CFD Module

User's Guide

5.3

COMSOL

CFD Module User's Guide

Version: COMSOL 5.3

Contact Information

Visit the Contact COMSOL page at www.comsol.com/contact to submit general inquiries, contact Technical Support, or search for an address and phone number. You can also visit the Worldwide Sales Offices page at www.comsol.com/contact/offices for address and contact information.

If you need to contact Support, an online request form is located at the COMSOL Access page at www.comsol.com/support/case. Other useful links include:

- Support Center: www.comsol.com/support
- Product Download: www.comsol.com/product-download
- Product Updates: www.comsol.com/support/updates
- COMSOL Blog: www.comsol.com/blogs
- Discussion Forum: www.comsol.com/community
- Events: www.comsol.com/events
- COMSOL Video Gallery: www.comsol.com/video
- Support Knowledge Base: www.comsol.com/support/knowledgebase

Contents

Chapter 1: Introduction

Chapter 2: Quick Start Guide

Chapter 3: Single-Phase Flow Interfaces

The Rotating Machinery, Laminar and Turbulent Flow

Chapter 4: Heat Transfer and Nonisothermal Flow

Interfaces

Chapter 5: Multiphase Flow Interfaces

Chapter 6: High Mach Number Flow Interfaces

Chapter 7: Porous Media and Subsurface Flow

Interfaces

Chapter 8: Chemical Species Transport Interfaces

Chapter 9: Thin-Film Flow Interfaces

Chapter 10: Mathematics, Moving Interface Branch

Chapter 11: Glossary

1

Introduction

This guide describes the CFD Module, an optional add-on package for COMSOL Multiphysics® that provides you with tools for computational fluid dynamics, CFD. The modeling of fluid flow is an increasingly important part in development of new equipment and processes.

This chapter introduces you to the capabilities of the module. A summary of the physics interfaces and where you can find documentation and model examples is also included. The last section is a brief overview with links to each chapter in this guide.

- About the CFD Module
- Overview of the User's Guide

About the CFD Module

In this section:

- Why CFD is Important for Modeling
- How the CFD Module Helps Improve Your Modeling
- Where Do I Access the Documentation and Application Libraries?

Why CFD is Important for Modeling

Computational fluid dynamics, CFD, is an integral part in a constantly growing number of development processes, and is a well established field within many different engineering disciplines; mechanical, chemical, civil, aeronautical, and also in more specialized areas such as biomedical engineering.

Often the flow itself is not the main focus in a simulation. Instead it is how the flow affects other process and application parameters that is important. The transport of species through the different parts of a chemical reactor, the effective cooling of a computer's hard drive and electronics, the dispersion of energy within the damping film of an accelerometer, the extent of nuclear waste spreading from a subterranean repository—all of these are applications for which the flow must be fully understood and is an integral part of the process's description and simulation.

In many situations, while the flow can add necessary operational parameters to a process or application, it is also affected by them. For example, a chemical reactor creates a pressure which disturbs the flow, the electronic heat affects the fluid's density and flow properties, the accelerometer elasticity imposes an oscillation on the flow, while the subterranean environment's poroelasticity changes the course of the flow.

A description combining several physics fields is often required to produce accurate models of real world applications involving fluid flow. Being able to effectively simulate such models increases the understanding of the studied processes and applications, which in turn leads to optimization of the flow and other parameters.

Historically, a sophisticated modeling tool was a privilege that only large companies could afford, for which the savings made in bulk production justified the computer software costs and need for CFD specialists. Today's engineers are educated in the use of software modeling tools, and are often expected to create realistic models of

advanced systems on their personal computers. This is where COMSOL Multiphysics can improve your modeling capabilities.

How the CFD Module Helps Improve Your Modeling

The CFD Module is an optional package that extends the COMSOL Multiphysics modeling environment with customized physics interfaces and functionality optimized for the analysis of all types of fluid flow. It is developed for a wide variety of users including researchers, developers, teachers, and students. It is not just a tool for CFD experts; it can be used by all engineers and scientists who work with systems in which momentum transport through fluid flow is an important part of a process or application.

The module uses the latest research possible to simulate fluid flow and it provides the most user-friendly simulation environment for CFD applications. The solvers and meshes are optimized for fluid-flow applications and have built-in robust stabilization methods.

The readily available coupling of heat and mass transport to fluid flow enables modeling of a wide range of industrial applications such as heat exchangers, turbines, separation units, and ventilation systems.

Ready-to-use interfaces enable you to model laminar and turbulent single- or multiphase flow. Functionality to treat coupled free and porous media flow, stirred vessels, and fluid structure interaction is also included.

Together with COMSOL Multiphysics and its other optional packages, the CFD Module takes flow simulations to a new level, allowing for arbitrary coupling to physics interfaces describing other physical phenomena, such as structural mechanics, electromagnetics, or even user-defined transport equations. This allows for unparalleled modeling capabilities for multiphysics applications involving fluid flow.

Like all COMSOL modules, the interfaces described in this guide include all the steps available for the modeling process, which are described in detail in the *COMSOL Multiphysics Reference Manual*:

- *Definitions* of parameters and component variables
- Creating, importing and manipulating the *geometry*
- Specifying the *materials* to include in the component
- Defining the *physics* of the fluid flow in domains and on boundaries, and coupling it to other physics

- Set up an appropriate *mesh* for the modeling domain with consideration given to the fluid-flow system's behavior

- Solving the equations that describe a system for stationary or dynamic behavior, or as a parametric or optimization *study*

- Collecting and analyzing *results* to present for further use in other analyses.

Once a model is defined, you can go back and make changes in all of the branches listed, while maintaining consistency in the other definitions throughout. You can restart the solver, for example, using the existing solution as an initial guess or even alter the geometry, while the equations and boundary conditions are kept consistent through the associative geometry feature.

Where Do I Access the Documentation and Application Libraries?

A number of internet resources have more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or context-based) help, and the application libraries are all accessed through the COMSOL Desktop.

> If you are reading the documentation as a PDF file on your computer, the blue links do not work to open an application or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to open other modules (as long as you have a license), application examples, and documentation sets.

THE DOCUMENTATION AND ONLINE HELP

The *COMSOL Multiphysics Reference Manual* describes the core physics interfaces and functionality included with the COMSOL Multiphysics license. This book also has instructions about how to use COMSOL Multiphysics and how to access the electronic Documentation and Help content.

Opening Topic-Based Help
The Help window is useful as it is connected to many of the features on the GUI. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then

displays information about that feature (or click a node in the Model Builder followed by the **Help** button (?). This is called *topic-based* (or *context) help*.

Win	To open the **Help** window: • In the **Model Builder**, **Application Builder**, or **Physics Builder** click a node or window and then press F1. • On any toolbar (for example, **Home**, **Definitions**, or **Geometry**), hover the mouse over a button (for example, **Add Physics** or **Build All**) and then press F1. • From the **File** menu, click **Help** (?). • In the upper-right corner of the COMSOL Desktop, click the **Help** (?) button.

Mac **Linux**	To open the **Help** window: • In the **Model Builder** or **Physics Builder** click a node or window and then press F1. • On the main toolbar, click the **Help** (?) button. • From the main menu, select **Help>Help**.

Opening the Documentation Window

Win	To open the **Documentation** window: • Press Ctrl+F1. • From the **File** menu select **Help>Documentation** (▪).

Mac **Linux**	To open the **Documentation** window: • Press Ctrl+F1. • On the main toolbar, click the **Documentation** (▪) button. • From the main menu, select **Help>Documentation**.

THE APPLICATION LIBRARIES WINDOW

Each application includes documentation with the theoretical background and step-by-step instructions to create a model application. The applications are available in COMSOL as MPH-files that you can open for further investigation. You can use the step-by-step instructions and the actual applications as a template for your own modeling and applications. In most models, SI units are used to describe the relevant properties, parameters, and dimensions in most examples, but other unit systems are available.

Once the Application Libraries window is opened, you can search by name or browse under a module folder name. Click to view a summary of the application and its properties, including options to open it or a PDF document.

⑦	The Application Libraries Window in the *COMSOL Multiphysics Reference Manual*.

Opening the Application Libraries Window
To open the **Application Libraries** window (▥):

Win	• From the **Home** toolbar, **Windows** menu, click (▥) **Applications Libraries**.
	• From the **File** menu select **Application Libraries**.
	To include the latest versions of model examples, from the **File>Help** menu, select (▥) **Update COMSOL Application Library**.

Mac	Select **Application Libraries** from the main **File>** or **Windows>** menus.
Linux	To include the latest versions of model examples, from the **Help** menu select (▥) **Update COMSOL Application Library**.

CONTACTING COMSOL BY EMAIL

For general product information, contact COMSOL at info@comsol.com.

To receive technical support from COMSOL for the COMSOL products, please contact your local COMSOL representative or send your questions to

support@comsol.com. An automatic notification and a case number are sent to you by email.

COMSOL ONLINE RESOURCES

COMSOL website	www.comsol.com
Contact COMSOL	www.comsol.com/contact
Support Center	www.comsol.com/support
Product Download	www.comsol.com/product-download
Product Updates	www.comsol.com/support/updates
COMSOL Blog	www.comsol.com/blogs
Discussion Forum	www.comsol.com/community
Events	www.comsol.com/events
COMSOL Video Gallery	www.comsol.com/video
Support Knowledge Base	www.comsol.com/support/knowledgebase

Overview of the User's Guide

The *CFD Module User's Guide* gets you started with modeling CFD systems using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions on how to use COMSOL in general are included with the *COMSOL Multiphysics Reference Manual*. For theory relating to the physics interfaces, see the end of each chapter.

> As detailed in the section Where Do I Access the Documentation and Application Libraries? this information can also be searched from the COMSOL Multiphysics software **Help** menu.

TABLE OF CONTENTS, GLOSSARY, AND INDEX

To help you navigate through this guide, see the Contents, Glossary, and Index.

QUICK START GUIDE

The Quick Start Guide includes some basic modeling strategies to get you started modeling fluid flow in your particular application area. For example, it gives some tips about how to control your material properties and how to set the optimal mesh to make solving the model easier and quicker. It also includes a summary of all the physics interfaces included with the CFD Module.

THE PHYSICS INTERFACES

The CFD Module both extends physics interfaces available with COMSOL Multiphysics and provides additional physics interfaces. As a result, the module contains a wide range of physics interfaces for modeling various types of momentum transport. You can simulate laminar and turbulent flow, Newtonian and non-Newtonian flow, isothermal and non-isothermal flow, multiphase flow, and flow in porous media. The CFD Module also provides interfaces for modeling flows that occur in thin-films or in bounded regions, and in stationary and rotating domains.

On top of this, the CFD Module includes physics interfaces for modeling heat transfer, and transport and reactions of chemical species. These are typical phenomena that occur in fluid flow and are strongly coupled to the flow field.

Single-Phase Flow

The Single-Phase Flow Interfaces chapter describes the many physics interfaces available for laminar and turbulent flow. Modeling Single-Phase Flow helps you choose the best Fluid Flow interface for your particular application.

Heat Transfer and Non-Isothermal Flow

The CFD Module includes physics interfaces for the simulation of heat transfer in fluid flow. As with all other physics models simulated in COMSOL Multiphysics, any description involving heat transfer can be directly coupled to any other physical process. This is particularly relevant for systems with fluid flow and mass transfer. The interfaces also allow you to account for heat sources and sinks, such as energy evolving from chemical reactions.

The Heat Transfer and Nonisothermal Flow Interfaces chapter describes these physics interfaces in greater detail. To help you select which physics interface to use see Modeling Heat Transfer in the CFD Module.

High Mach Flow

The High Mach Number Flow Interfaces chapter describes three versions of the same predefined multiphysics interface used to model laminar and turbulent compressible flows at high Mach numbers.

Multiphase Flow

The Multiphase Flow Interfaces chapter describes physics interfaces to model flows with more than one phase, for example flows with two fluids or flows with dispersed droplets or particles. To help you select which physics interface to use see Modeling Multiphase Flow.

Porous Media and Subsurface Flow

The Porous Media and Subsurface Flow Interfaces chapter describes the **Darcy's Law**, **Brinkman Equations**, and **Free and Porous Media Flow** interfaces. To help you select which physics interface to use see Modeling Porous Media and Subsurface Flow.

Thin-Film Flow

The Thin-Film Flow Interfaces chapter describes physics interfaces that model flow in thin regions such as lubrication shells and fluid bearings.

Chemical Species Transport

The Chemical Species Transport Interfaces chapter describes physics interfaces that are used for the simulation of chemical reactions, and mass or material transport through diffusion and convection. Modeling Chemical Species Transport helps you select the best physics interface to use.

The Mathematics Interfaces

Mathematics, Moving Interface Branch describes the **Phase Field** and **Level Set** interfaces found under the **Mathematics>Moving Interface** branch. In the CFD Module these physics features are integrated into the relevant physics interfaces.

2

Quick Start Guide

This chapter has some basic modeling strategies to get you started modeling fluid flow in your application area.

In this chapter:

• Modeling and Simulations of Fluid Flow

Modeling and Simulations of Fluid Flow

In this section:

- Modeling Strategy
- Geometric Complexities
- Material Properties
- Defining the Physics Interfaces and Features
- Meshing
- The Choice of Solver and Solver Settings
- The CFD Module Physics Interface Guide
- Common Physics Interface and Feature Settings and Nodes
- The Liquids and Gases Materials Database

	The Physics Interfaces and Building a COMSOL Multiphysics Model in the *COMSOL Multiphysics Reference Manual*

Modeling Strategy

Modeling and simulating fluid flow is a cost-effective way for engineers and scientists to understand, develop, optimize, and control designs and processes.

One of the most important things to consider before setting up a model is the accuracy that is required in the simulation results. This determines the level of complexity in the model.

Since fluid flow simulations are often computationally demanding, a multi-stage modeling strategy is usually required. This implies using a simplified model as a starting point in the project. Complexities can then be introduced gradually so that the effect of each refinement of the model description is well understood before introducing new complexities.

Complexities in the modeling process can be introduced at different stages in order to achieve the desired accuracy. They can be introduced in the description of the

geometry, the physical properties, and in the governing equations. The Model Builder, which shows the sequence of operations in the model tree, is designed with this strategy in mind.

In addition to fluid flow, COMSOL Multiphysics and the CFD Module have predefined couplings for fluid flow and other phenomena. Examples of these couplings are heat transfer for free convection and transport of chemical species in simulations of reacting flows. Set up your own couplings by defining mathematical expressions of the dependent variables (velocity, pressure, temperature, and so forth) in the physics interfaces for arbitrary multiphysics combinations.

Geometric Complexities

A complicated 3D CAD drawing is usually not the best starting point for the modeling process. A 2D representation of a cross section of the geometry can give valuable initial estimates of the flow field that can be used when setting up the full 3D model. For example, you might be able to determine the pressure variations and the nature of the flow, or whether or not a turbulence model is needed. This provides information about where in the final geometry the most amount of 'change' occurs, if a more advanced fluid-flow model and/or better resolution is required, and what parts of the modeling process are more sensitive than others.

Simplifying the geometry reduces the simulation time. Making use of symmetry planes can cut down the geometry to one half or even less of the original size. Rounding-off corners is another way to reduce mesh resolution. Resolving small geometric parts requires a fine mesh, but the parts themselves can have a negligible effects on the fluid field as a whole.

Geometry Modeling and CAD Tools in the *COMSOL Multiphysics Reference Manual*

Material Properties

Depending on the accuracy required in a simulation, the effort put in acquiring data for the fluid properties can also vary. In many cases, the dependencies of the fluid properties on pressure and temperature have to be taken into account.

For a pressure-driven flow, it is usually a good approach to first set up a model using constant density and viscosity, to get a first estimate of the flow and pressure fields.

Once the model works with constant properties it can be extended by adding the accurate expressions for density and viscosity.

For free convection the density variations drive the flow. The fluid properties' dependencies on the modeled variables, for example temperature, then have to be accounted for from the beginning. In difficult cases, with large temperature variations, it can be beneficial to run a time-dependent simulation even if the purpose of the simulation is to get the results at steady-state.

Defining the Physics Interfaces and Features

The CFD Module has physics interfaces for laminar and turbulent single-phase flow, multiphase flow, non-isothermal flow, high Mach number flow, thin-film flow, and porous media flow.

The choice of physics interface and features depends on the accuracy required in a simulation. A fluid that is weakly compressible could be approximated as incompressible if the required accuracy allows for it. A complex turbulence model can be replaced by a much simpler one, again if the resulting accuracy is sufficient. A first step to set up the physics is to start by making the model as simple as possible. The results from such a simulation can reveal useful pieces of information that help later when more complex steps are added to the physics.

The Fluid Flow interfaces can also be coupled to any other physics interface in a multiphysics model. When setting up such a complex multiphysics component involving fluid flow and other coupled physics, it is a good strategy to first define and solve one physics interface at a time. This allows for verification of the model setup, for example to check if the intended domain and boundary settings are reflected in the solution of each decoupled physics interface. The alternative, to debug the model setup with several coupled physics interfaces, can be time-consuming.

In steady-state multiphysics simulations, it can also be a good strategy to start by solving the model for each physics interface in a decoupled setup. The solutions from the decoupled models can then be used as initial guesses for the fully coupled model. This is especially recommended for highly nonlinear models. The Study node is designed for this modeling strategy.

> Building a COMSOL Multiphysics Model and Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Meshing

The mesh used in a fluid flow simulation depends on the fluid flow model and on the accuracy required in the simulation. A fluid flow model can inherently require a fine resolution in order to converge, even though the results might not require a correspondingly high accuracy. In such cases, it can be a good idea to change the fluid flow model. An example is the low-Reynolds number k-ε model which gives a very accurate description of the flow near solid walls, but requires a very fine mesh there. In many cases, the standard k-ε model with wall functions can deliver an accurate enough result at a much lower computational cost. In other cases, the requirement of accuracy in the results can limit the maximum element size.

There are a number of different mesh types and meshing strategies for fluid flow modeling in COMSOL Multiphysics.

UNSTRUCTURED MESHES

Free-meshing techniques generate unstructured meshes that can be used for most types of geometries. The mesh-generating algorithms are highly automated, often creating a good quality mesh from minimal user input. This mesh type is therefore a good choice when the geometry of the domain is evident but the behavior of the mathematical model in it is unknown. Yet, unstructured meshes tend to be isotropic or homogeneous in nature, so that they fail to take advantage of the different resolution requirements in the stream-wise and cross-stream directions.

STRUCTURED MESHES

In many ways, the properties of structured meshes complement those of the unstructured type. Structured meshes provide high quality meshes with few elements for sufficiently simple geometries. The properties of a structured mesh can furthermore be used to create very efficient numerical methods. Finally, it is often easier to control the mesh when high *anisotropy* or large variations in mesh size and distribution is required, as the size of a structured mesh can be easily increased linearly or geometrically with the dimensions of the computational domain.

SWEPT MESHES

Swept meshes are a particular form of structured meshes, sometimes denoted semistructured. These are generated in 3D by creating a mesh at a source face and then sweeping it along the domain to a destination face, such as from a cut in the cylindrical part of a polymerization reactor to its outlet face. A swept mesh is structured in the sweep direction, while the mesh at the source and destination faces can be either

structured or unstructured. As is the case for structured meshes, the model geometry determines if a swept mesh is applicable. Swept meshes are typically ideal when the cross section in the sweep direction is constant, which is the case for channels and pipes, for example. Revolving a mesh around a symmetry axis is another useful sweep operation.

BOUNDARY LAYER MESHES

A boundary layer mesh is a mesh with an element distribution that is stacked or dense in the direction normal to a boundary. It is created by inserting structured layers of elements along specific boundaries and merging the outer layer with the surrounding structured or unstructured mesh. This type of mesh is useful for many fluid flow applications especially when coupled to mass and energy transfer, where thin *boundary layers* need to be resolved. This is also the default physics-induced mesh for fluid flow.

MESH CONVERGENCE

Ideally, a mesh convergence analysis should be performed in order to estimate the accuracy of a simulation. This means that the mesh should be made twice as fine in each spatial direction and the simulation carried out once again on the refined mesh. If the change in critical solution parameters for the original mesh and the finer mesh is within the required tolerance, the solution can be regarded as being mesh-converged. For practical reasons, it is seldom possible to make the mesh twice as fine in each direction. Instead, some critical regions can be identified and the mesh is refined only there.

Q   Meshing in the *COMSOL Multiphysics Reference Manual*

The Choice of Solver and Solver Settings

The default solver for the Fluid Flow interfaces is optimized for a large variety of fluid flow conditions and applications. The suggested solver depends on the physics interface and the study type.

The default solver settings is a trade-off between performance and robustness. The more advanced the model, the more the solver can need tuning to obtain a solution. This is another reason why it is good to start with a reduced model description rather than the complete description.

2D models and small 3D models get so-called direct-solver suggestions. Direct solvers are robust but the memory requirement scales somewhere between $N^{1.5}$ and N^2 where

N is the number of degrees of freedom in the model. This means that a direct solver becomes prohibitively expensive for large problems. Large 3D models therefore get iterative solver suggestions per default. The memory requirement for an iterative solver optimally scales as N. The drawback with iterative solvers is that they are less robust than direct solvers. A model can converge with a direct solver but fail with an iterative solver. Large models therefore require more care when being set up than small models do.

For well-posed models, there are possibilities to tune the default solvers to gain performance. This is especially true for time-dependent models with a variety of solver settings providing options to reduce the computational time.

🔍	Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

The CFD Module Physics Interface Guide

The CFD Module extends the functionality of the physics interfaces of the base package for COMSOL Multiphysics. The details of the physics interfaces and study types for the CFD Module are listed in the table. The functionality of the COMSOL Multiphysics base package is listed in the *COMSOL Multiphysics Reference Manual*.

🔍	In the *COMSOL Multiphysics Reference Manual*: • Studies and Solvers • The Physics Interfaces • For a list of all the core physics interfaces included with a COMSOL Multiphysics license, see Physics Interface Guide.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE PRESET STUDY TYPE
⋮⋮ Chemical Species Transport				
Transport of Diluted Species[1]		tds	all dimensions	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE PRESET STUDY TYPE
Transport of Concentrated Species		tcs	all dimensions	stationary; time dependent
≋ Reacting Flow				
Laminar Flow	≋	—	3D, 2D, 2D axisymmetric	stationary; time dependent
≋ Turbulent Flow				
Turbulent Flow, k-ε	≋	—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω	≋	—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, SST	≋	—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, Low Re k-ε	≋	—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
≋ Reacting Flow in Porous Media				
Transport of Diluted Species		rfds	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species		rfcs	3D, 2D, 2D axisymmetric	stationary; time dependent
≋ Fluid Flow				
≋ Single-Phase Flow				
Creeping Flow	≋	spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow[1]	≋	spf	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE PRESET STUDY TYPE
≈≈ *Turbulent Flow*				
Turbulent Flow, Algebraic yPlus		spf	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, L-VEL		spf	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, k-ε		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, SST		spf	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, Low Re k-ε		spf	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, Spalart-Allmaras		spf	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, v2-f		spf	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
≈ *Rotating Machinery, Fluid Flow*				
Rotating Machinery, Laminar Flow		rmspf	3D, 2D	frozen rotor; time dependent
Rotating Machinery, Turbulent Flow, Algebraic yPlus		rmspf	3D, 2D	frozen rotor with initialization; transient with initialization
Rotating Machinery, Turbulent Flow, L-VEL		rmspf	3D, 2D	frozen rotor with initialization; transient with initialization
Rotating Machinery, Turbulent Flow, k-ε		rmspf	3D, 2D	frozen rotor; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE PRESET STUDY TYPE
Thin-Film Flow				
Thin-Film Flow, Shell		tffs	3D	stationary; time dependent; frequency domain; eigenfrequency
Thin-Film Flow, Domain		tff	2D	stationary; time dependent; frequency domain; eigenfrequency
Thin-Film Flow, Edge		tffs	2D and 2D axisymmetric	stationary; time dependent; frequency domain; eigenfrequency
Multiphase Flow				
Bubbly Flow				
Laminar Bubbly Flow		bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Bubbly Flow		bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model				
Mixture Model, Laminar Flow		mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, Turbulent Flow		mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Euler-Euler Model				
Euler-Euler Model, Laminar Flow		ee	3D, 2D, 2D axisymmetric	stationary; time dependent
Euler-Euler Model, Turbulent Flow		ee	3D, 2D, 2D axisymmetric	stationary; time dependent
Two-Phase Flow, Level Set				
Laminar Two-Phase Flow, Level Set		—	3D, 2D, 2D axisymmetric	transient with phase initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE PRESET STUDY TYPE
Turbulent Two-Phase Flow, Level Set		—	3D, 2D, 2D axisymmetric	transient with phase initialization
Two-Phase Flow, Phase Field				
Laminar Two-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	transient with phase initialization
Turbulent Two-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	transient with phase initialization
Three-Phase Flow, Phase Field				
Laminar, Three-Phase Flow, Phase Field		—	3D, 2D	time dependent
Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent
Two-Phase Darcy's Law		tpdl	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Flow				
Laminar Flow[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow				
Turbulent Flow, Algebraic yPlus[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, L-VEL[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE PRESET STUDY TYPE
Turbulent Flow, k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, SST[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, Low Re k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, Spalart-Allmaras[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
High Mach Number Flow				
High Mach Number Flow		hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ε		hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, Spalart-Allmaras		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Heat Transfer				
Heat Transfer in Fluids[1]		ht	all dimensions	stationary; time dependent
Heat Transfer in Porous Media		ht	all dimensions	stationary; time dependent
Conjugate Heat Transfer				
Laminar Flow[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE PRESET STUDY TYPE
≋ *Turbulent Flow*				
Turbulent Flow, Algebraic yPlus	≋	—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, L-VEL	≋	—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, k-ε[2]	≋	—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω[2]	≋	—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, Low Re k-ε[2]	≋	—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, SST[2]	≋	—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
Turbulent Flow, Spalart-Allmaras[2]	≋	—	3D, 2D, 2D axisymmetric	stationary with initialization; transient with initialization
△u **Mathematics**				
� **Moving Interface**				
Level Set	⦚	ls	all dimensions	transient with phase initialization
Phase Field	⦚	pf	all dimensions	time dependent; transient with phase initialization
Ternary Phase Field	⦚	terpf	3D, 2D, 2D axisymmetric	time dependent

[1] This physics interface is included with the core COMSOL package but has added functionality for this module.

[2] This physics interface is a predefined multiphysics coupling that automatically adds all the physics interfaces and coupling features required.

Common Physics Interface and Feature Settings and Nodes

There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in the same way no matter the physics interface or feature being used. There are also some physics feature nodes that display in COMSOL Multiphysics.

In each module's documentation, only unique or extra information is included; standard information and procedures are centralized in the *COMSOL Multiphysics Reference Manual*.

> In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Liquids and Gases Materials Database

The CFD Module includes an additional **Liquids and Gases** material database with temperature-dependent fluid properties.

> For detailed information about materials and the Liquids and Gases Materials Database, see Materials in the *COMSOL Multiphysics Reference Manual*.

3

Single-Phase Flow Interfaces

There are several fluid flow physics interfaces available as listed in The CFD Module Physics Interface Guide. This chapter describes the physics interfaces found under the **Fluid Flow>Single-Phase Flow** branch (≈). The section Modeling Single-Phase Flow helps to choose the best physics interface to start with.

In this chapter:

- The Creeping Flow, Laminar Flow, and Turbulent Flow Interfaces
- The Rotating Machinery, Laminar and Turbulent Flow Interfaces
- Theory for the Single-Phase Flow Interfaces
- Theory for the Turbulent Flow Interfaces
- Theory for the Rotating Machinery Interfaces
- The Wall Distance Interface is also available and described in the *COMSOL Multiphysics Reference Manual* including the theory and how it relates to fluid flow.

Modeling Single-Phase Flow

The descriptions in this section are structured based on the order displayed in the **Fluid Flow** branch. All the physics interfaces described in this section are found under the **Fluid Flow>Single-Phase Flow** branch ( ). Because most of the physics interfaces are integrated with each other, many physics features described cross reference to other physics interfaces. For example, nodes are usually available in both the laminar flow (Creeping Flow and Laminar Flow) and turbulent flow (Algebraic yPlus, L-VEL, k-ε, k-ω, SST, low Reynolds number k-ε, Spalart-Allmaras and v2-f turbulence models) interfaces.

In this section:

- Selecting the Right Physics Interface
- The Single-Phase Flow Interface Options
- Coupling to Other Physics Interfaces

> The Wall Distance Interface in the *COMSOL Multiphysics Reference Manual*

Selecting the Right Physics Interface

The Single-Phase Flow branch included with the CFD Module has a number of subbranches with physics interfaces that describe different types of single-phase fluid flow. One or more of these physics interfaces can be added, either singularly or in combination with other physics interfaces for mass transport and heat transfer, for example.

Different types of flow require different equations to describe them. If the type of flow to model is already known, then select it directly. However, when you are uncertain of the flow type, or because it is difficult to reach a solution easily, you can start instead with a simplified model and add complexity as the model is built. Then test your way forward and compare models and results. For single-phase flow, the Laminar Flow interface is a good place to start if this is the case.

In other cases, you may know exactly how a fluid behaves and which equations, models, or physics interfaces best describe it, but because the model is so complex it is difficult to reach an immediate solution. Simpler assumptions may need to be made to solve the problem, and other physics interfaces might be better to fine-tune the solution process for

the more complex problem. The next section gives you an overview of each of the
Single-Phase Flow interfaces to help you choose.

The Single-Phase Flow Interface Options

Several of the physics interfaces vary only by one or two default settings (see Table 3-1) in
the *Physical Model* section, which are selected either from a check box or drop-down list.
For the Single-Phase Flow branch, all except the Rotating Machinery interfaces have the
same *Name* (spf). The differences are based on the default settings required to model that
type of flow as described in Table 3-1. Figure 3-1 shows the **Settings** window for Laminar
Flow where you choose the type of compressibility (incompressible, weakly compressible
or compressible at *Mach numbers* below 0.3) and the turbulence model (or none for
laminar flow), and a check box to model Stokes flow by neglecting the inertial term.

TABLE 3-1: THE SINGLE-PHASE FLOW PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	TURBULENT MODEL TYPE	TURBULENCE MODEL	NEGLECT INERTIAL TERM (STOKES FLOW)
Creeping Flow	spf	Incompressible flow	None	n/a	Stokes Flow
Laminar Flow	spf	Incompressible flow	None	n/a	None
Turbulent Flow, Algebraic yPlus	spf	Incompressible flow	RANS	Algebraic yPlus	None
Turbulent Flow, L-VEL	spf	Incompressible flow	RANS	L-VEL	None
Turbulent Flow, k-ε	spf	Incompressible flow	RANS	k-ε	None
Turbulent Flow, k-ω	spf	Incompressible flow	RANS	k-ω	None
Turbulent Flow, SST	spf	Incompressible flow	RANS	SST	None
Turbulent Flow, Low Re k-ε	spf	Incompressible flow	RANS	Low Reynolds number k-ε	None
Turbulent Flow, Spalart-Allmaras	spf	Incompressible flow	RANS	Spalart-Allmaras	None
Turbulent Flow, v2-f	spf	Incompressible flow	RANS	v2-f	None

TABLE 3-1: THE SINGLE-PHASE FLOW PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	TURBULENT MODEL TYPE	TURBULENCE MODEL	NEGLECT INERTIAL TERM (STOKES FLOW)
Rotating Machinery, Laminar Flow	rmspf	Compressible flow (Ma<0.3)	None	None	None
Rotating Machinery, Turbulent Flow, Algebraic yPlus	rmspf	Compressible flow (Ma<0.3)	RANS	Algebraic yPlus	None
Rotating Machinery, Turbulent Flow, L-VEL	rmspf	Compressible flow (Ma<0.3)	RANS	L-VEL	None
Rotating Machinery, Turbulent Flow, k-ε	rmspf	Compressible flow (Ma<0.3)	None	RANS, k-ε	None

CREEPING FLOW

The Creeping Flow Interface (≡≡≡) models the Navier-Stokes equations without the contribution of the inertia term. This is often referred to as Stokes flow and is appropriate for flow at small Reynolds numbers, such as in very small channels or in microfluidic applications.

The Creeping Flow interface can also be activated by selecting a check box in the Laminar Flow interface. This physics interface can also model non-Newtonian fluids, using the Power Law and Carreau models, but not turbulence.

LAMINAR FLOW

The Laminar Flow Interface (≋) is used primarily to model flow at small to intermediate Reynolds numbers. The physics interface solves the Navier-Stokes equations, and by default assumes the flow to be incompressible; that is, the density is assumed to be constant.

Compressible flow is possible to model in this physics interface but you have to maintain control of the density and any of the mass balances that are deployed to accomplish this.

The Laminar Flow Interface allows you to model porous media flow or even mixed free- and porous media flow. A volume force due to gravity can optionally be included.

This physics interface also allows you to simulate a certain class of non-Newtonian fluid flows by modifying the dynamic viscosity in the Navier-Stokes equations. You can model the fluid using the power law and Carreau models or enter another expression that describes the dynamic viscosity appropriately.

You can also describe other material properties such as density by entering equations for its dependence on fluid composition and pressure (for compressible flow), or temperature. Many materials in the material libraries use temperature- and pressure-dependent property values. If the density is affected by temperature, a non-isothermal flow interface may be applicable (see The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces).
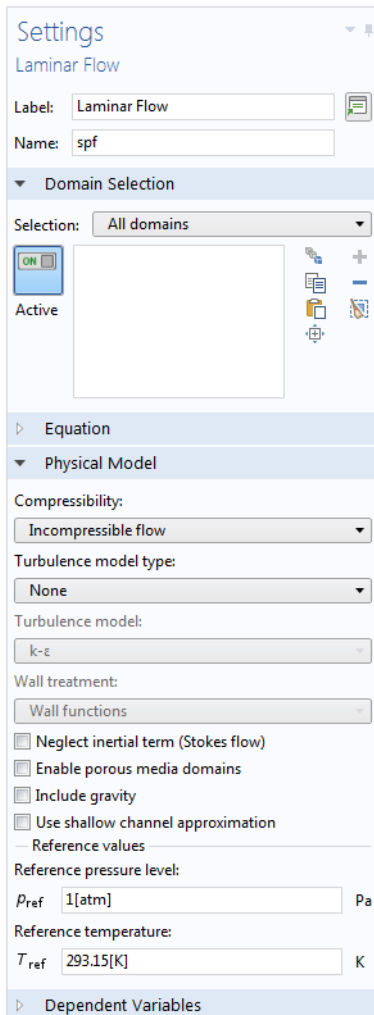
Figure 3-1: The Settings window for the Laminar Flow interface. Model incompressible or compressible flow, laminar or turbulent flow, Stokes flow and/or porous media flow. Combinations are also possible.

TURBULENT FLOW

The various forms of the Single-Phase Flow, Turbulent Flow interfaces (≋) model flow of large Reynolds numbers. The interfaces solve the Reynolds-averaged Navier-Stokes (RANS) equations for the filtered velocity field and filtered pressure as well as models for the turbulent viscosity. See The Creeping Flow, Laminar Flow, and Turbulent Flow

Interfaces for links to the physics interface information.

There are several turbulence models available: two algebraic turbulence models, the Algebraic yPlus and L-VEL models, and five transport-equation models, including a basic k-ε model, a k-ω model, an SST model, a Low Reynolds number k-ε model, the Spalart-Allmaras model, and the v2-f model. Each model has its merits and weaknesses. See the Theory for the Turbulent Flow Interfaces for more details.

Similarly to the Laminar Flow interface, incompressible flow is selected by default. If required, this can be changed to compressible flow. Non-Newtonian fluid models are not available for the Turbulent Flow interfaces.

ROTATING MACHINERY

The Rotating Machinery, Laminar and Turbulent Flow Interfaces ( ) model fluid flow in geometries with rotating parts. For example, stirred tanks, mixers, propellers and pumps.

Unlike the other physics interfaces under the Single-Phase Flow branch, the Rotating Machinery, Fluid Flow interface can not be activated directly from the Laminar Flow interface or any of the other physics interfaces. It supports compressible and incompressible flow, the flow of non-Newtonian fluids using the Power Law and Carreau models, as well as turbulence. This physics interface also supports creeping flow.

Coupling to Other Physics Interfaces

Often, you may want to simulate applications that couple fluid flow to another type of phenomenon described in another physics interface. Although this is not often another type of flow, it can still involve physics interfaces supported in the CFD Module and in the COMSOL Multiphysics base package. This is often the case for applications that include chemical reactions and mass transport (see Chemical Species Transport Interfaces), or energy transport, found in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of heat transfer, including radiation, can be found in the Heat Transfer Module, while a wider variety of tools for modeling chemical reactions and mass transport are found in the Chemical Reaction Engineering Module. Fluid flow is an important component for cooling electromagnetic phenomena, such as heat created through induction and microwave heating, which are simulated using the AC/DC Module and RF Module, respectively. Many applications involve the effect of fluid-imposed loads on structural applications, for example, fluid-structure interaction (FSI). The Structural Mechanics Module and MEMS Module have physics interfaces specifically for these multiphysics applications.

The Creeping Flow, Laminar Flow, and Turbulent Flow Interfaces

In this section:

- The Creeping Flow Interface
- The Laminar Flow Interface
- The Turbulent Flow, Algebraic yPlus Interface
- The Turbulent Flow, L-VEL Interface
- The Turbulent Flow, k-e Interface
- The Turbulent Flow, k-w Interface
- The Turbulent Flow, SST Interface
- The Turbulent Flow, Low Re k-e Interface
- The Turbulent Flow, Spalart-Allmaras Interface
- The Turbulent Flow, v2-f Interface

@	• Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow • Theory for the Single-Phase Flow Interfaces

In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings** sections, all accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Creeping Flow Interface

The **Creeping Flow (spf)** interface ( ) is used for simulating fluid flows at very low Reynolds numbers for which the inertial term in the Navier-Stokes equations can be neglected. Creeping flow, also referred to as Stokes flow, occurs in systems with high viscosity or small geometrical length scales (for example, in microfluidics and MEMS

devices). The fluid can be compressible or incompressible, as well as Newtonian or non-Newtonian.

The equations solved by the Creeping Flow interface are the Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Creeping Flow interface can be used for stationary and time-dependent analyses.

The main feature is the **Fluid Properties** node, which adds the Stokes equations and provides an interface for defining the fluid material and its properties. Except where noted below, see The Laminar Flow Interface for all other settings.

PHYSICAL MODEL

By default, the **Neglect inertial term (Stokes flow)** check box is selected. If unchecked, or, if the **Turbulence model type** is changed to **RANS**, the inertial terms are included in the computations.

DISCRETIZATION

By default, the Creeping Flow interface uses **P2+P1** elements**.** Contrary to general laminar and turbulent single-phase flow simulations employing purely linear P1+P1 elements, P2+P1 elements are well suited for most Creeping flow simulations but are not in general fully conservative. Full conservation properties and high accuracy is obtained by selecting P2+P2 or P3+P3 elements.

Observe that P1+P1, P2+P2 and P3+P3 discretizations (the so called equal order interpolations) require streamline diffusion to be active.

CONSISTENT STABILIZATION

This check box is selected by default and should remain selected for optimal performance. The consistent stabilization method does not perturb the original transport equation.

| | • The Laminar Flow Interface |
| 🔍 | • Theory for the Single-Phase Flow Interfaces |

The Laminar Flow Interface

The **Laminar Flow (spf)** interface (≋) is used to compute the velocity and pressure fields for the flow of a single-phase fluid in the laminar flow regime. A flow remains laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence. This critical

Reynolds number depends on the model, but a classical example is pipe flow where the critical Reynolds number is known to be approximately 2000.

The physics interface supports incompressible flow, weakly compressible flow (the density depends on temperature but not pressure) and compressible flow at low Mach numbers (typically less than 0.3). It also supports flow of non-Newtonian fluids.

The equations solved by the Laminar Flow interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Laminar Flow interface can be used for stationary and time-dependent analyses. Time-dependent studies should be used in the high-Reynolds number regime as these flows tend to become inherently unsteady.

When the Laminar Flow interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**. Other nodes, that implement, for example, boundary conditions and volume forces, can be added from the **Physics** toolbar or from the context menu displayed when right-clicking **Laminar Flow**.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Physics interface variables can be referred to using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `spf`.

About the Physics Interface Label Names
The label for a single-phase flow interface (the node name in the Model Builder) is dynamic and is re-set according to the turbulence model and the neglect inertial term (Stokes flow) property set at the physics interface level. The availability also depends on the software license.

For example, a Laminar Flow interface is added to the Model Tree. If the **Low Reynolds number k-ε** turbulence model is selected, the interface **Label** changes to **Turbulent Flow, Low Re k-ε**, which is the same Label that displays when the corresponding interface is added from the Model Wizard or Add Physics window.

If the **Neglect inertial term (Stokes flow)** check box is selected, then the Label changes to **Creeping Flow**, which is the same Label that displays when that interface is added from the Model Wizard or Add Physics window.

PHYSICAL MODEL

Compressibility
Depending of the fluid properties and the flow regime, three options are available for the **Compressibility** option. In general the computational complexity increases from **Incompressible flow** to **Weakly compressible flow** to **Compressible flow (Ma<0.3)** but the underlying hypotheses are increasingly more restrictive in the opposite direction.

When the **Incompressible flow** option (default) is selected, the incompressible form of the Navier-Stokes and continuity equations is applied. In addition, the fluid density is evaluated at the **Reference pressure level** and at the **Reference temperature** defined in **Reference values**. The fluid dynamic viscosity is evaluated at the **Reference temperature**.

The **Weakly compressible flow** option models compressible flow when the pressure dependency of the density can be neglected. When selected, the compressible form of the Navier-Stokes and continuity equations is applied. In addition, the fluid density is evaluated at the **Reference pressure level** defined in **Reference values**.

When the **Compressible flow (Ma<0.3)** option is selected, the compressible form of the Navier-Stokes and continuity equations is applied. $\mathrm{Ma} < 0.3$ indicates that the inlet and outlet conditions, as well as the stabilization, may not be suitable for transonic and supersonic flow. For more information, see The Mach Number Limit.

Turbulence Model Type
Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS** (Reynolds-Averaged Navier–Stokes).

Swirl Flow
The velocity component, u_φ, in the azimuthal direction can be included for 2D axisymmetric components by selecting the **Swirl flow** check box. While u_φ can be nonzero, there can be no gradients in the φ direction. Also see General Single-Phase Flow Theory.

Neglect Inertial Term (Stokes Flow)
For low Reynolds number flows, the inertial terms in the Navier-Stokes equations may be neglected.

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** check box is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. The **Fluid and Matrix Properties** can be applied on all domains or on a subset of the domains.

Include gravity

When the **Include gravity** check-box is selected a global **Gravity** feature is shown in the interface model tree and the buoyancy force is included in the Navier-Stokes equations.

When the **Include gravity** check box is selected, the option **Use reduced pressure** changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes are very small, otherwise the default formulation can be used. For more information, see Gravity.

	Natural convection is induced by variations in magnitude of the buoyancy force which is defined from the density. For incompressible flow the density is constant, hence the buoyancy force is homogeneous and natural convection can not be modeled. Nevertheless, using the **Nonisothermal Flow** multiphysics coupling, the buoyancy force is defined using the thermal expansion coefficient and the temperature. Hence in this case natural convection is accounted for following Boussinesq approximation.

Use Shallow Channel Approximation

For 2D components, selecting the **Use shallow channel approximation** check box enables modeling of fluid flow in shallow channels in microfluidics applications. Such channels often have an almost rectangular cross section where the **Channel thickness** d_z is much smaller than the channel width. Simple 2D components often fail to give correct results for this type of problems because they exclude the boundaries that have the greatest effect on the flow. The shallow channel approximation takes the effect of these boundaries into account by adding a drag term as a volume force to the momentum equation. The form of this term is

$$\mathbf{F}_\mu = -12\frac{\mu\mathbf{u}}{d_z^2} \tag{3-1}$$

where μ is the fluid's dynamic viscosity, $\mathbf{u}$ is the velocity field, and d_z is the channel thickness. This term represents the resistance that the parallel boundaries impose on the

flow; however, it does not account for any changes in velocity due to variations in the cross-sectional area of the channel.

Reference values
Reference values are global quantities used to evaluate the density and viscosity of the fluid when the **Incompressible flow** or the **Weakly compressible flow** option is selected and to define the gravity force.

Reference pressure level   There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A=p+p_{ref}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the reference density.

Reference temperature   The reference temperature is used to define the reference density.

Reference position   When **Include gravity** is selected, the reference position can be defined. It corresponds to the location where the total pressure (that includes the hydrostatic pressure) is equal to the **Reference pressure level.**

DEPENDENT VARIABLES
The following dependent variables (fields) are defined for this physics interface — the **Velocity field u** and its components, and the **Pressure** p.

The Projection Method for the Navier-Stokes Equations requires additional dependent variables. These are the **Corrected velocity field u_c** and the **Corrected pressure** p_c.

If required, the names of the field, component, and dependent variable may be edited. Editing the name of a scalar dependent variable changes both its field name and the dependent variable name. If a new field name coincides with the name of another field of the same type, the fields share degrees of freedom and dependent variable names. A new field name must not coincide with the name of a field of another type or with a component name belonging to some other field. Component names must be unique within a model except when two fields share a common field name.

ADVANCED SETTINGS
To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up

convergence. When selected, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

Q
- Pseudo Time Stepping for Laminar Flow Models
- The Projection Method for the Navier-Stokes Equations
- Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow
- Theory for the Single-Phase Flow Interfaces

DISCRETIZATION

The default discretization for Laminar Flow is **P1+P1** elements. That is piecewise linear interpolation for velocity and pressure. This is suitable for most flow problems.

Some higher order interpolations are also available and these can cost-effective options to obtain high accuracy for flows with low Reynolds numbers.

The **P2+P2** and **P3+P3** options, the equal order interpolation options, are the preferred higher order options since they have higher numerical accuracy than the mixed order options, **P2+P1** and **P3+P2**. The equal order interpolation options do however require streamline diffusion to be active.

▥
Flow Past a Cylinder: Application Library path
COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow

The Turbulent Flow, Algebraic yPlus Interface

The **Turbulent Flow, Algebraic yPlus (spf)** interface (≈≋) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Algebraic yPlus interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled wall distance. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation. When this physics interface is added, the following default nodes are also added in the

Model Builder—**Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-e Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

Wall Treatment
Algebraic yPlus employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Porous Media Domains
With the addition of various modules, the **Enable porous media domains** check box is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. Applying the **Fluid and Matrix Properties** on a subset of the domains enables studies of coupled porous-media flow and turbulent flow.

TURBULENCE MODEL PARAMETERS

The turbulence model parameters for the Algebraic yPlus model, κ_a and B_a, have been optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u**
- **Pressure** p
- **Reciprocal wall distance** G
- **Wall distance in viscous units** $yPlus$ (dimensionless)

The Algebraic yPlus interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Turbulent Flow, L-VEL Interface

The **Turbulent Flow, L-VEL (spf)** interface (⚏) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach number (typically less than 0.3).

The equations solved by the Turbulent Flow, L-VEL interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are included using an enhanced viscosity model based on the local wall distance, and the physics interface therefore includes a wall distance equation. When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**. Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-e Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

Wall Treatment
L-VEL employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Porous Media Domains
With the addition of various modules, the **Enable porous media domains** check box is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. Applying the **Fluid and Matrix Properties** on a subset of the domains enables studies of coupled porous-media flow and turbulent flow.

Turbulence model parameters, κ_l and E_l, have been optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Reciprocal wall distance** G
- **Tangential velocity in viscous units** $uPlus$ (dimensionless)

The L-VEL interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Turbulent Flow, k-ε Interface

The **Turbulent Flow, k-ε (spf)** interface (≋) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, k-ε interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. The flow near walls is modeled using wall functions.

The Turbulent Flow, k-ε interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equations and the transport equations for k and ε, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, and **Initial Values**.

Except where included below, see The Laminar Flow Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

Wall treatment for the k-ε model can only be set to **Wall functions**. More options becomes available by selecting another option under **Turbulence model**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1}, C_{e2}, C_μ, σ_k, σ_e, κ_v, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep

The Projection Method for the Navier-Stokes Equations requires additional dependent variables. These are the **Corrected velocity field u_c** and the **Corrected pressure** p_c.

ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. The **Turbulence variables scale parameters** subsection is available when the **Turbulence model type** is set to **RANS**.

In addition to the settings described for the Laminar Flow interface, enter a value for U_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The U_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is

generated. If you change the parameters, the new values take effect the next time you generate a new default solver

---

- The Laminar Flow Interface
- Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Theory for the Turbulent Flow Interfaces

- *Airflow Over an Ahmed Body*: Application Library path **CFD_Module/Single-Phase_Benchmarks/ahmed_body**
- *Solar Panel in Periodic Flow*: Application Library path **CFD_Module/Single-Phase_Tutorials/solar_panel**

The Turbulent Flow, k-ω Interface

The **Turbulent Flow, k-ω (spf)** interface (≋) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, k-ω interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Wilcox revised two-equation k-ω model with realizability constraints. The k-ω model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall.

The Turbulent Flow, k-ω interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equations and the transport equations for the turbulent kinetic energy k and the specific dissipation ω, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall**, and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-e Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The k-ω model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. The most robust, but least accurate option is select the **Wall functions** option.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough. Observe that the **Low Re** formulation requires the wall distance to be solved for prior to the flow.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are α, σ_k^*, σ_w, β_0, β_0^*, κ_v, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Specific dissipation rate** om

	Flow Through a Pipe Elbow: Application Library path **CFD_Module/Single-Phase_Benchmarks/pipe_elbow**

The Turbulent Flow, SST Interface

The **Turbulent Flow, SST (spf)** interface (🌊) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, SST interface are the Reynolds-averaged Navier-Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability constraints. The SST model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, SST interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-e Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment
The SST model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For this physics interface the parameters are a_1, β_0^*, β_1, β_2, γ_1, γ_2, σ_{k1}, σ_{k2}, σ_{w1}, and σ_{w2}.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Specific dissipation rate** om
- **Reciprocal wall distance** G

The **SST** interface requires a **Wall Distance Initialization** study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Turbulent Flow, Low Re k-ε Interface

The **Turbulent Flow, Low Re k-ε (spf)** interface (≋) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Low Re k-ε interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the AKN two-equation k-ε model with realizability constraints. The AKN model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, Low Re k-ε interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-e Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The AKN model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1}, C_{e2}, C_{μ}, σ_k, σ_e, and κ_v.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep
- **Reciprocal wall distance** G

The Low Reynolds number k-ε interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

Ⓠ
- The Laminar Flow Interface
- Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Theory for the Turbulent Flow Interfaces

The Turbulent Flow, Spalart-Allmaras Interface

The **Turbulent Flow, Spalart-Allmaras (spf)** interface (〰) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Spalart-Allmaras interface are the Reynolds-averaged Navier-Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Spalart-Allmaras one-equation model. The Spalart-Allmaras model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The Spalart-Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, Spalart-Allmaras interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equations and the transport equations for the undamped turbulent kinematic velocity $\tilde{v}$, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**— **Fluid Properties**, **Wall**, and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-e Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The Spalart-Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{b1}, C_{b2}, C_{v1}, σ_v, C_{w2}, C_{w3}, κ_v, and C_{rot}.

ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Under the **Turbulence variables scale parameters** subsection, the default v_{scale} is of the same order of magnitude as the kinematic viscosity of air at room temperature.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Reciprocal wall distance** G
- **Undamped turbulent kinematic viscosity** υ

The Spalart-Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Turbulent Flow, v2-f Interface

The **Turbulent Flow, v2-f (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, v2-f interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the v2-f transport-equation model with realizability constraints. The v2-f model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The physics interface includes a wall distance equation.

The Turbulent Flow, v2-f interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-e Interface for all the other settings.

PHYSICAL MODEL

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The v2-f model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are $C_{\mu v2f}$, C_τ, C_η, C_L, C_1, C_2, $C_{\varepsilon 1v2f}$, $C_{\varepsilon 2v2f}$, A_1, σ_{kv2f}, $\sigma_{\varepsilon v2f}$, $\sigma_{\zeta v2f}$, and κ_v.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p

- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep
- **Turbulent relative fluctuations** zeta
- **Elliptic blending function** alpha
- **Reciprocal wall distance** G

The v2-f interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

🔍	• The Laminar Flow Interface
	• Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
	• Theory for the Turbulent Flow Interfaces

Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

The following nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- Boundary Stress
- Fan
- Flow Continuity
- Fluid Properties
- Generate New Turbulence Model Interface
- Grille
- Gravity
- Initial Values
- Inlet
- Interior Fan
- Interior Wall

- Line Mass Source[1]
- Open Boundary
- Outlet
- Periodic Flow Condition
- Pipe Connection[1]
- Point Mass Source[1]
- Pressure Point Constraint
- Screen
- Symmetry
- Vacuum Pump
- Volume Force
- Wall

[1] A feature that may require an additional license

> For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations solved by the physics interface, except for volume forces which are added by the Volume Force feature. The node also provides an interface for defining the material properties of the fluid.

For the Turbulent Flow interfaces, the **Fluid Properties** node also adds the equations for the turbulence transport equations.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the single-phase flow interfaces are set to model isothermal flow. If a Heat Transfer interface is included in the component, the temperature field may alternatively be selected from this physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p+p_{ref}$, where p is the dependent pressure variable from the Navier-Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

FLUID PROPERTIES

Density

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible (at the physics interface level).

Dynamic Viscosity

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

Using the built-in variable for the shear rate magnitude, spf.sr, makes it possible to define arbitrary expressions of the dynamic viscosity as a function of the shear rate.

For laminar flow, the **Non-Newtonian power law** may be used to model the viscosity of a non-Newtonian fluid. The following model parameters are required for the **Non-Newtonian power law**:

- **Fluid consistency coefficient** m
- **Flow behavior index** n
- **Lower shear rate limit** $\dot{\gamma}_{\min}$

Alternatively, the **Non-Newtonian Carreau model** may be used to model the viscosity of a non-Newtonian fluid for laminar flow. The following Carreau model parameters are required:

- **Zero shear rate viscosity** μ_0
- **Infinite shear rate viscosity** $\mu_{\inf}$
- **Model parameter** λ and n

The non-Newtonian fluids models have a shear-rate dependent viscosity. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions. See Non-Newtonian Flow: The Power Law and the Carreau Model in the *CFD Module User's Guide*.

MIXING LENGTH LIMIT

For the Turbulent Flow, k-ε, Turbulent Flow, k-ω, and Rotating Machinery, Turbulent Flow k-ε interfaces, an upper limit on the mixing length is required.

When the **Mixing length limit** $l_{\mathrm{mix,lim}}$ is set to **Automatic**, it is evaluated to the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of

slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually.

DISTANCE EQUATION

For the Turbulent Flow, Low Reynolds number k-ε, Turbulent flow, Algebraic yPlus, Turbulent Flow, L-VEL, Turbulent flow, SST, the Turbulent Flow, Spalart-Allmaras, and the Turbulent Flow, v2-f interfaces, a Wall Distance interface is included.

When the **Reference length scale** l_{ref} is set to **Automatic,** it is evaluated to one tenth of the shortest side of the geometry bounding box. The solution to the wall distance equation is controlled by the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling because small objects would have too large an impact on the solution if the wall distance were measured exactly. The automatic value is usually a good choice but the value can become too high if the geometry consists of several slim entities. In such cases, it is recommended that the reference length scale is defined manually.

Volume Force

The **Volume Force** node specifies the volume force **F** on the right-hand side of the momentum equation.

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right] + \mathbf{F}$$

If several volume-force nodes are added to the same domain, then the sum of all contributions are added to the momentum equation.

Initial Values

The initial values serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver in a stationary simulation. Note that for a transient compressible-flow simulation employing a material for which the density depends on the pressure (such as air), discontinuities in the initial values trigger pressure waves even when the Mach number is small. The pressure waves must be resolved and this puts a restriction on the time step.

INITIAL VALUES

Initial values or expressions should be specified for the **Velocity field u** and the **Pressure** p.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p user input.

In the Turbulent Flow interfaces, initial values for the turbulence variables should also specified. Depending on the turbulent flow interface being used, additional initial values may be required for:

- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep
- **Reciprocal wall distance** G
- **Specific dissipation rate** om
- **Undamped turbulent kinematic viscosity** υ_0
- **Wall distance in viscous units** $yPlus$ (dimensionless). Under normal circumstances the default value need not be changed.
- **Tangential velocity in viscous units** $uPlus$ (dimensionless). Under normal circumstances the default value need not be changed.
- **Turbulent relative fluctuations** zeta
- **Elliptic blending function** alpha

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls. For turbulent flow, the description may involve wall functions and/or asymptotic expressions for certain turbulence variables.

BOUNDARY CONDITION

Select a **Boundary condition** for the wall.

- No Slip
- Slip

- Slip Velocity
- Leaking Wall

No Slip

No slip is the default boundary condition to model solid walls. A no slip wall is a wall where the fluid velocity relative to the wall velocity is zero. For a stationary wall that means that $\mathbf{u} = 0$.

For turbulent flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Physical Model** section of the interface settings.

When **Wall Treatment** is set to **Wall functions**, the **Apply wall roughness** option becomes available. When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. Select **Generic roughness** in order to specify more general roughness types.

- For **Sand roughness** an **Equivalent sand roughness height** k_{seq} should be specified.
- For **Generic roughness** a **Roughness height** k_{s} and a dimensionless **Roughness parameter** C_{s} should be specified.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Slip Velocity

In the microscale range, the flow condition at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a **Slip velocity** at the boundary. Two phenomena account for this velocity: noncontinuum effects and the flow induced by a thermal gradient along the boundary.

When the **Use viscous slip** check box is selected, the default **Slip length** L_{s} is **User defined**. Another value or expression may be entered if the default value is not applicable. For **Maxwell's model** values or expressions for the **Tangential momentum accommodation coefficient** a_{v} and the **Mean free path** λ should be specified. Tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

When the **Use thermal creep** check box is selected, a thermal creep contribution with **Thermal slip coefficient** σ_T is activated. Thermal slip coefficients are typically between 0.3 and 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

Slip velocity is available when **Turbulence Model** in the **Physical Model** section of the interface is set to **None**.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$ and adds a frictional force of the form

$$\mathbf{F}_{\text{fr}} = -\frac{\mu}{\beta}\mathbf{u}$$

where β is a slip length. The slip length is defined as $\beta = h_{\text{min}}/2$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements). The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance β outside of the wall.

The Navier Slip option is not available when selecting a turbulence model.

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_l$ through a perforated wall. The components of the **Fluid velocity** $\mathbf{u}_l$ on the leaking wall should be specified.

Leaking Wall is available when **Turbulence Model** in the **Physical Model** section of the interface is set to **None**.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{\text{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{\text{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u}_{\text{tr}}$ becomes equal to the frame movement. $\mathbf{u}_{\text{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u}_{\text{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall

to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall** $\mathbf{u}_w$ should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.

- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.

- For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the **Velocity of moving wall**, φ **component** v_w may also be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

	• Theory for the Wall Boundary Condition • Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Inlet

This condition should be used on boundaries for which there is a net flow into the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Outlet conditions when specifying an Inlet condition. For example, if the pressure is specified at the outlet, the velocity may be specified at the inlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties.

BOUNDARY CONDITION

The available **Boundary condition** options for an inlet are **Velocity**, **Laminar inflow**, **Mass flow**, and **Pressure**. After selecting a **Boundary Condition** from the list, a section with same or

a similar name displays underneath. For example, if **Velocity** is selected, a **Velocity** section, where further settings are defined, is displayed.

VELOCITY

The **Normal inflow velocity** is specified as $\mathbf{u} = -\mathbf{n}U_0$, where $\mathbf{n}$ is the boundary normal pointing out of the domain and U_0 is the normal inflow speed.

The **Velocity field** option sets the velocity vector to $\mathbf{u} = \mathbf{u}_0$. The components of the inlet velocity vector $\mathbf{u}_0$ should be defined for this choice.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure. If the reference pressure p_{ref}, defined at the physics interface level, is equal to 0, the value of the **Pressure** p_0, at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The **Suppress backflow** option adjusts the inlet pressure locally in order to prevent fluid from exiting the domain through the boundary. If you clear the suppress backflow option, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.

- **Flow direction** controls in which direction the fluid enters the domain.
    - For **Normal flow**, it prescribes zero tangential velocity component.
    - For **User defined**, an **Inflow velocity direction** $\mathbf{d_u}$ (dimensionless) should be specified. The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.

LAMINAR INFLOW

This boundary condition is applicable when the fluid enters the domain from a long pipe or channel, in which the laminar flow profile is fully developed. The normal stress at the inlet is determined from the flow conditions at the entrance to a fictitious channel of length L_{entr} appended to the boundary. The inflow can be specified by the **Average velocity** U_{av}, the **Flow rate** V_0, or the **Entrance pressure** p_{entr}.

For the **Entrance pressure** option, when **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{entr} user input.

For the **Average velocity** and **Flow rate** options, when **Include gravity** is selected in the interface **Physical model** section, **Use reduced pressure** should also be selected in the interface **Physical model** section because these two formulations are only valid with reduced pressure.

The **Entrance length** L_{entr} should be significantly greater than $0.06\mathrm{Re}D$, where Re is the Reynolds number and D is the inlet length scale (hydraulic diameter), in order that the flow can adjust to a fully developed laminar profile.

The **Constrain outer edges to zero** option forces the laminar profile to go to zero at the bounding points or edges of the inlet channel. Otherwise the velocity is defined by the boundary condition of the adjacent boundary in the computational domain. For example, if one end of a boundary with a **Laminar inflow** condition connects to a slip boundary, the laminar profile will have a maximum at that end.

MASS FLOW

The mass flow at an inlet can be specified by the **Mass flow rate,** the **Pointwise mass flux,** the **Standard flow rate**, or the **Standard flow rate (SCCM)**.

Mass Flow Rate

The **Mass flow rate** option sets the integrated mass flow across the entire boundary, the **Normal mass flow rate** to a specific value, m. The mass flow is assumed to be parallel to the boundary normal, and the tangential flow velocity is set to zero.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Pointwise Mass Flux

The **Pointwise mass flux** sets the mass flow parallel to the boundary normal. The tangential flow velocity is set to zero. The mass flux is a model input, which means that COMSOL Multiphysics can take its value from another physics interface when available. When **User defined** is selected a value or function M_f should be specified for the **Mass flux**.

Standard Flow Rate

The **Standard flow rate** Q_{sv} sets a standard volumetric flow rate, according to the SEMI standard E12-0303. The mass flow rate is specified as the volumetric flow rate of a gas at standard density — the **Mean molar mass** M_n divided by a **Standard molar volume** V_m (that is, the volume of one mole of a perfect gas at standard pressure and standard temperature). The flow occurs across the whole boundary in the direction of the boundary normal and is computed by a surface (3D) or line (2D) integral. The tangential flow velocity is set to zero.

The standard density can be defined directly, or by specifying a standard pressure and temperature, in which case the ideal gas law is assumed. The options in the **Standard flow rate defined by** list are:

- **Standard density**, for which the **Standard molar volume** V_m should be specified.

- **Standard pressure and temperature**, for which the **Standard pressure** P_{st} and the **Standard temperature** T_{st} should be defined.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Standard Flow Rate (SCCM)

The **Standard flow rate (SCCM)** boundary condition is equivalent to the **Standard flow rate** boundary condition, except that the flow rate is entered directly in SCCMs (standard cubic centimeters per minute) without the requirement to specify units. Here, the dimensionless **Number of SCCM units** Q_{sccm} should be specified.

TURBULENT FLOW SETTINGS

No additional inlet conditions are required for the algebraic turbulence models: Algebraic yPlus and L-VEL.

For the **Turbulent Flow, Spalart-Allmaras** interface, a value or expression for the **Undamped turbulent kinematic viscosity** v_0 should be specified.

For transport-equation turbulence models, apart from the Spalart-Allmaras turbulence model, the following settings are available under the **Specify turbulence length scale and intensity** option (see Table 3-2 for the default values):

- **Turbulent intensity** I_T

- **Turbulence length scale** L_T
- **Reference velocity scale** U_{ref}

For the v2-f turbulence model, the additional choice between **Isotropic_turbulence** and **Specify turbulence anisotropy** appears. For **Specify turbulence anisotropy**, a value for the turbulent relative fluctuations at the inlet, ζ_0, may be specified. When **Specify turbulence variables** is selected, values or expressions for the dependent turbulence variables should be defined. Availability is based on the physics interface and the boundary condition chosen.

- **Turbulent kinetic energy** k_0
- **Turbulent dissipation rate**, ε_0
- **Specific dissipation rate** ω_0
- **Turbulent relative fluctuations** ζ_0
- **Elliptic blending function** α_0

TABLE 3-2: DEFAULT VALUES FOR THE TURBULENT INTERFACES

NAME AND UNIT	VARIABLE	INLET	OPEN BOUNDARY	BOUNDARY STRESS
Turbulent intensity (dimensionless)	I_T	0.05	0.005	0.01
Turbulence length scale (m)	L_T	0.01	0.1	0.1
Reference velocity scale (m/s)	U_{ref}	1	1	1
Turbulent kinetic energy (m^2/s^2)	k_0	0.005	$2.5 \cdot 10^{-3}$	$1 \cdot 10^{-2}$
Turbulent dissipation rate (m^2/s^3)	ε_0	0.005	$1.1 \cdot 10^{-4}$	$1 \cdot 10^{-3}$
Specific dissipation rate (1/s)	ω_0	20	0.5	0.5
Undamped turbulent kinematic viscosity (m^2/s)	ν_0	3*spf5.nu		

About the Turbulent Intensity and Turbulence Length Scale Parameters
The **Turbulent intensity** I_T and **Turbulence length scale** L_T values are related to the turbulence variables via the following equations, Equation 3-2 for the Inlet and Equation 3-3 for the Open Boundary:

$$\text{Inlet } k = \frac{3}{2}(|\mathbf{U}|I_T)^2, \qquad \varepsilon = C_\mu^{3/4} \frac{k^{3/2}}{L_T} \tag{3-2}$$

$$\text{Open Boundary } k = \frac{3}{2}(I_T U_{\text{ref}})^2, \qquad \varepsilon = \frac{C_\mu^{3/4}}{L_T}\left(\frac{3(I_T U_{\text{ref}})^2}{2}\right)^{\frac{3}{2}} \tag{3-3}$$

For the Open Boundary and Boundary Stress options, and with any Turbulent Flow interface, inlet conditions for the turbulence variables also need to be specified. These conditions are used on the parts of the boundary where $\mathbf{u} \cdot \mathbf{n} < 0$, that is, where flow enters the computational domain.

For the **k-ω** and **SST** turbulence models the **Turbulent intensity** I_T and **Turbulence length scale** L_T values are related to the turbulence variables via the following equations, Equation 3-4 for the Inlet and Equation 3-5 for the Open Boundary:

$$\text{Inlet } k = \frac{3}{2}(|\mathbf{U}|I_T)^2, \qquad \omega = \frac{\sqrt{k}}{(\beta_0^*)^{1/4}L_T} \tag{3-4}$$

$$\text{Open Boundary } k = \frac{3}{2}(I_T U_{\text{ref}})^2, \qquad \omega = \frac{1}{(\beta_0^*)^{1/4}L_T}\sqrt{\left(\frac{3(I_T U_{\text{ref}})^2}{2}\right)} \tag{3-5}$$

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

②	• Prescribing Inlet and Outlet Conditions • Normal Stress Boundary Condition

②	For recommendations of physically sound values for the **Turbulent intensity** I_T and **Turbulence length scale** L_T, see Inlet Values for the Turbulence Length Scale and Turbulent Intensity.

▥	*Non-Newtonian Flow* (inlet): Application Library path **CFD_Module/Single-Phase_Tutorials/non_newtonian_flow**

Outlet

This condition should be used on boundaries for which there is a net outflow from the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Inlet conditions when specifying an Outlet condition. For example, if the velocity is specified at the inlet, the pressure may be specified at the outlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties. Selecting appropriate outlet conditions for the Navier-Stokes equations is a nontrivial task. Generally, if there is something interesting happening at an outflow boundary, the computational domain should be extended to include this phenomenon.

BOUNDARY CONDITION

The available **Boundary condition** options for an outlet are **Pressure, Laminar outflow**, and **Velocity**.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure. The tangential stress component is set to zero. If the reference pressure p_{ref}, defined at the physics interface level, is equal to 0, the value of the **Pressure** p_0, at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The **Normal flow** option changes the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.

- The **Suppress backflow** check box is selected by default. This option adjusts the outlet pressure in order to prevent fluid from entering the domain through the boundary.

VELOCITY

See the **Inlet** node Velocity section for the settings.

LAMINAR OUTFLOW

This boundary condition is applicable when the flow exits the domain into a long pipe or channel, at the end of which a laminar flow profile is fully developed. The normal stress at the outlet is determined from the flow conditions at the end of a fictitious channel

appended to the outlet boundary. The outflow can be specified by the **Average velocity** U_{av}, the **Flow rate** V_0, or the **Exit pressure** p_{exit}.

For the **Entrance pressure** option, when **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{exit} user input.

The **Exit length** L_{exit} should be significantly greater than 0.06ReD, where Re is the Reynolds number, and D is the outlet length scale (hydraulic diameter), in order that the flow can adjust to a fully developed laminar profile.

The **Constrain outer edges to zero** option forces the laminar profile to go to zero at the bounding points or edges of the outlet channel. Otherwise, the velocity is defined by the boundary condition of the adjacent boundary in the computational domain. For example, if one end of a boundary with a **Laminar outflow** condition connects to a slip boundary, the laminar profile will have a maximum at that end.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (👁) and selecting **Advanced Physics Options**.

> 🔍   Prescribing Inlet and Outlet Conditions

Symmetry

The **Symmetry** boundary condition prescribes no penetration and vanishing shear stresses. The boundary condition is a combination of a Dirichlet condition and a Neumann condition:

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad \left(-p\mathbf{I} + \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) \right)\mathbf{n} = \mathbf{0}$$

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = \mathbf{0}$$

for the compressible and incompressible formulations. The Dirichlet condition takes precedence over the Neumann condition, and the above equations are equivalent to the following equation for both the compressible and incompressible formulations:

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad \mathbf{K} - (\mathbf{K} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$
$$\mathbf{K} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n}$$

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at $r = 0$. The software automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the z direction and adds an **Axial Symmetry** node that implements these conditions on the axial symmetry boundaries only.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (![icon]) and selecting **Advanced Physics Options**.

Open Boundary

The **Open Boundary** condition describes boundaries in contact with a large volume of fluid. Fluid can both enter and leave the domain on boundaries with this type of condition.

BOUNDARY CONDITIONS

The **Boundary condition** options for open boundaries are **Normal stress** and **No viscous stress**.

Normal Stress

The **Normal stress** f_0 condition implicitly imposes $p \approx f_0$.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 user input.

No Viscous Stress

The **No Viscous Stress** condition specifies vanishing viscous stress on the boundary. This condition does not provide sufficient information to fully specify the flow at the open boundary and must at least be combined with pressure constraints at adjacent points.

The **No viscous stress** condition prescribes:

$$\left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right)\mathbf{n} = \mathbf{0}$$

$$\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} = \mathbf{0}$$

for the compressible and the incompressible formulations. This condition can be useful in some situations because it does not impose any constraint on the pressure. A typical example is a model with volume forces that give rise to pressure gradients that are hard to prescribe in advance. To make the model numerically stable, this boundary condition should be combined with a point constraint on the pressure.

This boundary condition is not compatible with the projection method equation form.

TURBULENCE CONDITIONS

See Turbulent Flow Settings.

Boundary Stress

The **Boundary Stress** node adds a boundary condition that represents a general class of conditions also known as traction boundary conditions.

BOUNDARY CONDITION

The **Boundary condition** options for the boundary stress are **General stress**, **Normal stress**, and **Normal stress, normal flow**.

General Stress

When **General stress** is selected, the components for the **Stress F** should be specified. The total stress on the boundary is set equal to the given stress **F**:

$$\left(-p\mathbf{I} + \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = \mathbf{F}$$

$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = \mathbf{F}$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n} - \mathbf{n} \cdot \mathbf{F} \tag{3-6}$$

If $\partial u_n/\partial n$ is small, Equation 3-6 states that $p \approx -\mathbf{n}\cdot\mathbf{F}$.

Normal Stress

Normal Stress is described for the Open Boundary node.

Normal Stress, Normal Flow

For **Normal stress, normal flow**, the magnitude of the **Normal stress** f_0 should be specified. The tangential velocity is set to zero on the boundary:

$$\mathbf{n}^T\left(-p\mathbf{I} + \left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = -f_0, \qquad \mathbf{t} \cdot \mathbf{u} = 0$$

$$\mathbf{n}^T(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -f_0, \qquad \mathbf{t} \cdot \mathbf{u} = 0$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n} + f_0 \qquad (3\text{-}7)$$

If $\partial u_n/\partial n$ is small, Equation 3-7 states that $p \approx f_0$.

This boundary condition is not compatible with the projection method equation form.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 or $p_{hydro}\mathbf{n}$ is added to $\mathbf{F}$ depending of the selected option.

Turbulent Boundary Type

The **Turbulent boundary type** options for this boundary condition are **Open boundary**, **Inlet**, and **Outlet**.

- For **Open boundary** parts of the boundary are expected to be outlets and other parts are expected to be to be inlets.

- The **Inlet** option should be selected when the whole boundary is expected to be an inlet.

- The **Outlet** option should be used when the whole boundary is expected to be an outflow boundary. In this case, homogeneous Neumann conditions are applied for the turbulence variables, that is, for k and ε

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla\varepsilon \cdot \mathbf{n} = 0$$

and additionally for the v2-f model

$$\nabla\alpha \cdot \mathbf{n} = 0 \qquad \nabla\zeta \cdot \mathbf{n} = 0$$

for k and ω

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla \omega \cdot \mathbf{n} = 0$$

or for the Spalart-Allmaras model

$$\nabla \tilde{\nu} \cdot \mathbf{n} = 0$$

TURBULENCE CONDITIONS

See Turbulent Flow Settings.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

If Normal Stress, Normal Flow is selected as the **Boundary condition**, then to **Apply reaction terms on** all dependent variables, the **All physics (symmetric)** option should be selected. Alternatively, the **Individual dependent variables** could be selected to restrict the reaction terms as needed.

Screen

The **Screen** condition models interior wire-gauzes, grilles, or perforated plates as thin permeable barriers. Common correlations are included for resistance and refraction coefficients. The Screen boundary condition can only be applied on interior boundaries.

SCREEN TYPE

The available options for the **Screen type** are **Wire gauze**, **Square mesh**, **Perforated plate**, and **User defined**. The settings are defined by the equations shown based on the selection (excluding User defined) which in turn adjusts what is available in the **Parameters** section.

PARAMETERS

If **Wire gauze**, **Square mesh**, or **Perforated plate** is selected as the **Screen type**, values or expressions for the **Solidity** σ_s (ratio of blocked area to total area of the screen) should be specified.

• For **Wire gauze** a value or expression for the **Wire diameter** d should also be specified.

- The **User defined** options requires the dimensionless **Resistance coefficient** K.

- For all screen types, the **Refraction** defaults to **Wire gauze**. With the **User defined** option, a different **Refraction coefficient** η (dimensionless) can be specified.

🔍	• Screen Boundary Condition
	• Theory for the Nonisothermal Screen Boundary Condition

Vacuum Pump

The **Vacuum Pump** node models the effective outlet pressure created by a vacuum pump device that is attached to the outlet.

PARAMETERS

The **Static pressure curve** option defines a lumped curve—**Linear**, **Static pressure curve data**, or **User defined**.

Linear

For the **Linear** option, values or expressions should be specified for the **Static pressure at no flow** p_{nf} and the **Free delivery flow rate** $V_{0,fd}$.

The static pressure curve value is equal to the static pressure at no flow rate when $V_0 < 0$ and equal to 0 when the flow rate is larger than the free delivery flow rate.

Static Pressure Curve Data

The **Static pressure curve data** option can be used to enter or load data under the **Static Pressure Curve Data** section below. The interpolation between points given in the **Static Pressure Curve Data** table is defined using the **Interpolation function type** list in the **Static Pressure Curve Interpolation** section.

User Defined

The **User defined** option can be used to enter a different value or expression. The flow rate across the selection where this boundary condition is applied is defined by `phys_id.V0` where `phys_id` is the name (for example, `phys_id` is `spf` by default for this physics interface). In order to avoid unexpected behavior, the function used for the fan curve is the maximum of the user-defined function and 0.

STATIC PRESSURE CURVE DATA

This section displays when **Static pressure curve data** is selected as the **Static pressure curve**. In the table, values or expressions for the **Flow rate** and **Static pressure curve** should be

specified. Alternatively, a text file can be imported by clicking the **Load from file** button
(📂) under the table.

UNITS

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. Units can be specified here for the **Flow rate** and **Static pressure curve**.

STATIC PRESSURE CURVE INTERPOLATION

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. The available options for the **Interpolation function type** are **Linear**, **Piecewise cubic**, and **Cubic spline**.

The extrapolation method always returns a constant value. In order to avoid problems with undefined data, the function used for the boundary condition is the maximum of the interpolated function and 0.

🔍	Vacuum Pump Boundary Condition

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group. Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, it is recommended to only include two boundaries.

No input is required when **Compressible flow (Ma<0.3)** is selected for **Compressibility** under the **Physical Model** section for the physics interface. Typically when a periodic boundary condition is used with a compressible flow, the pressure is the same at both boundaries and the flow is driven by a volume force.

PRESSURE DIFFERENCE

This section is available when **Incompressible flow** is selected for **Compressibility** under the **Physical Model** section for the physics interface.

A value or expression should be specified for the **Pressure difference**, $p_{src} - p_{dst}$. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (👁) and selecting **Advanced Physics Options**.

ORIENTATION OF SOURCE

For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

This boundary condition is not compatible with the projection method equation form.

Fan

The **Fan** condition is used to define the flow direction (inlet or outlet) and the fan parameters on exterior boundaries. The Interior Fan condition is available on interior boundaries.

FLOW DIRECTION

The **Flow direction** can be set to **Inlet** or **Outlet**. When a boundary has been selected, an arrow displays in the **Graphics** window to indicate the selected flow direction. The arrow can be updated if the selection changes by clicking any node in the **Model Builder** and then clicking the **Fan** node again to update the **Graphics** window.

The **Inlet Flow direction** controls in which direction the fluid enters the domain.

- For **Normal flow** it sets the tangential velocity component to zero.
- For **User defined** an **Inflow velocity direction** $\mathbf{d_u}$ (dimensionless) should be specified. The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.
- For **Swirl flow** (which is available for 3D or 2D axisymmetric when the **Swirl flow** check box in **Physical Model Properties** is checked) it specifies a swirl flow on the downstream side of the fan based on the **Rotation axis base point** $\mathbf{r}_{bp}$, **Revolutions per time** f, **Rotational direction** and **Swirl ratio** c_{sf}.

PARAMETERS

When **Inlet** is selected as the **Flow direction**, the **Input pressure** p_{input} defines the pressure at the fan inlet.

When **Outlet** is selected as the **Flow direction**, the **Exit pressure** p_{exit} defines the pressure at the fan outlet.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{input} or p_{exit} user input.

For either flow direction, **Static pressure curve** specifies a fan curve — **Linear**, **Static pressure curve data**, or **User defined**.

Linear

For both **Inlet** and **Outlet** flow directions, if **Linear** is selected, values or expressions for the **Static pressure at no flow** p_{nf} and the **Free delivery flow rate** $V_{0,\text{fd}}$ should be specified. The static pressure curve is equal to the static pressure at no flow rate when $V_0 < 0$ and equal to 0 when the flow rate is larger than the free delivery flow rate.

User Defined

With the **User defined** option, a different value or expression for the **Static pressure curve** can be specified. The flow rate across the selection where this boundary condition is applied is defined by `phys_id.V0` where `phys_id` is the name (for example, `phys_id` is `spf` by default for laminar single-phase flow). In order to avoid unexpected behavior, the function used for the fan curve returns the maximum of the user-defined function and 0.

Static Pressure Curve Data

The **Static pressure curve data** can be entered or loaded under the **Static Pressure Curve Data** section that displays for this option. The interpolation between points given in the table is defined using the **Interpolation function type** list in the **Static Pressure Curve Interpolation** section.

UNITS

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. Units can be specified for the **Flow rate** and **Static pressure**.

STATIC PRESSURE CURVE DATA

When **Static pressure curve data** is selected as the **Static pressure curve**, a table appears, where values or expressions the **Flow rate** and **Static pressure** can be specified or imported from a text file by clicking the **Load from file** button (📂) under the table. Units can be specified for the **Flow rate** and the **Static pressure curve**.

STATIC PRESSURE CURVE INTERPOLATION

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. The available options for the **Interpolation function type** are **Linear**, **Piecewise cubic**, and **Cubic spline**.

The extrapolation method always returns a constant value. In order to avoid problems with undefined data, the function used for the boundary condition returns the maximum of the interpolated function and 0.

TURBULENCE CONDITIONS ON FAN OUTLET

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε, specific dissipation rate, ω, or turbulent relative fluctuations, ζ, the values of the **Turbulent kinetic energy**, **Turbulent relative fluctuations** (for the v2-f turbulence model) and the **Turbulent dissipation rate** or **Specific dissipation rate** on the downstream side of the fan should be specified. Alternatively, the **Reference velocity scale** can be used to specify default values.

> 🔍   Fan and Grille Boundary Conditions

Interior Fan

The **Interior Fan** condition represents interior boundaries where a fan condition is set using a fan pressure curve to avoid an explicit representation of the fan. The **Interior Fan** defines a boundary condition on a slit for laminar flow. That means that the pressure and the velocity can be discontinuous across this boundary.

One side represents a flow inlet; the other side represents the fan outlet. The fan boundary condition ensures that the mass flow rate is conserved between its inlet and outlet:

$$\int_{\text{inlet}} \rho \mathbf{u} \cdot \mathbf{n} + \int_{\text{outlet}} \rho \mathbf{u} \cdot \mathbf{n} = 0$$

This boundary condition acts like a Pressure Conditions boundary condition on each side of the fan. The pressure at the fan outlet is fixed so that the mass flow rate is conserved. On the fan inlet the pressure is set to the pressure at the fan outlet minus the pressure drop induced by the fan. The pressure drop is defined from the static pressure curve, and is usually a function of the flow rate. To define a fan boundary condition on an exterior boundary, the Fan condition should be used instead.

INTERIOR FAN

The **Flow direction** can be defined by selecting **Along normal vector** or **Opposite to normal vector**. This defines which side of the boundary is the fan's inlet and which side is the fan's outlet.

TURBULENCE CONDITIONS ON FAN OUTLET

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε, specific dissipation rate, ω, or turbulent relative fluctuations, ζ, the values of the **Turbulent kinetic energy**, **Turbulent relative fluctuations** (for the v2-f turbulence model) and the **Turbulent dissipation rate** or **Specific dissipation rate** on the downstream side of the fan should be specified. Alternatively, the **Reference velocity scale** can be used to specify default values

After a boundary has been selected, an arrow displays in the **Graphics** window to indicate the selected flow direction. If the selection changes, the arrow can be updated by clicking any node in the **Model Builder** and then clicking the **Interior fan** node again to update the **Graphics** window.

The rest of the settings for this section are the same as for the Fan node. See Linear and Static Pressure Curve Data for details.

Fan Defined on an Interior Boundary

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an internal boundary. It allows discontinuities (velocity, pressure, and turbulence variables) across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-slip conditions on interior curves

and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed. The Interior Wall boundary condition is only available for single-phase flow. It is compatible with laminar and turbulent flow.

BOUNDARY CONDITION

The available **Boundary condition** options are **No slip** or **Slip**.

No Slip

The **No slip** condition models solid walls. No slip walls are walls where the fluid velocity relative to the wall is zero. For a interior stationary wall this means that $\mathbf{u} = 0$ on both sides of the wall..

For turbulent flows, the no slip conditions may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Physical Model** section of the interface settings.

When **Wall Treatment** is set to **Wall functions**, the **Apply wall roughness** option becomes available. When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. Select **Generic roughness** in order to specify more general roughness types.

- For **Sand roughness** an **Equivalent sand roughness height** k_{seq} should be specified.
- For **Generic roughness** a **Roughness height** k_{s} and a dimensionless **Roughness parameter** C_{s} should be specified.

Slip

The **Slip** condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It implicitly assumes that there are no viscous effects on either side of the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the important effect is to prevent the exchange of fluid between the regions separated by the interior wall.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{\text{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{\text{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u}_{\text{tr}}$ becomes equal to

the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

?	• Wall • Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

This boundary condition is not compatible with the projection method.

Grille

The **Grille** boundary condition models the pressure drop caused by having a grille that covers the inlet or outlet.

PARAMETERS

When **Inlet** is selected as the **Flow direction**, the **Input pressure** p_{input} defines the pressure at the fan inlet.

When **Outlet** is selected as the **Flow direction**, the **Exit pressure** p_{exit} defines the pressure at the fan outlet.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{input} or p_{exit} user input.

When **Quadratic loss** is selected for the **Static pressure curve**, the **Quadratic loss coefficient** qlc should be specified. qlc defines the static pressure curve which is a piecewise quadratic

function equal to 0 when the flow rate is < 0, equal to $V_0^2 \cdot qlc$ when the flow rate is > 0. See Fan for other settings for the Laminar Flow interface. Note that for the Turbulent Flow interfaces, **Quadratic loss** is the only available option for **Static pressure curve**.

TURBULENCE CONDITIONS

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε, specific dissipation rate, ω, or turbulent relative fluctuations, ζ, the **Specify turbulent length scale and intensity** and **Specify turbulence variables** options are available for the turbulence conditions on the downstream side of the grille. Alternatively, the **Reference velocity scale** can be used to specify default values.

🔍	Fan and Grille Boundary Conditions

Pipe Connection

This feature is available with a license for the Pipe Flow Module. For details, see Pipe Connection the in the *Pipe Flow Module User's Guide*.

Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

A Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Flow Continuity** node, additional Fallback feature subnodes can be added.

This boundary condition is not compatible with the projection method.

Pressure Point Constraint

The **Pressure Point Constraint** condition can be used to specify the pressure level. If it is not possible to specify the pressure level using a boundary condition, the pressure level must be set in some other way, for example, by specifying a fixed pressure at a point.

PRESSURE CONSTRAINT

The relative pressure value is set by specifying the **Pressure** p_0. Or, if the reference pressure p_{ref} defined at the physics interface level is equal to zero, p_0 represents the absolute pressure.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (![icon]) and selecting **Advanced Physics Options**.

Point Mass Source

This feature requires at least one of the following licenses: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Point Mass Source** feature models mass flow originating from an infinitely small domain centered around a point

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Batteries & Fuel Cells Module, there are two nodes: one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

SOURCE STRENGTH

The source **Mass flux**, $\dot{q}_p$ should be specified. A positive value results in mass being ejected from the point into the computational domain. A negative value results in mass being removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that a point source located on a symmetry plane has twice the given strength.

<table>
<tr><td>🔍</td><td>Mass Sources for Fluid Flow in the COMSOL Multiphysics Reference Manual</td></tr>
</table>

Line Mass Source

This feature requires at least one of the following licenses: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Line Mass Source** feature models mass flow originating from a tube region with infinitely small radius.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Batteries & Fuel Cells Module, there are two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the axis of symmetry
3D	Edges

SOURCE STRENGTH

The source **Mass flux**, $\dot{q}_l$, should be specified. A positive value results in mass being ejected from the line into the computational domain and a negative value means that mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This, for example, has the effect that a line source located on a symmetry plane has twice the given strength.

🔍	Mass Sources for Fluid Flow in the *COMSOL Multiphysics Reference Manual*

Generate New Turbulence Model Interface

This global feature requires a CFD Module license. It can be used to create a new turbulent flow interface based on the current laminar or turbulent flow interface. The new interface inherits the property values from the original interface except for the turbulence related ones. All the features in the original interface are also inherited by the newly created interface except for the **Generate New Turbulence Model Interface** feature itself and the **Initial Values** feature. The initial values of the new interface are either default values or estimates from the solution of the original interface depending on the settings in the **Generate New Turbulence Model Interface** feature.

MODEL GENERATION

This section contains a boolean input, **Copy only active settings**, which is selected by default. When selected, the disabled features and settings in the original model are not transferred to the new interface.

The **Create** button generates the new interface.

TURBULENCE MODEL INTERFACE

All available turbulence models can be selected from the drop-down list:

- Turbulent Flow, k-ε
- Turbulent Flow, Algebraic yPlus
- Turbulent Flow, *L-VEL*
- Turbulent Flow, k-ω
- Turbulent Flow, SST
- Turbulent Flow, Low Reynolds number k-ε
- Turbulent Flow, Spalart-Allmaras
- Turbulent Flow, v^2-f

The **Study** section contains two drop-down lists: **Study type** and **Initial value from study**. When Turbulent Flow, k-ε or Turbulent Flow, k-ω is selected as the **Turbulence Model Interface**, the **Study type** contains the following two options:

- **Stationary**
- **Time-dependent**

The default value is **Stationary**. For all other turbulence models, the available **Study type** options are:

- **Stationary with initialization**
- **Transient with initialization**

with default value **Stationary with initialization**. Note that the created new study only solves for the new turbulence interface.

Initial value from study contains a list of the studies that are currently in the model. It can also be set to **None**. If there is no study available, the default option is **None**. If there are available studies, the first study is the default option.

Gravity

This feature requires at least one of the following licenses: CFD Module, Heat Transfer Module.

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value.

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{const}\mathbf{e_z}$ in 2Daxi and 3D and $-g_{const}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

The Rotating Machinery, Laminar and Turbulent Flow Interfaces

The **Rotating Machinery, Laminar Flow (rmspf)** and **Rotating Machinery, Turbulent Flow (rmspf)** interfaces, found under the **Single-Phase Flow>Rotating Machinery** branch ( ) when adding a physics interface, are used for modeling flow where one or more of the boundaries rotate in a periodic fashion. This is used for mixers and propellers.

The physics interfaces support compressible and incompressible flow, the flow of non-Newtonian fluids described by the Power Law and Carreau models, and also turbulent flow. The physics interfaces also support creeping flow, although the shallow channel approximation is redundant.

In this section:

- The Rotating Machinery, Laminar Flow Interface
- The Rotating Machinery, Turbulent Flow, Algebraic yPlus Interface
- The Rotating Machinery, Turbulent Flow, L-VEL Interface
- The Rotating Machinery, Turbulent Flow, k-e Interface
- Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces

The Rotating Machinery, Laminar Flow Interface

The **Rotating Machinery, Laminar Flow (rmspf)** interface ( ), found under the **Single-Phase Flow>Rotating Machinery** branch ( ) when adding a physics interface, is used to simulate flow at low to moderate Reynolds numbers in geometries with one or more rotating parts. The physics interface supports incompressible and compressible flows at low Mach numbers (typically less than 0.3). It also supports modeling of non-Newtonian fluids. The physics interface is available for 3D and 2D components.

There are two study types available for this physics interface. Using the **Time Dependent** study type, rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and rotation is accounted for by the inclusion of centrifugal and Coriolis forces. In both types, the momentum balance is governed by the Navier-Stokes equations, and the mass conservation is governed by the continuity equation. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following default physics nodes are also added in the **Model Builder**—**Fluid Properties**, **Wall**, **Rotating Wall**, and **Initial Values.** Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Rotating Machinery, Laminar Flow** to select physics features from the context menu. See Rotating Domain, Initial Values, and Rotating Wall.

It should be noted that only one physics interface at a time can be used to control the solid body rotation in the machinery under investigation. If more than one rotating machinery interface is added to the same component, the last interface in the list (top to bottom) will control the rotation.

🔍	Pseudo Time Stepping for Laminar Flow Models

▥	*Laminar Flow in a Baffled Stirred Mixer*: Application Library path **CFD_Module/Single-Phase_Tutorials/baffled_mixer**

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `rmspf`.

In addition to the settings described below, see The Creeping Flow, Laminar Flow, and Turbulent Flow Interfaces for all the other settings available. See Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces for links to all the physics nodes.

ADVANCED SETTINGS

To display this section, click the **Show** button (▼) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Pseudo time stepping

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Frozen Rotor** equation form is used. (Frozen rotor is a pseudo stationary formulation.) When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** CFL_{loc} (dimensionless).

The Rotating Machinery, Turbulent Flow, Algebraic yPlus Interface

The **Rotating Machinery, Turbulent Flow, Algebraic yPlus (rmspf)** interface (⚞), found under the **Single-Phase Flow>Rotating Machinery** branch (⚞) when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Algebraic yPlus interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled wall distance. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

Two study types available for this physics interface. Using the **Transient with Initialization** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor with Initialization** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. Both study types includes an initial Wall Distance Initialization step in order to compute the wall distance. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder**—**Fluid Properties**, **Wall**, **Rotating Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Rotating Machinery, Turbulent Flow, Algebraic yPlus** to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the settings below, see the advanced settings for the The Rotating Machinery, Laminar Flow Interface, and the The Creeping Flow, Laminar Flow, and Turbulent Flow Interfaces.

The turbulence model parameters for the Algebraic yPlus model, κ_a and B_a, have been optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u**

- **Pressure** p

- **Reciprocal wall distance** G

- **Wall distance in viscous units** yPlus (dimensionless)

The Rotating Machinery, Turbulent Flow, L-VEL Interface

The **Rotating Machinery, Turbulent Flow, L-VEL (rmspf)** interface ( ), found under the **Single-Phase Flow>Rotating Machinery** branch ( ) when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, L-VEL interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled fluid flow velocity tangential to the nearest wall. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

Two study types available for this physics interface. Using the **Transient with Initialization** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor with Initialization** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. Both study types includes an initial Wall Distance Initialization step in order to compute the wall distance. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder**—**Fluid Properties**, **Wall**, **Rotating Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Rotating Machinery, Turbulent Flow, L-VEL** to select physics features from the context menu. For information about the available physics

features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the interface settings defined below, see the advanced settings for the The Rotating Machinery, Laminar Flow Interface, and the settings in The Creeping Flow, Laminar Flow, and Turbulent Flow Interfaces.

TURBULENCE MODEL PARAMETERS

The turbulence model parameters for the L-VEL model, κ_l and E_l, have been optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u**
- **Pressure** p
- **Reciprocal wall distance** G
- **Tangential velocity in viscous units** uPlus (dimensionless)

The Rotating Machinery, Turbulent Flow, k-ε Interface

The **Rotating Machinery, Turbulent Flow, k-ε (rmspf)** interface ( ), found under the **Single-Phase Flow>Rotating Machinery** branch ( ) when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible and compressible flows at low Mach numbers (typically less than 0.3).

The momentum balance is governed by the Navier-Stokes equations, and the mass conservation is governed by the continuity equation. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

There are two study types available for this physics interface. Using the **Time Dependent** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder**—**Fluid Properties**, **Wall**, **Rotating Wall**, and **Initial Values**. Then, from the

Physics toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Rotating Machinery, Turbulent Flow, k-ε** to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the defined settings below, see the advanced settings for the The Rotating Machinery, Laminar Flow Interface, and the settings in The Creeping Flow, Laminar Flow, and Turbulent Flow Interfaces.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1}, C_{e2}, C_μ, σ_k, σ_e, κ_v, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep

Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces

All versions of the Rotating Machinery, Fluid Flow interfaces include the following unique domain, boundary, point, and pair physics nodes.

- Wall
- Interior Wall
- Contact Angle
- Initial Values

- Rotating Domain
- Rotating Wall
- Rotating Interior Wall
- Stationary Free Surface

The nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

The following nodes, also available in the Rotating Machinery, Fluid Flow interfaces, are described for the Laminar Flow interface:

- No Viscous Stress
- Flow Continuity
- Fluid Properties
- Inlet
- Line Mass Source
- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Screen
- Symmetry
- Volume Force

Initial Values

The node prescribes initial values for the dependent variables solved for. The initial values can serve as initial conditions for a transient simulation, or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter values or expressions for the initial value of the **Velocity field u** and for the **Pressure** p.

When using a turbulence model, also enter values or expressions for the turbulence variables solved for.

Rotating Domain

This node defines a domain as rotating with respect to a stationary coordinate system. The mesh inside the domain, including external or internal boundaries, is defined to rotate as a solid body. The node prescribed the rotation rotational frequency and direction as well as the axis of rotation. If there is more than one rotating domain, these must not intersect.

The angular displacement, ω (SI unit: rad), of the rotating domain is computed from a specified angular velocity w (SI unit: rad/s) by solving the ODE

$$\frac{d\omega}{dt} = w(t).$$ (3-8)

Since the angular displacement is solved for, the domain rotation can be specified using any type of angular velocity (constant, analytic, interpolation function, and so forth).

3D Components

For 3D components, select the **Axis of rotation**, the z-axis is the default. If the x-axis is selected, it corresponds to a rotational axis $(1, 0, 0)$ with the origin as the base point. This is the same for the y-axis and z-axis. For **User defined** enter values for the **Rotation axis base point** $\mathbf{r}_{bp}$ and **Rotation axis direction** $\mathbf{r}_{ax}$.

Select a **Rotational frequency**—**Revolutions per time** (the default) or **Angular velocity**.

- For **Revolutions per time** enter a value or expression in the field and select a **Rotational direction**—**Positive angular velocity** or **Negative angular velocity**. The angular velocity in this case is defined as the input multiplied by $2 \cdot \pi$.

- For **Angular velocity** enter an **Angular velocity** w.

2D Components

For 2D components, enter coordinates for the **Rotation axis base point** $\mathbf{r}_{bp}$. The default is the origin $(0, 0)$.

Select a **Rotational frequency**—**Revolutions per time** or **Angular velocity**.

- For **Revolutions per time** enter a value or expression in the field and select a **Rotational direction**—**Clockwise** or **Counterclockwise**. The angular velocity in this case is defined as the input multiplied by $2 \cdot \pi$.

- For **Angular velocity** enter an **Angular velocity** w.

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls. For turbulent flow, the description may involve wall functions and/or asymptotic expressions for certain turbulence variables.

Select a **Boundary condition** for the wall.

- No Slip[1]
- Slip
- Sliding Wall
- Moving Wall
- Leaking Wall

- Slip Velocity
- Wall Functions[2]
- Sliding Wall (Wall Functions)
- Moving Wall (Wall Functions)

[1] The default for laminar flow.

[2] The default for turbulence model: k-ε.

No Slip

No slip is the default boundary condition for a stationary solid wall for laminar flow (and SST, Low Re k-ε, Algebraic yPlus, L-VEL, and Spalart-Allmaras turbulence models). The condition prescribes $\mathbf{u} = 0$; that is, the fluid at the wall is not moving.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Sliding Wall

The **Sliding wall** boundary condition is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall** $\mathbf{u}_w$ should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.

- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.

- For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the **Velocity of moving wall**, φ **component** v_w may also be specified.

Moving Wall

For an arbitrary wall movement, the condition $\mathbf{u} = \mathbf{u}_\text{w}$ may be prescribed. In this case, the components of the **Velocity of moving wall $\mathbf{u}_\text{w}$** should be specified.

Specifying this boundary condition does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_\text{l}$ through a perforated wall. The components of the **Fluid velocity $\mathbf{u}_\text{l}$** on the leaking wall should be specified.

Electroosmotic Velocity

When an electric field drives a flow along the boundary, the components for the **Electric field $\mathbf{E}$** along with the **Electroosmotic mobility** μ_eo should be defined. The **Built-in expression** for the **Electroosmotic mobility** requires values or expressions for the **Zeta potential** ζ and the **Relative permittivity** ε_r

This option requires the Microfluidics Module.

Slip Velocity

In the microscale range, the flow condition at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a **Slip velocity** at the boundary. Two phenomena account for this velocity: noncontinuum effects and the flow induced by a thermal gradient along the boundary. The components of **Velocity of moving wall: $\mathbf{u}_\text{w}$** should be specified. Zero values are used for a stationary wall.

When the **Use viscous slip** check box is selected, the default **Slip length L_s** is **User defined**. Another value or expression may be entered if the default value is not applicable. For **Maxwell's model** values or expressions for the **Tangential momentum accommodation coefficient** a_v and the **Mean free path** λ should be specified. Tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

When the **Use thermal creep** check box is selected, a thermal creep contribution with **Thermal slip coefficient** σ_T is activated. Thermal slip coefficients are typically between 0.3 and 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

This boundary condition is not compatible with the projection method.

Wall Functions

The **Wall functions** boundary condition replaces the no-slip condition on solid walls for certain turbulence models such as the k-ε and k-ω models. Wall functions are used to model the thin region with large gradients in flow variables near the wall.

When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. More general roughness types can be specified by selecting **Generic roughness**.

- For **Sand roughness** an **Equivalent sand roughness height** k_{seq} should be specified.
- For **Generic roughness** a **Roughness height** k_s and a dimensionless **Roughness parameter** C_s should be specified.

Sliding Wall (Wall Functions)

The **Sliding wall (wall functions)** boundary condition applies wall functions to a wall in a turbulent flow where the velocity magnitude in the tangential direction of the wall is prescribed. The tangential direction is determined in the same manner as in the Sliding Wall feature. The component values or expressions for the **Velocity of sliding wall** $\mathbf{u}_w$ should be specified.

The **Apply wall roughness** option is available for the **Sliding wall (wall functions)**. See Wall Functions for details.

Moving Wall (Wall Functions)

Applying this boundary condition does not automatically cause an associated geometry change. The **Moving wall (wall functions)** boundary condition applies wall functions to a wall with prescribed velocity $\mathbf{u}_w$ in a turbulent flow. Component values or expressions for the **Velocity of moving wall** $\mathbf{u}_w$ should be specified.

The **Apply wall roughness** option is available for the **Moving wall (wall functions)**. See Wall Functions for details.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (👁) and selecting **Advanced Physics Options**.

②	• Theory for the Wall Boundary Condition
	• Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an internal boundary. It allows discontinuities (velocity, pressure, and turbulence variables) across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-slip conditions on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed. The Interior Wall boundary condition is only available for single-phase flow. It is compatible with laminar and turbulent flow.

BOUNDARY CONDITION

The available **Boundary condition** options are **No slip** (for laminar flow), **Wall functions** (for turbulent flow), **Slip**, or **Moving wall**.

No Slip

The **No slip** condition prescribes $\mathbf{u} = 0$ on both sides of the boundary; that is, the fluid at the wall is not moving.

Wall Functions

For the k-ε turbulence model, the **Wall functions** boundary condition is used to model the thin region with large gradients in flow variables near a stationary, solid wall.

When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. More general roughness types can be specified by selecting **Generic roughness**.

- For **Sand roughness** an **Equivalent sand roughness height** k_{seq} should be specified.
- For **Generic roughness** a **Roughness height** k_s and adimensionless **Roughness parameter** C_s should be specified.

Slip

The **Slip** condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It implicitly assumes that there are no viscous effects on either side of the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the important effect is to prevent the exchange of fluid between the regions separated by the interior wall.

Moving Wall

Applying this boundary condition does not automatically cause an associated geometry change. An additional Moving Mesh interface must be added to physically track the wall movement in the spatial reference frame.

If the wall moves, so must the fluid on both sides of the wall. Hence, this boundary condition prescribes $\mathbf{u} = \mathbf{u}_w$. The components of the **Velocity of moving wall $\mathbf{u}_w$** should be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

	• Wall
	• Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Rotating Wall

This feature applies boundary conditions to external boundaries of a Rotating Domain. For laminar flow conditions corresponding to no slip (with respect to the rotating wall) are prescribed.

For turbulence models using wall functions, corresponding conditions accounting for the rotation of the wall are prescribed.

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

	References for the Single-Phase Flow, Turbulent Flow Interfaces

---

Rotating Interior Wall

This feature can be used to prescribe Rotating Wall conditions to internal (infinitely thin) walls of a Rotating Domain.

The feature is similar to the Rotating Wall boundary condition, except that it applies boundary conditions on both sides of an internal boundary. It allows for discontinuities in the dependent variables (velocity, pressure, turbulence) across the boundary.

The Rotating Interior Wall boundary condition is particularly useful to avoid meshing thin structures by instead introducing infinitely thin curves and surfaces in the mesh and applying rotating wall conditions on these.

🔍   References for the Single-Phase Flow, Turbulent Flow Interfaces

---

Stationary Free Surface

This postprocessing feature is used to estimate the deformation of a free surface from the pressure distribution on the boundary when using the **Frozen Rotor** or **Frozen Rotor with Initialization** study types. When computing the flow field, a slip condition together with a constant pressure level p_{ext} is applied on the boundary. The free surface deformation η_{FS} is evaluated from the linearized free surface condition in a separate study step, Stationary Free Surface, using the pressure from the Frozen Rotor study step.

$$p(\mathbf{x}_0) - p_{ext} + \hat{\mathbf{n}} \cdot \nabla p \big|_{\mathbf{x} = \mathbf{x}_0} \eta_{FS} = -\sigma \nabla_S^2 \eta_{FS} \qquad (3\text{-}9)$$

σ is the surface tension coefficient, $\mathbf{x} = \mathbf{x}_0$ represents the position of the undisturbed surface - the feature selection, and $\hat{\mathbf{n}}$ is its unit normal. The correct study sequence can be triggered by toggling the study window once a selection for the Stationary Free Surface feature has been made.

The Stationary Free Surface feature is supported by laminar and turbulent flow, and is applicable for small surface deformations (η_{FS} and its gradient should be small compared to the dimensions of the computational domain).

STATIONARY FREE SURFACE
Enter an **External pressure** p_{ext} corresponding to the average pressure level on the free surface.

SURFACE TENSION

The default **Surface tension coefficient** σ (SI unit: N/m) is **User defined**. It can also be specified from predefined libraries, by selecting **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**.

- For **Library coefficient, liquid/gas interface** select an option from the list — **Water/Air**, **Acetone/Air**, **Acetic acid/Air**, **Ethanol/Air**, **Ethylene glycol/Ethylene glycol vapor**, **Diethyl ether/Air**, **Glycerol/Air**, **Heptane/Nitrogen**, **Mercury/Mercury vapor**, or **Toluene/Air**.

- For **Library coefficient, liquid/liquid interface** select an option from the list — **Benzene/Water, 20°C**, **Corn oil/Water, 20°C**, **Ether/Water, 20°C**, **Hexane/Water, 20°C**, **Mercury/Water, 20°C**, or **Olive oil/Water, 20°C**.

Only one Stationary Free Surface feature can be applied in a Rotating Machinery, Fluid Flow interface, and it requires the study to be stationary (Frozen Rotor).

Contact Angle

This feature specifies the contact angle between the free surface and a solid wall. The Contact Angle feature is a subfeature to, and added under a Stationary Free Surface feature.

CONTACT ANGLE

Select an option from the **Specify contact angle list**—**Directly** (the default) or **Through Young's equation**.

- For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$.

- For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** χ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** χ_{s2} (SI unit: J/m^2).

Theory for the Single-Phase Flow Interfaces

> Also see [Theory for the Turbulent Flow Interfaces](#) and [Theory for the Rotating Machinery Interfaces](#).

The theory for the Single-Phase Flow, Laminar Flow interface is described in this section:

- General Single-Phase Flow Theory
- Compressible Flow
- Weakly Compressible Flow
- The Mach Number Limit
- Incompressible Flow
- The Reynolds Number
- Non-Newtonian Flow: The Power Law and the Carreau Model
- Gravity
- The Boussinesq Approximation
- Theory for the Wall Boundary Condition
- Prescribing Inlet and Outlet Conditions
- Laminar Inflow
- Laminar Outflow
- Mass Flow
- No Viscous Stress
- Normal Stress Boundary Condition
- Vacuum Pump Boundary Condition
- Fan Defined on an Interior Boundary
- Fan and Grille Boundary Conditions
- Screen Boundary Condition
- Mass Sources for Fluid Flow
- Numerical Stability — Stabilization Techniques for Fluid Flow

---

The theory about most boundary conditions is found in Ref. 2.

General Single-Phase Flow Theory

The Single-Phase Fluid Flow interfaces are based on the Navier-Stokes equations, which in their most general form read

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-10}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \boldsymbol{\tau}] + \mathbf{F} \tag{3-11}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T \right) = -(\nabla \cdot \mathbf{q}) + \boldsymbol{\tau}{:}\mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T} \bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p \right) + Q \tag{3-12}$$

where

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is pressure (SI unit: Pa)
- τ is the viscous stress tensor (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: N/m^3)
- C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- $\mathbf{q}$ is the heat flux vector (SI unit: W/m^2)
- Q contains the heat sources (SI unit: W/m^3)
- $\mathbf{S}$ is the strain-rate tensor:

$$\mathbf{S} = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

The operation ":" denotes a contraction between tensors defined by

$$\mathbf{a}:\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm} \qquad (3\text{-}13)$$

This is sometimes referred to as the double dot product.

Equation 3-10 is the continuity equation and represents conservation of mass. Equation 3-11 is a vector equation which represents conservation of momentum. Equation 3-12 describes the conservation of energy, formulated in terms of temperature. This is an intuitive formulation that facilitates boundary condition specifications.

To close the equation system, Equation 3-10 through Equation 3-12, constitutive relations are needed. For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

$$\boldsymbol{\tau} = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \qquad (3\text{-}14)$$

The dynamic viscosity, μ (SI unit: Pa·s), for a Newtonian fluid is allowed to depend on the thermodynamic state but not on the velocity field. All gases and many liquids can be considered Newtonian. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions. With the CFD Module, you can model flows of non-Newtonian fluids using the predefined power law and Carreau models, which describe the dynamic viscosity for non-Newtonian fluids. The Heat Transfer Module treats all fluids as Newtonian according to Equation 3-14. Other commonly used constitutive relations are Fourier's law of heat conduction and the ideal gas law.

In theory, the same equations describe both laminar and turbulent flows. In practice, however, the mesh resolution required to simulate turbulence with the Laminar Flow interface makes such an approach impractical.

There are several books where derivations of the Navier-Stokes equations and detailed explanations of concepts such as Newtonian fluids can be found. See, for example, the classical text by Batchelor (Ref. 3) and the more recent work by Panton (Ref. 4).

Many applications describe isothermal flows for which Equation 3-12 is decoupled from Equation 3-10 and Equation 3-11. Nonisothermal flow and the temperature equation are described in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 3-10 and Equation 3-11 requires $\partial/\partial\phi$ to be zero. That is, there must be no gradients in the azimuthal direction. A common additional assumption is however that $u_\phi=0$. In such cases, the ϕ-equation can be removed from Equation 3-11. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the ϕ-equation. The default 2D axisymmetric formulation of Equation 3-10 and Equation 3-11 therefore assumes that

$$\partial/\partial\phi = 0$$
$$u_\phi = 0$$

You can activate the **Swirl Flow** property which reduces the above assumptions to $\partial/\partial\phi = 0$ and reintroduces the ϕ-equation into Equation 3-11.

Compressible Flow

The equations of motion for a single-phase fluid are the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) = 0 \tag{3-15}$$

and the momentum equation:

$$\rho\frac{\partial\mathbf{u}}{\partial t} + \rho\mathbf{u} \cdot \nabla\mathbf{u} = -\nabla p + \nabla \cdot \left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right) + \mathbf{F} \tag{3-16}$$

These equations are applicable for incompressible as well as for compressible flow with density and viscosity variations.

Weakly Compressible Flow

The same equations as for Compressible Flow are applied for weakly compressible flow. The only difference is that the density is evaluated at the reference pressure. The density may be a function of other quantities, in particular it may be temperature dependent.

The weakly compressible flow equations are valid for incompressible as well as compressible flow with density variations independent of the pressure.

The Mach Number Limit

An important dimensionless number in fluid dynamics is the Mach number, Ma, defined by

$$\text{Ma} = \frac{|\mathbf{u}|}{a}$$

where a is the speed of sound. A flow is formally incompressible when $\text{Ma} = 0$. This is theoretically achieved by letting the speed of sound tend to infinity. The Navier-Stokes equations then have the mathematical property that pressure disturbances are instantaneously propagated throughout the entire domain. This results in a parabolic equation system.

The momentum equation, Equation 3-16, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 3-15, is hyperbolic for both steady and unsteady flow. The combined system of equations is thus hybrid parabolic-hyperbolic for unsteady flow and hybrid elliptic-hyperbolic for steady flow. An exception occurs when the viscous term in Equation 3-16 becomes vanishingly small, such as at an outflow boundary, in which case the momentum equation becomes locally hyperbolic. The number of boundary conditions to apply on the boundary then depends on the number of characteristics propagating into the computational domain. For the purely hyperbolic system, the number of characteristics propagating from the boundary into the domain changes as the Mach number passes through unity. Hence, the number of boundary conditions required to obtain a numerically well-posed system must also change. The compressible formulation of the laminar and turbulent interfaces uses the same boundary conditions as the incompressible formulation, which implies that the compressible interfaces are not suitable for flows with a Mach number larger than or equal to one.

The practical Mach number limit is lower than one, however. The main reason is that the numerical scheme (stabilization and boundary conditions) of the Laminar Flow interface does not recognize the direction and speed of pressure waves. The fully compressible Navier-Stokes equations do, for example, start to display very sharp gradients already at moderate Mach numbers. But the stabilization for the single-phase flow interface does not necessarily capture these gradients. It is impossible to give an exact limit where the low Mach number regime ends and the moderate Mach number regime begins, but a rule of thumb is that the Mach number effects start to appear at $\text{Ma} = 0.3$. For this reason, the compressible formulation is referred to as *Compressible flow (Ma<0.3)* in COMSOL Multiphysics. To model high Mach number flows, use on of The High Mach Number Flow Interfaces.

Incompressible Flow

When the temperature variations in the flow are small, a single-phase fluid can often be assumed incompressible; that is, ρ is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant ρ, Equation 3-15 reduces to

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{3-17}$$

and Equation 3-16 becomes

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} \tag{3-18}$$

In order to apply the incompressible flow formulation, the density is evaluated at the reference pressure level, and both the density and viscosity are evaluated at the reference temperature. However, if the density is a function of other quantities such as a concentration field, the user has to make sure that the density is defined as constant when the incompressible flow formulation is used.

The Reynolds Number

A fundamental characteristic in analyses of fluid flow is the Reynolds number:

$$\mathrm{Re} = \frac{\rho U L}{\mu}$$

where U denotes a velocity scale, and L denotes a representative length. The Reynolds number represents the ratio between inertial and viscous forces. At low Reynolds numbers, viscous forces dominate and tend to damp out all disturbances, which leads to laminar flow. At high Reynolds numbers, the damping in the system is very low, giving small disturbances the possibility to grow by nonlinear interactions. If the Reynolds number is high enough, the flow field eventually ends up in a chaotic state called turbulence.

Observe that the Reynolds number can have different meanings depending on the length scale and velocity scale. To be able to compare two Reynolds numbers, they must be based on equivalent length and velocity scales.

The Fluid Flow interfaces automatically calculate the local cell Reynolds number $\mathrm{Re}^c = \rho|\mathbf{u}|h/(2\mu)$ using the element length h for L and the magnitude of the velocity vector u for the velocity scale U. This Reynolds number is not related to the character of the flow field, but to the stability of the numerical discretization. The risk for numerical oscillations

in the solution increases as Re^c grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as: `spf.cellRe`).

Non-Newtonian Flow: The Power Law and the Carreau Model

The viscous stress tensor is directly dependent on the shear rate tensor and can be written as:

$$\boldsymbol{\tau} = \mu\dot{\boldsymbol{\gamma}} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$$

$$\boldsymbol{\tau} = \mu\dot{\boldsymbol{\gamma}}$$

using the compressible and incompressible formulations. Here $\dot{\boldsymbol{\gamma}}$ denotes the strain-rate tensor defined by:

$$\dot{\boldsymbol{\gamma}} = (\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

Its magnitude, the shear rate, is:

$$\dot{\gamma} = |\dot{\boldsymbol{\gamma}}| = \sqrt{\frac{1}{2}\dot{\boldsymbol{\gamma}}{:}\dot{\boldsymbol{\gamma}}}$$

where the contraction operator ":" is defined by

$$\mathbf{a}{:}\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm}$$

For a *non-Newtonian fluid*, the dynamic viscosity is assumed to be a function of the shear rate:

$$\mu = \mu(\dot{\gamma})$$

The Laminar Flow interfaces have the following predefined models to prescribe a non-Newtonian viscosity—the power law and the Carreau model.

POWER LAW

The power law model is an example of a generalized Newtonian model. It prescribes

$$\mu = m\dot{\gamma}^{n-1} \tag{3-19}$$

where m and n are scalars that can be set to arbitrary values. For $n > 1$, the power law describes a shear thickening (dilatant) fluid. For $n < 1$, it describes a shear thinning

(pseudoplastic) fluid. A value of n equal to one gives the expression for a *Newtonian fluid*.

Equation 3-19 predicts an infinite viscosity at zero shear rate for $n < 1$. This is however never the case physically. Instead, most fluids have a constant viscosity for shear rates smaller than 10^{-2} s^{-1} (Ref. 19). Since infinite viscosity also makes models using Equation 3-19 difficult to solve, COMSOL Multiphysics implements the power law model as

$$\mu = m\max(\dot{\gamma}, \dot{\gamma}_{min})^{n-1} \tag{3-20}$$

where $\dot{\gamma}_{min}$ is a lower limit for the evaluation of the shear rate magnitude. The default value for $\dot{\gamma}_{min}$ is 10^{-2} s^{-1}, but can be given an arbitrary value or expression using the corresponding text field.

CARREAU MODEL

The Carreau model defines the viscosity in terms of the following four-parameter expression

$$\mu = \mu_\infty + (\mu_0 - \mu_{inf})[1 + (\lambda\dot{\gamma})^2]^{\frac{(n-1)}{2}} \tag{3-21}$$

where λ is a parameter with the unit of time, μ_0 is the zero shear rate viscosity, μ_{inf} is the infinite shear-rate viscosity, and n is a dimensionless parameter. This expression is able to describe the viscosity for most stationary polymer flows.

Gravity

DEFINITION

The gravity force is defined from the acceleration of gravity vector, $\mathbf{g}$, and the density, ρ. Under usual conditions and in Cartesian coordinates with the z-axis in the vertical direction,

$$\mathbf{g} = \begin{pmatrix} 0 \\ 0 \\ -g_{const} \end{pmatrix}.$$

When gravity is considered, a volume force equal to $\rho\mathbf{g}$ is included in the momentum equation. For example, for laminar weakly compressible flow, it reads:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} \ = \ \nabla \cdot \left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) + \mathbf{F} + \rho \mathbf{g} \qquad (3\text{-}22)$$

Introducing a constant reference density ρ_{ref}, and assuming that $\mathbf{g}$ is homogeneous, this equation is equivalently written:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} =$$

$$\nabla \cdot \left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} + \rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) \right) + \mathbf{F} + (\rho - \rho_{\text{ref}})\mathbf{g}$$

$$(3\text{-}23)$$

where $\mathbf{r}$ is the position vector and $\mathbf{r}_{\text{ref}}$ is an arbitrary reference position vector.

From this equation, it is convenient to define the reduced pressure which accounts for the hydrostatic pressure, $\tilde{p} \ = \ p - \rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}})$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} \ = \ \nabla \cdot \left(-\tilde{p}\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) + \mathbf{F} + (\rho - \rho_{\text{ref}})\mathbf{g} \ \ (3\text{-}24)$$

In Equation 3-24, the gravity force is written $(\rho - \rho_{\text{ref}})\mathbf{g}$. Assuming that the density is a function of the temperature only $(\rho - \rho_{\text{ref}})\mathbf{g} \ = \ (\rho(T) - \rho(T_{\text{ref}}))\mathbf{g}$. A first order Taylor approximation gives $(\rho - \rho_{\text{ref}})\mathbf{g} \approx -\rho(T_{\text{ref}})\alpha_p(T_{\text{ref}})(T - T_{\text{ref}})\mathbf{g}$ where

$$\alpha_p(T_{\text{ref}}) \ = \ -\frac{1}{\rho}\frac{\partial \rho}{\partial T}\bigg|_{T_{\text{ref}}}$$

is the thermal expansion coefficient.

Using the same approach, the gravity force in Equation 3-22 can be rewritten as $\rho \mathbf{g} \approx -\rho(T_{\text{ref}})(1 - \alpha_p(T_{\text{ref}})(T - T_{\text{ref}}))\mathbf{g}$.

INCOMPRESSIBLE FLOW

For incompressible flow the fluid properties are assumed to be constant (Boussinesq's approximation). Hence it is natural to define the reference density, ρ_{ref}, such that $\rho = \rho_{\text{ref}} = \rho(T_{\text{ref}}, p_{\text{ref}})$ and $\mu_{\text{ref}} = \mu(T_{\text{ref}})$ which makes it possible to simplify equation Equation 3-24:

$$\rho_{\text{ref}}\frac{\partial \mathbf{u}}{\partial t} + \rho_{\text{ref}}\mathbf{u} \cdot \nabla \mathbf{u} \ = \ \nabla \cdot (-\tilde{p}\mathbf{I} + \mu_{\text{ref}}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) + \mathbf{F}$$

In some cases, even when the flow is modeled as incompressible, buoyancy should be accounted for. Using the approximation of the gravity force based on the thermal expansion coefficient (which is relevant in this case: since the density changes are small, the

first order approximation is reasonably accurate), it is possible to rewrite the momentum equation with constant density and a buoyancy force:

$$\rho_{ref}\frac{\partial \mathbf{u}}{\partial t} + \rho_{ref}\mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot (-\tilde{p}\mathbf{I} + \mu_{ref}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) + \mathbf{F}$$
$$-\rho_{ref}\alpha_p(T_{ref})(T - T_{ref})\mathbf{g}$$

WEAKLY COMPRESSIBLE FLOW

For weakly compressible flow the assumption is that the density depends only on the temperature. In particular, the pressure dependency of the density is neglected, and the density is evaluated at the reference pressure: $\rho=\rho(T,p_{ref})$. With the relative pressure as dependent variable, Equation 3-22 is used

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right) + \mathbf{F} + \rho\mathbf{g}$$

With the reduced pressure as dependent variable, Equation 3-24 is used:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-\tilde{p}\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right) + \mathbf{F} + (\rho - \rho_{ref})\mathbf{g}$$

COMPRESSIBLE FLOW

For compressible flow the density may depend on any other variable, in particular on the temperature and the pressure. Similar equations are used as for the Weakly Compressible Flow case except that the density is not evaluated at the reference pressure.

NONISOTHERMAL FLOW COUPLING

For consistency, when the **Nonisothermal Flow** coupling is active, the assumptions made for the single phase flow interface are also made in the heat transfer interface:

- Incompressible flow: the Boussinesq approximation implies that the thermal conductivity and heat capacity are also constant.
- Weakly Compressible flow: the density is evaluated at p_{ref} in the heat interface too.
- Compressible flow: no change.

PRESSURE FORMULATION

When the relative pressure is used (default option) the interface dependent variable represents the relative pressure and the absolute pressure is defined as $p_A = p_{ref} + p$. When the pressure is used to define a boundary condition (for example when p_0 defines the pressure condition at an outlet), it represents the relative pressure. Hence defining the

outlet pressure as $p_{\text{hydro, approx}} = -\rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}})$ compensates for the gravity force for an ambient reference pressure of 0Pa when the density is constant, there is no external force, and provided p_{ref}, $\mathbf{g}$ and $\mathbf{r}_0$ are defined consistently.

When the reduced pressure is used, the interface dependent variable (named p by default) represents the reduced pressure. The absolute pressure is then defined as $p_A = p_{\text{ref}} - \rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) + p$. In this case when the pressure is used to define a boundary condition (for example to define a pressure condition at an outlet), its value corresponds to the reduced pressure. Hence, the prescribed pressure compensates for an approximate hydrostatic pressure, $p_{\text{hydro, approx}} = -\rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}})$ which is exact only when the density is constant and there is no external force.

PRESSURE BOUNDARY CONDITION

For an immobile fluid the momentum equation simplifies to $\nabla \cdot (p\mathbf{I}) = \mathbf{F} + \rho\mathbf{g}$ or $\nabla \cdot (-\tilde{p}\mathbf{I}) = \mathbf{F} + (\rho - \rho_{\text{ref}})\mathbf{g}$ depending on the pressure formulation.

For incompressible flow, assuming there are no external forces, this leads respectively to $p = -\rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) + p_0$ or $p = p_0$.

For weakly compressible flow and compressible flow, since the density varies, there is no corresponding explicit expression. We have $p = \int_{\mathbf{r}_{\text{ref}}}^{\mathbf{r}} \rho\mathbf{g} \cdot d\mathbf{r} + p_0$ and $\tilde{p} = \int_{\mathbf{r}_{\text{ref}}}^{\mathbf{r}} (\rho - \rho_{\text{ref}})\mathbf{g} \cdot d\mathbf{r} + p_0$.

In practice, these integrals can be problematic to evaluate. Hence, whenever possible, it is recommended to locate the pressure boundary in a region where the approximate definition of the hydrostatic pressure is applicable, or to define a boundary that is perpendicular to the gravity vector.

If it is not possible and if the pressure conditions cannot be determined, you can use a no viscous stress condition (available in the Open Boundary feature).

The Boussinesq Approximation

The Boussinesq approximation is a way to treat certain simple cases of buoyant flow without having to use the compressible formulation of the Navier-Stokes equations.

The Boussinesq approximation assumes that variations in density have no effect on the flow field except that they give rise to a buoyancy force. The density is assigned a reference value, ρ_0, everywhere except in the volume force term, which is set to

$$\mathbf{F} = (\rho_0 + \Delta\rho)\mathbf{g} \tag{3-25}$$

where $\mathbf{g}$ is the gravity vector. A further simplification is often possible. Because $\mathbf{g}$ can be written in terms of a potential, Φ, Equation 3-25 can be written as:

$$\mathbf{F} = -\nabla(\rho_0\Phi) + \Delta\rho\mathbf{g}$$

The first part can be canceled out by splitting the true pressure, p, into a hydrodynamic component, P, and a hydrostatic component, $-\rho_0\Phi$. Equation 3-17 and Equation 3-18 are expressed in terms of the hydrodynamic pressure $P = p + \rho_0\Phi$:

$$\rho\nabla \cdot \mathbf{u} = 0 \tag{3-26}$$

$$\rho_0\frac{\partial\mathbf{u}}{\partial t} + (\rho_0\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla P + \nabla \cdot (\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) + \mathbf{g}\Delta\rho \tag{3-27}$$

To obtain the Boussinesq approximation on this form, the flow must be defined as **Incompressible** with the **Include gravity** and **Use reduced pressure** options selected in the flow interface, and the **Nonisothermal Flow** multiphysics feature should be used to coupled the heat transfer and fluid flow interfaces.

In practice, the shift from p to P can be ignored except where the pressure appears in boundary conditions. The pressure that is specified at boundaries is the reduced pressure in this case. For example, at a vertical outflow or inflow boundary, the reduced pressure is typically a constant, whereas the true pressure is a function of the vertical coordinate.

The system formed by Equation 3-26 and Equation 3-27 has its limitations. The main assumption is that the density fluctuations must be small; that is, $\Delta\rho/\rho_0 \ll 1$. There are also some more subtle constraints that, for example, make the Boussinesq approximation unsuitable for systems of very large dimensions. An excellent discussion of the Boussinesq approximation and its limitations appears in Chapter 14 of Ref. 10.

Theory for the Wall Boundary Condition

See Wall for the node settings.

SLIP

The Slip condition assumes that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this is a reasonable approximation if the important effect of the wall is to prevent fluid from leaving the domain. Mathematically, the constraint can be formulated as:

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = \mathbf{0}$$

The no-penetration term takes precedence over the Neumann part of the condition and the above expression is therefore equivalent to

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{K} - (\mathbf{K} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$
$$\mathbf{K} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T})\mathbf{n}$$

expressing that there is no flow across the boundary and no viscous stress in the tangential direction.

For a moving wall with translational velocity $\mathbf{u}_{tr}$, $\mathbf{u}$ in the above equations is replaced by the relative velocity $\mathbf{u}_{rel} = \mathbf{u} - \mathbf{u}_{tr}$.

For turbulent flow, turbulence variables are in general subject to homogeneous Neumann conditions. For example

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla \varepsilon \cdot \mathbf{n} = 0$$

for the k-ε model.

SLIDING WALL

The sliding wall option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

- In 2D, the tangential direction is unambiguously defined by the direction of the boundary, but the situation becomes more complicated in 3D. For this reason, this boundary condition has slightly different definitions in the different space dimensions.

- For 2D and 2D axisymmetric components, the velocity is given as a scalar U_w and the condition prescribes

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{u} \cdot \mathbf{t} = U_w$$

  where $\mathbf{t} = (n_y, -n_x)$ for 2D and $\mathbf{t} = (n_z, -n_r)$ for axial symmetry.

- For 3D components, the velocity is set equal to a given vector $\mathbf{u}_w$ projected onto the boundary plane:

$$\mathbf{u} = \frac{\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w)\mathbf{n}}{\left\| \mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w)\mathbf{n} \right\|} \left\| \mathbf{u}_w \right\|$$

The normalization makes $\mathbf{u}$ have the same magnitude as $\mathbf{u}_w$ even if $\mathbf{u}_w$ is not exactly parallel to the wall.

SLIP VELOCITY

In the microscale range, the flow at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a slip velocity at the boundary. Two phenomena account for this velocity: violation of the continuum hypothesis for the viscosity and flow induced by a thermal gradient along the boundary.

The following equation relates the viscosity-induced jump in tangential velocity to the tangential shear stress along the boundary:

$$\Delta u = \frac{1}{\beta} \tau_{n, t}$$

For gaseous fluids, the coefficient β is given by

$$\beta = \frac{\mu}{\left(\dfrac{2 - \alpha_v}{\alpha_v}\right)\lambda}$$

where μ is the fluid's dynamic viscosity (SI unit: Pa·s), α_v represents the tangential momentum accommodation coefficient (TMAC) (dimensionless), and λ is the molecules' mean free path (SI unit: m). The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 15.

A simpler expression for β is

$$\beta = \frac{\mu}{L_s}$$

where L_s, the slip length (SI unit: m), is a straight channel measure of the distance from the boundary to the virtual point outside the flow domain where the flow profile extrapolates to zero. This equation holds for both liquids and gases.

Thermal creep results from a temperature gradient along the boundary. The following equation relates the thermally-induced jump in tangential velocity to the tangential gradient of the natural logarithm of the temperature along the boundary:

$$\Delta u = \sigma_T \frac{\mu}{\rho} \nabla_t \log T$$

where σ_T is the thermal slip coefficient (dimensionless) and ρ is the density of the fluid. The thermal slip coefficients range between 0.3 and 1.0 and can be found in Ref. 15.

Combining the previous relationships results in the following equation:

$$\mathbf{u} - \mathbf{u}_{w,\,t} \;=\; \frac{L_s}{\mu}\tau_{n,\,t} + \sigma_{\mathrm{T}}\frac{\mu}{\rho T}\nabla_t T$$

Relate the tangential shear stress to the viscous boundary force by

$$\tau_{n,\,t} \;=\; \mathbf{K} - (\mathbf{n} \cdot \mathbf{K})\mathbf{n}$$

where the components of $\mathbf{K}$ are the Lagrange multipliers that are used to implement the boundary condition. Similarly, the tangential temperature gradient results from the difference of the gradient and its normal projection:

$$\nabla_t T \;=\; \nabla T - (\mathbf{n} \cdot \nabla T)\mathbf{n}$$

Use Viscous Slip

When viscous slip is used, select Maxwell's model to calculate L_{s} using:

$$L_s \;=\; \left(\frac{2 - \alpha_{\mathrm{v}}}{\alpha_{\mathrm{v}}}\right)\lambda$$

Also see Wall for the node settings.

Prescribing Inlet and Outlet Conditions

The Navier-Stokes equations can show large variations in mathematical behavior, ranging from almost completely elliptic to almost completely hyperbolic. This has implications when it comes to prescribing admissible boundary conditions. There is also a discrepancy between mathematically valid boundary conditions and practically useful boundary conditions. See Inlet and Outlet for the node settings.

INLET CONDITIONS

An inlet requires specification of the velocity components. The most robust way to do this is to prescribe a velocity field using a Velocity condition.

A common alternative to prescribing the complete velocity field is to prescribe a pressure and all but one velocity component. The pressure cannot be specified pointwise because this is mathematically over-constraining. Instead the pressure can be specified via a stress condition:

$$-p + 2\mu\frac{\partial u_n}{\partial n} \;=\; F_n \tag{3-28}$$

where $\partial u_n/\partial n$ is the normal derivative of the normal velocity component. Equation 3-28 is prescribed by the Pressure condition in the Inlet and Outlet features and the Normal stress condition in the Open Boundary and Boundary Stress features. Equation 3-28 is mathematically more stringent compared to specifying the pressure pointwise and at the same time cannot guarantee that p obtains the desired value. In practice, p is close to F_n, except for low Reynolds number flows where viscous effects are the only effects that balance the pressure. In addition to Equation 3-28, all but one velocity component must be specified. For low Reynolds numbers, this can be specified by a vanishing tangential stress condition:

$$\mu\frac{\partial u_t}{\partial n} = 0$$

which is what the Normal stress condition does. Vanishing tangential stress becomes a less well-posed inlet condition as the Reynolds number increases. The Pressure condition in the Inlet feature therefore requires a flow direction to be prescribed, which provides a well-posed condition independent of Reynolds number.

OUTLET CONDITIONS

The most common approach is to prescribe a pressure via a normal stress condition on the outlet. This is often accompanied by a vanishing tangential stress condition:

$$\mu\frac{\partial u_t}{\partial n} = 0$$

where $\partial u_t/\partial n$ is the normal derivative of the tangential velocity field. It is also possible to prescribe u_t to be zero. The latter option should be used with care since it can have a significant effect on the upstream solution.

The elliptic character of the Navier-Stokes equations mathematically permit specifying a complete velocity field at an outlet. This can, however, be difficult to apply in practice. The reason being that it is hard to prescribe the outlet velocity so that it is consistent with the interior solution at each point. The adjustment to the specified velocity then occurs across an outlet boundary layer. The thickness of this boundary layer depends on the Reynolds number; the higher the Reynolds number, the thinner the boundary layer.

ALTERNATIVE FORMULATIONS

COMSOL provides several specialized boundary conditions that either provide detailed control over the flow at the boundary or that simulate specific devices. In practice they

often prescribe a velocity or a pressure, but calculate the prescribed values using for example ODEs.

| ![icon] | Normal Stress Boundary Condition |

Laminar Inflow

In order to prescribe a fully developed inlet velocity profile, this boundary condition adds a weak form contribution and constraints corresponding to unidirectional flow perpendicular to the boundary. The applied condition corresponds to the situation shown in Figure 3-2: a fictitious domain of length L_{entr} is assumed to be attached to the inlet of the computational domain. The domain is an extrusion of the inlet boundary, which means that laminar inflow requires the inlet to be flat. The boundary condition uses the assumption that the flow in this fictitious domain is *fully developed laminar flow*. The "wall" boundary conditions for the fictitious domain is inherited from the real domain, Ω, unless the option to constrain outer edges or endpoints to zero is selected in which case the fictitious "walls" are no-slip walls.
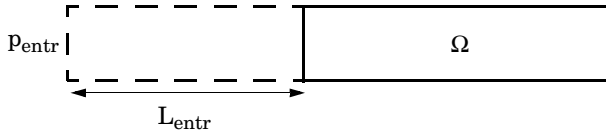
Figure 3-2: An example of the physical situation simulated when using the Laminar inflow boundary condition. Ω is the actual computational domain while the dashed domain is a fictitious domain.

If an average inlet velocity or inlet volume flow is specified instead of the pressure, COMSOL Multiphysics adds an ODE that calculates a pressure, p_{entr}, such that the desired inlet velocity or volume flow is obtained.

Laminar Outflow

In order to prescribe an outlet velocity profile, this boundary condition adds a weak form contribution and constraints corresponding to unidirectional flow perpendicular to the boundary. The applied condition corresponds to the situation shown in Figure 3-3: assume that a fictitious domain of length L_{exit} is attached to the outlet of the computational domain. The domain is an extrusion of the outlet boundary, which means

that laminar outflow requires the outlet to be flat. The boundary condition uses the assumption that the flow in this fictitious domain is *fully developed laminar flow*. The "wall" boundary conditions for the fictitious domain is inherited from the real domain, Ω, unless the option to constrain outer edges or endpoints to zero is selected in which case the fictitious "walls" are no-slip walls.
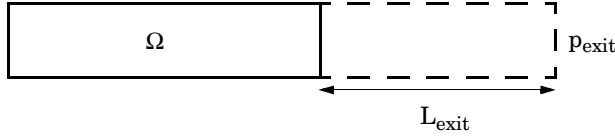
Figure 3-3: An example of the physical situation simulated when using the Laminar outflow boundary condition. Ω is the actual computational domain while the dashed domain is a fictitious domain.

If the average outlet velocity or outlet volume flow is specified instead of the pressure, the software adds an ODE that calculates p_{exit} such that the desired outlet velocity or volume flow is obtained.

Mass Flow

The **Mass Flow** boundary condition constrains the mass flowing into the domain across an inlet boundary. The mass flow can be specified in a number of ways.

POINTWISE MASS FLUX

The pointwise mass flux sets the velocity at the boundary to:

$$\mathbf{u} = -\frac{m_f}{\rho}\mathbf{n}$$

where m_f is the normal mass flux and ρ is the density.

MASS FLOW RATE

The mass flow rate boundary condition sets the total mass flow through the boundary according to:

$$-\int_{\partial\Omega} d_{bc}\rho(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = m$$

where d_{bc} (only present in the 2D Cartesian axis system) is the boundary thickness normal to the fluid-flow domain and m is the total mass flow rate.

In addition to the constraint on the total flow across the boundary, the tangential velocity components are set to zero on the boundary

$$\mathbf{u} \times \mathbf{n} = \mathbf{0} \tag{3-29}$$

STANDARD FLOW RATE

The standard flow rate boundary condition specifies the mass flow as a standard volumetric flow rate. The mass flow through the boundary is set by the equation:

$$-\int_{\partial\Omega} d_{\mathrm{bc}} \frac{\rho}{\rho_{\mathrm{st}}} (\mathbf{u} \cdot \mathbf{n}) \mathrm{d}S = Q_{\mathrm{sv}}$$

where d_{bc} (only present in the 2D component Cartesian axis system) is the boundary thickness normal to the fluid-flow domain, ρ_{st} is the standard density, and Q_{sv} is the standard flow rate. The standard density is defined by one of the following equations:

$$\rho_{\mathrm{st}} = \frac{M_n}{V_n}$$

$$\rho_{\mathrm{st}} = \frac{p_{\mathrm{st}} M_n}{R T_{\mathrm{st}}}$$

where M_n is the mean molar mass of the fluid, V_n is the standard molar volume, p_{st} is the standard pressure, R is the universal molar gas constant, and T_{st} is the standard temperature.

Equation 3-29 or Equation 3-30 is also enforced for compressible and incompressible flow, respectively, ensuring that the normal component of the viscous stress and the tangential component of the velocity are zero at the boundary.

No Viscous Stress

For this module, and in addition to the Pressure, No Viscous Stress boundary condition, the viscous stress condition sets the viscous stress to zero:

$$\left(\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \mathbf{n} = \mathbf{0}$$

$$(\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \mathbf{n} = \mathbf{0}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

The condition is not a sufficient outlet condition since it lacks information about the outlet pressure. It must hence be combined with pressure point constraints on one or several points or lines surrounding the outlet.

This boundary condition is numerically the least stable outlet condition, but can still be beneficial if the outlet pressure is nonconstant due to, for example, a nonlinear volume force.

Normal Stress Boundary Condition

The total stress on the boundary is set equal to a stress vector of magnitude f_0, oriented in the negative normal direction:

$$\left(-p\mathbf{I} + \left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = -f_0\mathbf{n}$$

$$(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -f_0\mathbf{n}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This implies that the total stress in the tangential direction is zero. This boundary condition implicitly sets a constraint on the pressure which for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n} + f_0 \tag{3-30}$$

If $\partial u_n/\partial n$ is small, Equation 3-30 states that $p \approx f_0$.

The Normal Stress condition is the mathematically correct version of the Pressure Conditions condition (Ref. 4), but it is numerically less stable.

Pressure Boundary Condition

For single-phase flow, a mathematically correct natural boundary condition for outlets is

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -p_0\mathbf{n} \tag{3-31}$$

$$(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n} \tag{3-32}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This is a normal stress condition together with a no-tangential-stress condition. When $\mu > 0$, Equation 3-31 or Equation 3-32 can be supplemented with a tangential velocity condition

$$\mathbf{u} \cdot \mathbf{t} = 0 \tag{3-33}$$

If so, the no-tangential-stress condition is overridden. An issue with Equation 3-31 or Equation 3-32 is that it does not strongly enforce unidirectional flow on the boundary. If the prescribed pressure on an outlet is too high, parts of the outlet can actually have inflow. This is not as much of an issue for the Navier-Stokes equations as it is an issue for scalar transport equations solved along with the Navier-Stokes equations. Hence, when applying the **Pressure** boundary condition at an outlet or inlet you can further constrain the flow. With the Suppress backflow option

$$\begin{aligned} \left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right)\mathbf{n} &= -\hat{p}_0\mathbf{n} \\ (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} &= -\hat{p}_0\mathbf{n} \\ \hat{p}_0 &\leq p_0 \end{aligned} \tag{3-34}$$

the normal stress is adjusted to keep

$$\mathbf{u} \cdot \mathbf{n} \geq 0 \tag{3-35}$$

Equation 3-34 effectively means that the prescribed pressure is p_0 if $\mathbf{u} \cdot \mathbf{n} \geq 0$, but smaller at locations where $\mathbf{u} \cdot \mathbf{n} < 0$. This means that Equation 3-34 does not completely prevent backflow, but the backflow is substantially reduced. Backflow is suppressed also when external forces are acting on the fluid, provided the magnitude of these forces are of the same order as the dynamic pressure at the outlet.

A pressure condition can also be applied at an inlet. In this case, either the normal stress is prescribed

$$\begin{aligned} \mathbf{n}^T\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right)\mathbf{n} &= -\hat{p}_0 \\ \mathbf{n}^T(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} &= -\hat{p}_0 \\ \hat{p}_0 &\geq p_0 \end{aligned} \tag{3-36}$$

together with the tangential condition in Equation 3-33, or, a general flow direction is prescribed.

$$\mathbf{r}_{\mathbf{u}}^T\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0(\mathbf{r}_{\mathbf{u}} \cdot \mathbf{n})$$

$$\mathbf{r}_{\mathbf{u}}^T(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -\hat{p}_0(\mathbf{r}_{\mathbf{u}} \cdot \mathbf{n})$$

$$\hat{p}_0 \geq p_0 \tag{3-37}$$

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{r}_{\mathbf{u}})\mathbf{r}_{\mathbf{u}} = \mathbf{0}, \ \mathbf{r}_{\mathbf{u}} = \frac{\mathbf{d}_{\mathbf{u}}}{\|\mathbf{d}_{\mathbf{u}}\|}$$

The ">" option is used with suppress backflow to have $\mathbf{u} \cdot \mathbf{n} \leq 0$ or $\mathbf{u} \cdot \mathbf{r}_{\mathbf{u}} \geq 0$.

See Inlet, Outlet, Open Boundary, and No Viscous Stress for the individual node settings. Note that some modules have additional theory sections describing options available with that module.

Vacuum Pump Boundary Condition

Vacuum pumps (devices) can be represented using lumped curves implemented as boundary conditions. These simplifications also imply some assumptions. In particular, it is assumed that a given boundary can only be either an inlet or an outlet. Such a boundary should not be a mix of inlets/outlets nor switch between them during a simulation.

Manufacturers usually provide curves that describe the static pressure as a function of flow rate for a vacuum pump. Also see Vacuum Pump for the node settings.

DEFINING A DEVICE AT AN OUTLET

In this case (see Figure 3-4), the device's inlet is the interior face situated between the blue (cube) and green (circle) domains while its outlet is an external boundary, here the circular boundary of the green domain. The lumped curve gives the flow rate as a function of the pressure difference between the interior face and the external boundary. This boundary condition implementation follows the Pressure Boundary Condition for outlets with the Suppress backflow option:

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0\mathbf{n}$$

$$\hat{p}_0 \leq p_{\text{vacuum pump}}(V_0) - p_{\text{ref}} \tag{3-38}$$

Here, V_0 is the flow rate across the boundary and $p_{\text{vacuum pump}}(V_0)$ is the static pressure function of flow rate for the vacuum pump. p_{ref} is the reference pressure that ensure that the absolute pressure is set to $p_{\text{vacuum pump}}$. In vacuum pump models the reference pressure may be set to 0 Pa since the absolute pressure is close to 0 Pa by opposition to ambient conditions where p_{ref} is often set to 1 atm. Equation 3-38 corresponds to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla \cdot \mathbf{u})$ vanishes. In 2D the thickness in the third direction, Dz, is used to define the flow rate. Vacuum pumps are modeled as rectangles in this case.
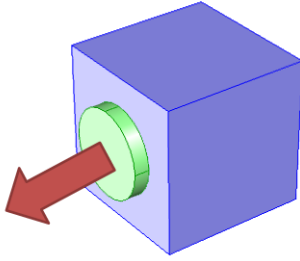
Figure 3-4: A vacuum pump at the outlet. The arrow represents the flow direction, the green circle represents the vacuum pump (that should not be part of the model), and the blue cube represents the modeled domain with an outlet boundary condition described by a lumped curve for the attached vacuum pump.

Fan Defined on an Interior Boundary

In this case, the inlet and outlet of the device are both interior boundaries (see Figure 3-5). The boundaries are called dev_in and dev_out. The boundary conditions are described as follows:

- The inlet of the device is an outlet boundary condition for the modeled domain. For this outlet side, on dev_in, a pressure condition is set. The value of the pressure is set to the sum of the mean value of the pressure on dev_out and the pressure drop across the device. The pressure drop is calculated from a lumped curve using the flow rate evaluated on dev_in.

- For the inlet side, on `dev_out`, a pressure boundary condition is defined. The pressure value is set so that the flow rate is equal on `dev_in` and `dev_out`. An ODE is added to compute the pressure value.

- When a turbulence model with transport equations for the turbulence quantities is applied, the turbulent kinetic energy, k, and dissipation rate, ε, specific dissipation rate, ω, or turbulent relative fluctuations, ζ, must be specified on the downstream side of the fan. The turbulence conditions are specific to the design and operating conditions of the fan. A reference velocity scale U_{ref} is available in order to set default values.

$$k_{0init} = 0.015 U_{ref}^2, \quad \varepsilon_{0init} = \frac{C_\mu^{3/4} k_{0init}^{3/2}}{l_{ref}} \tag{3-39}$$

| | In both cases, the boundary condition implementation follows the Pressure Boundary Condition for outlet or inlet with the Suppress backflow option. |

| | See Interior Fan for node settings. |
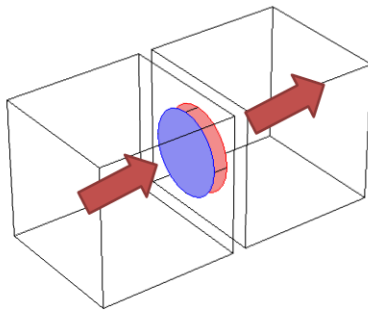
Figure 3-5: A device between two boundaries. The red arrows represent the flow direction, the cylindrical part represents the device (that should be not be part of the model), and the two cubes are the domain that are modeled with a particular inlet boundary condition to account for the device.

Fan and Grille Boundary Conditions

Fans, pumps, or grilles (devices) can be represented using lumped curves implemented as boundary conditions. These simplifications also imply some assumptions. In particular, it is assumed that a given boundary can only be either an inlet or an outlet. Such a boundary should not be a mix of inlets/outlets, nor switch between them during a simulation.

Manufacturers usually provide curves that describe the static pressure as a function of flow rate for a fan. See Fan and Grille for the node settings.

DEFINING A DEVICE AT AN INLET

In this case, the device's inlet is an external boundary, represented by the external circular boundary of the green domain on Figure 3-6. The device's outlet is an interior face situated between the green and blue domains in Figure 3-6. The lumped curve gives the flow rate as a function of the pressure difference between the external boundary and the interior face. This boundary condition implementation follows the Pressure Boundary Condition for inlets with the Suppress backflow option:

$$\mathbf{n}^{\mathrm{T}}\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0$$
$$\hat{p}_0 \geq p_{\mathrm{input}} + \Delta p_{\mathrm{fan}}(V_0) \tag{3-40}$$

The Grille boundary condition sets the following conditions:

$$\mathbf{n}^{\mathrm{T}}\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0$$
$$\hat{p}_0 \geq p_{\mathrm{input}} + \Delta p_{\mathrm{grille}}(V_0) \tag{3-41}$$

Here, V_0 is the flow rate across the boundary, p_{input} is the pressure at the device's inlet, and $\Delta p_{\mathrm{fan}}(V_0)$ and $\Delta p_{\mathrm{grille}}(V_0)$ are the static pressure functions of flow rate for the fan and the grille. Equation 3-40 and Equation 3-41 correspond to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla\cdot\mathbf{u})$ vanishes. When a turbulence model with a transport equation for the turbulent kinetic energy is applied, the term $-(2/3)\rho k$ appears on the left-hand sides of Equation 3-40 and Equation 3-41. In such cases the turbulent kinetic energy, k, the turbulent relative fluctuations, ζ (for the v2-f turbulence model), and dissipation rate, ε, or specific dissipation rate, ω, must be specified on the downstream side. The turbulence conditions are specific to the design and operating conditions of the fan or grille. For the Fan condition, a reference velocity scale U_{ref} is available in order to set default values according to Equation 3-39. For the Grille boundary condition the

turbulence quantities on the downstream side are specified by defining a loss coefficient $K = 2\Delta p_{\text{grille}}/\rho(\mathbf{u} \cdot \mathbf{n})^2$, from which a refraction coefficient is derived using Equation 3-54. Equation 3-47 through Equation 3-49 are then used to relate upstream and downstream turbulence quantities.

When an algebraic turbulence model, such as the Algebraic yPlus or L-VEL model, is used, the turbulence is only implicitly affected by the device through the change in the local Reynolds number.

The flow direction is enforced to be normal to the boundary by default. However, it is possible to define an arbitrary inflow velocity direction. In such case, Equation 3-40 and Equation 3-41 are modified similarly to Equation 3-37. In 2D, the thickness in the third direction, Dz, is used to define the flow rate. Fans are modeled as rectangles in this case.

For 3D and 2D axisymmetry when the swirl flow is included, it is possible to define a swirl on the downstream side of the fan. It sets the following boundary conditions:

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0$$

$$\mathbf{u} \cdot \mathbf{t} = \mathbf{u}_{\text{swirl}} = c_{\text{sf}}2\pi f\mathbf{n} \times (\mathbf{r} - \mathbf{r}_{\text{pb}})$$

$$\hat{p}_0 \geq p_{\text{input}} + \Delta p_{\text{fan}}$$

Here, the swirl ratio c_{sf} is a positive number less than 1, defining the ratio of the rotation transferred from the fan to the flow, f is the number of revolutions per time for the fan, and $\mathbf{r}_{\text{rb}}$ is the rotation axis base point.
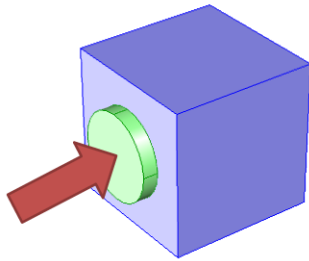
Figure 3-6: A device at the inlet. The arrow represents the flow direction, the green circle represents the device (that should not be part of the model), and the blue cube represents the modeled domain with an inlet boundary condition described by a lumped curve for the attached device.

DEFINING A DEVICE AT AN OUTLET

In this case (see Figure 3-15), the fan's inlet is the interior face situated between the blue (cube) and green (circle) domain while its outlet is an external boundary, here the circular boundary of the green domain. The lumped curve gives the flow rate as a function of the pressure difference between the interior face and the external boundary. This boundary condition implementation follows the Pressure Boundary Condition for outlets with the Suppress backflow option:

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0\mathbf{n}$$

$$\hat{p}_0 \leq p_{\text{exit}} - \Delta p_{\text{fan}}(V_0)$$

(3-42)

The Grille boundary condition sets the following conditions:

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0\mathbf{n}$$

$$\hat{p}_0 \leq p_{\text{exit}} - \Delta p_{\text{grille}}(V_0)$$

(3-43)

Here, V_0 is the flow rate across the boundary, p_{exit} is the pressure at the device outlet, and $\Delta p_{\text{fan}}(V_0)$ and $\Delta p_{\text{grille}}(V_0)$ are the static pressure function of flow rate for the fan and the grille. Equation 3-42 and Equation 3-43 correspond to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla\cdot\mathbf{u})\mathbf{n}$ vanishes. When a turbulence model with a transport equation for the turbulence kinetic energy is applied, the term $-(2/3)\rho k\mathbf{n}$ appears on the left-hand sides of Equation 3-42 and Equation 3-43. In 2D the thickness in the third direction, Dz, is used to define the flow rate. Fans are modeled as rectangles in this case.
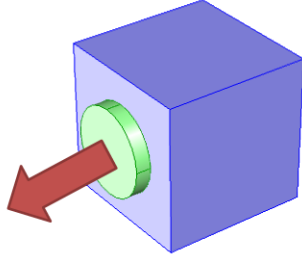
Figure 3-7: A fan at the outlet. The arrow represents the flow direction, the green circle represents the fan (that should not be part of the model), and the blue cube represents the modeled domain with an outlet boundary condition described by a lumped curve for the attached fan.

Screen Boundary Condition

The word "screen" refers to a barrier with distributed perforations such as a wire gauze, grille, or perforated plate. The screen is assumed to have a width, which is small compared to the resolved length-scales of the flow field and can thus be modeled as an edge (in 2D) or surface (in 3D). This idea permits an economic implementation of the screen, where the details of the barrier need not be resolved. The general influence of a screen on the flow field is a loss in the normal momentum component, a change in direction (related to a suppression of the tangential velocity component), attenuation of the turbulence kinetic energy and preservation of the turbulence length scale (Ref. 16). The conditions across the screen are expressed as,

$$[\rho \mathbf{u} \cdot \mathbf{n}]_{-}^{+} = 0 \tag{3-44}$$

$$\left[\rho(\mathbf{u} \cdot \mathbf{n})^2 + p - \mathbf{n}^T \left\{ (\mu + \mu_T) \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) - \frac{2}{3} \rho k \mathbf{I} \right\} \mathbf{n} \right]_{-}^{+}$$
$$= -\frac{K}{2} \rho_{-} (\mathbf{u}_{-} \cdot \mathbf{n})^2 \tag{3-45}$$

$$\mathbf{n} \times \mathbf{u}_{+} = \eta (\mathbf{n} \times \mathbf{u}_{-}) \tag{3-46}$$

$$k_{+} = \eta^2 k_{-} \tag{3-47}$$

and, depending on the turbulence model in use, either,

$$\varepsilon_+ = \eta^3 \varepsilon_-$$

(3-48)

or,

$$\omega_+ = \eta \omega_-$$

(3-49)

− and + refer to the upstream and downstream side of the screen, whereas K and η are the screen resistance and refraction coefficients. Isotropic turbulence is expected on the downstream side of the screen, hence,

$$\zeta_+ = \frac{2}{3}$$

(3-50)

is enforced when the v2-f turbulence model is used.

The attenuation of the turbulence kinetic energy (Equation 3-47) is based on the suppression of the tangential velocity (Equation 3-46) and the changes in ε and ω are determined by the assumption of preservation of the turbulence length-scale across the screen.

When an algebraic turbulence model, such as the Algebraic yPlus or L-VEL model, is used, the turbulence is only implicitly affected by the device through the change in the local Reynolds number.

The Screen feature provides three commonly used correlations for K (Ref. 17). The following correlation is valid for wire gauzes

$$K = (0.52 + 0.66/\text{Re}_d^{4/3})((1-\sigma_s)^{-2} - 1), \text{Re}_d = |\mathbf{u}|d/\nu$$

(3-51)

Here σ_s is the solidity (ratio of blocked area to total area of the screen) and d is the diameter of the wires. For a square mesh, the following correlation is applied,

$$K = 0.98((1-\sigma_s)^{-2} - 1)^{1.09}$$

(3-52)

and for a perforated plate,

$$K = 0.94((1-\sigma_s)^{-2} - 1)^{1.28}$$

(3-53)

The following correlation for wire gauzes (Ref. 18) gives reasonable values for η for a wide range of applications and has been included in the implementation,

$$\eta = \sqrt{\frac{K^2}{16} + 1} - \frac{K}{4} \tag{3-54}$$

🔍	See Screen for the node settings. Also see Theory for the Nonisothermal Screen Boundary Condition for the nonisothermal- version of these physics interfaces.

Mass Sources for Fluid Flow

There are two types of mass sources in a Single-Phase Flow interface: point sources and line sources.

📑	These features require at least one of the following licenses: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

POINT SOURCE

A point source is theoretically formed by taking a mass injection/ejection, $\dot{Q}$ (SI unit: $kg/(m^3 \cdot s)$), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_p$ (SI unit: kg/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q} = \dot{q}_p \tag{3-55}$$

An alternative way to form a point source/sink is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant, results in the same point source. For this alternative approach, effects resulting from the physical object volume, such as drag and fluid displacement, need to be neglected.

The weak contribution

$$\dot{q}_p \text{test}(p)$$

is added to a point in the geometry. As can be seen from Equation 3-55, $\dot{Q}$ must tend to plus or minus infinity as δV tends to zero. This means that in theory the pressure also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 3-55 corresponds to a finite pressure in a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region, but also a more extreme pressure value. It is important not to mesh too finely around a point source since the resulting pressure can result in unphysical values for the density, for example. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}$ (SI unit: $kg/(m^3 \cdot s)$), located within a tube with cross-sectional area δS and then letting δS tend to zero, while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_l$ (SI unit: $kg/(m \cdot s)$), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_l \tag{3-56}$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects on the fluid resulting from the physical object volume are neglected.

The weak contribution

$$\dot{q}_l \text{test}(p)$$

is added to lines in 3D or to points in 2D (which represent cut-through views of lines). Line sources can also be added to the axisymmetry line in 2D axisymmetry components. It cannot, however, be added to geometrical lines in 2D because they represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

🔍	For feature node information, see Line Mass Source and Point Mass Source in the *COMSOL Multiphysics Reference Manual*.

❗	For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Batteries & Fuel Cells Module, these shared physics nodes are renamed as follows: • The **Line Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**). • The **Point Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

Numerical Stability — Stabilization Techniques for Fluid Flow

The momentum equation (Equation 3-16 or Equation 3-18) is a (nonlinear) convection-diffusion equation. Such equations can easily become unstable if discretized using the Galerkin finite element method. Stabilized finite element methods are usually necessary in order to obtain physical solutions. The stabilization settings are found in the main Fluid Flow interface features. To display this section, click the **Show** button (👁) and select **Stabilization**.

There are three types of stabilization methods available for Navier-Stokes — *streamline diffusion*, *crosswind diffusion*, and *isotropic diffusion*. Streamline diffusion and crosswind diffusion are consistent stabilization methods, whereas isotropic diffusion is an inconsistent stabilization method.

For optimal functionality, the exact weak formulations of and constants in the streamline diffusion and crosswind diffusion methods depend on the order of the shape functions (basis functions) for the elements. The values of constants in the streamline diffusion and crosswind diffusion methods follow Ref. 5 and Ref. 6.

STREAMLINE DIFFUSION

For strongly coupled systems of equations, the streamline diffusion method must be applied to the system as a whole rather than to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 7) and were later extended to Galerkin

least-squares (GLS) applied to the Navier-Stokes equations (Ref. 8). This is the streamline diffusion formulation that COMSOL Multiphysics supports. The time-scale tensor is the diagonal tensor presented in Ref. 9.

Streamline diffusion is active by default because it is necessary when convection is dominating the flow.

The governing equations for incompressible flow are subject to the Babuska-Brezzi condition, which states that the shape functions (basis functions) for pressure must be of lower order than the shape functions for velocity. If the incompressible Navier-Stokes equations are stabilized by streamline diffusion, it is possible to use equal-order interpolation. Hence, streamline diffusion is necessary when using first-order elements for both velocity and pressure. This applies also if the model is solved using geometric multigrid (either as a solver or as a preconditioner) and at least one multigrid hierarchy level uses linear Lagrange elements.

CROSSWIND DIFFUSION

Crosswind diffusion can also be formulated for systems of equations, and when applied to the Navier-Stokes equations it becomes a shock-capturing operator. COMSOL Multiphysics supports the formulation in Ref. 8 with a shock-capturing viscosity of the Hughes-Mallet type Ref. 7.

Incompressible flows do not contain shock waves, but crosswind diffusion is still useful for introducing extra diffusion in sharp boundary layers and shear layers that otherwise would require a very fine mesh to resolve.

Crosswind diffusion is active by default as it makes it easier to obtain a solution even if the problem is fully resolved by the mesh. Crosswind diffusion also enables the iterative solvers to use inexpensive presmoothers. If crosswind diffusion is deactivated, more expensive preconditioners must be used instead.

ISOTROPIC DIFFUSION

Isotropic diffusion adds diffusion to the Navier-Stokes equations. Isotropic diffusion significantly reduces the accuracy of the solution but does a very good job at reducing oscillations. The stability of the continuity equation is not improved.

Numerical Stabilization and Iterative in the *COMSOL Multiphysics Reference Manual*

Solvers for Laminar Flow

The Navier-Stokes equations constitute a nonlinear equation system. A nonlinear solver must hence be applied to solve the problem. The nonlinear solver iterates to reach the final solution. In each iteration, a linearized version of the nonlinear system is solved using a linear solver. In the time-dependent case, a time marching method must also be applied. The default suggestions for each of these solver elements are discussed below.

NONLINEAR SOLVER

The nonlinear solver method depends on if the model solves a stationary or a time-dependent problem.

Stationary Solver

In the stationary case, a fully coupled, damped Newton method is applied. The initial damping factor is low since a full Newton step can be harmful unless the initial values are close to the final solution. The nonlinear solver algorithm automatically regulates the damping factor in order to reach a converged solution.

For advanced models, the automatically damped Newton method might not be robust enough. A pseudo time-stepping algorithm can then be invoked. See Pseudo Time Stepping for Laminar Flow Models.

Time-Dependent Solver

In the time-dependent case, the initial guess for each time step is (loosely speaking) the previous time step, which is a very good initial value for the nonlinear solver. The automatic damping algorithm is then not necessary. The damping factor in the Newton method is instead set to a constant value slightly smaller than one. Also, for the same reason, it suffices to update the Jacobian once per time-step.

It is seldom worth the extra computational cost to update the Jacobian more than once per time step. For most models it is more efficient to restrict the maximum time step or possibly lower the damping factor in the Newton method.

LINEAR SOLVER

The linearized Navier-Stokes equation system has saddle point character, unless the density depends on the pressure. This means that the Jacobian matrix has zeros on the diagonal. Even when the density depends on the pressure, the equation system effectively shares many numerical properties with a saddle point system.

For small 2D and 3D models, the default solver suggestion is a direct solver. Direct solvers can handle most nonsingular systems and are very robust and also very fast for small

models. Unfortunately, they become slow for large models and their memory requirement scales as somewhere between $N^{1.5}$ and N^2, where N is the number of degrees of freedom in the model. The default suggestion for large 2D and 3D models is therefore the iterative GMRES solver. The memory requirement for an iterative solver optimally scales as N.

GMRES is accelerated by a multigrid method, per default the Smoothed Aggregation Algebraic Mutligrid (SAAMG) method. The cost of SAAMG is typically very low compared to the number of GMRES iterations necessary if no multigrid method is used. As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, Geometric Multigrid (GMG) requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared memory computations with many cores. When the default linear solver is GMRES, an optional, but deactivated, linear solver node is available where GMRES is accelerated by GMG.

Multigrid methods need smoothers, but the saddle point character of the linear system restricts the number of applicable smoothers. The choices are further restricted by the anisotropic meshes frequently encountered in fluid-flow problems. The efficiency of the smoothers is highly dependent on the numerical stabilization. Iterative solvers perform at their best when both Streamline Diffusion and Crosswind Diffusion are active.

The default smoother for P1+P1 elements is SCGS. This is an efficient and robust smoother specially designed to solve saddle point systems on meshes that contain anisotropic elements. The SCGS smoother works well even without crosswind diffusion. SCGS can sometimes work for higher-order elements, especially if **Method** in the SCGS settings is set to **Mesh element lines**. But there is no guarantee for this, so the default smoother for P2+P1 elements and P3+P2 elements is an SOR Line smoother. SOR Line handles mesh anisotropy but does not formally address the saddle point character. It does, however, function in practice provided that streamline diffusion and crosswind diffusion are both active.

A different kind of saddle point character can arise if the equation system contains ODE variables. Some advanced boundary conditions, for example Laminar Inflow, can add equations with such variables. These variables must be treated with the Vanka algorithm. SCGS includes an option to invoke Vanka. Models with higher-order elements must apply SCGS or use the Vanka smoother. The latter is the default suggestion for higher-order elements, but it does not work optimally for anisotropic meshes.

TIME-DEPENDENT SOLVERS

The default time-dependent solver for Navier-Stokes is the BDF method with maximum order set to two. Higher BDF orders are not stable for transport problems in general nor for Navier-Stokes in particular.

BDF methods have been used for a long time and are known for their stability. However, they can have severe damping effects, especially the lower-order methods. Hence, if robustness is not an issue, a model can benefit from using the generalized-α method instead. Generalized-α is a solver which has properties similar to those of the second-order BDF solver but it is much less diffusive.

Both BDF and generalized-α are per default set to automatically adjust the time step. While this works well for many models, extra efficiency and accuracy can often be gained by specifying a maximum time step. It is also often beneficial to specify an initial time step to make the solver progress smoothly in the beginning of the time series.

ⓠ	In the *COMSOL Multiphysics Reference Manual*: • Time-Dependent Solver • Multigrid, Direct, Iterative, SCGS, SOR Line, and Vanka • Stationary Solver

Pseudo Time Stepping for Laminar Flow Models

A stationary formulation has per definition no time derivatives and Equation 3-18 reduces to:

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F} \tag{3-57}$$

Solving Equation 3-57 requires a starting guess that is close enough to the final solution. If no such guess is at hand, the fully transient problem can be solved instead. This is, however, a rather costly approach in terms of computational time. An intermediate approach is to add a fictitious time derivative to Equation 3-57:

$$\rho\frac{\mathbf{u} - \text{nojac}(\mathbf{u})}{\Delta \tilde{t}} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$$

where $\Delta \tilde{t}$ is a *pseudo time step*. Since $\mathbf{u}$–nojac($\mathbf{u}$) is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a step of size Δt of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step $\tilde{\Delta t}$ can be chosen individually for each element based on the local CFL number:

$$\tilde{\Delta t} = \mathrm{CFL}_{\mathrm{loc}} \frac{h}{|\mathbf{u}|}$$

where h is the mesh cell size. A small CFL number means a small time step. It is practical to start with a small CFL number and gradually increase it as the solution approaches steady state.

If the automatic expression for $\mathrm{CFL}_{\mathrm{loc}}$ is set to the built-in variable `CFLCMP`, then the automatic setting suggests a PID regulator for the pseudo time step in the default solver. The PID regulator starts with a small CFL number and increases $\mathrm{CFL}_{\mathrm{loc}}$ as the solution comes closer to convergence.

The default manual expression is

$$
\begin{aligned}
& 1.3^{\min(\text{niterCMP},\, 9)} + \\
& \mathrm{if}(\text{niterCMP} > 20,\, 9 \cdot 1.3^{\min(\text{niterCMP} - 20,\, 9)},\, 0) + \\
& \mathrm{if}(\text{niterCMP} > 40,\, 90 \cdot 1.3^{\min(\text{niterCMP} - 40,\, 9)},\, 0)
\end{aligned}
\tag{3-58}
$$

The variable `niterCMP` is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. $\mathrm{CFL}_{\mathrm{loc}}$ starts at 1.3 and increases by 30% each iteration until it reaches $1.3^9 \approx 10.6$. It remains there until iteration number 20 at which it starts to increase until it reaches approximately 106. A final increase after iteration number 40 then takes it to 1060. Equation 3-58 can, for some advanced flows, increase $\mathrm{CFL}_{\mathrm{loc}}$ too slowly or too quickly. $\mathrm{CFL}_{\mathrm{loc}}$ can then be tuned for the specific application.

For details about the CFL regulator, see Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual.*

The Projection Method for the Navier-Stokes Equations

A well-known approach to solve the Navier-Stokes equations is the pressure-correction method. This type of method is a so-called segregated method, and it generally requires far less memory than the COMSOL Multiphysics default formulation. Several versions of the original method have been developed (see Ref. 12, for example). COMSOL uses

incremental pressure-correction schemes.

> **!** This formulation is only available for time-dependent problems and requires the time discrete solver. It is available for the Laminar Flow and Turbulent Flow, k-ε interfaces.

This method reformulates the Navier-Stokes equations so that it is possible to solve for one variable at a time in sequence. Let $\mathbf{u}$ and p be the velocity and pressure variables and $\mathbf{u}_c$ and p_c the corrected velocity and pressure variables, respectively. The pressure-correction algorithm solves the Navier-Stokes equations using the following steps:

1 Solve in sequence for all $\mathbf{u}$ components following equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u}_c^n \cdot \nabla \mathbf{u}^{n+1} = -\nabla p^n + \nabla \cdot \left(\mu (\nabla \mathbf{u}^{n+1} + (\nabla \mathbf{u}^{n+1})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}^{n+1}) \mathbf{I} \right) + \mathbf{F}$$

where the superscript denotes the time-step index, and $\frac{\partial \mathbf{u}}{\partial t}$ is discretized using a BDF method up to second order where the $\mathbf{u}$ values from previous time steps are replaced by $\mathbf{u}_c$ values. To first order it is discretized as:

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}_c^n}{\text{timestep}}$$

2 Solve Poisson's equation to adjust the pressure:

$$\text{timestep} \Delta (p^{n+1} - p^n) = -\frac{\partial \rho}{\partial t} - \nabla \cdot \rho \mathbf{u}^{n+1} \tag{3-59}$$

3 Update the corrected velocity:

$$\mathbf{u}_c^{n+1} = \mathbf{u}^{n+1} - \frac{\text{timestep}}{\rho} \nabla (p^{n+1} - p^n)$$

For incompressible flows, the

$$\frac{2}{3} \mu (\nabla \cdot \mathbf{u}^{n+1}) \mathbf{I}$$

term in Equation 3-58 and the $\frac{\partial \rho}{\partial t}$ term in Equation 3-59 are excluded.

Due to the specific time discretization scheme, this algorithm is only available with the time discrete solver.

Because the velocity components and the pressure are solved in a segregated way, some boundary conditions have a different implementation or might not be available with the

projection method. In such cases, this is mentioned in the documentation for each boundary condition.

When the projection method is used for turbulent flows or with multiphysics couplings, the same algorithm is used for the velocity and pressure variables. Extra steps are needed to solve the other variables. By default the equation form used for these variables is the time-dependent form, and the time derivative is automatically discretized using a second-order BDF method.

Discontinuous Galerkin Formulation

Some boundary conditions are implemented using a discontinuous Galerkin formulation. These boundary conditions include

- Wall – Slip, Sliding walls and moving walls (that is, walls with non-zero translational velocity).
- Periodic Flow Condition
- Flow Continuity

The formulation used in the Fluid Flow interfaces in COMSOL Multiphysics is the Symmetric Interior Penalty Galerkin method (SIPG). The SIPG method can be regarded to satisfy the boundary conditions in an integral sense rather than pointwise. More information on SIPG can be found in Ref. 13.

In particular, the SIPG formulation includes a penalty parameter that must be large enough for the formulation to be coercive. The higher the value, the better the boundary condition is fulfilled, but a too high value results in an ill-conditioned equation system. The penalty parameter in COMSOL Multiphysics is implemented according to Ref. 14.

Particle Tracing in Fluid Flow

The Particle Tracing Module is available to assist with these types of modeling problems.

It is possible to model particle tracing with COMSOL Multiphysics provided that the impact of the particles on the flow field is negligible. First compute the flow field, and then, as an analysis step, calculate the motion of the particles. The motion of a particle is defined by Newton's second law

$$m\frac{d^2\mathbf{x}}{dt^2} = \mathbf{F}\left(t, \mathbf{x}, \frac{d\mathbf{x}}{dt}\right)$$

where $\mathbf{x}$ is the position of the particle, m the particle mass, and $\mathbf{F}$ is the sum of all forces acting on the particle. Examples of forces acting on a particle in a fluid are the drag force, the buoyancy force, and the gravity force. The drag force represents the force that a fluid exerts on a particle due to a difference in velocity between the fluid and the particle. It includes the viscous drag, the added mass, and the Basset history term. Several empirical expressions have been suggested for the drag force. One of those is the one proposed by Khan and Richardson (Ref. 11). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

$$\mathrm{Re}_p = \frac{|\mathbf{u} - \mathbf{u}_p| 2r\rho}{\mu}$$

where $\mathbf{u}$ is the velocity of the fluid, $\mathbf{u}_p$ the particle velocity, r the particle radius, ρ the fluid density, and μ the dynamic viscosity of the fluid. The empirical expression for the drag force according to Khan and Richardson is

$$\mathbf{F} = \pi r^2 \rho |\mathbf{u} - \mathbf{u}_p| (\mathbf{u} - \mathbf{u}_p) [1.84 \mathrm{Re}_p^{-0.31} + 0.293 \mathrm{Re}_p^{0.06}]^{3.45}$$

The model *Flow Past a Cylinder* (Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow**) demonstrates how to add and set up particle tracing in a plot group using the **Particle Tracing with Mass** node. It uses the predefined Khan-Richardson model for the drag force and neglects gravity and buoyancy forces.

References for the Single-Phase Flow, Laminar Flow Interfaces

1. G.G. Stokes, Trans. Camb. Phil. Soc., 8, 287-305, 1845

2. P.M. Gresho and R.L. Sani, *Incompressible Flow and the Finite Element Method, Volume 2: Isothermal Laminar Flow*, John Wiley & Sons, 2000.

3. G.K. Batchelor, *An Introduction To Fluid Dynamics*, Cambridge University Press, 1967.

4. R.L. Panton, *Incompressible Flow*, 2nd ed., John Wiley & Sons, 1996.

5. I. Harari and T.J.R. Hughes, "What are C and h? Inequalities for the Analysis and Design of Finite Element Methods," *Comp. Meth. Appl. Mech. Engrg*, vol. 97, pp. 157–192, 1992.

6. Y. Bazilevs, V.M. Calo, T.E. Tezduyar, and T.J.R. Hughes, "*YZβ* Discontinuity Capturing for Advection-dominated Processes with Application to Arterial Drug Delivery," *Int.J.Num. Meth. Fluids*, vol. 54, pp. 593–608, 2007.

7. T.J.R. Hughes and M. Mallet, "A New Finite Element Formulation for Computational Fluid Dynamics: III. The Generalized Streamline Operator for Multidimensional Advective-Diffusive System," *Comp. Meth. Appl. Mech. Engrg*, vol. 58, pp. 305–328, 1986.

8. G. Hauke and T.J.R. Hughes, "A Unified Approach to Compressible and Incompressible Flows," *Comp. Meth. Appl. Mech. Engrg*, vol. 113, pp. 389–395, 1994.

9. G. Hauke, "Simple Stabilizing Matrices for the Computation of Compressible Flows in Primitive Variables," *Comp. Meth. Appl. Mech. Engrg*, vol. 190, pp. 6881–6893, 2001.

10. D.J. Tritton, *Physical Fluid Dynamics*, 2nd ed., Oxford University Press, 1988.

11. J.M. Coulson and J.F. Richardson, "Particle Technology and Separation Processes," *Chemical Engineering, Volume 2*, Butterworth-Heinemann, 2002.

12. J.L. Guermond, P. Minev, and J. Shen, "An overview of projection methods for incompressible flows," *Comp. Meth. Appl. Mech. Engrg*, vol. 195, pp. 6011–6045, 2006.

13. B. Rivière, *Discontinuous Galerkin Methods for Solving Elliptic and Parabolic Equations*, SIAM, 2008.

14. Y. Epshteyn and B. Rivière, "Estimation of penalty parameters for symmetric interior penalty Galerkin methods," *J. Computational and Applied Mathematics*, vol. 206, pp. 843–872, 2007.

15. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

16. G.B. Schubauer, W.G. Spangenberg, and P.S. Klebanoff, "Aerodynamic Characteristics of Damping Screens," *NACA Technical note 2001*, Jan. 1950.

17. P.E. Roach, "The Generation of Nearly Isotropic Turbulence by Means of Grids," *Int. J. Heat and Fluid Flow*, vol. 8, pp. 82–92, 1986.

18. J.C. Gibbings, "The Pyramid Gauze Diffuser," *Ing. Arch.*, vol. 42, pp. 225–233, 1973.

19. R.P. Chhabra and J.F. Richardson, *Non-Newtonian Flow and Applied Rheology*, 2nd ed., Elsevier, 2008.

Theory for the Turbulent Flow Interfaces

The theory for the Single-Phase Flow, Turbulent Flow interfaces is described in this section:

- Turbulence Modeling
- The Algebraic yPlus Turbulence Model
- The L-VEL Turbulence Model
- The k-e Turbulence Model
- The k-w Turbulence Model
- The SST Turbulence Model
- The Low Reynolds Number k-e Turbulence Model
- The Spalart-Allmaras Turbulence Model
- The v2-f Turbulence Model
- Inlet Values for the Turbulence Length Scale and Turbulent Intensity
- Theory for the Pressure, No Viscous Stress Boundary Condition
- Initial Values for Generate New Turbulence Model Interfaces
- Solvers for Turbulent Flow
- Pseudo Time Stepping for Turbulent Flow Models
- References for the Single-Phase Flow, Turbulent Flow Interfaces

Q	Theory for the Single-Phase Flow Interfaces

Turbulence Modeling

Turbulence is a property of the flow field and it is characterized by a wide range of flow scales: the largest occurring scales, which depend on the geometry, the smallest, quickly fluctuating scales, and all the scales in between. The propensity for an isothermal flow to become turbulent is measured by the Reynolds number

$$\mathrm{Re} = \frac{\rho U L}{\mu} \tag{3-60}$$

where μ is the dynamic viscosity, ρ the density, and U and L are velocity and length scales of the flow, respectively. Flows with high Reynolds numbers tend to become turbulent. Most engineering applications belong to this category of flows.

The Navier-Stokes equations can be used for turbulent flow simulations, although this would require a large number of elements in order to capture the wide range of scales in the flow. An alternative approach is to divide the flow quantities into mean values and fluctuations. When solving for the mean-flow quantities, the effect of the fluctuations is modeled using a turbulence closure. The idea behind this approach is that solving the model for the turbulence closure is numerically less expensive than resolving all the turbulence scales. Different turbulence closures invoke different assumptions on the modeled fluctuations, resulting in various degrees of accuracy for different flow cases.

This module includes Reynolds-averaged Navier-Stokes (RANS) models which is the model type most commonly used in industrial flow applications.

REYNOLDS-AVERAGED NAVIER-STOKES (RANS) EQUATIONS

The following assumes that the fluid is incompressible and Newtonian in which case the Navier-Stokes equations take the form:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} \tag{3-61}$$

$$\rho \nabla \cdot \mathbf{u} = 0$$

Once the flow has become turbulent, all quantities fluctuate in time and space. It is seldom worth the extreme computational cost to obtain detailed information about the fluctuations. An averaged representation often provides sufficient information about the flow.

The Reynolds-averaged representation of turbulent flows divides the flow quantities into an averaged value and a fluctuating part,

$$\phi = \bar{\phi} + \phi'$$

where ϕ can represent any scalar quantity of the flow. In general, the mean value can vary in space and time. This is exemplified in Figure 3-8, which shows time averaging of one component of the velocity vector for nonstationary turbulence. The unfiltered flow has a time scale Δt_1. After a time filter with width $\Delta t_2 \gg \Delta t_1$ has been applied, there is a fluctuating part, u'_i, and an average part, U_i. Because the flow field also varies on a time

scale longer than Δt_2, U_i is still time-dependent but is much smoother than the unfiltered velocity u_i.
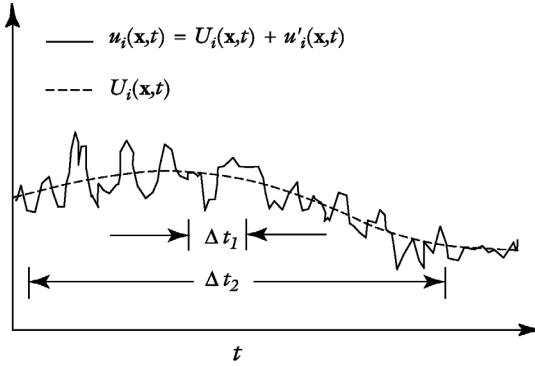
Figure 3-8: The unfiltered velocity component u_i, with a time scale Δt_1, and the averaged velocity component, U_i, with time scale Δt_2.

Decomposition of the flow field into an averaged part and a fluctuating part, followed by insertion into the Navier-Stokes equation, and averaging, gives the Reynolds-averaged Navier-Stokes (RANS) equations:

$$\rho\frac{\partial \mathbf{U}}{\partial t} + \rho\mathbf{U} \cdot \nabla\mathbf{U} + \nabla \cdot \overline{(\rho\mathbf{u'} \otimes \mathbf{u'})} = -\nabla P + \nabla \cdot \mu(\nabla\mathbf{U} + (\nabla\mathbf{U})^T) + \mathbf{F} \qquad (3\text{-}62)$$

$$\rho\nabla \cdot \mathbf{U} = 0$$

where $\mathbf{U}$ is the averaged velocity field and $\otimes$ is the outer vector product. A comparison with Equation 3-61 indicates that the only difference is the appearance of the last term on the left-hand side of Equation 3-62. This term represents the interaction between the fluctuating parts of the velocity field and is called the Reynolds stress tensor. This means that to obtain the mean flow characteristics, information about the small-scale structure of the flow is needed. In this case, that information is the correlation between fluctuations in all three directions.

EDDY VISCOSITY

The most common way to model turbulence is to assume that the turbulence is of a purely diffusive nature. The deviating part of the Reynolds stress is then expressed as

$$\rho(\overline{\mathbf{u'} \otimes \mathbf{u'}}) - \frac{\rho}{3}\text{trace}(\overline{\mathbf{u'} \otimes \mathbf{u'}})I = -\mu_T(\nabla\mathbf{U} + (\nabla\mathbf{U})^T)$$

where μ_T is the *eddy viscosity*, also known as the turbulent viscosity. The spherical part can be written

$$\frac{\rho}{3}\text{trace}(\overline{\mathbf{u'} \otimes \mathbf{u'}})I = \frac{2}{3}\rho k$$

where k is the turbulent kinetic energy. In simulations of incompressible flows, this term is included in the pressure, but when the absolute pressure level is of importance (in compressible flows, for example) this term must be explicitly included.

TURBULENT COMPRESSIBLE FLOW

If the Reynolds average is applied to the compressible form of the Navier-Stokes equations, terms of the form

$$\overline{\rho' u'}$$

appear and need to be modeled. To avoid this, a density-based average, known as the Favre average, is introduced:

$$\tilde{u}_i = \frac{1}{\overline{\rho}} \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} \rho(\mathbf{x},\tau)u_i(\mathbf{x},\tau) \, d\tau \tag{3-63}$$

It follows from Equation 3-63 that

$$\overline{\rho}\tilde{u}_i = \overline{\rho u_i} \tag{3-64}$$

and a variable, u_i, is decomposed into a mass-averaged component, $\tilde{u}_i$, and a fluctuating component, u_i'', according to

$$u_i = \tilde{u}_i + u_i'' \tag{3-65}$$

Using Equation 3-64 and Equation 3-65 along with some modeling assumptions for compressible flows (Ref. 7), Equation 3-16 and Equation 3-17 can be written on the form

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\tilde{u}_i) = 0$$

$$\overline{\rho}\frac{\partial \tilde{u}_i}{\partial t} + \overline{\rho}\tilde{u}_j\frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\mu\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij} - \overline{\rho u_j'' u_i''}\right) + \overline{F}_i \tag{3-66}$$

The Favre-averaged Reynolds stress tensor is modeled using the same argument as for incompressible flows:

$$-\overline{\rho u_j'' u_i''} = \mu_T \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \left(\mu_T \frac{\partial \tilde{u}_k}{\partial x_k} + \overline{\rho} k \right) \delta_{ij}$$

where k is the turbulent kinetic energy. Comparing Equation 3-66 to its incompressible counterpart (Equation 3-62), it can be seen that except for the term

$$-(2/3)\overline{\rho} k \delta_{ij}$$

the compressible and incompressible formulations are exactly the same, except that the free variables are $\tilde{u}_i$ instead of

$$U_i = \overline{u}_i$$

More information about modeling turbulent compressible flows can be found in Ref. 1 and Ref. 7.

The turbulent transport equations are used in their fully compressible formulations (Ref. 8).

The Algebraic yPlus Turbulence Model

The *algebraic yPlus turbulence model* is an algebraic turbulence model based on the distance to the nearest wall. The model is based on Prandtl's mixing-length theory and is suitable for internal flows. It is less mesh sensitive than transport-equation models like Spalart-Allmaras or the k-ε model. In what follows, let y be the coordinate normal to the wall, and U the velocity parallel to the wall. Using a mixing length formulation, the balance for the shear stress in the wall layer may be approximated as

$$\left(\mu + \rho l_{\text{mix}}^2 \left| \frac{\partial U}{\partial y} \right| \right) \frac{\partial U}{\partial y} = \rho u_\tau^2$$

which, expressed on dimensionless form, reduces to

$$\left(1 + l_{\text{mix}}^{+2} \left| \frac{\partial u^+}{\partial y^+} \right| \right) \frac{\partial u^+}{\partial y^+} = 1 \tag{3-67}$$

where $y^+ = y u_\tau / \nu$, $u^+ = U/u_\tau$ and $u_\tau = \sqrt{\tau_w / \rho}$ is the friction velocity. Close to the wall, the mixing length must be zero such that $u^+ = y^+$, and far away from the wall, $l_{\text{mix}}^+ \approx \kappa y^+$ such that $u^+ = (1/\kappa)\log(y^+) + B$. To obtain the correct behavior, the mixing length is chosen to be

$$l^+_{mix} = \begin{cases} 0 & y^+ \le y^* \\ \kappa(y^+ - y^*) & y^+ > y^* \end{cases} \tag{3-68}$$

where y^* is to be determined. Inserting Equation 3-68 into Equation 3-67

$$\frac{\partial u^+}{\partial y^+} = \begin{cases} 1 & y^+ \le y^* \\ \dfrac{\sqrt{1 + 4\kappa^2(y^+ - y^*)^2} - 1}{2\kappa^2(y^+ - y^*)^2} & y^+ > y^* \end{cases} \tag{3-69}$$

Integrating Equation 3-69

$$u^+ = \begin{cases} y^+ & y^+ \le y^* \\ y^* + \dfrac{1 - \sqrt{1 + 4\kappa^2(y^+ - y^*)^2}}{2\kappa^2(y^+ - y^*)} & \\ \quad + \dfrac{1}{\kappa}\log(\sqrt{1 + 4\kappa^2(y^+ - y^*)^2} + 2\kappa(y^+ - y^*)) & y^+ > y^* \end{cases} \tag{3-70}$$

For large values of y^+, Equation 3-70 reduces to

$$u^+ = \frac{1}{\kappa}\log(y^+) + \frac{1}{\kappa}(\log(4\kappa) - 1) + y^*$$

Comparing the above expression with the logarithmic law of the wall

$$u^+ = \frac{1}{\kappa}\log(y^+) + B$$

the value of the constant y^* is obtained as

$$y^* = B - \frac{1}{\kappa}(\log(4\kappa) - 1)$$

The dimensionless effective viscosity can be evaluated from

$$
\nu^+ = \begin{cases} 1 & y^+ \le y^* \\ 1 + \kappa^2(y^+ - y^*)^2 \left| \dfrac{\partial u^+}{\partial y^+} \right| = \dfrac{1 + \sqrt{1 + 4\kappa^2(y^+ - y^*)^2}}{2} & y^+ > y^* \end{cases}
$$
(3-71)

This requires the local value of y^+, which is obtained from the Reynolds number

$$
\mathrm{Re} = \frac{Uy}{\nu} = \frac{Uyu_\tau}{u_\tau \, \nu} = u^+ y^+ =
$$

$$
\begin{cases} y^{+2} & y^+ \le y^* \\[2mm] y^+\left(y^* + \dfrac{1 - \sqrt{1 + 4\kappa^2(y^+ - y^*)^2}}{2\kappa^2(y^+ - y^*)} + \dfrac{1}{\kappa}\log\left(\sqrt{1 + 4\kappa^2(y^+ - y^*)^2} + 2\kappa(y^+ - y^*)\right) \right) & \\[4mm] & y^+ > y^* \end{cases}
$$
(3-72)

The nonlinear algebraic Equation 3-72 has to be solved at each node point to evaluate the effective viscosity from Equation 3-71. The local Reynolds number $\mathrm{Re} = Uy/\nu$ is formed with the local absolute value of the velocity and the distance to the nearest wall. This implicitly assumes that the main flow direction is parallel to the wall.

WALL DISTANCE

The wall distance, y is provided by a mathematical Wall Distance interface that is included when using the Algebraic yPlus model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Transient study step.

WALL BOUNDARY CONDITION

Low Reynolds Number Wall Treatment
The Algebraic yPlus turbulence model is consistent with a no slip boundary condition, that is $\mathbf{u}=\mathbf{0}$. Since the turbulence model is algebraic, no additional boundary condition is

needed. This boundary conditions is applied for Wall Treatment equal to **Low Re**.

The low-Reynolds-number formulation of the Algebraic yPlus model can be considered to be well resolved at a wall if l_c^+ is of order unity. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell and can be evaluated as the boundary variable: **lplus_cc**.

Automatic Wall Treatment

The default boundary treatment for Algebraic yPlus is the **Automatic** wall treatment. The automatic wall treatment assumes that there is a small gap, $\delta_w = h_w/2$, between the computational domain and the physical wall. Here, h_w is the height of the mesh cell adjacent to the wall. wall (see Figure 3-9).
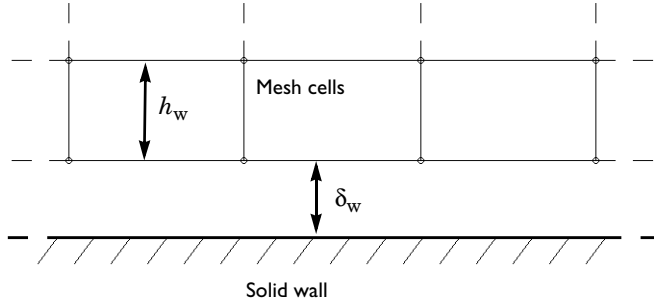
Figure 3-9: The computational domain is located a distance δ_w from the wall.

The boundary conditions for the velocity is a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \sigma - (\mathbf{n} \cdot \sigma \cdot \mathbf{n})\mathbf{n} = -\rho u_\tau^2 \frac{\mathbf{u}}{|\mathbf{u}|}$$

where

$$\sigma = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

and

$$u_\tau = \frac{\mathbf{u}}{u^+}$$

The automatic wall treatment tends to the low-Reynolds-number formulation when h_w tends to zero, and it becomes a wall function formulation when the resolution in viscous

units, $\Delta_w{}^+$ increases. The resolution in viscous units is available as a postprocessing variable, `Delta_wPlus`.

See also Wall for boundary condition details.

	In the *COMSOL Multiphysics Reference Manual*:
Ⓠ	• The Wall Distance Interface
	• Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization

---

The L-VEL Turbulence Model

The *L-VEL (Length-VELocity) turbulence model* is an algebraic turbulence model often used in electronic cooling applications. It is less mesh sensitive than transport-equation models like Spalart-Allmaras or the k-ε model. It was developed by Agonafer et al. (Ref. 22) for internal flows and uses an extension of the logarithmic law of the wall which applies all the way down to the wall

$$y^+ = u^+ + \frac{1}{E}\left(e^{\kappa u^+} - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6} - \frac{(\kappa u^+)^4}{24}\right) \tag{3-73}$$

where $y^+ = yu_\tau/\nu$, $u^+ = U/u_\tau$, U is the local flow speed, y is the distance to the nearest wall, ν is the kinematic viscosity and u_τ is the friction velocity. κ is the von Kàrman constant and E=8.6 is another constant needed to fit the logarithmic law of the wall. The shear stress in the wall layer is given by

$$\rho(\nu + \nu_T)\frac{\partial U}{\partial y} = \rho u_\tau^2 \Rightarrow 1 + \frac{\nu_T}{\nu} = \frac{u_\tau^2}{\nu}\frac{1}{\partial U/\partial y} = \frac{1}{\partial(U/u_\tau)/\partial(yu_\tau/\nu)} \Rightarrow$$

$$\nu^+ = \frac{1}{\partial u^+/\partial y^+}$$

Differentiating Equation 3-73 with respect to y^+, the dimensionless effective viscosity is obtained as

$$\nu^+ = 1 + \frac{\kappa}{E}\left(e^{\kappa u^+} - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6}\right) \tag{3-74}$$

If the local value of u^+ is known, the effective viscosity can be evaluated from Equation 3-74. The value of u^+ is obtained by forming a local Reynolds number

$$\text{Re} = \frac{Uy}{\nu} = \frac{Uy}{u_\tau}\frac{u_\tau}{\nu} = u^+ y^+ =$$

$$= u^+\left(u^+ + \frac{1}{E}\left(e^{\kappa u^+} - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6} - \frac{(\kappa u^+)^4}{24}\right)\right)$$

(3-75)

where the last expression follows from Equation 3-73. Hence, the nonlinear algebraic Equation 3-75 has to be solved at each node point to evaluate the effective viscosity. The local Reynolds number $\text{Re} = Uy/\nu$ is formed with the local absolute value of the velocity and the distance to the nearest wall. This implicitly assumes that the main flow direction is parallel to the wall.

WALL DISTANCE

The wall distance, y is provided by a mathematical Wall Distance interface that is included when using the L-VEL model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Transient study step.

WALL BOUNDARY CONDITION

Low Reynolds Number Wall Treatment
The L-VEL turbulence model is consistent with a no slip boundary condition, that is **u=0**. Since the turbulence model is algebraic, no additional boundary condition is needed. This boundary conditions is applied for Wall Treatment equal to **Low Re**.

The L-VEL model can be considered to be well resolved at a wall if l_c^+ is of order unity. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell and can be evaluated as the boundary variable: **lplus_cc**.

Automatic Wall Treatment
The default boundary treatment for Algebraic yPlus is the **Automatic** wall treatment. The details are described in Wall boundary condition for The Algebraic yPlus Turbulence Model.

See also Wall for boundary condition details.

	In the *COMSOL Multiphysics Reference Manual:*
⊘	• The Wall Distance Interface • Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization

The k-ε Turbulence Model

The k-ε model is one of the most used turbulence models for industrial applications. This module includes the standard k-ε model (Ref. 1). The model introduces two additional transport equations and two dependent variables: the turbulent kinetic energy, k, and the turbulent dissipation rate, ε. The turbulent viscosity is modeled as

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon} \tag{3-76}$$

where C_μ is a model constant.

The transport equation for k reads:

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon \tag{3-77}$$

where the production term is

$$P_k = \mu_T \left(\nabla \mathbf{u} : (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}(\nabla \cdot \mathbf{u})^2 \right) - \frac{2}{3}\rho k \nabla \cdot \mathbf{u} \tag{3-78}$$

The transport equation for ε reads:

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} \tag{3-79}$$

The model constants in Equation 3-76, Equation 3-77, and Equation 3-79 are determined from experimental data (Ref. 1) and the values are listed in Table 3-3.

TABLE 3-3: MODEL CONSTANTS

CONSTANT	VALUE
C_μ	0.09
$C_{\varepsilon 1}$	1.44

TABLE 3-3: MODEL CONSTANTS

CONSTANT	VALUE
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3

MIXING LENGTH LIMIT

Equation 3-77 and Equation 3-79 cannot be implemented directly as written. There is, for example, nothing that prevents division by zero. The equations are instead implemented as suggested in Ref. 10. The implementation includes an upper limit on the mixing length, $l_{\text{mix}}^{\lim}$:

$$l_{\text{mix}} = \max\left(C_\mu \frac{k^{3/2}}{\varepsilon}, l_{\text{mix}}^{\lim}\right) \tag{3-80}$$

The mixing length is used to calculated the turbulent viscosity. $l_{\text{mix}}^{\lim}$ should not be active in a converged solution but is merely a tool to obtain convergence.

REALIZABILITY CONSTRAINTS

The eddy-viscosity model of the Reynolds stress tensor can be written

$$\rho \overline{u_i u_j} = -2\mu_T S_{ij} + \frac{2}{3}\rho k \delta_{ij}$$

where δ_{ij} is the Kronecker delta and S_{ij} is the strain-rate tensor. The diagonal elements of the Reynolds stress tensor must be nonnegative, but calculating μ_T from Equation 3-76 does not guarantee this. To assert that

$$\rho \overline{u_i u_i} \geq 0 \quad \forall i$$

the turbulent viscosity is subjected to a realizability constraint. The constraint for 2D and 2D axisymmetry without swirl is:

$$\mu_T \leq \frac{\rho k \sqrt{2}}{3\sqrt{S_{ij}S_{ij}}} \tag{3-81}$$

and for 3D and 2D axisymmetry with swirl flow it reads:

$$\mu_T \leq \frac{\rho k}{\sqrt{6}\sqrt{S_{ij}S_{ij}}} \tag{3-82}$$

Combining equation Equation 3-81 with Equation 3-76 and the definition of the mixing length gives a limit on the mixing length scale:

$$l_{\text{mix}} \leq \sqrt{\frac{2}{3}} \frac{\sqrt{k}}{\sqrt{S_{ij}S_{ij}}} \tag{3-83}$$

Equivalently, combining Equation 3-82 with Equation 3-76 and Equation 3-80 gives:

$$l_{\text{mix}} \leq \frac{1}{\sqrt{6}} \frac{\sqrt{k}}{\sqrt{S_{ij}S_{ij}}} \tag{3-84}$$

This means there are two limitations on l_{mix}: the realizability constraint and the imposed limit via Equation 3-80.

The effect of not applying a realizability constraint is typically excessive turbulence production. The effect is most clearly visible at stagnation points. To avoid such artifacts, the realizability constraint is always applied for the RANS models. More details can be found in Ref. 4, Ref. 5, and Ref. 6.

MODEL LIMITATIONS

The k-ε turbulence model relies on several assumptions, the most important of which is that the Reynolds number is high enough. It is also important that the turbulence is in equilibrium in boundary layers, which means that production equals dissipation. These assumptions limit the accuracy of the model because they are not always true. It does not, for example, respond correctly to flows with adverse pressure gradients and can result in under-prediction of the spatial extent of recirculation zones (Ref. 1). Furthermore, in simulations of rotating flows, the model often shows poor agreement with experimental data (Ref. 2). In most cases, the limited accuracy is a fair trade-off for the amount of computational resources saved compared to using more complicated turbulence models.

WALL FUNCTIONS

The flow close to a solid wall is for a turbulent flow very different from the free stream. This means that the assumptions used to derive the k-ε model are not valid close to walls. While it is possible to modify the k-ε model so that it describes the flow in wall regions (see The Low Reynolds Number k-e Turbulence Model), this is not always desirable because of the very high resolution requirements that follow. Instead, analytical expressions are used to describe the flow near the walls. These expressions are known as wall functions.

The wall functions in COMSOL Multiphysics are such that the computational domain is assumed to be located a distance δ_w from the wall as shown in Figure 3-9. The distance δ_w is automatically computed so that

$$\delta_w^+ = \rho u_\tau \delta_w / \mu$$

where $u_\tau = C_\mu^{1/4}\sqrt{k}$ is the friction velocity, is 11.06. This corresponds to the distance from the wall where the logarithmic layer meets the viscous sublayer (or to some extent would meet it if there were no buffer layer in between). δ_w is limited from below so that it never becomes smaller than half the height of the boundary mesh cell. This means that δ_w^+ can become larger than 11.06 if the mesh is relatively coarse.

Always investigate the solution to check that δ_w is small compared to the dimensions of the geometry. Also check that δ_w^+ is 11.06 on most of the walls. If δ_w^+ is much larger than 11.06 over a significant part of the walls, the accuracy might become compromised. Both the wall lift-off, δ_w, and the wall lift-off in viscous units, δ_w^+, are available as results and analysis variables.

The boundary conditions for the velocity is a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \sigma - (\mathbf{n} \cdot \sigma \cdot \mathbf{n})\mathbf{n} = -\rho u_\tau \frac{\mathbf{u}}{u^+}$$

where

$$\sigma = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

is the viscous stress tensor and

$$u_\tau = \max\left(\frac{|\mathbf{u}|}{\frac{1}{\kappa_v}\ln \delta_w^+ + B}, C_\mu^{1/4}\sqrt{k} \right)$$

where in turn, κ_v, is the von Kárman constant (default value 0.41) and B is a constant that by default is set to 5.2.

The turbulent kinetic energy is subject to a homogeneous Neumann condition $\mathbf{n} \cdot \nabla k = 0$ and the boundary condition for ε reads:

$$\varepsilon = \frac{C_\mu^{3/4} k^{3/2}}{\kappa_v \delta_w}$$

See Ref. 10 and Ref. 11 for further details.

WALL FUNCTIONS FOR ROUGH WALLS

The physics interfaces: Wall, Interior Wall, Rotating Wall, and Rotating Interior Wall have an option to apply wall roughness by modifying the wall functions. Cebeci (Ref. 20) suggested a model which adjusts the friction velocity for surface roughness,

$$u_\tau = \frac{|\mathbf{u}|}{\frac{1}{\kappa_v}\ln\delta_w^+ + B - \Delta B} \tag{3-85}$$

where

$$\Delta B = \begin{cases} 0 & k_s^+ \leq 2.25 \\ \frac{1}{\kappa_v}\ln\left[\frac{k_s^+ - 2.25}{87.75} + C_s k_s^+\right]\sin[0.4258(\ln k_s^+ - 0.811)] & 2.25 \leq k_s^+ \leq 90 \\ \frac{1}{\kappa_v}\ln(1 + C_s k_s^+) & k_s^+ \geq 90 \end{cases}$$

k_s^+ is the roughness height in viscous units,

$$k_s^+ = \frac{\rho C_\mu^{1/4}\sqrt{k}}{\mu}k_s$$

The roughness height, k_s, is the peak-to-peak value of the surface variations and the wall is relocated to their mean level.
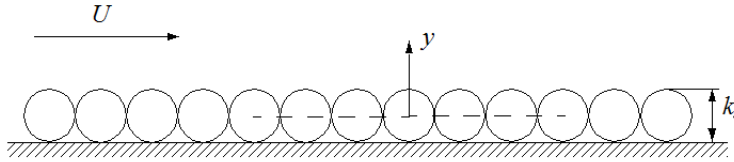
Figure 3-10: Definitions of the roughness height and the modified wall location.

Hence, when Equation 3-85 is used the lift-off is modified according to,

$$\delta_w^+ = max\{11.06,\ k_s^+/2,\ h^+/2\}$$

where h^+ is the height of the boundary mesh cell in viscous units. C_s is a parameter that depends on the shape and distribution of the roughness elements. When the turbulence parameters κ_v and B have the values 0.41 and 5.2, respectively, and $C_s = 0.26$, k_s

corresponds to the *equivalent sand roughness height*, k_{seq}, as introduced by Nikuradse (Ref. 21). A few characteristic values of the equivalent sand roughness height are given in Table 3-4 below,

TABLE 3-4: EQUIVALENT SAND ROUGHNESS HEIGHTS k_{seq}

SURFACE TYPE	EQUIVALENT SAND ROUGHNESS HEIGHT
Steel, new	50 µm
Galvanized steel	0.13 mm
Riveted steel	0.9-9 mm
Cast iron, new	0.25 mm
Galvanized iron	0.15-0.30 mm
Cast iron, rusted	1.0-1.5 mm
Bituminized steel or iron, new	30-50 µm
Glass	0.3 µm
Drawn tubing	1.5 µm
Wood, new	0.5 mm
Concrete, new	0.3-3 mm

Use other values of the roughness parameter C_s and roughness height k_s to specify generic surface roughnesses.

INITIAL VALUES

The default initial values for a stationary simulation are (Ref. 10),

$$\mathbf{u} = 0$$
$$p = 0$$
$$k = \left(\frac{10 \cdot \mu}{\rho(0.1 \cdot l_{mix}^{lim})}\right)^2$$
$$\varepsilon = \frac{C_\mu k_{init}^{3/2}}{0.1 \cdot l_{mix}^{lim}}$$

where l_{mix}^{lim} is the mixing length limit. For time-dependent simulations, the initial value for k is instead

$$k = \left(\frac{\mu}{\rho(0.1 \cdot l_{mix}^{lim})}\right)^2$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The k-ε equations are derived under the assumption that the flow has a high enough Reynolds number. If this assumption is not fulfilled, both k and ε have very small magnitudes and behave chaotically in the manner that the relative values of k and ε can change by large amounts due to small changes in the flow field.

A time-dependent simulation of a turbulent flow can include a period when the flow is not fully turbulent. A typical example is the startup phase when for example an inlet velocity or a pressure difference is gradually increased. To sort out numerical fluctuations in k and ε during such periods, the default time-dependent solver for the k-ε model employs unscaled absolute tolerances for k and ε. The tolerances are set to

$$k_{\text{scale}} = (0.01 U_{\text{scale}})^2$$
$$\varepsilon_{\text{scale}} = 0.09 k_{\text{sclae}}^{3/2} / (L_{\text{fact}} \cdot l_{\text{bb, min}})$$

(3-86)

where U_{scale} and L_{fact} are input parameters available in the Advanced Settings section of the physics interface node. Their default values are 1 m/s and 0.035 respectively. $l_{\text{bb,min}}$ is the shortest side of the geometry bounding box. Equation 3-86 is closely related to the expressions for k and ε on inlet boundaries (see Equation 3-142).

The practical implication of Equation 3-86 is that variations in k and ε smaller than k_{scale} and $\varepsilon_{\text{scale}}$ respectively, are regarded as numerical noise.

The k-ω Turbulence Model

The k-ω model solves for the turbulent kinetic energy, k, and for the dissipation per unit turbulent kinetic energy, ω. ω is also commonly know as the specific dissipation rate. The CFD Module has the Wilcox revised k-ω model (Ref. 1)

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = P_k - \rho \beta^* k \omega + \nabla \cdot ((\mu + \sigma^* \mu_T) \nabla k)$$
$$\rho \frac{\partial \omega}{\partial t} + \rho \mathbf{u} \cdot \nabla \omega = \alpha \frac{\omega}{k} P_k - \rho \beta \omega^2 + \nabla \cdot ((\mu + \sigma \mu_T) \nabla \omega)$$

(3-87)

where

$$\mu_T = \rho \frac{k}{\omega}$$

(3-88)

$$\alpha = \frac{13}{25} \quad \beta = \beta_0 f_\beta \quad \beta^* = \beta_0^* f_\beta \quad \sigma = \frac{1}{2} \quad \sigma^* = \frac{1}{2}$$

$$\beta_0 = \frac{13}{125} \quad f_\beta = \frac{1 + 70\chi_\omega}{1 + 80\chi_\omega} \quad \chi_\omega = \left| \frac{\Omega_{ij}\Omega_{jk}S_{ki}}{(\beta_0^*\omega)^3} \right|$$

$$\beta_0^* = \frac{9}{100} \quad f_{\beta^*} = \begin{cases} 1 & \chi_k \leq 0 \\ \dfrac{1 + 680\chi_k^2}{1 + 400\chi_k^2} & \chi_k > 0 \end{cases} \quad \chi_k = \frac{1}{\omega^3}(\nabla k \cdot \nabla \omega) \qquad (3\text{-}89)$$

where in turn Ω_{ij} is the mean rotation-rate tensor

$$\Omega_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

and S_{ij} is the mean strain-rate tensor

$$S_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

P_k is given by Equation 3-78. The following auxiliary relations for the dissipation, ε, and the turbulent mixing length, l_*, are also used:

$$\varepsilon = \beta^* \omega k \quad l_{\text{mix}} = \frac{\sqrt{k}}{\omega} \qquad (3\text{-}90)$$

MIXING LENGTH LIMIT AND REALIZABILITY CONSTRAINTS

The implementation of the k-ω model relies on the same concepts as the k-ε model (Ref. 10). This means that the following approximations have been used:

$$\frac{\omega}{k} \approx \frac{\rho}{\max(\mu_T, \text{eps})}$$

$$\frac{1}{\omega} = \frac{\sqrt{k}}{\omega\sqrt{k}} = \frac{l_{\text{mix}}}{\sqrt{k}} = l_{\text{mix}}\left(\frac{\rho l_{\text{mix}}}{\mu_T}\right) \approx \frac{l_{\text{mix}}^2 \rho}{\max(\mu_T, \text{eps})}$$

$$l_{\text{mix}} = \min\left(\frac{\sqrt{k}}{\omega}, l_{\text{mix}}^{\lim}, l_{\text{r}}\right)$$

where l_{r} is the limit given by the realizability constraints (Equation 3-83 and Equation 3-84).

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. For the specific dissipation, these solutions read

$$\omega_{\text{visc}} = \frac{6\nu}{\beta_0 \delta_w^2} \qquad \omega_{\log} = \frac{u_\tau}{\sqrt{\beta_0^*}\kappa_v \delta_w} \tag{3-91}$$

The corresponding expressions for the velocity is

$$u_\tau^{\text{visc}} = \sqrt{\frac{\nu U_\parallel}{\delta_w}} \qquad u_\tau^{\log} = \frac{U_\parallel}{\frac{1}{\kappa_v}\log(\delta_w^+) + B} \tag{3-92}$$

where δ_w is the distance to the nearest wall, κ_v, is the von Kárman constant (default value 0.41), $U_\parallel$ is the velocity parallel to the wall and B is a constant that by default is set to 5.2. Menter et al. (Ref. 9) suggested the following smooth blending expressions for ω and u_τ:

$$\omega = \sqrt{\omega_{\text{visc}}^2 + \omega_{\log}^2} \tag{3-93}$$

and

$$u_\tau = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u_\tau^{\log})^4} \tag{3-94}$$

These expression can be combined with the lift-off concept shown in Figure 3-9 which gives $\delta_w = h_w/2$. The wall condition for ω is given by Equation 3-93 and the conditions

for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \sigma - (\mathbf{n} \cdot \sigma \cdot \mathbf{n})\mathbf{n} = -\rho u_\tau \frac{\mathbf{u}}{u^+} \tag{3-95}$$

The k-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all δ_w^+.

The system given by Equation 3-85 through Equation 3-95 are however non-linear in u_τ and not very stable. To circumvent this, a variable $u^{*, \log}$ is introduced (see Ref. 10 and Ref. 11) such that

$$u^{*, \log} = \sqrt[4]{\beta_0^*} \sqrt{k} \tag{3-96}$$

This is then used in an alternative expression for the friction velocity:

$$u^* = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u^{*, \log})^4} \tag{3-97}$$

Equation 3-97 is in turn is used to calculate an alternative dimensionless wall distance

$$\delta_w^* = \frac{u^* \delta_w}{\nu} \tag{3-98}$$

Equation 3-97 is used instead of u_τ in the expression for $\omega_{\log}$ and Equation 3-98 is used instead of δ_w^+ in the expression for $u_\tau^{\log}$. The traction condition in Equation 3-95 is replaced by

$$\mathbf{n} \cdot \sigma - (\mathbf{n} \cdot \sigma \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^+} \tag{3-99}$$

Observe that the variable u^+ is calculated using equation Equation 3-94.

The resulting wall resolution, δ_w^+, is available as the postprocessing variable `Delta_wPlus`.

Wall Functions

When Wall Treatment is set to Wall functions, wall boundaries are treated with the same type of boundary conditions as for the k-ε model (see Wall Functions) with C_μ replaced by β_0^* and the boundary condition for ω given by

$$\omega_w = \frac{\rho k}{\kappa \delta_w^+ \mu} \tag{3-100}$$

Low Reynolds Number

The k-ω turbulence model can be integrated all the way down to the wall and is consistent with the no-slip condition $\mathbf{u} = 0$. Since all velocities must disappear on the wall, so must k. Hence, $k=0$ on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_w \to 0} \omega = \frac{6\mu}{\rho \beta_0 l_w^2} \qquad (3\text{-}101)$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-101 (using the variable ω_w, which only exists in those cells). Accurate solutions in the near-wall region require that,

$$l_w^+ = \rho u_\tau l_w / \mu \sim 1 \qquad (3\text{-}102)$$

where u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \qquad (3\text{-}103)$$

The boundary variable **Distance to cell center in viscous units**, `lplus_cc`, is available to ensure that the mesh is fine enough. According to Equation 3-102, l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

Since the ω_w requires the wall distance, a wall distance equation must be solved prior to solving a k-ω model with low-Reynolds-number wall treatment.

INITIAL VALUES

The default initial values are the same as for the k-ε model (see Initial Values) but with the initial value of ω given by

$$\omega_{\text{init}} = \frac{\sqrt{k_{\text{init}}}}{0.1 \cdot l_{\text{mix}}^{\text{lim}}}$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The k-ω model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations) except that the scale for ω is given by

$$\omega_{\text{scale}} = \frac{\sqrt{k_{\text{scale}}}}{L_{\text{fact}} \cdot l_{\text{bb, min}}}$$

The k-ω model can in many cases give results that are superior to those obtained with the k-ε model (Ref. 1). It behaves, for example, much better for flat plate flows with adverse or favorable pressure gradients. However, there are two main drawbacks. The first is that the k-ω model can display a relatively strong sensitivity to free stream inlet values of ω. The other is that the k-ω model is numerically less robust than the k-ε model.

The SST Turbulence Model

To combine the superior behavior of the k-ω model in the near-wall region with the robustness of the k-ε model, Menter (Ref. 17) introduced the SST (Shear Stress Transport) model which interpolates between the two. The version of the SST model in the CFD Module includes a few well-tested (Ref. 16, Ref. 18) modifications, such as production limiters for both k and ω, the use of S instead of Ω in the limiter for μ_T and a sharper cut-off for the cross-diffusion term.

It is also a low Reynolds number model, that is, it does not apply wall functions. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate. The model equations are formulated in terms k and ω,

$$\rho\frac{\partial k}{\partial t} + \rho\mathbf{u} \cdot \nabla k = P - \rho\beta_0^* k\omega + \nabla \cdot ((\mu + \sigma_k\mu_T)\nabla k)$$

$$\rho\frac{\partial \omega}{\partial t} + \rho\mathbf{u} \cdot \nabla\omega = \frac{\rho\gamma}{\mu_T}P - \rho\beta\omega^2 + \nabla \cdot ((\mu + \sigma_\omega\mu_T)\nabla\omega) + 2(1 - f_{v1})\frac{\rho\sigma_{\omega2}}{\omega}\nabla\omega \cdot \nabla k$$

$$(3\text{-}104)$$

where,

$$P = \min(P_k, 10\rho\beta_0^* k\omega) \tag{3-105}$$

and P_k is given in Equation 3-78. The turbulent viscosity is given by,

$$\mu_T = \frac{\rho a_1 k}{\max(a_1\omega, Sf_{v2})} \tag{3-106}$$

where S is the characteristic magnitude of the mean velocity gradients,

$$S = \sqrt{2S_{ij}S_{ij}} \tag{3-107}$$

The model constants are defined through interpolation of appropriate inner and outer values,

$$\phi = f_{v1}\phi_1 + (1 - f_{v1})\phi_2 \quad \text{for} \quad \phi = \beta, \gamma, \sigma_k, \sigma_\omega \tag{3-108}$$

The interpolation functions f_{v1} and f_{v2} are defined as,

$$f_{v1} = \tanh(\theta_1^4)$$

$$\theta_1 = \min\left[\max\left(\frac{\sqrt{k}}{\beta_0^*\omega l_w}, \frac{500\mu}{\rho\omega l_w^2}\right), \frac{4\rho\sigma_{\omega 2}k}{CD_{k\omega}l_w^2}\right] \tag{3-109}$$

$$CD_{k\omega} = \max\left(\frac{2\rho\sigma_{\omega 2}}{\omega}\nabla\omega \cdot \nabla k, 10^{-10}\right)$$

and,

$$f_{v2} = \tanh(\theta_2^2)$$

$$\theta_2 = \max\left(\frac{2\sqrt{k}}{\beta_0^*\omega l_w}, \frac{500\mu}{\rho\omega l_w^2}\right) \tag{3-110}$$

where l_w is the distance to the closest wall.

Realizability Constraints are applied to the SST model.

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the SST model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Transient study step.

The default model constants are given by,

$$\beta_1 = 0.075, \quad \gamma_1 = 5/9, \quad \sigma_{k1} = 0.85, \quad \sigma_{\omega 1} = 0.5$$
$$\beta_2 = 0.0828, \quad \gamma_2 = 0.44, \quad \sigma_{k2} = 1.0, \quad \sigma_{\omega 2} = 0.856 \qquad (3\text{-}111)$$
$$\beta_0^* = 0.09, \quad a_1 = 0.31$$

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

When Wall Treatment is set to **Automatic** the same type of formulation described for the k-ω model is applied at the boundary but with β_1 instead of β_0. See Automatic Wall Treatment for more details.

Low Reynolds Number

The SST model is low-Reynolds-number model, so the equations can be integrated all the way through the boundary layer to the wall, which allows for a no slip condition to be applied to the velocity, that is **u=0**.

Since all velocities must disappear on the wall, so must k. Hence, $k=0$ on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_w \to 0} \omega = \frac{6\mu}{\rho \beta_1 l_w^2} \qquad (3\text{-}112)$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-101 (using the variable ω_w, which only exists in those cells). Accurate solutions in the near-wall region require that,

$$l_w^+ = \rho u_\tau l_w / \mu \sim 1 \qquad (3\text{-}113)$$

where u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \qquad (3\text{-}114)$$

The boundary variable **Distance to cell center in viscous units**, `lplus_cc`, is available to ensure that the mesh is fine enough. According to Equation 3-102, l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the SST model.

The SST model was originally developed for exterior aerodynamic simulations. The recommended far-field boundary conditions (Ref. 17) can be expressed as,

$$\frac{10^{-5}U_\infty^2}{Re_L} < k_\infty < \frac{0.1\,U_\infty^2}{Re_L}$$
$$\frac{U_\infty}{L} < \omega_\infty < 10\frac{U_\infty}{L}$$

(3-115)

where L is the approximate length of the computational domain.

INITIAL VALUES

The SST model has the same default initial guess as the standard k-ω model (see Initial Values) but with l_{mix}^{lim} replaced by l_{ref}.

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The SST model applies absolute scales of the same type as the k-ω model (see Scaling for Time-Dependent Simulations).

	In the *COMSOL Multiphysics Reference Manual:*
ℚ	• The Wall Distance Interface
	• Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization

---

The Low Reynolds Number k-ε Turbulence Model

When the accuracy provided by wall functions in the k-ε model is not enough, a so called *low Reynolds number* model can be used. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate.

Most low Reynolds number k-ε models adapt the turbulence transport equations by introducing damping functions. This module includes the AKN model (after the inventors Abe, Kondoh, and Nagano; Ref. 12). The AKN k-ε model for compressible flows reads (Ref. 8 and Ref. 12):

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - f_\varepsilon C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k}$$

(3-116)

where

$$P_k = \mu_T \left(\nabla \mathbf{u} : (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u})^2 \right) - \frac{2}{3} \rho k \nabla \cdot \mathbf{u}$$

$$\mu_T = \rho f_\mu C_\mu \frac{k^2}{\varepsilon}$$

$$f_\mu = (1 - e^{-l^*/14})^2 \cdot \left(1 + \frac{5}{R_t^{3/4}} e^{-(R_t/200)^2} \right)$$

(3-117)

$$f_\varepsilon = (1 - e^{-l^*/3.1})^2 \cdot (1 - 0.3 e^{-(R_t/6.5)^2})$$

$$l^* = (\rho u_\varepsilon l_w)/\mu \quad R_t = \rho k^2/(\mu \varepsilon) \quad u_\varepsilon = (\mu \varepsilon/\rho)^{1/4}$$

and

$$C_{\varepsilon 1} = 1.5 \quad C_{\varepsilon 2} = 1.9 \quad C_\mu = 0.09 \quad \sigma_k = 1.4 \quad \sigma_\varepsilon = 1.4 \qquad (3\text{-}118)$$

l_w is the distance to the closest wall.

Realizability Constraints are applied to the low Reynolds number k-ε model.

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the low Reynolds number k-ε model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Transient study step.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. A formulation for ω-based methods was described by Menter et al. in Ref. 9. The Low-Reynolds number model uses a similar formulation and defines

$$u_\tau^{\text{visc}} = \sqrt{\frac{\nu U_{\|}}{\delta_w}} \quad u^{*,\log} = \sqrt[4]{C_\mu}\sqrt{k} \tag{3-119}$$

and

$$u^* = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u^{*,\log})^4} \tag{3-120}$$

δ_w is the distance to the closest wall. The boundary conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \sigma - (\mathbf{n} \cdot \sigma \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^+} \tag{3-121}$$

In Equation 3-121, $u^+ = U_{\|}/u_\tau$ with

$$u_\tau = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u_\tau^{\log})^4} \tag{3-122}$$

where in turn

$$u_\tau^{\log} = \frac{U_{\|}}{\frac{1}{\kappa_v}\log(\delta_w^+) + B} \tag{3-123}$$

Here, κ_v, is the von Kárman constant (default value 0.41), $U_{\|}$ is the velocity parallel to the wall and B is a constant that by default is set to 5.2.

These expression can be combined with the lift-off concept shown in Figure 3-9 which gives $\delta_w = h_w/2$. The k-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all δ_w^+.

The conditions for the turbulent dissipation, ε, is given by the Wolfshtein model which is commonly employed in two-layer k-ε implementations (Ref. 13):

$$\varepsilon = \frac{k^{3/2}}{l_\varepsilon}$$

$$l_\varepsilon = C_l \delta_w (1 - e^{-\mathrm{Re}_{\delta_w}/A_\varepsilon}) \qquad C_l = \kappa_v C_\mu^{-3/4} \qquad \qquad (3\text{-}124)$$

$$A_\varepsilon = 2C_l \qquad \qquad \mathrm{Re}_y = \frac{\delta_w \sqrt{k}}{\nu}$$

The resulting wall resolution, δ_w^+, is available as the postprocessing variable. `Delta_wPlus`.

Low Reynolds Number Wall Treatment

The damping terms in the equations for k and ε allow for a no slip condition to be applied to the velocity, that is **u=0** which is the case when Wall Treatment is set to **Low Re**.

Since all velocities must disappear on the wall, so must k. Hence, $k=0$ on the wall.

The correct wall boundary condition for ε is

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$$

where n is the wall normal direction. This condition is however numerically very unstable. Therefore, ε is not solved for in the cells adjacent to a solid wall and instead the analytical relation

$$\varepsilon = 2\frac{\mu}{\rho}\frac{k}{l_w^2} \qquad \qquad (3\text{-}125)$$

is prescribed in those cells (using the variable ε_w, which only exists in those cells). Equation 3-125 can be derived as the first term in a series expansion of

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$$

For the expansion to be valid, it is required that

$$l_c^+ < 0.5$$

l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell. The boundary variable **Distance to cell center in viscous units**, `lplus_cc`, is available to ensure that the mesh is fine enough. Observe that it is unlikely that a solution is obtained at all if

$$l_c^+ \gg 0.5$$

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the low-Reynolds number k-ε model.

INITIAL VALUES

The low-Reynolds number k-ε model has the same default initial guess as the standard k-ε model (see Initial Values) but with l_{mix}^{lim} replaced by l_{ref}.

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

In some cases, especially for stationary solutions, a fast way to convergence is to first solve the model using the ordinary k-ε model and then to use that solution as an initial guess for the low-Reynolds number k-ε model. The procedure is then as follows:

1 Solve the model using the k-ε model.

2 Switch to the low-Reynolds number k-ε model.

3 Add a new **Stationary with Initialization** study.

4 In the **Wall Distance Initialization** study step, set **Values of variables not solved for** to **Solution** from the first study. This is to propagate the solution from the first study down to the second step in the new study.

5 Solve the new study.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The low-Reynolds number k-ε model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations).

☑	In the *COMSOL Multiphysics Reference Manual:* • The Wall Distance Interface Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization

The Spalart-Allmaras Turbulence Model

The *Spalart-Allmaras turbulence model* is a one-equation turbulence model designed mainly for aerodynamic applications. It is a low Reynolds number model, that is, it does

not utilize wall functions. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate.

The model gives satisfactory results for many engineering applications, in particular for airfoil and turbine blade applications for which it is calibrated. It is however not appropriate for applications involving jet-like free shear regions. It also has some nonphysical properties. For example, it predicts zero decay rate for the eddy viscosity in a uniform free-stream (Ref. 1).

Compared to the low Reynolds number k-ε model, the Spalart-Allmaras model is generally considered more robust and is often used as a way to obtain an initial solution for more advanced models. It can give reasonable results on relatively coarse meshes for which the low Reynolds number k-ε model does not converge or even diverges.

This module includes the standard version of the Spalart-Allmaras model without the trip term (see Ref. 1 and Ref. 14). The model solves for the undamped turbulent kinematic viscosity, $\tilde{v}$:

$$\frac{\partial \tilde{v}}{\partial t} + \mathbf{u} \cdot \nabla \tilde{v} = c_{b1}\tilde{S}\tilde{v} - c_{w1}f_w\left(\frac{\tilde{v}}{l_w}\right)^2 + \frac{1}{\sigma}\nabla \cdot ((v + \tilde{v})\nabla \tilde{v}) + \frac{c_{b2}}{\sigma}\nabla \tilde{v} \cdot \nabla \tilde{v} \qquad (3\text{-}126)$$

The model includes the following auxiliary variables

$$c_{w1} = \frac{c_{b1}}{\kappa_v^2} + \frac{1 + c_{b2}}{\sigma}, \quad \chi = \frac{\tilde{v}}{v}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}$$

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_w = g\left(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6}\right)^{1/6}, \quad g = r + c_{w2}(r^6 - r)$$

$$r = \min\left(\frac{\tilde{v}}{\tilde{S}\kappa_v^2 l_w^2}, 10\right), \quad \tilde{S} = \max\left(\Omega + C_{\mathrm{Rot}}\min(0, S - \Omega) + \frac{\tilde{v}}{\kappa_v^2 l_w^2}f_{v2}, 0.3\Omega\right)$$

$$S = \sqrt{2S_{ij}S_{ij}} \qquad \Omega = \sqrt{2\Omega_{ij}\Omega_{ij}}$$

where

$$S_{ij} = 0.5(\nabla\mathbf{u} + \nabla\mathbf{u}^T) \qquad \Omega_{ij} = 0.5(\nabla\mathbf{u} - \nabla\mathbf{u}^T)$$

are the mean strain rate and mean rotation rate tensors, l_w, is the distance to the closest wall and $v = \mu/\rho$ is the kinematic viscosity. The turbulent viscosity is calculated by

$$\mu_T = \rho \tilde{v} f_{v1}$$

The default values for the modeling parameters are:

$$c_{b1} = 0.1355 \quad c_{b2} = 0.622 \quad c_{v2} = 7.1 \quad \sigma = 2/3$$
$$c_{w2} = 0.3 \quad\quad c_{w3} = 2 \quad\quad \kappa_v = 0.41 \quad C_{Rot} = 2.0$$

The implementation of the production term $\tilde{S}$ includes the rotation correction suggested in Ref. 14. See also Ref. 15. The terms r and $\tilde{S}$ are furthermore regularized according to Ref. 14.

Pseudo Time Stepping for Turbulent Flow Models is by default applied to the stationary form of the Spalart-Allmaras model.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment
For the Spalart-Allmaras turbulence model, the following relation is valid from the wall all the way through the log layer (Ref. 24):

$$\tilde{v} = \kappa_v \delta_w u_\tau \quad \Leftrightarrow \quad \tilde{v}^+ = \frac{\tilde{v}}{v} = \frac{\kappa_v \delta_w u_\tau}{v} = \kappa_v \delta_w^+ \tag{3-127}$$

δ_w^+ from Equation 3-127 can be used in Equation 3-92 to calculate u_τ^{log} which in turn gives u_τ through Equation 3-94. With u_τ, the boundary condition for $\tilde{v}$ is given by $\tilde{v} = \kappa_v \delta_w u_\tau$.

These relations are applied to the lift-off concept shown in Figure 3-9 which gives $\delta_w = h_w/2$. The boundary conditions for the momentum equations are a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$ and the traction condition given by Equation 3-95.

The resulting wall resolution, δ_w^+, is available as the postprocessing variable. `Delta_wPlus`.

Low Reynolds Number Wall Treatment
The Spalart-Allmaras model is consistent with a no slip boundary condition, that is $\mathbf{u}=0$. Since, there can be no fluctuations on the wall, the boundary condition for $\tilde{v}$ is $\tilde{v} = 0$.

The Spalart-Allmaras model can be considered to be well resolved at a wall if l_c^+ is of order unity. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell and can be evaluated as the boundary variable:

Distance to cell center in viscous units, `lplus_cc`. See also Wall for boundary condition details.

INITIAL VALUES

The default initial values for the Spalart-Allmaras version of the physics interface are:

$$\mathbf{u} = 0$$
$$p = 0$$
$$\tilde{\nu} = \frac{\mu}{\rho}$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The Spalart-Allmaras model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations) except that the scale for $\tilde{\nu}$ is given directly by the ν_{scale} parameter available in the advanced section of the physics interface node. The default value for ν_{scale} is $5 \cdot 10^{-6}$ m^2/s.

The v2-f Turbulence Model

For the v2-f model, the turbulent viscosity is based on the velocity fluctuations, $\overline{v^2}$, normal to the streamlines. This makes it possible to model turbulence anisotropy, and to separate between low-Reynolds number effects and wall blockage. Non-local effects of the pressure fluctuations on the turbulent fields are included by applying elliptic relaxation to the pressure strain term (Ref. 25, Ref. 26). The formulation implemented in COMSOL, solves for the normalized velocity fluctuations,

$$\zeta = \frac{\overline{v^2}}{k} \tag{3-128}$$

and an elliptic blending function, α, which is used to combine near-wall effects with those in the far-field. The complete model for compressible flow reads,

$$\rho\frac{\partial k}{\partial t} + \rho\mathbf{u} \cdot \nabla k = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_{kv2f}}\right)\nabla k\right) + P_k - \rho\varepsilon$$

$$\rho\frac{\partial\varepsilon}{\partial t} + \rho\mathbf{u} \cdot \nabla\varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_{\varepsilon v2f}}\right)\nabla\varepsilon\right) + \frac{1}{\tau}(C'_{\varepsilon 1}P_k - C'_{\varepsilon 2}\rho\varepsilon)$$

$$\frac{\partial\zeta}{\partial t} + \rho\mathbf{u} \cdot \zeta = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_{\zeta v2f}}\right)\nabla\zeta\right) + \frac{2}{k}\left(\alpha^3\mu + \frac{\mu_T}{\sigma_{kv2f}}\right)\nabla k \cdot \nabla\zeta \qquad \text{(3-129)}$$

$$-\frac{\zeta}{k}P_k + \alpha^3 f_h + (1-\alpha^3)f_w$$

$$\nabla^2\alpha = \frac{\alpha - 1}{L^2}$$

where

$$P_k = \mu_T\left(\nabla\mathbf{u}{:}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}(\nabla \cdot \mathbf{u})^2\right) - \frac{2}{3}\rho k\nabla \cdot \mathbf{u}$$

$$\mu_T = \rho C_{\mu v2f} k\zeta\tau$$

$$f_h = -\frac{\rho}{\tau}\left(C_1 - 1 + C_2\frac{P_k}{\rho\varepsilon}\right)\left(\zeta - \frac{2}{3}\right) \qquad \text{(3-130)}$$

$$f_w = -\rho\frac{\zeta}{k}\varepsilon$$

$$L = C_L\max\left[\frac{k^{3/2}}{\varepsilon}, C_\eta\left(\frac{\nu^3}{\varepsilon}\right)^{1/4}\right] \quad \tau = \max\left[\frac{k}{\varepsilon}, C_\tau\sqrt{\frac{\nu}{\varepsilon}}\right]$$

where $\nu = \mu/\rho$. The modified coefficients in the ε-equation are given by

$$C'_{\varepsilon 1} = C_{\varepsilon 1 v2f}\left(1 + A_1(1-\alpha^3)\frac{1}{\sqrt{\zeta}}\right)$$

$$C'_{\varepsilon 2} = C_{\varepsilon 2 v2f} + \alpha^3(1 - C_{\varepsilon 2 v2f})\tanh\left(\left|\frac{\mu_T\nabla^2 k}{\rho\varepsilon}\right|^{3/2}\right) \qquad \text{(3-131)}$$

with the default turbulence parameters

$$\begin{array}{llll}
C_{\varepsilon 1 v2f} = 1.44 & C_{\varepsilon 2 v2f} = 1.83 & C_{\mu v2f} = 0.22 & \sigma_{kv2f} = \sigma_{\zeta v2f} = 1 \\
\sigma_\varepsilon = 1.22 & C_1 = 1.7 & C_2 = 1.2 & C_\eta = 86 \\
C_\tau = 6 & A_1 = 0.04 & &
\end{array} \qquad \text{(3-132)}$$

Realizability Constraints are applied to the turbulent viscosity.

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the v2-f model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Transient study step.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. A formulation for ω-based methods was described by Menter et al. in Ref. 9. The v2-f model uses a similar formulation and defines

$$u_\tau^{\text{visc}} = \sqrt{\frac{\nu U_{\parallel}}{\delta_w}} \qquad u^{*,\log} = \sqrt[4]{C_{\mu v2f}} \zeta \sqrt{k} \tag{3-133}$$

and

$$u^* = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u^{*,\log})^4} \tag{3-134}$$

δ_w is the distance to the closest wall. The boundary conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \sigma - (\mathbf{n} \cdot \sigma \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^+} \tag{3-135}$$

In Equation 3-135, $u^+ = U_{\parallel}/u_\tau$ with

$$u_\tau = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u_\tau^{\log})^4} \tag{3-136}$$

where in turn

$$u_\tau^{\log} = \frac{U_\parallel}{\frac{1}{\kappa_v}\log(\delta_w^+) + B} \tag{3-137}$$

Here, κ_v, is the von Kármán constant (default value 0.41), $U_\parallel$ is the velocity parallel to the wall and B is a constant that by default is set to 5.2.

These expression can be combined with the lift-off concept shown in Figure 3-9 which gives $\delta_w = h_w/2$. The k-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all δ_w^+.

The conditions for the turbulent dissipation rate, ε, is similar to that in the Wolfshtein model which is commonly employed in two-layer k-ε implementations (Ref. 13):

$$\varepsilon = \frac{(C_{\mu v2f}\zeta_0)^{3/4}k^{3/2}}{l_\varepsilon}$$

$$l_\varepsilon = L(1 - e^{-\sqrt{Re_L}(\delta_w/L)})^2 \tag{3-138}$$

$$Re_y = \frac{(C_{\mu v2f}\zeta_0)^{3/4}\sqrt{k}L}{2\nu}$$

where

$$\zeta_0 = \frac{2}{3}\left(1 - \frac{1}{C_1 + C_2}\right) \tag{3-139}$$

The boundary conditions applied on ζ and α are given by

$$\zeta = \zeta_0\frac{\delta_w^2}{\delta_w^2 + L^2} \qquad \alpha = 1 - e^{-\delta_w/L} \tag{3-140}$$

The resulting wall resolution, δ_w^+, is available as the postprocessing variable. `Delta_wPlus`.

Low Reynolds Number Wall Treatment
The no slip condition, that is $\mathbf{u} = \mathbf{0}$ is applied when Wall Treatment is set to **Low Re**.

Since all velocities must disappear on the wall, so must k and ζ (since $k \sim y^2$ and $\overline{v^2} \sim y^4$). Hence, $k = 0$ and $\zeta = 0$ on the wall. By definition, $\alpha = 0$ on the wall.

The correct wall boundary condition for ε is

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$$

where n is the wall normal direction. This condition is however numerically very unstable. Therefore, ε is not solved for in the cells adjacent to a solid wall and instead the analytical relation

$$\varepsilon = 2\frac{\mu}{\rho}\frac{k}{l_w^2} \tag{3-141}$$

is prescribed in those cells (using the variable ε_w, which only exists in those cells). Equation 3-125 can be derived as the first term in a series expansion of

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$$

For the expansion to be valid, it is required that

$$l_c^+ < 0.5$$

l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell. The boundary variable **Distance to cell center in viscous units**, lplus_cc, is available to ensure that the mesh is fine enough. Observe that it is unlikely that a solution is obtained at all if

$$l_c^+ \gg 0.5$$

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the v2-f model.

INITIAL VALUES

The v2-f model has the same default initial guess as the standard k-ε model (see Initial Values) but with l_{mix}^{lim} replaced by l_{ref}. The default initial values for ζ and α are 2/3 and 1 respectively.

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

In some cases, especially for stationary solutions, a fast way to convergence is to first solve the model using the ordinary k-ε model and then to use that solution as an initial guess for the v2-f model. The procedure is then as follows:

1 Solve the model using the k-ε model.

2 Switch to the v2-f model.

3 Add a new **Stationary with Initialization** study.

4 In the **Wall Distance Initialization** study step, set **Values of variables not solved for** to **Solution** from the first study. This is to propagate the solution from the first study down to the second step in the new study.

5 Solve the new study.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The v2-f model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations).

In the *COMSOL Multiphysics Reference Manual:*

- The Wall Distance Interface
- Stationary with Initialization, Transient with Initialization, and Wall Distance Initialization

---

Inlet Values for the Turbulence Length Scale and Turbulent Intensity

If inlet data for the turbulence variables are not available, crude approximations for k, ε, ω and ζ can be obtained from the following formulas:

$$k = \frac{3}{2}(|\mathbf{U}|I_{\mathrm{T}})^2$$

$$\varepsilon = C_\mu^{3/4}\frac{k^{3/2}}{L_{\mathrm{T}}}$$

$$\omega = \frac{\sqrt{k}}{(\beta_0^*)^{1/4}L_T}$$

$$\zeta = \frac{2}{3}$$

(3-142)

where I_{T} is the turbulent intensity and L_{T} is the turbulence length scale.

A value of 10^{-3} (0.1%) is a low turbulent intensity I_T. Good wind tunnels can produce values as low as $5 \cdot 10^{-4}$ (0.05%). Fully turbulent flows usually have intensities between 0.05 (5%) and 0.1 (10%).

The turbulence length scale L_T is a measure of the size of the eddies that are not resolved. For free-stream flows these are typically very small (on the order of centimeters). The length scale cannot be zero, however, because that would imply infinite dissipation. Use Table 3-5 as a guideline when specifying L_T (Ref. 3) where l_w is the wall distance, and

$$l_w^+ = l_w/l^*$$

TABLE 3-5: TURBULENCE LENGTH SCALES FOR TWO-DIMENSIONAL FLOWS

FLOW CASE	L_T	L
Mixing layer	$0.07L$	Layer width
Plane jet	$0.09L$	Jet half width
Wake	$0.08L$	Wake width
Axisymmetric jet	$0.075L$	Jet half width
Boundary layer ($\partial p/\partial x = 0$) – Viscous sublayer and log-layer – Outer layer	$\kappa l_w(1 - \exp(-l_w^+/26))$ $0.09L$	Boundary layer thickness
Pipes and channels (fully developed flows)	$0.07L$	Pipe diameter or hydraulic diameter or channel width

Theory for the Pressure, No Viscous Stress Boundary Condition

For this module, the turbulent intensity I_T, turbulence length scale L_T, and reference velocity scale U_{ref} values are related to the turbulence variables via

$$k = \frac{3}{2}(I_T U_{ref})^2, \quad \varepsilon = \frac{C_\mu^{3/4}}{L_T}\left(\frac{3(I_T U_{ref})^2}{2}\right)^{\frac{3}{2}}, \quad \omega = \sqrt{\frac{3}{2}}\frac{I_T U_{ref}}{(\beta_0^*)^{1/4}L_T}, \quad \zeta = \frac{2}{3}$$

?	For recommendations of physically sound values see Inlet Values for the Turbulence Length Scale and Turbulent Intensity. Also see Inlet and Outlet for the node settings.

Initial Values for Generate New Turbulence Model Interfaces

A major advantage with the **Generate New Turbulence Model Interface** feature is that it can express initial values for the new turbulence model in terms of the original model. This makes it possible to first solve a problem using a simple, but robust, turbulence model, such as the k-ε model, and then switch to a more advanced model.

Unless the **Initial value from study** is not **None**, the **Generate New Turbulence Model Interface** initial values for velocity and pressure are taken directly from the solution of the parent model. The initial values of turbulent dependent variables are estimated by using the solution from the selected study:

- When the parent model is a Laminar Flow model, or when **Initial value from study** is not **None**, turbulent dependent variables get their default initial values.

- Initial values of dependent variables that exist in both the parent model and the generated model are taken directly from the selected study.

- When the parent model is Turbulent Flow, k-ε or Turbulent Flow, Low Reynolds k-ε and the generated model is Turbulent Flow, k-ω or SST, the initial value for ω is

$$\omega_{\text{init}} = 1/(\max(\text{eps}, \eta_T))\rho k$$

- When the parent model is k-ω or SST, and the generated model is k-ε or Low Reynolds k-ε or v2f, the initial value of ε is

$$\varepsilon_{\text{init}} = 1/(\max(\text{eps}, \eta_T))\rho k^2 c_\mu$$

- When the parent model is Algebraic yPlus, and the generated model is k-ε or Low Reynolds k-ε, the initial values of k and ε are:

$$k_{\text{init}} = \upsilon_T{}^2/(\sqrt{c_\mu}L_T)$$

$$\varepsilon_{\text{init}} = (c_\mu{}^{3/4}/L_T)k^{3/2}$$

where $L_T = \max(\kappa_a y, (y^*\upsilon)/u_T)$ and $u_T = |\mathbf{u}|/(\max(\text{eps}, u^+))$.

- When the parent model is Algebraic yPlus and the generated model is k-ω or SST, the initial value of k and ω are

$$k_{\text{init}} = \upsilon_T / (\sqrt{\beta^*}_0 L_T)^2$$

$$\omega_{\text{init}} = \sqrt{k} / (\beta^*_0{}^{1/4} L_T)$$

where $L_T = \max(\kappa_a y, (y^* \upsilon)/u_T)$ and $u_T = |\mathbf{u}|/(\max(\text{eps}, u^+))$.

- When the parent model is L-VEL, and the current model is k-ε or Low Reynolds k-ε, the initial value of k and ε are

$$k_{\text{init}} = \upsilon_T{}^2 / (\sqrt{c_\mu} L_T)$$

$$\varepsilon_{\text{init}} = (c_\mu{}^{3/4}/L_T) k^{3/2}$$

where $L_T = \max(\kappa_l y, (\kappa_l \upsilon E_l)/u_T)$.

- When the parent model is L-VEL, and the generated model is k-ω and SST, the initial values of k and omega are

$$k_{\text{init}} = \upsilon_T{}^2 / (\sqrt{\beta^*}_0 L_T)$$

$$\omega_{\text{init}} = (\sqrt{k}) / (\beta^*_0{}^{1/4} L_T)$$

- When the parent model is Spalart-Allmaras and the current model is k-ε or Low Reynolds k-ε, the initial value of k and ε are:

$$k_{\text{init}} = (f_{v1}{}^2 / (\sqrt{C_\mu})) \cdot \min((\tilde{\nu}/(\max(\kappa_\nu y, \text{eps})))^2, \nu |\Omega|)$$

$$\varepsilon_{\text{init}} = (\chi^8 / (\chi^3 + c_{v1}^3)^3) \cdot \min((1/\nu)(\tilde{\nu}/(\max(\kappa_\nu y, \text{eps})))^4, \nu |\Omega|)$$

- When the parent model is Spalart-Allmaras and the generated model is k-ω or SST the initial values of k and ω are

$$k_{\text{init}} = (f_{v1}^2/(\sqrt{\beta^*}_0)) \cdot \min(\tilde{v}/(\max(\kappa_v y, \text{eps}))^2, v|\Omega|)$$

$$\omega_{\text{init}} = (1/(\sqrt{\beta^*}_0))(\chi^2/(\chi^3 + c_{v1}^3)^2) \cdot \min((1/v)(\tilde{v}/(\max(\kappa_v y, \text{eps})))^2, v|\Omega|)$$

- When the generated model is Spalart-Allamas turbulent mode, and the parent model any turbulence model but Spalart-Allamas, the initial value of the dependent variable is $\tilde{v}_{\text{init}} = \mu_T/\rho$.

Solvers for Turbulent Flow

The nonlinear system that the Navier-Stokes (RANS) and turbulence transport equations constitute can become ill-conditioned if solved using a fully coupled solver. Turbulent flows are therefore solved using a segregated approach (Ref. 19): Navier-Stokes in one group and the turbulence transport equations in another.

For each iteration in the Navier-Stokes group, two or three iterations are performed for the turbulence transport equations. This is necessary to make sure that the very nonlinear source terms in the turbulence transport equations are in balance before performing another iteration for the Navier-Stokes group.

The default iterative solver for the turbulence transport equations is a damped Newton method with constant damping factor. In each iteration, a linearized version of the nonlinear system is solved using GMRES accelerated by Smoothed Aggregated Algebraic Multigrid (SAAMG). The default smoother is SOR Line.

As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, Geometric Multigrid (GMG) requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared memory computations with many cores. When the default linear solver is GMRES, an optional, but deactivated, linear solver node is available where GMRES is accelerated by GMG.

- Pseudo Time Stepping for Turbulent Flow Models
- Multigrid, Stationary Solver, Iterative, and SOR Line in the *COMSOL Multiphysics Reference Manual*

Pseudo Time Stepping for Turbulent Flow Models

The default stationary solver applies pseudo time stepping for both 2D and 3D models. This improves the robustness of the nonlinear iterations as well as the condition number for the linear equation system. The latter is especially important for large 3D models where iterative solvers must be applied. The turbulence equations use the same $\tilde{\Delta t}$ as the momentum equations.

The default manual expression for CFL_{loc} is, for 2D models:

$$1.3^{\min(\text{niterCMP-1},\,9)} +$$
$$\text{if}(\text{niterCMP} > 25,\, 9 \cdot 1.3^{\min(\text{niterCMP} - 25,\, 9)},\, 0) +$$
$$\text{if}(\text{niterCMP} > 50,\, 90 \cdot 1.3^{\min(\text{niterCMP} - 50,\, 9)},\, 0)$$

and for 3D models:

$$1.3^{\min(\text{niterCMP-1},\,9)} +$$
$$\text{if}(\text{niterCMP} > 30,\, 9 \cdot 1.3^{\min(\text{niterCMP} - 30,\, 9)},\, 0) +$$
$$\text{if}(\text{niterCMP} > 60,\, 90 \cdot 1.3^{\min(\text{niterCMP} - 60,\, 9)},\, 0)$$

References for the Single-Phase Flow, Turbulent Flow Interfaces

1. D.C. Wilcox, *Turbulence Modeling for CFD*, 2nd ed., DCW Industries, 1998.

2. D.M. Driver and H.L. Seegmiller, "Features of a Reattaching Turbulent Shear Layer in Diverging Channel Flow," *AIAA Journal*, vol. 23, pp. 163–171, 1985.

3. H.K. Versteeg and W. Malalasekera, *An Introduction to Computational Fluid Dynamics*, Prentice Hall, 1995.

4. A. Durbin, "On the k-ε Stagnation Point Anomaly," *Int. J. Heat and Fluid Flow*, vol. 17, pp. 89–90, 1986.

5. A, Svenningsson, *Turbulence Transport Modeling in Gas Turbine Related Applications*," doctoral dissertation, Department of Applied Mechanics, Chalmers University of Technology, 2006.

6. C.H. Park and S.O. Park, "On the Limiters of Two-equation Turbulence Models," *Int. J. Computational Fluid Dynamics*, vol. 19, no. 1, pp. 79–86, 2005.

7. J. Larsson, *Numerical Simulation of Turbulent Flows for Turbine Blade Heat Transfer*, doctoral dissertation, Chalmers University of Technology, Sweden, 1998.

8. L. Ignat, D. Pelletier, and F. Ilinca, "A Universal Formulation of Two-equation Models for Adaptive Computation of Turbulent Flows," *Computer Methods in Applied Mechanics and Engineering*, vol. 189, pp. 1119–1139, 2000.

9. F. Menter, J.C. Ferreira, T. Esch and B. Konno, "The SST Turbulence Model with Improved Wall Treatment for Heat Transfer Predictions in Gas Turbines," *Proceedings of the International Gas Turbine Congress*, IGTC2003-TS-059, Nov. 2-7, 2003.

10. D. Kuzmin, O. Mierka, and S. Turek, "On the Implementation of the k-ε Turbulence Model in Incompressible Flow Solvers Based on a Finite Element Discretization," *Int.J. Computing Science and Mathematics*, vol. 1, no. 2–4, pp. 193–206, 2007.

11. H. Grotjans and F.R. Menter, "Wall Functions for General Application CFD Codes," *ECCOMAS 98, Proceedings of the Fourth European Computational Fluid Dynamics Conference*, John Wiley & Sons, pp. 1112–1117, 1998.

12. K. Abe, T. Kondoh, and Y. Nagano, "A New Turbulence Model for Predicting Fluid Flow and Heat Transfer in Separating and Reattaching Flows—I. Flow Field Calculations," *Int. J. Heat and Mass Transfer*, vol. 37, no. 1, pp. 139–151, 1994.

13. H.C. Chen and V.C. Patel, "Near-Wall Turbulence Models for Complex Flows Including Separation," *AIAA Journal*, Vol. 26, No. 6, pp. 641-648, 1988.

14. "The Spalart-Allmaras Turbulence Model," http://turbmodels.larc.nasa.gov/spalart.html.

15. J. Dacles-Mariani, G.G. Zilliac and J.S. Chow, "Numerical/Experimental Study of a Wingtip Vortex in the Near Field", *AIAA Journal*, vol. 33, no. 9, 1995.

16. "The Menter Shear Stress Transport Turbulence Model," http://turbmodels.larc.nasa.gov/sst.html.

17. F.R. Menter, "Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications," *AIAA Journal*, vol. 32, no. 8, 1994.

18. F.R. Menter, M. Kuntz, and R. Langtry, "Ten Years of Industrial Experience with the SST Turbulence Model," *Turbulence Heat and Mass Transfer*, vol. 4, 2003.

19. M. Vázquez, M. Ravachol, F. Chalot, and M. Mallet, "The Robustness Issue on Multigrid Schemes Applied to the Navier-Stokes Equations for Laminar and Turbulent, Incompressible and Compressible Flows," *Int. J.for Numerical Methods in Fluids*, vol. 45, pp. 555–579, 2004.

20. T. Cebeci, *Analysis of Turbulent Flows*, 2nd ed., Elsevier, Amsterdam, 2004.

21. J. Nikuradse, "Strömungsgesetze in rauhen Rohren", *Forschg. Arb. Ing.-Wes.*, no. 361, 1933.

22. D. Agonafer, L. Gan-Li and D.B. Spalding, "LVEL turbulence model for conjugate heat transfer at low Reynolds numbers", EEP 6, *ASME International Mechanical Congress and Exposition*, Atlanta, 1996.

23. L. Prandtl, "Über die ausgebildete Turbulenz", ZAMM 5, 1925.

24. P.R. Spalart and S.R. Allmaras, "A one-equation turbulence model for aerodynamic flows," *La Aerospatiale*, no. 1, pp. 5-21, 1994.

25. P.A. Durbin, "Application of a near-wall turbulence model to boundary layers and heat transfer," *Int. J. Heat and Fluid Flow*, vol. 14, no. 4, 1993.

26. K. Hanjalic, M. Popovac and M. Hadziabdic, "*A robust near-wall elliptic-relaxation eddy-viscosity turbulence model for CFD,*" Int. J. Heat and Fluid Flow, vol. 25, no. 6, 2004.

Theory for the Rotating Machinery Interfaces

Both the Rotating Machinery, Laminar Flow and Rotating Machinery, Turbulent Flow interfaces model flow in geometries with rotating parts. For example, stirred tanks, mixers, and pumps.

The Navier-Stokes equations formulated in a rotating coordinate system read (Ref. 1 and Ref. 2)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{3-143}$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho (\mathbf{v} \cdot \nabla) \mathbf{v} + 2\rho \mathbf{\Omega} \times \mathbf{v} =$$

$$\nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} - \rho \left(\frac{\partial \mathbf{\Omega}}{\partial t} \times \mathbf{r} + \mathbf{\Omega} \times (\mathbf{\Omega} \times \mathbf{r}) \right) \tag{3-144}$$

where $\mathbf{v}$ is the velocity vector in the rotating coordinate system, $\mathbf{r}$ is the position vector, and $\mathbf{\Omega}$ is the angular velocity vector. The relation between $\mathbf{v}$ and the velocity vector in the stationary coordinate system is

$$\mathbf{u} = \mathbf{v} + \frac{\partial \mathbf{r}}{\partial t}$$

The Rotating Machinery, Fluid Flow interfaces solve Equation 3-143 and Equation 3-144, but reformulated in terms of a non-rotating coordinate system; that is, they solve for $\mathbf{u}$. This is achieved by invoking the Arbitrary Lagrangian-Eulerian Formulation (ALE) machinery. In rotating domains, $\mathbf{x} = \mathbf{x}(\mathbf{\Omega}, t)$ as prescribed in the Rotating Domain features. The Navier-Stokes equations on rotating domains then read

$$\frac{\partial \rho}{\partial T} - \frac{\partial \mathbf{x}}{\partial T} \cdot \nabla \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-145}$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial T} - \frac{\partial \mathbf{x}}{\partial T} \cdot \nabla \mathbf{u} \right) + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} \tag{3-146}$$

The derivative operator $\partial\rho/\partial T$ is the mesh time derivative of the density and appears in the equation view as `d(rmspf.rho,TIME)`. Analogously, $\partial\mathbf{u}/\partial T$ is the mesh time derivative of the velocity. The variable `TIME` replaces t as the variable for time.

The user input for a rotating domain prescribes the angular frequency, w. To calculate $\boldsymbol{\Omega}$, the physics interfaces set up an ODE variable for the angular displacement ω. The equation for ω is

$$\frac{d\omega}{dt} = w \tag{3-147}$$

$\boldsymbol{\Omega}$, is defined as w times the normalized axis of rotation. In 2D, the axis of rotation is the z direction while it in 3D is specified in the Rotating Domain features. If the model contains several rotating domains, each domain has its own angular displacement ODE variable.

In non-rotating domains, the ordinary Navier-Stokes equations are solved. The rotating and fixed parts need to be coupled together by an identity pair, where a continuity boundary condition is applied.

Boundary conditions in the rotating parts must be specified correctly. For example, walls that rotate must be prescribed as rotating walls. Walls in rotating domains can also be prescribed as non-rotating, but in that case, $\boldsymbol{\Omega} \times \mathbf{n}$, where $\mathbf{n}$ is the wall normal, must be tangential to the wall.

@ | Arbitrary Lagrangian-Eulerian Formulation (ALE) in the *COMSOL Multiphysics Reference Manual*

Frozen Rotor

Equation 3-145 through Equation 3-147 must be solved using a Time Dependent study. This can be computationally expensive. The Rotating Machinery, Fluid Flow interfaces therefore support the so-called frozen rotor approach. The frozen rotor approach assumes that the flow in the rotating domain, expressed in the rotating coordinate system, is fully developed. Equation 3-143 then reduces to

$$\nabla \cdot (\rho\mathbf{v}) = 0 \tag{3-148}$$

and Equation 3-144 to

$$\rho(\mathbf{v} \cdot \nabla)\mathbf{v} + 2\rho\boldsymbol{\Omega} \times \mathbf{v} = \\ \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} - \rho\boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \mathbf{r}) \tag{3-149}$$

Frozen rotor is both a study type and an equation form. When solving a rotating machinery model using a Frozen Rotor study step, the Rotating Machinery, Fluid Flow interfaces effectively solve Equation 3-149 and Equation 3-149 in a "rotating" domain, but "rotating" domains do not rotate at all. Boundary conditions remain transformed as if the domains were rotating, but the domains remain fixed, or frozen, in position. As in the time-dependent case, the Rotating Machinery, Fluid Flow interfaces solve for the velocity vector in the stationary coordinate system, $\mathbf{u}$, rather than for $\mathbf{v}$.

To make Equation 3-145 and Equation 3-146 equivalent to Equation 3-148 and Equation 3-149, the Frozen Rotor study step defines a parameter TIME, which by default is set to zero (TIME appears in the Parameters node under Global Definitions). Equation 3-147 is replaced by

$$\omega = w\,\mathrm{TIME}$$

Since TIME is a parameter and $\mathbf{x}$ is a function of TIME, $\partial\mathbf{x}/\partial\mathrm{T}$ evaluates to its correct value. Finally, $\partial\rho/\partial\mathrm{T} = 0$ and the mesh time derivative of the velocity is replaced by

$$\frac{\partial\mathbf{u}}{\partial\mathrm{T}} = \boldsymbol{\Omega} \times \mathbf{u}$$

In nonrotating domains, the ordinary, stationary Navier-Stokes equations are solved. The Frozen Rotor study step invokes a stationary solver to solve the resulting equation system.

The frozen rotor approach can in special cases give the same solution as solving Equation 3-145 through Equation 3-147 to steady state. This is the case if, for example, the whole geometry is rotating, or if the model is invariant with respect to the position of the rotating domain relative to the nonrotating domain. The latter is the case for a fan placed in the middle of a straight, cylindrical duct.

In most cases, however, there is no steady-state solution to the rotating machinery problem. Only a pseudo-steady state where the solution varies periodically around some average solution. In those cases, the frozen rotor approach gives an approximate solution to the pseudo-steady state. The approximation depends on the position in which the rotor is frozen, and the method cannot capture transient effects (see Ref. 3 and Ref. 4). An estimate of the effect of the rotor position can be obtained by making a parametric sweep over TIME.

The frozen rotor approach is very useful for attaining initial values for time-dependent simulations. Starting from a frozen rotor solution, the pseudo-steady state can be reached within a few revolutions, while starting from $\mathbf{u} = \mathbf{0}$ can require tens of revolutions. See, for example, Ref. 5.

Only interfaces that explicitly support frozen rotors are included in a Frozen Rotor study step.

> 🔍   Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Setting Up a Rotating Machinery Model

The Rotating Machinery, Fluid Flow interfaces primarily handle two types of geometries with rotating parts.

The first type is where the whole geometry rotates. Typical examples are individual parts in turbo machinery and lab-on-a-chip devices. For such cases, apply a Rotating Domain feature to all domains in the geometry.

The other type is geometries where it is possible to divide the modeled device into rotationally invariant geometries. The operation can be, for example, to rotate an impeller in a baffled tank, as in Figure 3-11 where the impeller rotates from position 1 to 2.

The first step to set up these type of models is to divide the geometry into two parts, as shown in Step 1a. Draw the geometry using separate domains for fixed and rotating parts. If you intend to do a time-dependent simulation, activate the assembly (using an assembly instead of a union, see Geometry Modeling and CAD Tools in the *COMSOL Multiphysics Reference Manual*) and create identity pairs, which makes it possible to treat the domains as separate parts in an assembly.

The second step is to specify the parts to model using Rotating Domain features and the ones to model using a fixed frame (Step 1b).

Once this is done, proceed to the usual steps of setting the fluid properties, boundary conditions. Apply a Flow Continuity to assembly pairs (Step 2a). Then mesh and solve the problem.
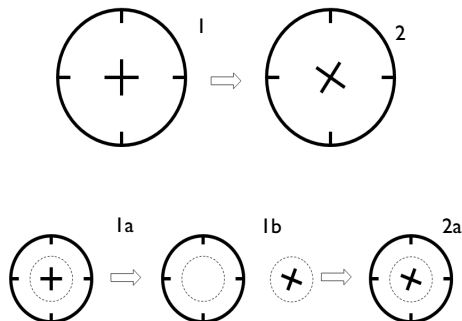
Figure 3-11: The modeling procedure in the Rotating Machinery, Fluid Flow interface.

References

1. H.P. Greenspan, *The Theory of Rotating Fluids*, Breukelen Press, 1990.

2. G.K. Batchelor, *An Introduction to Fluid Dynamics*, Cambridge University Press, 2000.

3. CFD Online, *Best practice guidelines for turbomachinery CFD*, http://www.cfd-online.com/Wiki/Best_practice_guidelines_for_turbomachinery_CFD.

4. A. Brucato, M. Ciofalo, F. Grisafi, and G. Micale, "Numerical Prediction of Flow Fields in Baffled Stirred Vessels: A Comparison of Alternative Modelling Approaches", *Chemical Engineering Science*, vol. 53, no. 21, pp. 3653–3684, 1998.

5. J.-P. Torré, D.F. Fletcher, T. Lasuye, and C. Xuereb, "Single and Multiphase CFD Approaches for Modelling Partially Baffled Stirred Vessels: Comparison of Experimental Data with Numerical Predictions", *Chemical Engineering Science*, vol. 62, no. 22, pp. 6246–6262, 2007.

4

Heat Transfer and Nonisothermal Flow Interfaces

There are several physics interfaces included in the CFD Module to model heat transfer and nonisothermal flow. This chapter describes the physics interfaces found under the **Heat Transfer** branch (⦀) as well as those under the **Fluid Flow>Nonisothermal Flow** branch ( ). The Modeling Heat Transfer in the CFD Module section helps you choose the best physics interface to start with.

- Modeling Heat Transfer in the CFD Module
- The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces
- Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

The documentation of all features in the Heat Transfer in Porous Media interface is now found in the *Heat Transfer Module User's Guide*, specifically in the following sections:

- The Heat Transfer Module Interfaces
- The Heat Transfer in Porous Media Interface
- Theory for the Heat Transfer Module
- Theory for Heat Transfer in Porous Media

Modeling Heat Transfer in the CFD Module

Heat transfer is an important phenomenon in many industrial processes. Often, a fluid plays a major role in transporting the heat and a detailed description of the flow field is necessary to accurately describe such processes. Typical examples are heating and cooling operations. Chemical reactions and phase changes are other commonly occurring phenomena. The temperature, in turn, affects the fluid properties and can alter the flow field. Natural convection is an example of this.

In this section:

- Selecting the Right Physics Interface
- Coupling to Other Physics Interfaces

Selecting the Right Physics Interface

The **Heat Transfer** branch (![icon]) included with this module has a number of physics interfaces that can be used to model energy transport. One or more of these can be added; either by themselves or together with other physics interfaces, typically flow physics interfaces.

While the standard COMSOL Multiphysics package includes physics interfaces for simulating heat transfer through conduction and convection, this module provides extra functionality within the standard Heat Transfer interfaces. The CFD Module also includes additional Heat Transfer interfaces such as The Heat Transfer in Porous Media Interface.

For heat transfer in single-phase flows, the CFD Module provides the **Nonisothermal Flow** (![icon]) (located under the **Fluid Flow** branch) and **Conjugate Heat Transfer** (![icon]) (located under the **Heat Transfer** branch) interfaces. There are several versions of these interfaces that combine heat transfer with either laminar or turbulent flow. The multiphysics interfaces automatically couple the flow and heat equations and they also provide functionality, such as support for turbulent heat transfer, that is not readily available when adding the interfaces separately.

HEAT TRANSFER IN SOLIDS OR FLUIDS, AND JOULE HEATING

The **Heat Transfer in Solids** ( ), **Heat Transfer in Fluids** ( ) (general convection and conduction), and **Electromagnetic Heating>Joule Heating** interfaces ( ), all belong to the COMSOL Multiphysics base package.

HEAT TRANSFER IN POROUS MEDIA

The **Heat Transfer in Porous Media** interface ( ) is an extension of a the generic heat transfer interface that includes modeling heat transfer through convection, conduction and radiation, conjugate heat transfer, and nonisothermal flow. The ability to define material properties, boundary conditions, and more for porous media heat transfer is also activated by selecting the **Heat transfer in porous media** check box on any heat transfer interface.

NONISOTHERMAL FLOW AND CONJUGATE HEAT TRANSFER

The **Nonisothermal Flow** ( ) and **Conjugate Heat Transfer** ( ) interfaces solve the Navier-Stokes equations together with an energy balance. They can also solve for heat transfer in solids.

Nonisothermal Flow and Conjugate Heat Transfer differ by their default features. The default heat transfer domain feature for Nonisothermal Flow is a Heat Transfer in Fluids node while Conjugate Heat Transfer has a Heat Transfer in Solids node as its default domain feature.

The Laminar Flow versions of the physics interfaces are used primarily to model slowly flowing fluids in environments where energy transport is also an important part of the system and application, and must be coupled or connected to the fluid flow in some way. Stokes' law (creeping flow) can be activated from the Nonisothermal Flow, Laminar Flow and Conjugate Heat Transfer, Laminar Flow interfaces if wanted. If you expect the flow to become turbulent, select one of the versions of the turbulent flow interfaces. Each physics interface includes a RANS turbulence model to calculate the turbulence and algebraic models for the turbulent Prandtl number.

The Nonisothermal Flow and Conjugate Heat Transfer interfaces can solve the fully compressible form of the Navier-Stokes equations. But boundary conditions and stabilizations are provided for Mach numbers less than 0.3. If you expect the Mach number in your model to become higher than 0.3, use The High Mach Number Flow Interfaces.

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple heat transfer in turbulent flow to another type of phenomenon described by another physics interface. This can, for example, include chemical reactions and mass transport, as covered by the physics interfaces in the Chemical Species Transport branch.

Furthermore, the Chemical Reaction Engineering Module includes, not only support for setting up and simulating chemical reactions, but also for simulating reaction kinetics through the temperature-dependent Arrhenius Expression and Mass Action Law. This physics interface also includes support for including and calculating thermodynamic data as temperature-dependent expressions, for both reaction kinetics and fluid-flow.

In addition, if you also have the Heat Transfer Module, it includes more detailed descriptions and tools for simulating energy transport, such as surface-to-surface and participating media radiation.

Fluid Damper: Application Library path
CFD_Module/Nonisothermal_Flow/fluid_damper

A variety of modeling techniques are discussed in the following sections of the *Heat Transfer Module User's Guide*:

- Heat Transfer Variables
- Using the Boundary Conditions for the Heat Transfer Interfaces
- Handling Frames in Heat Transfer
- Heat Transfer and Fluid Flow Coupling
- Solver Settings

Also see The Heat Transfer Module Interfaces and Theory for the Heat Transfer Module.

The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces

In this section:

Advantages of Using the Multiphysics Interfaces

The Nonisothermal Flow and Conjugate Heat Transfer interfaces combine the heat equation with either laminar flow or turbulent flow and use either a **Heat Transfer in Fluids** or **Heat Transfer in Solids** domain model. The advantage of using the multiphysics interfaces is that predefined couplings are available in both directions. In particular, physics interfaces use the same definition of the density, which can therefore be a function of both pressure and temperature. Solving this coupled system of equations usually requires numerical stabilization accounting for the couplings, which the predefined multiphysics interfaces also set up.

> ⊙ See also Heat Transfer and Fluid Flow Coupling in the *Heat Transfer Module User's Manual* for more information.

The Nonisothermal Flow, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the **Fluid Flow>Nonisothermal Flow** branch of the **Model Wizard** or **Add Physics** windows, one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) and **Heat Transfer** are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

⚙   The Multiphysics Node in the *COMSOL Multiphysics Reference Manual*.

- The **Laminar Flow** interface (≋) combines a Heat Transfer in Fluids interface with a Laminar Flow interface.
- The **Turbulent Flow, Algebraic yPlus** interface (≋) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface (≋) combines a Heat Transfer in Fluids interface with a Turbulent Flow, L-VEL interface.
- The **Turbulent Flow, k-ε** interface (≋) combines a Heat Transfer in Fluids interface with a Turbulent Flow, k-ε interface.
- The **Turbulent Flow, k-ω** interface (≋) combines a Heat Transfer in Fluids interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, SST** interface (≋) combines a Heat Transfer in Fluids interface with a Turbulent Flow, SST interface.
- The **Turbulent Flow, Low Re k-ε** interface (≋) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, Spalart-Allmaras** interface (≋) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Spalart-Allmaras interface.

The Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the **Heat Transfer>Conjugate Heat Transfer** branch of the **Model Wizard** or **Add Physics** windows, **Heat Transfer** and one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

> 🔍   The Multiphysics Node in the *COMSOL Multiphysics Reference Manual*.

- The **Laminar Flow** interface (🌊) combines a Heat Transfer in Solids interface with a Laminar Flow interface.
- The **Turbulent Flow, Algebraic yPlus** interface (🌊) combines a Heat Transfer in Solids interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface (🌊) combines a Heat Transfer in Solids interface with a Turbulent Flow, L-VEL interface.
- The **Turbulent Flow, k-ε** interface (🌊) combines a Heat Transfer in Solids interface with a Turbulent Flow, k-ε interface.
- The **Turbulent Flow, k-ω** interface (🌊) combines a Heat Transfer in Solids interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, Low Re k-ε** interface (🌊)combines a Heat Transfer in Solids interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, SST** interface (🌊) combines a Heat Transfer in Solids interface with a Turbulent Flow, SST interface.
- The **Turbulent Flow, Spalart-Allmaras** interface (🌊) combines a Heat Transfer in Solids interface with a Turbulent Flow, Spalart-Allmaras interface.

Settings for Physics Interfaces and Coupling Features

When physics interfaces are added using the predefined couplings, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Heat Transfer in Fluids** and **Laminar Flow** interfaces are added, COMSOL Multiphysics adds an empty **Multiphysics** node. When you right-click this

node, you can choose from the available coupling features, **Nonisothermal Flow**, **Temperature Coupling**, and **Flow Coupling**, but the modified settings are not included.

TABLE 4-1: MODIFIED SETTINGS FOR THE NONISOTHERMAL FLOW INTERFACES

PHYSICS OR COUPLING INTERFACE	MODIFIED SETTINGS (IF ANY)
Heat Transfer in Solids	Discretization order from temperature Lagrange shape function is 1.
	A **Heat Transfer in Fluids** feature is added with a default editable selection set to **All domains**.
Heat Transfer in Fluids	none
Nonisothermal Flow	The **Fluid flow** and **Heat transfer** interfaces are preselected
	The **Compressibility** option of the fluid flow interface is set to **Weakly Compressible**

Coupling Features

The Nonisothermal Flow and Flow Coupling multiphysics coupling nodes are described in this section. See Temperature Coupling in the *COMSOL Multiphysics Reference Manual*.

	Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

HEAT TRANSFER IN FLUIDS (NONISOTHERMAL FLOW)

The available physics features for The Heat Transfer in Fluids Interface are listed in the section Feature Nodes for the Heat Transfer in Fluids Interface. Also see Fluid for details about that feature.

HEAT TRANSFER IN SOLIDS (CONJUGATE HEAT TRANSFER)

The available physics features for The Heat Transfer in Solids Interface are listed in the section Feature Nodes for the Heat Transfer in Solids Interface. Also see Solid for details about that feature.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, ALGEBRAIC YPLUS

The available physics features for The Turbulent Flow, Algebraic yPlus Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, L-VEL

The available physics features for The Turbulent Flow, L-VEL Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ε

The available physics features for The Turbulent Flow, k-e Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ω

The available physics features for The Turbulent Flow, k-w Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE k-ε

The available physics features for The Turbulent Flow, Low Re k-e Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

The available physics features for The Turbulent Flow, Spalart-Allmaras Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

Nonisothermal Flow

Use the **Nonisothermal Flow** (≋) multiphysics coupling to simulate fluid flows where the fluid properties depend on temperature. Models can also include heat transfer in solids or in porous media as well as surface-to-surface radiation and radiation in participating media, with the Heat Transfer Module. The physics interface supports low Mach numbers (typically less than 0.3).

The Nonisothermal Flow, Laminar Flow interface solves for conservation of energy, mass and momentum in fluids and porous media and for conservation of energy in solids. It synchronizes the features from the **Heat Transfer** and **Fluid Flow** interfaces when a turbulent flow regime is defined. It also complements the **Screen** and **Interior Fan** feature from the flow interface to account for thermal effects.

💡	When the **Nonisothermal Flow** is used, there is no need to add **Flow Coupling** or **Temperature Coupling**. Indeed, **Nonisothermal Flow** combines the effects of both of them. In addition it also accounts for the multiphysics stabilization terms and for the heat transfer changes in the turbulent regime (for example, thermal wall functions), for work due to pressure forces and viscous dissipation, and for natural convection, including Boussinesq approximation.

📑 The multiphysics stabilizations (streamline diffusion and crosswind diffusion) are controlled by the Fluid Flow interface. For example, the multiphysics streamline diffusion can be disabled in a **Laminar Flow** physics node, in the **Stabilization** section. The stabilization selected in the Heat Transfer physics interface has no effect if the multiphysics coupling stabilization is active, but remains active if not. However, the isotropic diffusion is not a multiphysics stabilization and is controlled by each physics interface.

Finally, when one of the physics interfaces or the multiphysics coupling is not solved in a study step, then the stabilization of each solved physics is used instead of the coupled stabilization, and the solver suggestions are uncoupled.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is nitf1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the nonisothermal flow, or select **All domains** as needed.

HEAT TRANSFER TURBULENCE MODEL

Select an option from the **Heat transport turbulence model** list: **Kays-Crawford** (the default), **Extended Kays-Crawford**, or **User-defined turbulent Prandtl number**.

For **Extended Kays-Crawford**, enter a **Reynolds number at infinity** $\mathrm{Re}_{\mathrm{inf}}$ (dimensionless).

For **User-defined turbulent Prandtl number**, enter a **Turbulent Prandtl number** pr_{T} (dimensionless).

When the flow interface uses a RANS turbulence model, the conductive heat flux is defined as

$$q = -(k + k_{\mathrm{T}})\nabla T$$

with the turbulent thermal conductivity defined as

$$k_{\mathrm{T}} = \frac{\mu_{\mathrm{T}} C_p}{Pr_{\mathrm{T}}}$$

where μ_{T} is defined by the flow interface, and Pr_{T} depends on the **Heat transport turbulence model**. See Turbulent Conductivity for details.

MATERIAL PROPERTIES

Select an option from the **Specify density** list — **From heat transfer interface** (the default), **From fluid flow interface**, or **Custom**.

For **Custom, linearized density**, enter the **Reference density** ρ_{ref} (SI unit: kg/m^3) and the **Coefficient of thermal expansion** α_p (SI unit: 1/K), or select **From material,** or select a variable in the list if available. When **Custom, linearized density** is selected, regardless how the properties are defined they should be constant. If material properties are not constant you should consider using any of the other options to define the density.

For **Custom**, enter a **Density** ρ (SI unit: kg/m^3), or select a density in the list if available.

The density definition in the **Nonisothermal Flow** node ensure that the same definition of the density is used on the fluid flow and heat transfer interfaces. When the fluid flow compressibility setting is set to **Incompressible** then the thermal conductivity and the heat capacity are evaluated at the **Reference temperature** defined in the fluid flow interface. When **Include gravity** is selected and the **Compressibility** is set to **Incompressible flow** in the fluid interface properties, the gravity forces are defined using the coefficient of thermal expansion. Along with the fact that the material properties are evaluated for a constant temperature and pressure, this gravity force definition corresponds to Boussinesq approximation. Unless the density is defined as **Custom, linearized density** the coefficient of thermal expansion is evaluated from the fluid density.

FLOW HEATING

Select the **Include work done by pressure changes** check box to account for the heat source due to pressure changes:

$$Q_p = \alpha_p \left(\frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p \right)$$

By default this option is not selected, however it should be selected for compressible fluids as soon as significant pressure gradients occur.

Select the **Include viscous dissipation** check box to account for the heat source corresponding to viscous heating. This option is not selected by default. Because it may induce an extra computational cost it should be only selected in application where such effect is expected. If no information on this is available, selecting the option ensure that energy balance for the heat and the flow equation is respected.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Heat transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.

- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Heat Transfer in Fluids** is deleted, then the **Heat transfer** list defaults to **None** as there is nothing to couple to.

| ⚠ | When an interface is selected from the **Heat transfer** list, some of its model inputs are forced with values from the **Nonisothermal Flow** node. In addition, it defines how the turbulence has to be accounted for, depending on the **Fluid flow** interface's turbulence settings. Therefore, each heat transfer or fluid flow interface should be used in at most one **Nonisothermal Flow** node. In cases where multiple fluid flow interfaces are used, an equal number of heat transfer interfaces and **Nonisothermal Flow** nodes are needed to define proper multiphysics couplings. |

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Heat transfer** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Approaches in the *COMSOL Multiphysics Reference Manual.*

Flow Coupling

The **Flow Coupling** multiphysics coupling ( ) defines **u** and p variables in order to set the model inputs in the Heat Transfer interface (or when applicable, a chemical species transport interface). In addition it provides all the fluids quantities that may be needed by the Heat Transfer interface (for example, viscosity, turbulence parameters, and so on).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is fc1.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. By default, the applicable physics interface is selected in the **Source** list to apply the **Destination** to its physics interface to establish the coupling.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Heat Transfer in**

Solids is deleted, then the **Destination** list defaults to **None** as there is nothing to couple to.

When the **Destination** interface is a heat transfer interface, the Nonisothermal Flow coupling node should be preferred to **Flow Coupling**. Indeed, **Nonisothermal Flow** brings an optimized stabilization; supports natural convection, including Boussinesq approximation; supports turbulent flow (wall functions, effective thermal conductivity); and handles work due to the pressure forces and viscous dissipation.

When the **Destination** interface is a chemical species transport interface, a **Reacting Flow** coupling node should be used instead of **Flow Coupling**. See The Reacting Flow Multiphysics Interfaces for more details.

If a physics interface is deleted and then added to the model again, and in order to re-establish the coupling, you need to choose the physics interface again from the lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present physics interface. See Multiphysics Modeling Approaches in the *COMSOL Multiphysics Reference Manual*.

Marangoni Effect

The **Marangoni Effect** multiphysics coupling (🔴) accounts for Marangoni convection. Marangoni convection occurs when the surface tension of an interface (generally liquid-air) depends on the concentration of a species or on the temperature distribution. In the case of temperature dependence, the Marangoni effect is also called thermo-capillary convection. It is of primary importance in the fields of welding, crystal growth, and electron beam melting of metals.

The Marangoni effect is a shear stress which depends on the tangential temperature gradient and should be implemented as such. It has the following contribution described by forces induced on the fluid/fluid interface:

$$\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right]\mathbf{n} = \gamma\nabla_{\mathbf{t}}T$$

where γ is the temperature derivative of the surface tension σ (N/(m·K)). Note that this formulation is intended for laminar flow regimes only.

S E T T I N G S

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is me1.

S U R F A C E   T E N S I O N

Select a **Surface tension coefficient type** — **Library coefficient, liquid/gas interface** or **User defined** (the default).

- For **Library coefficient, liquid/gas interface** choose an option from the **Library surface tension coefficient** list.

- For **User defined** enter a **Surface tension coefficient** σ (SI unit: N/m).

M A R A N G O N I   E F F E C T

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Heat transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.

- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Heat Transfer in**

Fluids is deleted, then the **Heat transfer** list defaults to **None** as there is nothing to couple to.

| | If a physics interface is deleted and then added to the model again, then in order to re-establish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Heat transfer** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Approaches in the *COMSOL Multiphysics Reference Manual*. |

Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

In this section:

- The Nonisothermal Flow and Conjugate Heat Transfer Equations
- Turbulent Nonisothermal Flow Theory
- Theory for the Nonisothermal Screen Boundary Condition
- Theory for the Interior Fan Boundary Condition
- References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

The Nonisothermal Flow and Conjugate Heat Transfer Equations

In industrial applications it is common that the density of a process fluid varies. These variations can have a number of different sources but the most common one is the presence of an inhomogeneous temperature field. This module includes the Nonisothermal Flow predefined multiphysics coupling to simulate systems in which the density varies with temperature.

Other situations where the density might vary includes chemical reactions, for instance where reactants associate or dissociate.

The Nonisothermal Flow and Conjugate Heat Transfer interfaces contain the fully compressible formulation of the continuity and momentum equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left(\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F}$$

(4-1)

where

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is the pressure (SI unit: Pa)

- μ is the dynamic viscosity (SI unit: Pa·s)
- **F** is the body force vector (SI unit: N/m^3)

It also solves the heat equation, which for a fluid is given by

$$\rho C_p\left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T\right) = -(\nabla \cdot \mathbf{q}) + \mathbf{\tau}{:}\mathbf{S} - \frac{T}{\rho}\frac{\partial \rho}{\partial T}\bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p\right) + Q$$

where in addition to the quantities above

- C_p is the specific heat capacity at constant pressure (SI unit: J/(kgK))
- T is the absolute temperature (SI unit: K)
- **q** is the heat flux by conduction (SI unit: W/m^2)
- τ is the viscous stress tensor (SI unit: Pa)
- **S** is the strain-rate tensor (SI unit: 1/s)

$$\mathbf{S} = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

- Q contains heat sources other than viscous heating (SI unit: W/m^3)

The *work done by pressure changes* term

$$\alpha_p T\left(\frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p\right) \text{ with } \alpha_p = -\frac{1}{\rho}\frac{\partial \rho}{\partial T}\bigg|_p.$$

and the *viscous heating* term

$$\mathbf{\tau}{:}\mathbf{S}$$

are not included by default because they are usually negligible. These terms can, however, be added by selection corresponding check-boxes in the Nonisothermal Flow feature. For a detailed discussion of the fundamentals of heat transfer in fluids, see Ref. 3.

The physics interface also supports heat transfer in solids:

$$\rho C_p\frac{\partial T}{\partial t} = -(\nabla \cdot \mathbf{q}) + Q + Q_{\text{ted}}$$

where Q_{ted} is the thermoelastic damping heat source (SI unit: $W/(m^3)$). This term is not included by default but must be added by selecting corresponding check-box.

Turbulent Nonisothermal Flow Theory

Turbulent energy transport is conceptually more complicated than energy transport in laminar flows since the turbulence is also a form of energy.

Equations for compressible turbulence are derived using the Favre average. The Favre average of a variable T is denoted $\tilde{T}$ and is defined by

$$\tilde{T} = \frac{\overline{\rho T}}{\bar{\rho}}$$

where the bar denotes the usual Reynolds average. The full field is then decomposed as

$$T = \tilde{T} + T''$$

With this notation the equation for total internal energy, e, becomes

$$\frac{\partial}{\partial t}\left(\bar{\rho}\left(\tilde{e} + \frac{\tilde{u}_i \tilde{u}_i}{2}\right) + \frac{\overline{\rho u_i'' u_i''}}{2}\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\left(\tilde{h} + \frac{\tilde{u}_i \tilde{u}_i}{2}\right) + \tilde{u}_j\frac{\overline{\rho u_i'' u_i''}}{2}\right) =$$

$$\frac{\partial}{\partial x_j}\left(-q_j - \overline{\rho u_j'' h''} + \overline{\tau_{ij} u_i''} - \frac{\overline{\rho u_j'' u_i'' u_i''}}{2}\right) + \frac{\partial}{\partial x_j}(\tilde{u}_i(\overline{\tau_{ij}} - \overline{\rho u_i'' u_j''})) \tag{4-2}$$

where h is the enthalpy. The vector

$$q_j = -\lambda \frac{\partial T}{\partial x_j} \tag{4-3}$$

is the laminar conductive heat flux and

$$\tau_{ij} = 2\mu S_{ij} - \frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}$$

is the laminar, viscous stress tensor. Notice that the thermal conductivity is denoted λ.

The modeling assumptions are in large part analogous to those for incompressible turbulence modeling. The stress tensor

$$-\overline{\rho u_i'' u''}_j$$

is modeled using the *Boussinesq approximation*:

$$-\overline{\rho u_i'' u''}_j = \bar{\rho}\tau_{ij} = 2\mu_T\left(\tilde{S}_{ij} - \frac{1}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right) - \frac{2}{3}\bar{\rho}k\delta_{ij} \tag{4-4}$$

where k is the turbulent kinetic energy, which in turn is defined by

$$\bar{\rho}k = \frac{1}{2}\overline{\rho u_i'' u_i''} \tag{4-5}$$

The correlation between u_j'' and h'' in Equation 4-2 is the turbulent transport of heat. It is modeled analogously to the laminar conductive heat flux

$$\overline{\rho u_j'' h''} = q^T_j = -\lambda_T\frac{\partial \tilde{T}}{\partial x_j} = -\frac{\mu_T C_p}{Pr_T}\frac{\partial \tilde{T}}{\partial x_j} \tag{4-6}$$

The molecular diffusion term,

$$\overline{\tau_{ij}u_i''}$$

and turbulent transport term,

$$\overline{\rho u_j'' u_i'' u_i''}/2$$

are modeled by a generalization of the molecular diffusion and turbulent transport terms found in the incompressible k equation

$$\overline{\tau_{ij}u_i''} - \frac{\overline{\rho u_j'' u_i'' u_i''}}{2} = \left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j} \tag{4-7}$$

Inserting Equation 4-3, Equation 4-4, Equation 4-5, Equation 4-6 and Equation 4-7 into Equation 4-2 gives

$$\frac{\partial}{\partial t}\left(\bar{\rho}\left(\tilde{e} + \frac{\tilde{u}_i \tilde{u}_i}{2} + k\right)\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\left(\tilde{h} + \frac{\tilde{u}_i \tilde{u}_i}{2} + k\right)\right) =$$

$$\frac{\partial}{\partial x_j}\left(-q_j - q^T{}_j + \left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\tilde{u}_i(\bar{\tau}_{ij} + \bar{\rho}\tau^T{}_{ij})) \tag{4-8}$$

The Favre average can also be applied to the momentum equation, which, using Equation 4-4, can be written

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{u}_i) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} + \bar{\rho}\tau^T{}_{ij}) \tag{4-9}$$

Taking the inner product between $\tilde{u}_i$ and Equation 4-9 results in an equation for the resolved kinetic energy, which can be subtracted from Equation 4-8 with the following result:

$$\frac{\partial}{\partial t}(\bar{\rho}(\tilde{e} + k)) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j(\tilde{e} + k)) = -\bar{p}\frac{\partial\tilde{u}_j}{\partial x_j} +$$

$$\frac{\partial}{\partial x_j}\left(-q_j - q^T{}_j + \left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\tilde{u}_i(\bar{\tau}_{ij} + \bar{\rho}\tau^T{}_{ij})) \tag{4-10}$$

where the relation

$$\tilde{h} = \tilde{e} + \bar{p}/\bar{\rho}$$

has been used.

According to Wilcox (Ref. 1), it is usually a good approximation to neglect the contributions of k for flows with Mach numbers up to the supersonic range. This gives the following approximation of Equation 4-10 is

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{e}) = -\bar{p}\frac{\partial\tilde{u}_j}{\partial x_j} + \frac{\partial}{\partial x_j}(-q_j - q^T{}_j) + \frac{\partial}{\partial x_j}(\tilde{u}_i(\bar{\tau}_{ij} + \bar{\rho}\tau^T{}_{ij})) \tag{4-11}$$

Larsson (Ref. 2) suggests to make the split

$$\bar{\tau}_{ij} = \tilde{\tau}_{ij} + \bar{\tau_{ij}''}$$

Since

$$\tilde{\tau}_{ij} \gg \overline{\tau_{ij}''}$$

for all applications of engineering interest, it follows that

$$\overline{\tau_{ij}} \approx \tilde{\tau}_{ij}$$

and consequently

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{e}) = -\bar{p}\frac{\partial \tilde{u}_j}{\partial x_j} + \frac{\partial}{\partial x_j}\left((\lambda + \lambda_T)\frac{\partial \tilde{T}}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\tilde{u}_i\tilde{\tau}_{ij}^{\text{Tot}}) \qquad (4\text{-}12)$$

where

$$\tilde{\tau}_{ij}^{\text{Tot}} = (\mu + \mu_T)\left(2\tilde{S}_{ij} - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)$$

Equation 4-12 is completely analogous to the laminar energy equation and can be expanded using the same theory (see for example Ref. 3):

$$\bar{\rho}C_p\left(\frac{\partial \tilde{T}}{\partial t} + \tilde{u}_j\frac{\partial \tilde{T}}{\partial x_j}\right) = \frac{\partial}{\partial x_j}\left((\lambda + \lambda_T)\frac{\partial \tilde{T}}{\partial x_j}\right) + \tilde{\tau}_{ij}\tilde{S}_{ij} - \frac{\tilde{T}}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial T}\bigg|_{\bar{p}}\left(\frac{\partial \bar{p}}{\partial t} + \tilde{u}_j\frac{\partial \bar{p}}{\partial x_j}\right)$$

which is the temperature equation solved in the turbulent Nonisothermal Flow and Conjugate Heat Transfer interfaces.

TURBULENT CONDUCTIVITY

Kays-Crawford
This is a relatively exact model for Pr_T, while still quite simple. In Ref. 4, it is compared to other models for Pr_T and found to be a good approximation for most kinds of turbulent wall bounded flows except for turbulent flow of liquid metals. The model is given by

$$\text{Pr}_T = \left(\frac{1}{2\text{Pr}_{T\infty}} + \frac{0.3}{\sqrt{\text{Pr}_{T\infty}}}\frac{C_p\mu_T}{\lambda} - \left(0.3\frac{C_p\mu_T}{\lambda}\right)^2\left(1 - e^{-\lambda/(0.3C_p\mu_T\sqrt{\text{Pr}_{T\infty}})}\right)\right)^{-1} \qquad (4\text{-}13)$$

where the Prandtl number at infinity is $\text{Pr}_{T\infty} = 0.85$ and λ is the conductivity.

Extended Kays-Crawford

Weigand and others (Ref. 5) suggested an extension of Equation 4-13 to liquid metals by introducing

$$\mathrm{Pr}_{T\infty} = 0.85 + \frac{100\lambda}{C_p\mu\mathrm{Re}_\infty^{0.888}}$$

where Re_∞, the Reynolds number at infinity must be provided either as a constant or as a function of the flow field. This is entered in the Model Inputs section of the Fluid feature.

TEMPERATURE CONDITION FOR AUTOMATIC WALL TREATMENT AND WALL FUNCTIONS

Both automatic wall treatment and wall functions introduce a theoretical gap between the solid wall and the computational domain for the fluid and temperature fields. See Wall Boundary Conditions described for the The Algebraic yPlus Turbulence Model and The k-e Turbulence Model). This theoretical gap applies also to the temperature fields but is most often ignored when the computational geometry is drawn.

The heat flux between the fluid with temperature T_f and a wall with temperature T_w, is:

$$q_{wf} = \frac{\rho C_p u_\tau (T_w - T_f)}{T^+}$$

where ρ is the fluid density, C_p is the fluid heat capacity, u_τ is the friction velocity given by the wall treatment. T^+ is the dimensionless temperature and is given by (Ref. 6):

$$T^+ = \begin{cases} \mathrm{Pr}\delta_w^+ & \text{for } \delta_w^+ < \delta_{w1}^+ \\ \left(15\mathrm{Pr}^{2/3} - \dfrac{500}{\delta_w^{+2}}\right) & \text{for } \delta_{w1}^+ \leq \delta_w^+ < \delta_{w2}^+ \\ \dfrac{\mathrm{Pr}_T}{\kappa}\ln\delta_w^+ + \beta & \text{for } \delta_{w2}^+ \leq \delta_w^+ \end{cases}$$

where in turn

$$\delta_w^+ = \frac{\delta_w \rho \sqrt{C_\mu^{1/2} k}}{\mu} \qquad\qquad \delta_{w1}^+ = \frac{10}{\text{Pr}^{1/3}}$$

$$\delta_{w2}^+ = 10 \sqrt{10 \frac{\kappa}{\text{Pr}_T}} \qquad\qquad \text{Pr} = \frac{C_p \mu}{\lambda}$$

$$\beta = 15 \text{Pr}^{2/3} - \frac{\text{Pr}_T}{2\kappa} \left(1 + \ln\left(1000 \frac{\kappa}{\text{Pr}_T} \right) \right)$$

λ is the thermal conductivity, and κ is the von Karman constant equal to 0.41.

The distance between the computational fluid domain and the wall, δ_w, is always $h_w/2$ for automatic wall treatment where h_w is the hight of the mesh cell adjacent to the wall. $h_w/2$ is almost always very small compared to any geometrical quantity of interest, at least if a boundary layer mesh is used. For wall function, δ_w is at least $h_w/2$ and can be bigger if necessary to keep δ_w^+ higher than 11.06. So the computational results for wall functions should be checked so that the distance between the computational fluid domain and the wall, δ_w, is everywhere small compared to any geometrical quantity of interest. The distance δ_w is available for evaluation on boundaries.

Theory for the Nonisothermal Screen Boundary Condition

When the Nonisothermal Flow multiphysics coupling feature is active, the conditions that apply across a screen in isothermal flow are complemented by:

$$[H_0]_-^+ = 0 \qquad\qquad (4\text{-}14)$$

where H_0 is the total enthalpy.

	• See Screen for the feature node details.
	• Also see Screen Boundary Condition described for the single-phase flow interfaces.

Theory for the Interior Fan Boundary Condition

When the Nonisothermal Flow multiphysics coupling feature is active, the conditions that apply across an interior fan are complemented by:

• If direction is Along normal vector, the outlet temperature is T_avg where T_avg is the weighted averaged temperature defined as:

$$T_{\mathrm{avg}} = \frac{\int_{\Gamma}(\mathrm{down}(\mathbf{u} \cdot \mathbf{n}\rho C_p T))dS}{\max\left(\varepsilon, \int_{\Gamma}(\mathrm{down}(\mathbf{u} \cdot \mathbf{n}\rho C_p T))dS\right)}$$

- If the direction is opposite to normal vector, the outlet temperature is `T_avg` where `T_avg` is:

$$T_{\mathrm{avg}} = \frac{\int_{\Gamma}(\mathrm{up}(\mathbf{u} \cdot \mathbf{n}\rho C_p T))dS}{\max\left(\varepsilon, \int_{\Gamma}(\mathrm{up}(\mathbf{u} \cdot \mathbf{n}\rho C_p T))dS\right)}$$

References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

1. D.C. Wilcox, *Turbulence Modeling for CFD*, 2nd ed., DCW Industries, 1998.

2. J. Larsson, *Numerical Simulation of Turbulent Flows for Turbine Blade Heat Transfer*, Doctoral Thesis for the Degree of Doctor of Philosophy, Chalmers University of Technology, Sweden, 1998.

3. R.L. Panton, *Incompressible Flow*, 2nd ed., John Wiley & Sons, 1996.

4. W.M. Kays, "Turbulent Prandtl Number — Where Are We?", *ASME Journal of Heat Transfer*, vol. 116, pp. 284–295, 1994.

5. B. Weigand, J.R. Ferguson, and M.E. Crawford, "An Extended Kays and Crawford Turbulent Prandtl Number Model," *Int. J. Heat and Mass Transfer*, vol. 40, no. 17, pp. 4191–4196, 1997.

6. D. Lacasse, È. Turgeon, and D. Pelletier, "On the Judicious Use of the k—ε Model, Wall Functions and Adaptivity," *Int. J. Thermal Sciences,* vol. 43, pp. 925–938, 2004.

5

Multiphase Flow Interfaces

This chapter discusses the physics interfaces found under the **Fluid Flow>Multiphase Flow** branch ( ). The section Modeling Multiphase Flow helps you choose the best physics interface to start with.

In this chapter:

- The Two-Phase Flow, Level Set and Phase Field Interfaces
- The Three-Phase Flow, Phase Field Interface
- The Bubbly Flow Interfaces
- The Mixture Model Interfaces
- The Euler-Euler Model Interfaces
- Theory for the Two-Phase Flow Interfaces
- Theory for the Three-Phase Flow Interface
- Theory for the Bubbly Flow Interfaces
- Theory for the Mixture Model Interfaces
- Theory for the Euler-Euler Model Interfaces

Modeling Multiphase Flow

In this section:

- Selecting the Right Physics Interface
- The Multiphase Flow Interface Options
- The Relationship Between the Physics Interfaces
- Coupling to Other Physics Interfaces

🗒	Certain types of multiphase flow can be described using the Phase Field and Level Set interfaces found under the **Mathematics>Moving Interface** branch (▍). In this module these physics features are already integrated into the relevant Fluid Flow interfaces.

🔍	• The Physics Interfaces in the *COMSOL Multiphysics Reference Manual* • Mathematics, Moving Interface Branch

Selecting the Right Physics Interface

The **Multiphase Flow** branch (◣) included with this module has a number of subbranches to describe momentum transport for multiphase flow. One or more physics interfaces can be added; either singularly or in combination with other physics interfaces for applications such as mass transfer and energy (heat) transfer.

Different types of flow require different equations to describe them. If you know the type of flow to model, then select it directly. However, when you are not certain of the flow type, or when it is difficult to obtain a solution, you can instead start with a simplified model and add complexity as you build the model. Then you can successively advance forward, comparing models and results.

The Bubbly Flow, Mixture Model and Euler-Euler Model interfaces are appropriate when you want to simulate a flow with many particles, droplets, or bubbles immersed in a liquid. With these physics interfaces, you do not track each particle in detail. Instead you solve for the averaged volume fraction. If you are interested in the exact motion of individual

bubbles, including how the fluid interface deforms due to, for instance, surface tension, use any of the Two-Phase Flow interfaces.

To model the detailed dynamics of fluid interfaces, either use the level set method or the phase field method. In general, it is not obvious which one of these to use when the flow is convection-dominating. However when the flow is diffusion-dominating, for example, phase-separation, only phase field should be used.

Three-phase flow can be simulated using the Laminar Three-Phase Flow, Phase Field interface.

The Multiphase Flow Interface Options

For any of the Multiphase Flow interfaces, you can assume either laminar or turbulent flow as the starting point. This enables you to make the appropriate mathematical model assumptions required to solve the flow. Turbulence is modeled using the standard k-ε model

The Relationship Between the Physics Interfaces

Several of the interfaces vary only by one or two default settings (see Table 5-1, Table 5-2, and Table 5-4) in the Physical Model section, which are selected either from a check box or a list. For the **Multiphase Flow** branch, the **Bubbly Flow (bf)**, **Mixture Model (mm)** and **Euler-Euler Model (ee)** subbranches have two physics interfaces each and both have the same Name. All the Two-Phase Flow interfaces contain a multiphysics coupling feature with a name as (tpf). The **Three-Phase Flow, Phase Field** branch contains a single interface for laminar flow.

BUBBLY FLOW

TABLE 5-1: BUBBLY FLOW PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	LOW GAS CONCENTRATION	TURBULENT MODEL TYPE	SOLVE FOR INTERFACIAL AREA
Laminar Bubbly Flow	bf	Yes	None	No
Turbulent Bubbly Flow	bf	Yes	RANS, k-ε	No

The **Bubbly Flow** ( ) branch interfaces are used primarily to model two-phase flow where the fluids are gas-liquid mixtures, and gas content is less than 10%. The Laminar Bubbly Flow Interface ( ) and The Turbulent Bubbly Flow Interface ( ) solve the flow equations, whether described by the Navier-Stokes equations or the RANS equations with the k-ε turbulence model, and where the momentum equation is corrected by a term

induced by the slip velocity. The slip velocity can be described by the Hadamard-Rybczynski drag law for small spherical bubbles, a nonlinear drag law taking surface tension into account for larger bubbles, or by defining it on your own.

By default, the physics interfaces assume that the volume fraction of the gas is less than 0.1. It is then valid to approximate the liquid velocity as incompressible. This is significantly easier to solve numerically. It is possible, though, to use the complete continuity equation.

The physics interfaces also allow you to define your own relations for the density of both phases and for the dynamic viscosity of the gas phase. Definitions of non-Newtonian fluid flow through the power law and Carreau models are however not possible. You can also model mass transfer between the two phases, using the two-film theory or your own expression for interfacial mass transfer.

MIXTURE MODEL INTERFACES

TABLE 5-2: MIXTURE MODEL PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	DISPERSED PHASE	SLIP MODEL	TURBULENCE MODEL TYPE	SOLVE FOR INTERFACIAL AREA
Mixture Model, Laminar Flow	mm	Solid particles	Homogeneous flow	None	No
Mixture Model, Turbulent Flow	mm	Solid particles	Homogeneous flow	RANS, k-ε	No

The **Mixture Model** (⋙) branch interfaces are similar to the **Bubbly Flow** interfaces except that both phases are assumed to be incompressible. Examples include solid particles dispersed in a liquid, and liquid droplets dispersed in another liquid when the two liquids are immiscible.

Like the Bubbly Flow interfaces, The Mixture Model, Laminar Flow Interface (⋙) and The Mixture Model, Turbulent Flow Interface (⋙) solve the flow equations, whether described by the Navier-Stokes equations or the RANS equations with the k-ε turbulence model, and where the momentum equation is corrected by a term induced by the slip velocity. The slip velocity can be described by the Hadamard-Rybczynski, Schiller-Naumann or Haider-Levenspiel method, or by defining it on your own.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. Definitions of non-Newtonian fluid flow through the power law and Carreau models are however not possible. The dynamic viscosity of the mixture can either be of Krieger type (which uses a maximum packing concentration), volume-averaged (for gas-liquid, liquid-liquid systems), or a user-defined expression.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature. The physics interfaces also enable you to model mass transfer between the two phases, using the two-film theory or your own expression for interfacial mass transfer.

EULER-EULER MODEL INTERFACES

TABLE 5-3: EULER-EULER MODEL PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	DIPERSED PHASE	DRAG MODEL	TURBULENCE MODEL TYPE
Euler-Euler Model, Laminar Flow	ee	Solid particles	Schiller-Naumann	None
Euler-Euler Model, Turbulent Flow	ee	Solid particles	Schiller-Naumann	RANS, k-ε

The **Euler-Euler Model** ( ) branch interfaces are used to model the flow of two continuous and fully interpenetrating phases. For both phases the conservation equations are averaged over volumes, which are small compared to the computational domain, but large compared to the dispersed phase particles, droplets or bubbles. The Euler-Euler Model, Laminar Flow interface solves two sets of conservation equations, one for each phase. The Euler-Euler Model, Turbulent Flow Interface additionally solves transport equations for the turbulence quantities, either using a mixture averaged turbulence models or solving separate transport equations for the turbulence quantities of each phase. The drag model can be described by the Hadamard-Rybczynski, Schiller-Naumann, Haider-Levenspiel or Gidaspow method, or by defining it on your own.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. Definitions of non-Newtonian fluid flow through the power law and Carreau models are however not possible. Predefined expressions for the dynamic viscosity of Krieger type (which uses a maximum packing concentration), are available.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature.

TABLE 5-4: TWO-PHASE FLOW AND THREE-PHASE FLOW PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	COMPRESSIBILITY	TURBULENCE MODEL TYPE	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-Phase Flow, Level Set	-	Two-phase flow, level set	Incompressible flow	None	False
Turbulent, Two-Phase Flow, Level Set	-	Two-phase flow, level set	Incompressible flow	RANS, k-ε RANS, k-ω	False
Laminar, Two-Phase Flow, Phase Field	-	Two-phase flow, phase field	Incompressible flow	None	False
Turbulent, Two-Phase Flow, Phase Field	-	Two-phase flow, phase field	Incompressible flow	RANS, k-ε RANS, k-ω	False
Laminar Three-Phase Flow, Phase Field	-	Three-phase flow, phase field	Incompressible flow	None	False

Two-Phase Flow, Level Set

The Laminar Two-Phase Flow, Level Set Interface ( ) and The Turbulent Two-Phase Flow, Level Set Interface ( ), found under the **Two-Phase Flow, Level Set** branch ( ), are used primarily to model two fluids separated by a fluid interface. The moving interface is tracked in detail using the level set method. Surface tension acting on the fluid interface is automatically included in the fluid-flow equations.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Level Set interface. You can also choose to model incompressible flow, and simplify the equations to be solved. Stokes' law is an option.

Specify the density and viscosity for each of the two fluids. For any of the two fluids, you can easily use non-Newtonian models based on the power law or Carreau model, or by using an arbitrary user-defined expression.

Two-Phase Flow, Phase Field

The Laminar Three-Phase Flow, Phase Field Interface ( ) and The Turbulent Two-Phase Flow, Phase Field Interface ( ) found under the **Two-Phase Flow, Phase Field** branch ( ), also model two fluids separated by a fluid interface. You can easily switch

between the physics interfaces, which can be useful if you are not sure which physics interface provides the best description. Library surface tension coefficients between a number of common substances are also available.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Phase Field interfaces. You can also model incompressible flow and simplify the equations to be solved. Stokes flow is also an option.

Specify the density and viscosity for each of the two fluids. For any of the two fluids, you can easily use non-Newtonian models based on the power law or Carreau model, or by using an arbitrary user-defined expression.

Three-Phase Flow, Phase Field
The Laminar Three-Phase Flow, Phase Field Interface found under the **Three-Phase Flow, Phase Field** branch ( ) models flows of three incompressible fluids separated by sharp interfaces. Library surface tension coefficients between a number of common substances are also available.

Specify the density and viscosity for each of the three fluids. For any of the fluids, you can easily use non-Newtonian models based on the power law or Carreau model, or by using an arbitrary user-defined expression.

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple fluid flow to another type of phenomenon described in another physics interface. Although this is not often another type of flow, it can still involve physics interfaces supported in the CFD Module or in the COMSOL Multiphysics base package. This typically occurs in cases where applications include chemical reactions and mass transport, as included in Chemical Species Transport Interfaces, or energy transport, found in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of heat transfer, such as those involving radiation, can be found in the Heat Transfer Module, while tools for modeling chemical reactions and mass transport are available in the Chemical Reaction Engineering Module.

The Two-Phase Flow, Level Set and Phase Field Interfaces

The following sections list all the physics interfaces and the physics features associated with them under the **Multiphase Flow** branch (![icon]). The descriptions follow a structured order as defined by the order in the branch. Because many of the physics interfaces are integrated with each other, some nodes described also cross reference to other physics interfaces.

![question icon]	Selecting the Right Physics Interface

This section includes the following topics:

- The Laminar Two-Phase Flow, Level Set Interface
- The Turbulent Two-Phase Flow, Level Set Interface
- Two-Phase Flow, Level Set Coupling Features
- The Wetted Wall Coupling Feature
- The Laminar Two-Phase Flow, Phase Field Interface
- The Turbulent Two-Phase Flow, Phase Field Interface
- The Two-Phase Flow, Phase Field Coupling Features
- Domain, Boundary, Point, and Pair Nodes for the Laminar and Turbulent Flow, Two-Phase, Level Set and Phase Field Interfaces

---

![question icon]	• Mathematics, Moving Interface Branch

The Laminar Two-Phase Flow, Level Set Interface

The **Laminar Two-Phase Flow, Level Set** interface (![icon]) found under the **Multiphase Flow>Two-Phase Flow, Level Set** branch (![icon]), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Laminar Two-Phase Flow, Level Set** multiphysics interface, a **Laminar Flow** and a **Level Set** interface are added to the Model Builder. In addition the **Multiphysics** node, a multiphysics coupling feature **Two-Phase Flow, Level Set** is added automatically. Another multiphysics coupling feature **Wetted Wall** can be added when needed.

Simulations using the Laminar Two-Phase Flow, Level Set interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Turbulence Model
By default the **Turbulence model type** selected is **None.** If **RANS** is selected, the property **Turbulence model** will be activated, and allow to select **k-ε** or **k-ω** turbulent model.

Multiphysics Coupling Option
Laminar Flow interface coupled to a Laminar Two-Phase Flow, Level Set interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar Two-Phase Flow, Level Set interface **Multiphysics coupling option** is automatically set to **Level Set**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \tag{5-1}$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces.

$\circledast$	• Theory for the Two-Phase Flow Interfaces • Theory for the Single-Phase Flow Interfaces

The Turbulent Two-Phase Flow, Level Set Interface

The **Turbulent Two-Phase Flow, Level Set** interface (⬡) found under the **Multiphase Flow>Two-Phase Flow, Level Set** branch (⬡), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Turbulent Two-Phase Flow, Level Set** multiphysics interface, a **Laminar Flow** and a **Level Set** interface are added to the Model Builder. In addition the **Multiphysics** node,

a multiphysics coupling feature **Two-Phase Flow, Level Set** is added automatically. Another multiphysics coupling feature **Wetted Wall** can be added when needed.

Simulations using the Turbulent Two-Phase Flow, Level Set interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Turbulence Model
By default the **Turbulence model type** selected is **RANS.** The property **Turbulence model** will be activated, and allow to select **k-ε** or **k-ω** turbulent model. If **None** is selected for **Turbulence model type**, it becomes a laminar model.

Multiphysics coupling option
Laminar Flow interface coupled to a Laminar Two-Phase Flow, Level Set interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar Two-Phase Flow, Level Set interface **Multiphysics coupling option** is automatically set to **Level Set**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \tag{5-2}$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces.

	• Theory for the Two-Phase Flow Interfaces
ⓠ	• Theory for the Single-Phase Flow Interfaces

Two-Phase Flow, Level Set Coupling Features

The **Laminar Two-Phase Flow, Level Set,** (🪣) and **Turbulent Two-Phase Flow, Level Set,** (🪣) interfaces contain a multiphysics coupling feature, **Two-Phase Flow, Level Set**, which is added automatically.

The multiphysics coupling feature **Two-Phase Flow, Level Set** defines density and dynamic viscosity of the flow used in the **Laminar Flow** and **Turbulent Flow** interfaces, and defines the surface tension on the interface in form of a volume force used in momentum equation. It also enable the **Level set** interface use the velocity field calculated from **Laminar Flow** or **Turbulent Flow** interfaces to convect the interface.

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Level Set** in the model) is tpf1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

FLUID PROPERTIES

Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2** respectively.

To specify the properties of **Fluid 1** from a material, select the appropriate material in the **Fluid 1** list. Also make sure that the **Density of fluid 1** ρ_1 and **Dynamic viscosity of fluid 1** μ_1 are both set to **From Material**.

The non-Newtonian power-law and Carreau models can alternatively be used to specify the dynamic viscosities of the two fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid 1** ρ_1 or the **Dynamic viscosity of fluid 1** μ_1 drop down list and enter the expression in the corresponding edit field.

Similarly, the properties of **Fluid 2** can be specified.

⚠️ Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2.

The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two

fluids. For this reason selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

SURFACE TENSION

Select the **Neglect surface tension in momentum equation** check box to neglect surface tension.

Select a **Surface tension coefficient** σ (SI unit: N/m):

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air**, **Glycerol/Air** and so forth).

- For **User defined** enter a value or expression for the surface tension coefficient σ(SI unit: N/m).

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

The Wetted Wall Coupling Feature

The **Laminar Two-Phase Flow, Level Set,** (⬛) and **Turbulent Two-Phase Flow, Level Set,** (⬛) interfaces contain an optional multiphysics coupling boundary feature, **Wetted Wall**. It is an exclusive feature which overrides the **Wall** feature of Laminar Flow or Turbulence Flow interfaces together with the **No Flow** feature of Level Set interface.

The **Wetted wall** boundary condition is suitable for walls in contact with the fluid-fluid interface. If this boundary condition is used, the fluid-fluid interface can move along the wall.

This boundary condition enforces the no-penetration condition $\mathbf{u} \cdot \mathbf{n}_{\mathrm{wall}} = 0$ and adds a frictional force of the form

$$\mathbf{F}_{\mathrm{fr}} = -\frac{\mu}{\beta}\mathbf{u}$$

where β is the slip length. For numerical calculations it is suitable to set $\beta = h$, where h is the mesh element size. The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance β outside the wall (see Figure 5-1).

Finally, the boundary condition adds the following weak boundary term:

$$\int_{\partial\Omega} \text{test}(\mathbf{u}) \cdot [\sigma(\mathbf{n}_{\text{wall}} - (\mathbf{n}\cos\theta_w))\delta]dS$$

The boundary term results from the partial integration of the surface tension force in the momentum equation. Define the contact angle θ_w (that is, the angle between the fluid interface and the wall). Figure 5-1 illustrates the definition of the contact angle.
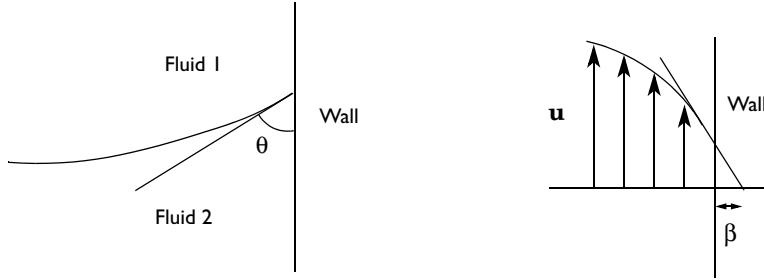
Figure 5-1: Definition of the contact angle θ at interface/wall contact points (left) and an illustration of the slip length β (right).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first multiphysics coupling feature **Wetted Wall** in the model) is ww1.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = 0$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall

to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

WETTED WALL

Here define the following two properties for the wetted wall:

- Enter a value or expression for the **Contact angle** θ_w. The default is `pi/2` ($\pi/2$) rad.

- Enter a value or expression for the **Slip length** β (SI unit: m). The default is `h`, which is the variable for the local mesh element size h.

🔍	• Theory for the Two-Phase Flow Interfaces

The Laminar Two-Phase Flow, Phase Field Interface

The **Laminar Two-Phase Flow, Phase Field** interface (🝠) found under the **Multiphase Flow>Two-Phase Flow, Phase Field** branch (🝠), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Laminar Two-Phase Flow, Phase Field** multiphysics interface, a **Laminar Flow** and a **Phase Field** interface are added to the Model Builder. In addition the **Multiphysics** node, a multiphysics coupling feature **Two-Phase Flow, Phase Field** is added automatically. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall function here is not implemented as a separated multiphase coupling boundary feature, but as the default **Wetted Wall** feature of **Phase Field** interface.

🔍	Wetted Wall

Simulations using the Laminar Two-Phase Flow, Phase Field interface are always time-dependent since the position of an interface is almost always dependent on its history.

Turbulence Model

By default the **Turbulence model type** selected is **None.** If **RANS** is selected, the property **Turbulence model** will be activated, and allow to select **k-ε** or **k-ω** turbulent model.

Multiphysics Coupling Option

Laminar Flow or Turbulent Flow interface coupled to a Laminar or Turbulent Two-Phase Flow, Phase Field interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar or Turbulent Two-Phase Flow, Phase Field interface, a **Multiphysics coupling option** is automatically set to **Phase Field**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \tag{5-3}$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces

---

> 🔍   Theory for the Two-Phase Flow Interfaces

The Turbulent Two-Phase Flow, Phase Field Interface

The **Turbulent Two-Phase Flow, Phase Field** interface (🌢) found under the **Multiphase Flow>Two-Phase Flow, Phase Field** branch (🌢), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Turbulent Two-Phase Flow, Phase Field** multiphysics interface, a **Turbulent Flow** and a **Phase Field** interface are added to the Model Builder. In addition the **Multiphysics** node, a multiphysics coupling feature **Two-Phase Flow, Phase Field** is added automatically. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall function here is not implemented as a separated multiphase coupling boundary feature, but as the default **Wetted Wall** feature of **Phase Field** interface.

> 🔍   Wetted Wall

Simulations using the Laminar Two-Phase Flow, Phase Field interface are always time-dependent since the position of an interface is almost always dependent on its history.

INTERFACE PROPERTIES

Turbulence Model
By default the **Turbulence model type** selected is **RANS.** The property **Turbulence model** allows the user to select **k-ε** or **k-ω** turbulent model If **RANS** is selected. When **None** is selected for **Turbulence model type**, it will become a laminar model.

Multiphysics Coupling Option
Laminar Flow or Turbulent Flow interface coupled to a Laminar or Turbulent Two-Phase Flow, Phase Field interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar or Turbulent Two-Phase Flow, Phase Field interface, a **Multiphysics coupling option** is automatically set to **Phase Field**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \qquad (5\text{-}4)$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces

🔍	Theory for the Two-Phase Flow Interfaces

The Two-Phase Flow, Phase Field Coupling Features

The **Laminar Two-Phase Flow, Phase Field,** (🔵) and **Turbulent Two-Phase Flow, Phase Field,** (🔵) interfaces contain a multiphysics coupling feature, **Two-Phase Flow, Phase Field**, which is added automatically.

The multiphysics coupling feature **Two-Phase Flow, Phase Field** defines density and dynamic viscosity of the flow used in the **Laminar Flow** and **Turbulent Flow** interfaces, and defines the surface tension on the interface in form of a volume force used in momentum equation. It also enable the **Phase Field** interface use the velocity field calculated from **Laminar Flow** or **Turbulent Flow** interfaces to convect the interface.

SETTINGS
The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Phase Field** in the model) is tpf1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

FLUID PROPERTIES

Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid 1** from a material, select the appropriate material in the **Fluid 1** list. Also make sure that the **Density of fluid 1** ρ_1 and **Dynamic viscosity of fluid 1** μ_1 are both set to **From Material**.

The non-Newtonian power-law and Carreau models can alternatively be used to specify the dynamic viscosities of the two fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid 1** ρ_1 or the **Dynamic viscosity of fluid 1** μ_1 drop down list and enter the expression in the corresponding edit field.

Similarly, the properties of **Fluid 2** can be specified.

> ⚠ Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2.

The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

The fluid defined as Fluid 1 affects the wetting characteristics on wetted walls. See the Wetted Wall node for details.

SURFACE TENSION

Select the **Neglect surface tension in momentum equation** check box to neglect surface tension.

Select a **Surface tension coefficient** σ (SI unit: N/m):

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air**, **Glycerol/Air** and so forth).

- For **User defined** enter a value or expression for the surface tension coefficient σ (SI unit: N/m).

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

🔍	• Theory for the Two-Phase Flow Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar and Turbulent Flow, Two-Phase, Level Set and Phase Field Interfaces

The Two-Phase Flow, Level Set and Phase Field Interfaces are multiphysics interfaces combining Laminar Flow or Turbulent Flow interfaces together with Level Set or Phase Field interfaces.

LAMINAR FLOW

The available physics features for the Laminar Flow interface are listed in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW

The available physics features for The Turbulent Flow Interface are also listed in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LEVEL SET

The available physics features for the Level Set Interface are listed in Domain, Boundary, and Pair Nodes for the Level Set Interface.

PHASE FIELD

The available physics features for the Phase Field Interface are listed in Domain, Boundary, and Pair Nodes for the Phase Field Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Three-Phase Flow, Phase Field Interface

This section includes the following topics:

- The Laminar Three-Phase Flow, Phase Field Interface
- The Three-Phase Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

---

Q | • Mathematics, Moving Interface Branch

The Laminar Three-Phase Flow, Phase Field Interface

The **Laminar Three-Phase Flow, Phase Field** interface (⬤), found under the **Multiphase Flow>Three-Phase Flow, Phase Field** branch (⬤), is a multiphysics interface designed to track the interfaces between three immiscible and incompressible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The density of each fluid is assumed to be constant, but the there is no restriction on the density differences between the separate fluids.

When adding the **Laminar Three-Phase Flow, Phase Field** multiphysics interface, a **Laminar Flow** and a **Ternary Phase Field** interface are added to the Model Builder. In addition the **Multiphysics** node, including the multiphysics coupling feature **Three-Phase Flow, Phase Field** is added.

Q | The Multiphysics Node in the *COMSOL Multiphysics Reference Manual.*

Simulations using the Laminar Three-Phase Flow, Phase Field interface are always time-dependent since the position of an interface is almost always dependent of its history.

Turbulence Model

Since the Three-Phase Flow, Phase Field interface assumes laminar flow, the Turbulence Model property in the Laminar Flow interface is deactivated when the interface is added as a part of a multiphysics interface.

Multiphysics Coupling Option

Laminar Flow interfaces coupled to a Three-Phase Flow, Phase Field interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Three-Phase Flow, Phase Field interface **Multiphysics coupling option** is automatically set to **Ternary Phase Field**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\frac{\partial \log \rho}{\partial t} + \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \log \rho = 0 \tag{5-5}$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces.

The Three-Phase Flow, Phase Field Coupling Feature

Use the **Three-Phase Flow, Phase Field** (⬡) multiphysics coupling to simulate the flow of a three immiscible fluids while explicitly tracking the interface separating each pair of the fluids.

The Three-Phase Flow interface solves Navier-Stokes equations for the conservation of momentum, and a continuity equation for the conservation of mass. The positions of the interfaces separating the fluid phases are tracked by solving four additional transport equations: two equations governing phase field variables and two equations for the corresponding generalized chemical potentials. The movement of the fluid-fluid interfaces is determined by minimization of free energy.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `tfpf1`.

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the three-phase flow, or select **All domains** as needed.

FLUID PROPERTIES
Use the corresponding section to specify the properties of all three fluids. The fluids are denoted **Fluid A**, **Fluid B**, and **Fluid C**, respectively.

To specify the properties of **Fluid A** from a material, select the appropriate material in the **Fluid A** list. Also make sure that the **Density of fluid A** ρ_A and **Dynamic viscosity of fluid A** μ_A are both set to **From Material**.

The non-Newtonian power-law and Carreau models can alternatively be used to specify the dynamic viscosities of the three fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid A** ρ_A or the **Dynamic viscosity of fluid A** μ_A drop down list and enter the expression in the corresponding edit field.

COUPLED INTERFACES
This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

> ⊕   • Theory for the Two-Phase Flow Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

The Three-Phase Flow, Phase Field Interface is a multiphysics interface combining The Laminar Flow Interface and the The Ternary Phase Field Interface.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

TERNARY PHASE-FIELD

The available physics features for The Ternary Phase Field Interface are listed in Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Bubbly Flow Interfaces

In this section:

- The Laminar Bubbly Flow Interface
- The Turbulent Bubbly Flow Interface
- Domain and Boundary Nodes for the Laminar and Turbulent Bubbly Flow Interfaces

The Laminar Bubbly Flow Interface

The **Laminar Bubbly Flow (bf)** interface ( ), found under the **Multiphase Flow>Bubbly Flow** branch ( ) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at low and moderate Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is computed from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density.

The physics interface can also model the distribution of the number density, that is, the number of bubbles per unit volume which in turn can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for laminar bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Laminar Bubbly Flow**, **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Laminar Bubbly Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `bf`.

PHYSICAL MODEL

Specify if the gas concentration is low and whether or not to solve for the interfacial area.

Low Gas Concentration
The **Low gas concentration** check box is selected by default. This approximation is valid if the gas volume fraction is low and its density does not have any significant effects on the continuity equation in The Bubbly Flow Equations (Equation 5-22 becomes Equation 5-23).

Turbulence Model Type
By default no turbulence model is used.

Solve For Interfacial Area
To add a transport equation for the bubble density in order to determine the interfacial area, select the **Solve for interfacial area** check box.

Reference Pressure Level
Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

Swirl Flow
For 2D axisymmetric models, select the **Swirl flow** check box to include the swirl velocity component — that is, the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction. Also see General Single-Phase Flow Theory (2D Axisymmetric Formulations).

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** `rhogeff` (SI unit: kg/m^3), and the **Number density, gas phase** `nd` (SI unit: $1/\text{m}^3$). The names can be changed but the names of fields and dependent variables must be unique within a component.

To display this section, click the **Show** button (⟅) and select **Stabilization**. This section contains the settings for stabilization of the momentum transport (the fluid flow) in the **Momentum transport** area and stabilization of the equation for the dispersed phase in the **Gas phase transport** area.

Consistent streamline and crosswind diffusion is applied by default to both gas and momentum transport. Additional inconsistent stabilization terms may be added when required, either as isotropic diffusion or in the streamline direction only. Isotropic diffusion (shock capturing, $O(h^2)$) requires a scale for the effective gas density. An appropriate scale is the maximum value.

ADVANCED SETTINGS

To display this section, click the **Show** button (⟅) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression**—**Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** CFL_{loc} (dimensionless).

⟲	• Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual* • Domain and Boundary Nodes for the Laminar and Turbulent Bubbly Flow Interfaces • Theory for the Bubbly Flow Interfaces • The Turbulent Bubbly Flow Interface

---

The Turbulent Bubbly Flow Interface

The **Turbulent Bubbly Flow (bf)** interface (≋), found under the **Multiphase Flow>Bubbly Flow** branch (≋) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of

Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints and bubble-induced turbulence production. Flow close to walls is modeled using wall functions.

The physics interface can also model the distribution of the number density (that is, the number of bubbles per unit volume), which in turn can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Turbulent Bubbly Flow**, **Fluid Properties**, **Wall** (the default boundary types are **Wall functions** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Turbulent Bubbly Flow** to select physics features from the context menu.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface.

PHYSICAL MODEL

Specify if the gas concentration is low and whether or not to solve for the interfacial area.

Low Gas Concentration
Select the **Low gas concentration** check box if the gas volume fraction is low (ϕ_g less than a few percent). It is then generally valid to replace the continuity equation in The Bubbly Flow Equations see Equation 5-23 with Equation 5-26). This option is selected by default.

Turbulence Model Type
By default a **k-ε** turbulence model is used.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: kg/m^3), the

Turbulent dissipation rate ep (SI unit: m^2/s^3), the **Turbulent kinetic energy** k (SI unit: m^2/s^2), and the **Number density, gas phase** nd (SI unit: $1/m^3$).

The names of variables can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**. The settings for this section are the same as for The Laminar Bubbly Flow Interface with the addition of this section: stabilization for the turbulence variables in the **Turbulence equations** area.

When using a turbulence model, streamline and crosswind diffusion are by default applied to the turbulence equations.

DISCRETIZATION

P1+P1 is not permitted unless streamline diffusion is active for the momentum transport.

$\mathbb{Q}$	• Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual* • Domain and Boundary Nodes for the Laminar and Turbulent Bubbly Flow Interfaces • Theory for the Bubbly Flow Interfaces

---

▦	*Flow in an Airlift Loop Reactor*: path **CFD_Module/Multiphase_Benchmarks/airlift_loop_reactor**

Domain and Boundary Nodes for the Laminar and Turbulent Bubbly Flow Interfaces

For both The Laminar Bubbly Flow Interface and The Turbulent Bubbly Flow Interface these domain and boundary nodes are available from the **Physics** ribbon toolbar (Windows

users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

DOMAIN

- Fluid Properties
- Gravity
- Initial Values
- Mass Transfer
- Volume Force (described for The Laminar Flow Interface)

BOUNDARY

	The sections describe the available boundary conditions for the liquid and the gas. In all equations, **n** denotes the outward pointing unit vector normal to the boundary.

The boundary types for the liquid flow variables, described in this section, are:

- Inlet
- Outlet
- Symmetry
- Wall (the default boundary condition)

In addition to the boundary conditions for the liquid, the following boundary conditions for the gas are available for all boundary condition types except symmetry:

- Gas Concentration (the default condition for inlets)
- Gas Flux
- Gas Outlet (the default condition for outlets)

- No Gas Flux (the default condition for walls)
- Symmetry

ⓠ	Gas Boundary Condition Equations

🠋	For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Fluid Properties

The **Fluid Properties** node contains the material properties for the liquid and the gas. It also contains settings for the slip model.

MATERIALS

Select the materials to use for the material properties of the liquid and the gas (when they are set to take their value from the material). The default is to use the **Domain material** for both the **Liquid** and the **Gas**. Select another material to use that material's properties for the liquid or gas as needed.

LIQUID PROPERTIES

The default **Density, liquid phase** ρ_l (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression.

The default **Dynamic viscosity, liquid phase** μ_l (SI unit: Pa·s) uses values **From material**; the value is then defined for the material selected in the **Materials** section for the continuous phase. For **User defined** enter another value or expression.

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity.

GAS PROPERTIES

The default **Density, gas phase** ρ_g (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression.

Enter the **Bubble diameter** d_b (SI unit: m). The default value is 10^{-3} m (1 mm).

Select a **Slip model**—**Homogeneous flow** (the default), **Pressure-drag balance**, or **User defined**.

Homogeneous flow assumes that the velocity of the two phases are equal; that is, $\mathbf{u}_{\text{slip}} = 0$. For **User defined** enter different values or expressions for the components of the **Slip velocity** $\mathbf{u}_{\text{slip}}$ (SI unit: m/s).

For **Pressure-drag balance** it uses a model based on the assumption that the pressure forces on a bubble are balanced by the drag force:

$$\frac{3}{4}\frac{C_{\text{d}}}{d_{\text{b}}}\rho_{\text{l}}\big|\mathbf{u}_{\text{slip}}\big|\mathbf{u}_{\text{slip}} = -\nabla p$$

Here d_{b} (SI unit: m) is the bubble diameter, and C_{d} (dimensionless) is the drag coefficient.

Select a **Drag coefficient model**:

- **Small spherical bubbles (Hadamard-Rybczynski)** for bubbles with a diameter smaller than 2 mm.
- **Large bubbles** for gas bubbles with a diameter larger than 2 mm. Then enter the **Surface tension coefficient** σ (SI unit N/m). The default is 0.07 N/m.
- **Air bubbles in tap water (Schwarz-Turner)** for air bubbles of 1–10 mm mean diameter in water.
- **User defined** to enter a different value or expression for the **Drag coefficient** C_d (dimensionless). The default value is 1.

Q | See the Slip Model theory section.

MIXING LENGTH LIMIT

This section is available for The Turbulent Bubbly Flow Interface.

When the **Mixing length limit** $l_{\text{mix,lim}}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression.

Gravity

The **Gravity** node adds the force $\rho\mathbf{g}$ to the right-hand side of the momentum transport equation. Gravity nodes are mutually exclusive, that is, there can only be one active Gravity node per domain.

GRAVITY

Enter the components of the **Gravity vector**, $\mathbf{g}$ (SI unit: m/s^2). For 2D components the default Gravity vector is defined as $(0, -g\_const)$. Here g_const is a physical constant equal to 9.8066 m/s^2. For 3D and 2D axisymmetric components, the gravity acts in the negative z direction by default.

Mass Transfer

Add a **Mass Transfer** node to include mass transfer from the gas to the liquid.

MASS TRANSFER

Select a **Mass transfer model** — **Two-film theory** model or **User defined**. For **User defined** enter a value or expression for the **Mass transfer from gas to liquid** m_{gl} (SI unit: $kg/(m^3{\cdot}s)$). The default is 0 $kg/(m^3{\cdot}s)$.

For **Two-film theory** enter values for the **Mass transfer coefficient** k (SI unit: m/s), **Henry's constant** H (SI unit: $Pa{\cdot}m^3/mol$), the **Dissolved gas concentration** c (SI unit: mol/m^3), and the **Molecular weight of species** M (SI unit: kg/mol). Refer to the theory below for more information.

Henry's law gives the equilibrium concentration c^* of gas dissolved in liquid:

$$c^* = \frac{p + p_{\mathrm{ref}}}{H}$$

where H is Henry's constant. The molar flux per interfacial area, N (SI unit: $mol/(s{\cdot}m^2)$), is determined by

$$N = k(c^* - c)$$

where k is the Mass transfer coefficient and c is the Dissolved gas concentration in liquid.

The mass transfer from gas to liquid, m_{gl}, is given by

$$m_{gl} = NMa$$

where M is the Molecular weight of species and a is the interfacial area per volume (SI unit: m^2/m^3).

> 🔍   Also see Theory for the Bubbly Flow Interfaces for details about how a is computed.

For two-film theory, you also need to solve for the concentration of the dissolved gas;

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}_1) \ = \ \nabla \cdot (D\nabla c) + \frac{m_{gl}}{M}$$

which can be done by adding a Transport of Diluted Species interface.

Initial Values

The **Initial Values** node adds initial values for the flow variables and the effective gas density that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field. liquid phase u** (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0. Also enter a value or expression for the **Effective gas density** $rhogeff$ (SI unit: kg/m^3). The default is 0 kg/m^3.

If the **Solve for interfacial area** check box is selected in The Laminar Bubbly Flow Interface or The Turbulent Bubbly Flow Interface enter an initial value for the **Number density, gas phase** nd (SI unit: $1/m^3$). The default is 0 $1/m^3$.

For The Turbulent Bubbly Flow Interface also enter initial values for the **Turbulent dissipation rate** ep (SI unit: m^2/s^3), and **Turbulent kinetic energy** k (SI unit: m^2/s^2).

Wall

The **Wall** node adds a selection of boundary conditions that describe the existence of a solid wall. The Wall node by default specifies no gas flux for the gas phase.

> 🔍   Gas Boundary Condition Equations

LIQUID BOUNDARY CONDITION

The **Liquid boundary condition** is specified as follows.

- For The Laminar Bubbly Flow Interface, select **No slip** (the default) or **Slip**.

- For The Turbulent Bubbly Flow Interface, select **Wall functions** (the default) or **Slip**.

No Slip
Sets the liquid velocity to zero at the wall:

$$\mathbf{u}_l = 0$$

This is the default boundary condition for the liquid.

Slip
Sets the velocity component normal to the wall to zero:

$$\mathbf{u}_l \cdot \mathbf{n} = 0$$

Wall Functions
This boundary condition models a no slip condition for solid walls in a turbulent flow. Wall functions are used to model the thin region with large gradients in the flow variables near the wall.

Click to select the **Apply wall roughness** check box to apply the roughness correction. When the check box is selected, the default **Roughness model** is **Sand roughness**, which is derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

- For **Sand roughness** enter an **Equivalent sand roughness height** k_{seq} (SI unit: m). The default is 3.2 micrometers.

- For **Generic roughness** enter a **Roughness height** k_s (SI unit: m). The default is 3.2 micrometers. Then enter a **Roughness parameters** C_s (dimensionless). The default is 0.26.

> 🔍   References for the Single-Phase Flow, Turbulent Flow Interfaces

---

GAS BOUNDARY CONDITION

From the list, select a **Gas boundary condition** for the gas phase on the wall—**No gas flux** (the default), **Gas concentration**, **Gas outlet**, **Gas flux**, or **Symmetry**.

Gas Concentration

For **Gas concentration** enter the **Effective gas density** $\rho_g \phi_{g0}$ (SI unit: kg/m^3). The default is 0 kg/m^3. If **Solve for interfacial area** is selected, also select either the **Bubble number density** (the default) or the **Bubble diameter and gas density** button.

- For **Bubble number density** enter the **Bubble number density** n_0 (SI unit: 1/m^3). The default is 1000 1/m^3.

- For **Bubble diameter and gas density** enter the **Bubble diameter** d_b (SI unit: m) (the default is 1 mm) and **Density, gas phase** ρ_g (SI unit: kg/m^3) (the default is 1 kg/m^3).

Gas Flux

For **Gas flux** enter the **Gas mass flux** $N_{\rho_g \phi_g}$ (SI unit: kg/(m^2·s)) (the default is 0 kg/(m^2·s)) and if the **Solve for interfacial area** check box is selected on the physics interface, the **Number density flux** N_n (SI unit: 1/(m^2·s)). The default is 0 (1/(m^2·s)).

Inlet

The **Inlet** node adds a selection of boundary conditions that describe inlets in fluid-flow simulations.

<div>❓</div> [Gas Boundary Condition Equations](#)

LIQUID BOUNDARY CONDITION

Select a **Liquid boundary condition**—**Velocity** (the default), **Pressure**, or for [The Laminar Bubbly Flow Interface](#), **Laminar inflow** is also an option.

VELOCITY

For **Velocity** click the **Normal inflow velocity** (the default) or **Velocity field** buttons.

- For **Normal inflow velocity** enter a value or expression for U_0 (SI unit: m/s).

- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{u}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{u}_l = \mathbf{u}_0$$

PRESSURE

This condition specifies the normal stress which in most cases is approximately equal to the pressure. Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a

relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.

- The **Suppress backflow** check box is selected by default. This option adjusts the inlet pressure, $\hat{p}_0 \geq p_0$, locally in order to prevent fluid from exiting the domain through the boundary. If suppress backflow is deselected, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.

- **Flow direction** controls in which direction the fluid enters the domain.

  - For **Normal flow** (the default) it prescribes zero tangential velocity component.

  - For **User defined** define an **Inflow velocity direction**, $\mathbf{d_u}$ (dimensionless). The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.

LAMINAR INFLOW

This section is available for The Laminar Bubbly Flow Interface and when **Laminar inflow** is selected as the **Liquid boundary condition**.

Select a **Laminar inflow option** — **Average velocity** (the default), **Flow rate**, or **Entrance pressure**.

For any selection, also choose the **Constrain outer edges to zero** check box to force the laminar profile to go to zero at the bounding points or edges of the inlet channel. Otherwise the velocity is defined by the boundary condition of the adjacent boundary in the model. For example, if one end of a boundary with a laminar inflow condition connects to a slip boundary condition, the laminar profile has a maximum at that end.

Then:

- For **Average velocity** enter U_{av} (SI unit: m/s). Enter an **Entrance length** L_{entr} (SI unit: m). The default is 1 m.

- For **Flow rate** enter an **Entrance length** L_{entr} (SI unit: m, default 1 m), **Entrance thickness** D_z (SI unit: m), and **Flow rate** V_0 (SI unit: m^3/s).

- For **Entrance pressure** enter an **Entrance pressure** p_{entr} (SI unit: Pa) and an **Entrance length** L_{entr} (SI unit: m).

GAS BOUNDARY CONDITION

These settings are the same as for Wall. See Gas Boundary Condition. The only difference is that **Gas concentration** is the default.

This section is available for The Turbulent Bubbly Flow Interface so that the inlet conditions for the turbulence variables (k and ε) can be specified. Except for Equation 5-6, of the settings information is the same as that described for single-phase flow.

The turbulent length scale L_T and turbulence intensity I_T are related to the turbulence variables via

$$k = \frac{3}{2}(|\mathbf{U}|I_T)^2, \qquad \varepsilon = C_\mu^{3/4}\frac{k^{3/2}}{L_T} \tag{5-6}$$

Outlet

The **Outlet** node adds a set of boundary conditions that describe outlets in fluid-flow simulations; that is, the conditions at boundaries where the fluid exits the domain.

LIQUID BOUNDARY CONDITION

Select a **Liquid boundary condition** — **Pressure** (the default), **Velocity**, or for The Laminar Bubbly Flow Interface, **Laminar outflow** is also an option.

PRESSURE CONDITIONS

The **Pressure** condition specifies the normal stress which in most cases is approximately equal to the pressure. The tangential stress component is set to 0 N/m^2.

- Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.

- Select the **Normal flow** check box to change the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.

The **Suppress backflow** check box is selected by default. This option adjusts the outlet pressure in order to prevent fluid from entering the domain through the boundary.

VELOCITY

For **Velocity** click the **Velocity field** (the default) or **Normal outflow velocity** buttons.

- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{u}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{u}_1 = \mathbf{u}_0$$

- For **Normal outflow velocity** enter a value or expression for U_0 (SI unit: m/s).

GAS BOUNDARY CONDITION

The settings for the **Gas boundary condition** are the same as for Wall. See Gas Boundary Condition.

When the **Gas boundary condition** is set to **Gas outlet**, the **Exterior gas condition(s)** section contains an input field for the **Effective gas density** on the downstream side of the outlet. If **Solve for interfacial area** is selected at the physics interface level, additional input fields appear for the **Bubble number density** or the **Bubble diameter and gas density** on the downstream side of the outlet.

LAMINAR OUTFLOW

This section is available for The Laminar Bubbly Flow Interface when **Laminar outflow** is selected as the **Liquid boundary condition**.

Select a **Laminar outflow option** — **Average velocity** (the default), **Flow rate**, or **Exit pressure**. For any selection, also choose the **Constrain outer edges to zero** check box to force the laminar profile to go to zero at the bounding points or edges of the inlet channel. Otherwise the velocity is defined by the boundary condition of the adjacent boundary in the model.

For example, if one end of a boundary with a laminar inflow condition connects to a slip boundary condition, then the laminar profile has a maximum at that end.

- For **Average velocity** enter an **Average velocity** U_{av} (SI unit: m/s) the default is 0. Enter an **Exit length** L_{exit} (SI unit: m). The default is 1 m.
- For **Flow rate** enter an **Exit length** L_{exit} (SI unit: m). The default is 1 m. Enter a **Flow rate** V_0 (SI unit: m^3/s).
- For **Entrance pressure** enter an **Exit length** L_{exit} (SI unit: m). The default is 1 m. Enter an **Exit pressure** p_{exit} (SI unit: Pa).

Symmetry

The **Symmetry** node adds boundary conditions that describe symmetry boundaries in fluid-flow simulations. The boundary condition for symmetry boundaries prescribes no penetration and vanishing shear stresses:

$$\mathbf{u}_1 \cdot \mathbf{n} = 0, \qquad \mathbf{t}^T\left(\phi_1(\mu_1 + \mu_T)\left(\nabla\mathbf{u}_1 + \nabla\mathbf{u}_1^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_1)\mathbf{I}\right)\right)\mathbf{n} = 0$$

BOUNDARY SELECTION

A boundary condition for 2D axial symmetry is not required.

For the symmetry axis at $r = 0$, the software automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the z direction and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Gas Boundary Condition Equations

In addition to the boundary conditions for the liquid, specify boundary conditions for the gas on Wall, Inlet, and Outlet nodes. Select a **Gas Boundary Condition**:

Gas Concentration

Using this boundary condition, specify the effective gas density.

$$\tilde{\rho}_g = \tilde{\rho}_g^0$$

Gas Outlet

This boundary condition is appropriate for boundaries where the gas phase flows outward with the gas velocity, $\mathbf{u}_g$, at the boundary.

Gas Flux

Using this boundary condition, specify the gas mass flux through the boundary:

$$-\mathbf{n} \cdot (\tilde{\rho}_g\mathbf{u}_g) = N_{\rho_g\phi_g}$$

Symmetry

This boundary condition, which is useful on boundaries that represent a symmetry line for the gas flow, sets the gas flux through the boundary to zero:

$$\mathbf{n} \cdot (\tilde{\rho}_g\mathbf{u}_g) = 0$$

No Gas Flux

This boundary condition represents boundaries where the gas flux through the boundary is zero:

$$\mathbf{n} \cdot (\phi_d\mathbf{u}_d) = 0$$

The Mixture Model Interfaces

In this section:

The Mixture Model, Laminar Flow Interface

The **Mixture Model, Laminar Flow (mm)** interface ( ), found under the **Multiphase Flow>Mixture Model** branch ( ) when adding a physics interface, is used to model the flow at low and moderate Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Laminar Flow interface solves one set of Navier-Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

The main physics node is the Mixture Properties feature, which adds the equations for the mixture and provides an interface for defining the fluid materials for the continuous and dispersed phases as well as which slip model and mixture viscosity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder**—**Mixture Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Mixture Model, Laminar Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is mm.

PHYSICAL MODEL

Specify the characteristics of the dispersed phase, the model for the slip velocity, and whether or not to solve for the interfacial area.

Dispersed Phase

To characterize the **Dispersed phase**, select **Solid particles** (the default) or **Liquid droplets/bubbles**.

The selection from this list is further defined for the Mixture Properties node under the Mixture Model section.

Slip Model

To compute the slip velocity $\mathbf{u}_{\text{slip}}$ (SI unit: m/s), select a **Slip model** — **Homogeneous flow** (the default), **Hadamard-Rybczynski**, **Schiller-Naumann**, **Haider-Levenspiel**, or **User defined**.

- The **Homogeneous flow** model assumes that the velocities of the two phases are equal, that is, $\mathbf{u}_{\text{slip}} = 0$.

- In most cases there is a significant difference in the velocity fields due to the buoyancy of the dispersed phase. Use one of the predefined slip models for such cases.

- For **User defined** specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data. For the Mixture Properties node under the Mixture Model section, enter the **Slip velocity field** $\mathbf{u}_{\text{slip}}$ (SI unit: m/s).

Turbulence Model Type

The default selection is **None**.

Solve For Interfacial Area

To add a transport equation for the number density of the dispersed particles, in order to determine the interfacial area, select the **Solve for interfacial area** check box (by default not selected.

For the Mass Transfer rate, use a two-film theory model, which includes the interfacial area per unit volume between the two phases. It is possible to compute the interfacial area per unit volume if the number density n (that is, the number of dispersed particles per volume)

is known. Select the **Solve for interfacial area** check box to add the following equation for the number density n:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}_d) = 0$$

This equation states that a dispersed phase particle cannot disappear, appear, or merge with other particles, although it can expand or shrink.

The Mixture Model, Laminar Flow Interface calculates the interfacial area a (SI unit: m^2/m^3) from

$$a = (4n\pi)^{1/3}(3\phi_d)^{2/3}$$

Reference Pressure Level
Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm].

Swirl Flow
For 2D axisymmetric components, select the **Swirl flow** check box to include the swirl velocity component — that is, the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction

---

  General Single-Phase Flow Theory (2D Axisymmetric Formulations)

DEPENDENT VARIABLES
Enter values for the dependent variables (field variables):

- **Velocity field, mixture u** (SI unit: m/s)

- **Pressure** p (SI unit: Pa)

- **Volume fraction, dispersed phase** $phid$ (dimensionless)

- **Squared slip velocity** *slipvel*

- **Number density, dispersed phase** nd (SI unit: $1/m^3$).

The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION AND INCONSISTENT STABILIZATION
To display this section, click the **Show** button ( ) and select **Stabilization**.

The consistent stabilizations **Streamline diffusion** and **Crosswind diffusion** are by default applied to the **Navier-Stokes and gas transport equations**. In addition, when the flow is turbulent, the consistent stabilizations are also applied to the **Turbulence**.

Isotropic shock capturing, $O(h^2)$ for the dispersed phase needs a scale for the volume fraction of the dispersed phase. A suitable scale is the maximum value of the dispersed phase volume fraction.

ADVANCED SETTINGS

To display this section, click the **Show** button (![icon]) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Penalty Diffusion can be used to suppress negative values of the dispersed volume fraction. Including this term has been observed to slow down convergence and it is therefore disabled by default

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression**—**Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** CFL_{loc} (dimensionless).

⚲
- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Domain and Boundary Nodes for the Mixture Model Laminar and Turbulent Flow Interfaces
- The Mixture Model, Turbulent Flow Interface
- Slip Velocity Models and Theory for the Mixture Model Interfaces

---

▥
Two-Phase Flow Modeling of a Dense Suspension: path
CFD_Module/Multiphase_Benchmarks/dense_suspension

The Mixture Model, Turbulent Flow Interface

The **Mixture Model, Turbulent Flow (mm)** interface (![icon]), found under the **Multiphase Flow>Mixture Model** branch (![icon]) when adding a physics interface, is used to model the

flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Turbulent Flow interface solves one set of Navier-Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface.

PHYSICAL MODEL

The default **Turbulence model type** is **RANS, k-ε**.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture u** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** $phid$ (dimensionless)
- **Squared slip velocity** $slipvel$
- **Number density, dispersed phase** nd (SI unit: $1/\text{m}^3$)
- **Turbulent kinetic energy** k (SI unit: m^2/s^2)
- **Turbulent dissipation rate** ε (SI unit: m^2/s^3)

The names can be changed but the names of fields and dependent variables must be unique within a component.

	• Domain and Boundary Nodes for the Mixture Model Laminar and Turbulent Flow Interfaces
Q	• Slip Velocity Models
	• Theory for the Mixture Model Interfaces

Domain and Boundary Nodes for the Mixture Model Laminar and Turbulent Flow Interfaces

For both The Mixture Model, Laminar Flow Interface and The Mixture Model, Turbulent Flow Interface the following domain and boundary nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

DOMAIN

- Gravity
- Initial Values
- Mass Transfer
- Mixture Properties
- Volume Force (described for The Laminar Flow Interface)

BOUNDARY

Boundary conditions for the mixture velocity, pressure and dispersed phase volume fraction need to be specified. The following boundary condition types are available for The Mixture Model, Laminar Flow Interface and The Mixture Model, Turbulent Flow Interface:

- Inlet
- Outlet

- Symmetry
- Wall (the default boundary condition feature).

For the flow variables, the velocity and the pressure, the boundary conditions correspond to those defined for single phase flow (see Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow). There is also a point constraint for the pressure, which is useful if no other boundary condition in the model includes a pressure level constraint.

The following boundary conditions for the dispersed phase are available for all boundary condition types except symmetry. These are described in more detail in the Theory for the Mixture Model Interfaces.

- **Dispersed phase concentration** (the default condition for inlets)
- **Dispersed phase flux**
- **Dispersed phase outlet** (the default condition for outlets)
- **No dispersed phase flux** (the default condition for walls)
- **Symmetry**

	For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.

Mixture Properties

The **Mixture Properties** node contains the material properties for the continuous phase and the dispersed phase. It also contains settings for the viscosity model.

MATERIALS

Select the fluid materials to use for the material properties. The default material used for both **Continuous phase** and **Dispersed phase** is the **Domain material**. Select another material (when available).

CONTINUOUS PHASE PROPERTIES

The default **Density, continuous phase** ρ_c (SI unit: kg/m^3) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case the default is $0 \ kg/m^3$.

The default **Dynamic viscosity, continuous phase** μ_c (SI unit: Pa·s), uses values **From material**. It describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. For **User defined** enter another value or expression. In this case, the default is 0 Pa·s.

DISPERSED PHASE PROPERTIES

The default **Density, dispersed phase** ρ_d (SI unit: kg/m^3) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case, the default is 0 kg/m^3.

Enter the **Diameter of particles/droplets** d_d (SI unit: m). The default is 10^{-3} m (1 mm). If **Haider-Levenspiel** is selected for the **Slip model** under **Physical Model**, enter a value between 0 and 1 for the **Sphericity** (dimensionless). The default is 1.

If **Liquid droplets/bubbles** is selected from the **Dispersed phase** list for either The Mixture Model, Laminar Flow Interface or The Mixture Model, Turbulent Flow Interface, then **Dynamic viscosity, dispersed phase** μ_d (SI unit: Pa·s) is also available. The default uses values **From material** (as selected in the **Materials** section) or select **User defined** to enter another value or expression. In this case, the default is 0 Pa·s.

MIXTURE MODEL

The options in this section are based on the selection made from the **Dispersed phase** list for either The Mixture Model, Laminar Flow Interface or The Mixture Model, Turbulent Flow Interface.

Slip Velocity Field

When a **User defined Slip model** is selected for the physics interface, specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data. Enter the **Slip velocity field** $\mathbf{u}_{slip}$ (SI unit: m/s).

Mixture Viscosity Model

Select the **Mixture viscosity model**.

- When **Solid particles** is the **Dispersed phase**, select either **Krieger type** (the default) or **User defined**.

- When **Liquid droplets/bubbles** is the **Dispersed phase**, select **Krieger type** (the default), **User defined**, or **Volume averaged**.

User Defined

For **User defined** enter a value or expression for the **Dynamic viscosity** μ (SI unit: Pa·s). The default is 0 Pa·s. When using this option, make sure to limit the viscosity to bounded positive values.

Krieger Type

When **Krieger type** is selected, enter a value or expression for the **Maximum packing concentration** ϕ_{max} (dimensionless). The default is 0.62.

Select Krieger type to model the most generally valid expression for the mixture viscosity:

$$\mu = \mu_c\left(1 - \frac{\phi_d}{\phi_{max}}\right)^{-2,5\phi_{max}\mu^*}$$

where ϕ_{max} is the maximum packing concentration, which for solid particles is approximately 0.62. The dimensionless parameter $\mu^* = 1$ for solid particles and

$$\mu^* = \frac{\mu_d + 0,4\mu_c}{\mu_d + \mu_c}$$

for droplets and bubbles. When applying the Krieger type viscosity model, ϕ_d is replaced by $\min(\phi_d, 0.999\phi_{max})$ for better robustness.

Volume Averaged

Select **Volume averaged** to model the mixture viscosity of liquid-liquid mixtures, which uses the following equation for the viscosity:

$$\mu = \phi_d\mu_d + \phi_c\mu_c$$

The Mixture Model interfaces always employ the mixture viscosity in the particle Reynolds number expression used to calculate the slip velocity, thereby accounting for the increase in viscous drag due to particle-particle interactions.

MIXING LENGTH LIMIT

This section is available for The Mixture Model, Turbulent Flow Interface.

Select how the **Mixing length limit** $l_{mix,lim}$ (SI unit: m) is defined—**Automatic** (default) or **Manual**:

• For **Automatic** the mixing length limit is automatically evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of

slim entities, this measure can give a too high value. In such cases, it is recommended that it is defined manually.

- For **Manual** it defines a different value or expression. The default is 1 (that is, one unit length of the model unit system).

Initial Values

The **Initial Values** node adds initial values for the mixture velocity, pressure, and volume fraction of the dispersed phase, that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter values or expressions for the following dependent variables:

- **Velocity field, mixture**, the components of **u** (SI unit: m/s). The defaults are 0 m/s.
- **Pressure** p (SI unit: Pa). The default is 0 Pa.
- **Volume fraction, dispersed phase** (dimensionless). The default is 0.
- If the **Solve for interfacial area** check box is selected for the physics interface, enter an initial value for the **Number density, dispersed phase** nd (SI unit: $1/m^3$). The default is $0\ 1/m^3$.
- If a **Schiller-Naumann** or a **Haider-Levenspiel** slip model is used in the physics interface, enter an initial value for the **Squared slip velocity** $slipvel$ (SI unit: m^2/s^2). The default is $0.081\ m^2/s^2$.

For The Mixture Model, Turbulent Flow Interface also enter values or expressions for:

- **Turbulent dissipation rate** ep (SI unit: m^2/s^3). The default is `mm.epinit`.
- **Turbulent kinetic energy** k (SI unit: m^2/s^2). The default is `mm.kinit`.

> **!** The following sections describe the available boundary conditions for the mixture and the dispersed phase volume fraction. In all equations, **n** denotes the outward pointing unit vector normal to the boundary.

Wall

The **Wall** node has boundary conditions available that describe the existence of a solid wall.

MIXTURE BOUNDARY CONDITION

Select a **Mixture boundary condition**—**No slip** (laminar flow only), **Slip**, or **Wall functions** (turbulent flow only).

Slip

Select **Slip** to set the velocity component normal to the wall to zero $\mathbf{u} \cdot \mathbf{n} = 0$.

No Slip

No slip is the default boundary condition for The Mixture Model, Laminar Flow Interface and prescribes $\mathbf{u} = 0$, that is, the fluid at the wall is not moving.

Wall Functions

Wall functions is the default boundary condition for The Mixture Model, Turbulent Flow Interface. It models a no slip condition for a solid wall in turbulent flow. Wall functions are used to model the thin region with high gradients in the flow variables near the wall.

This boundary condition models a no slip condition for solid walls in a turbulent flow. Wall functions are used to model the thin region with large gradients in the flow variables near the wall.

Click to select the **Apply wall roughness** check box to apply the roughness correction. When the check box is selected, the default **Roughness model** is **Sand roughness**, which is derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

- For **Sand roughness** enter an **Equivalent sand roughness height** k_{seq} (SI unit: m). The default is 3.2 μm.

- For **Generic roughness** enter a **Roughness height** k_{s} (SI unit: m). The default is 3.2 μm. Enter a **Roughness parameter** C_{s} (dimensionless). The default is 0.26.

> 🔍   References for the Single-Phase Flow, Turbulent Flow Interfaces

---

DISPERSED PHASE BOUNDARY CONDITION

Select a **Dispersed phase boundary condition** — **No dispersed phase flux**, **Dispersed phase concentration**, **Dispersed phase outlet**, **Dispersed phase flux**, or **Symmetry**.

- For **Dispersed phase concentration** enter a **Dispersed phase volume fraction** ϕ_{d0} (dimensionless). The default is 0. When **Solve for interfacial area** is selected under the **Physical Model** section, click either the **Dispersed phase number density** n_0 (SI unit:

$1/m^3$) or **Diameter of particles/droplets** d_d (SI unit: m) button and enter a value or expression for n_0 (the default is $5 \times 10^6 \ 1/m^3$) or d_d (the default is 1 mm).

- For **Dispersed phase flux** enter values or expression for the **Dispersed phase flux** $N_{\phi d}$ (SI unit: m/s) and, if **Solve for interfacial area** is selected under the **Physical Model** section, the **Number density flux** N_n (SI unit: $1/(m^2 \cdot s)$). The defaults are 0 m/s and 0 $1/(m^2 \cdot s)$, respectively.

⍰	Dispersed Phase Boundary Conditions Equations

Mass Transfer

Use the **Mass Transfer** node to include mass transfer from the dispersed phase to the continuous phase.

MASS TRANSFER

Select a **Mass transfer model** — **User defined** (the default) or **Two-film theory**. For **User defined** enter a value or expression for the **Mass transfer from dispersed to continuous phase** m_{dc} (SI unit: $kg/(m^3 \cdot s)$). The default is 0 $kg/(m^3 \cdot s)$.

Two-film Theory

For **Two-film theory** enter values or expressions for each of the following:

- **Mass transfer coefficient** k (SI unit: m/s). The default is 0 m/s.
- **Species concentration in dispersed phase** c_d (SI unit: mol/m^3). The default is 0 mol/m^3.
- **Species concentration in continuous phase** c_c (SI unit: mol/m^3). The default is 0 mol/m^3.
- **Molecular weight of species** M (SI unit: kg/mol). The default is 0 kg/mol.

The mass transfer is modeled as

$$m_{dc} = k(c_d - c_c)Ma$$

where k denotes the mass transfer rate, and c_d and c_c are the species concentrations in the dispersed and the continuous phase, respectively. M is the species' molecular weight, and a is the interfacial area per unit volume between the two phases.

Interfacial Area

When the **Solve for interfacial area** check box is selected for either The Mixture Model, Laminar Flow Interface or The Turbulent Bubbly Flow Interface (under the **Physical Model** section), it is also possible to compute the interfacial area per unit volume. When **Solve for interfacial area** is selected, the following equation for the number density n of dispersed particles is added:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}_{\mathrm{d}}) = 0$$

This equation states that a dispersed phase particle cannot disappear, appear, or merge with other particles, although it can expand or shrink.

The Mixture Model interfaces calculate the interfacial area a (SI unit: $\mathrm{m}^2/\mathrm{m}^3$) from the following equation:

$$a = (4n\pi)^{1/3}(3\phi_{\mathrm{d}})^{2/3}$$

Gravity

The **Gravity** node adds the force $\rho\mathbf{g}$ to the right-hand side of the momentum transport equation.

GRAVITY

Enter the components of the **Gravity vector**, $\mathbf{g}$ (SI unit: $\mathrm{m/s}^2$). The default value is $(0, \texttt{-g\_const})$ where $\texttt{g\_const}$ is a physical constant equal to $9.8066 \ \mathrm{m/s}^2$.

Ω	For 2D components, gravity acts in the negative y direction by default. For example, in a 2D component, the y component is $\texttt{-g\_const}$ and the other component is 0. In this setting, $\texttt{g\_const}$ is a predefined physical constant for the standard gravity (acceleration due to gravity at sea level).

	For 3D and 2D axisymmetric components, gravity acts in the negative z direction by default. For example, in a 3D component, the z component is $\texttt{-g\_const}$ and the other components are 0. In this setting, $\texttt{g\_const}$ is a predefined physical constant for the standard gravity (acceleration due to gravity at sea level).

Inlet

The **Inlet** node adds a set of boundary conditions that describe inlets in fluid-flow simulations. Define the **Velocity** boundary condition (the default mixture boundary condition for inlet boundaries) or the **Pressure** condition.

MIXTURE BOUNDARY CONDITION

Select a **Mixture boundary condition** for the inlet — **Velocity** (the default) or **Pressure**.

VELOCITY

For **Velocity** click the **Normal inflow velocity** (the default) or **Velocity field** buttons.

- For **Normal inflow velocity** enter a value or expression for U_0 (SI unit: m/s).

- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{u}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{u} = \mathbf{u}_0$$

PRESSURE

This condition specifies the normal stress which in most cases is approximately equal to the pressure. Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.

- The **Suppress backflow** check box is selected by default. This option adjusts the inlet pressure, $\hat{p}_0 \ge p_0$, locally in order to prevent fluid from exiting the domain through the boundary. If suppress backflow is deselected, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.

- **Flow direction** controls in which direction the fluid enters the domain.

  - For **Normal flow** (the default) it prescribes zero tangential velocity component.

  - For **User defined** define an **Inflow velocity direction**, $\mathbf{d_u}$ (dimensionless). The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.

DISPERSED PHASE BOUNDARY CONDITION

The default is **Dispersed phase concentration**. See Wall > Dispersed Phase Boundary Condition for the settings.

See Dispersed Phase Boundary Conditions Equations for more information.

For The Mixture Model, Turbulent Flow Interface the following is also available.

Click the **Specify turbulent length scale and intensity** or **Specify turbulence variables** button.

- For **Specify turbulent length scale and intensity** enter a value for the **Turbulent intensity** I_T (dimensionless) and **Turbulence length scale** L_T (SI unit: m). When **Pressure** is selected, also enter a **Reference velocity scale** U_{ref} (SI unit: m/s).

- For **Specify turbulence variables** enter values or expressions for the **Turbulent kinetic energy** k_0 (SI unit: m^2/s^2) and **Turbulent dissipation rate** ε_0 (SI unit: m^2/s^3).

Outlet

The **Outlet** node adds a selection of boundary conditions that describe outlets in fluid-flow simulations; that is, the conditions at boundaries where the fluid exits the domain.

MIXTURE BOUNDARY CONDITION

Select a **Mixture boundary condition** for the outlet — **Pressure** (the default) or **Velocity**.

PRESSURE CONDITIONS

The **Pressure** condition specifies the normal stress which in most cases is approximately equal to the pressure. The tangential stress component is set to $0 \ N/m^2$.

- Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.

- Select the **Normal flow** check box to change the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.

The **Suppress backflow** check box is selected by default. This option adjusts the outlet pressure in order to prevent fluid from entering the domain through the boundary.

VELOCITY

For **Velocity** click the **Normal outflow velocity** (the default) or **Velocity field** buttons.

- For **Normal outflow velocity** enter a value or expression for U_0 (SI unit: m/s).

- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{u}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{u} = \mathbf{u}_0$$

The default is **Dispersed phase outlet**. See Wall > Dispersed Phase Boundary Condition for the settings.

When the **Dispersed phase boundary condition** is set to **Dispersed phase outlet**, the **Exterior dispersed phase condition(s)** section contains an input field for the **Dispersed phase volume fraction** on the downstream side of the outlet. If **Solve for interfacial area** is selected at the physics interface level, additional input fields appear for the **Dispersed phase number density** or the **Diameter of particles/droplets** on the downstream side of the outlet.

See Dispersed Phase Boundary Conditions Equations for more information.

Symmetry

The **Symmetry** node adds boundary conditions that describe symmetry boundaries in fluid-flow simulations. The boundary condition for symmetry boundaries prescribes no penetration and vanishing tangential stress:

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{t}^T(\rho c_{\mathrm{d}}(1 - c_{\mathrm{d}})\mathbf{u}_{\mathrm{slip}}\mathbf{u}_{\mathrm{slip}} + \tau_{\mathrm{Gm}})\mathbf{n} = 0$$

BOUNDARY SELECTION

A boundary condition for 2D axial symmetry is not required.

For the symmetry axis at $r = 0$, the program automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the z direction and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

The Euler-Euler Model Interfaces

In this section:

The Euler-Euler Model, Laminar Flow interface

The **Euler-Euler Model, Laminar Flow (ee)** interface (⬡), found under the **Multiphase Flow>Euler-Euler Model** branch (⬡) when adding a physics interface, can be used to simulate the flow of two continuous and fully interpenetrating incompressible phases (see Ref. 1 under the Theory for the Euler-Euler Model Interfaces). The physics interface can model flow at low and moderate Reynolds numbers. Typical applications are fluidized beds (solid particles in gas), sedimentation (solid particles in liquid), or transport of liquid droplets or bubbles in a liquid.

The physics interface solves two sets of Navier-Stokes equations, one for each phase, in order to calculate the velocity field for each phase. The phases interchange momentum as described by a drag model. The pressure is calculated from a mixture-averaged continuity equation and the volume fraction of the dispersed phase is tracked with a transport equation.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Phase Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Euler-Euler Model, Laminar Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is ee.

DISPERSED PHASE

Select a **Dispersed phase** — **Solid particles** or **Liquid droplets/bubbles**.

When **Solid particles** is selected, the Solid Pressure section is available in the Phase Properties node. Also see Dispersed Phase in the theory section.

PHYSICAL MODEL

The pressure solved for by the interface may represent the absolute pressure, or a relative pressure. The absolute pressure, used for example by the material properties, is defined by the interface as the sum of the **Reference pressure level** p_{ref} and the pressure solved for.

DEPENDENT VARIABLES

The dependent variables (field variables) are:

- **Velocity field, continuous phase uc**
- **Velocity field, dispersed phase ud**
- **Pressure** p
- **Volume fraction, dispersed phase** $phid$

The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION

To display this section, click the **Show** button (🔁) and select **Stabilization**.

INCONSISTENT STABILIZATION

To display this section, click the **Show** button (🔁) and select **Stabilization**.

Inconsistent stabilization can be activated independently for the momentum equation for the continuous phase, the momentum equation for the dispersed phase, and for the dispersed phase transport equation respectively by selecting the corresponding check box. Each inconsistent stabilization contribution has a tuning parameter.

ADVANCED SETTINGS

To display this section, click the **Show** button (🔁) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected,

also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** CFL_{loc} (dimensionless).

DISCRETIZATION

To display this section, click the **Show** button ( ) and select **Discretization**.

The Euler-Euler Model, Laminar Flow interface supports three options for the basis functions: **P1+P1** (the default option), **P2+P1**, and **P3+P2**. They all represent Lagrangian basis functions of different orders:

- **P1+P1** – Linear basis functions for all degrees of freedom. Linear basis functions are computationally less expensive than the higher-order options and are also more robust. This option requires that **Streamline diffusion** is activated for both of the momentum equations.

- **P2+P1** – Quadratic basis functions for all degrees of freedom except the pressure which is described by linear basis functions. Higher order elements, as compared to linear elements, are a computationally effective way to obtain high accuracy but only if the flow is well resolved. This requirement is most likely fulfilled for flows with very low velocities and/or small length scales.

- **P3+P2** – Cubic basis functions for all degrees of freedom except the pressure which is described by quadratic basis functions. This option is computationally very expensive and the least robust one but it is also the option with the highest formal accuracy.

Specify the **Value type when using splitting of complex variables** — **Real** (the default) or **Complex**.

MIXING LENGTH LIMIT

This section is available for The Euler-Euler Model, Turbulent Flow Interface.

When the **Mixing length limit** $l_{\text{mix,lim}}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases,

it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression.

Q
- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Isotropic Diffusion in the *COMSOL Multiphysics Reference Manual*
- Domain, Boundary, Point, and Pair Nodes for the Euler-Euler Model Interfaces
- Theory for the Euler-Euler Model Interfaces

▥
Circulating Fluidized Bed: path
CFD_Module/Multiphase_Tutorials/fluidized_bed

The Euler-Euler Model, Turbulent Flow Interface

The **Euler-Euler Model, Turbulent Flow (ee)** interface ( ), found under the **Multiphase Flow>Euler-Euler Model** branch ( ) when adding a physics interface, can be used to simulate high Reynolds number flow of a two-phase mixture containing a continuous and a dispersed phase. The Euler-Euler model assumes that both phases are continuous, fully interpenetrating, and incompressible (see Theory for the Euler-Euler Model Interfaces). Typical applications for the interface are fluidized beds (solid particles in gas), sedimentation (solid particles in liquid), or transport of liquid droplets or bubbles in a liquid.

The physics interface solves two sets of Navier-Stokes equations, one for each phase, in order to calculate the velocity field for each phase. The phases interchange momentum as described by a drag model. The pressure is calculated from a mixture-averaged continuity equation and the volume fraction of the dispersed phase is tracked with a transport equation.

Two-phase turbulence is modeled using the standard two-equation k-ε model with realizability constraints. The interface includes the possibility to solve one set of k-ε equations for the two-phase mixture, or to solve two sets of k-ε equations, one for each phase. Flow close to walls is modeled using wall functions.

Except where indicated below, the settings for this physics interface are the same as for The Euler-Euler Model, Laminar Flow interface.

PHYSICAL MODEL

Turbulence Model Type
The default **Turbulence model type** is **RANS, k-ε**.

Two-phase turbulence
By default the **Two-Phase Turbulence** is defined as **Mixture**. This implies that one set of k-ε equations are solved for. To instead solve for two sets of k-ε equations, one for each fluid phase, select **Phase specific** (see Turbulent Two-Phase Flow Modeling).

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Turbulent Two-Phase Flow Modeling.

DEPENDENT VARIABLES

The following dependent variables (field variables) are defined for this interface:

- **Velocity field, continuous phase uc**
- **Velocity field, dispersed phase ud**
- **Pressure** p
- **Turbulent kinetic energy, mixture** k
- **Turbulent dissipation rate, mixture** ep

- **Turbulent kinetic energy, continuous phase** kc
- **Turbulent dissipation rate, continuous phase** epc
- **Turbulent kinetic energy, dispersed phase** kd
- **Turbulent dissipation rate, dispersed phase** epd

The names can be changed but the names of fields and dependent variables must be unique within a component.

Domain, Boundary, Point, and Pair Nodes for the Euler-Euler Model Interfaces

The Euler-Euler Model Interfaces has the following domain, boundary, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- Gravity
- Initial Values
- Inlet

- Outlet
- Phase Properties
- Volume Force
- Wall

The following nodes are described for the Laminar Flow interface:

- Pressure Point Constraint
- Symmetry

> **!**
>
> In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Phase Properties

The **Phase Properties** node has the material properties settings for the pure continuous and dispersed phases. It also has settings for the viscosity models for each of the two interpenetrating phases and the drag model. When the dispersed phase consists of solid particles, it also has settings for the solid pressure model.

MATERIALS

Select the materials to use for the material properties of the continuous phase and the dispersed phase respectively (when they are defined to take their values **From material**). By default, both the **Continuous phase** and **Dispersed phase** use the **Domain material**. This corresponds to the material currently applied to the domain in question.

Other materials present can be selected from the **Continuous phase** or **Dispersed phase** list in order to use that material's properties for the liquid or gas, respectively.

CONTINUOUS PHASE PROPERTIES

Density, Continuous Phase

The default **Density, continuous phase** ρ_c (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression.

Dynamic Viscosity, Pure Continuous Phase

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. The dynamic viscosity of the pure continuous phase refers to the viscosity the fluid would have in the absence of the dispersed phase.

The default **Dynamic viscosity, pure continuous phase** μ_c (SI unit: Pa·s) uses values **From material**. The value of the viscosity is then the value defined for the material selected in the **Materials** section for the continuous phase. For **User defined** define a different value or expression.

DISPERSED PHASE PROPERTIES

The default **Density, dispersed phase** ρ_d (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression.

Enter a value or expression for the **Diameter of particles/droplets** d_d (SI unit: m). The default is 10^{-3} m (1 mm).

The **Dynamic viscosity, pure dispersed phase** μ_d (SI unit: Pa·s) field is available when **Liquid droplets/bubbles** is selected as the **Dispersed phase** in The Euler-Euler Model Interfaces.

The default uses values **From material**. The value of the viscosity is then the value defined for the material selected in the **Materials** section for the dispersed phase. For **User defined** define a different value or expression.

VISCOSITY MODEL

Select a **Viscosity model—Calculate from mixture velocity** (the default) or **User defined**.

• For **Calculate from mixture viscosity** select a **Mixture viscosity model—Krieger type** (the default) or **User defined**. For **Krieger type**, enter an expression or value for the **Maximum packing concentration** ϕ_{max} (dimensionless). The default is 0.62 when the dispersed

phase is solid particles and 1 when the dispersed phase is liquid droplets/bubbles. For **User defined**, enter a value or expression for the **Dynamic viscosity** μ.

- For **User defined** enter a value or expression for the **Dynamic viscosity, dispersed phase** μ_d. The default expression, muinit, corresponds to the Krieger type viscosity.

DRAG MODEL

The models for the interphase drag force $\mathbf{F}_\mathrm{drag}$ are available and described in The Euler-Euler Model Equations. When the dispersed phase corresponds to **Solid particles**, the **Gidaspow**, **Schiller-Naumann**, **Haider-Levenspiel**, and **Hadamard-Rybczynzki** models are available. For **Liquid droplets/bubbles**, the **Schiller-Naumann**, **Haider-Levenspiel** and **Hadamard-Rybczynzki** models are available.

Select a **Drag model**—**Gidaspow**, **Schiller-Naumann**, **Haider-Levenspiel**, **Hadamard-Rybczynzki**, or **User defined**. For **User defined** enter a value or expression for the **Drag force coefficient** β. For **Haider-Levenspiel** enter a value between 0 and 1 for the **Sphericity** S_p (dimensionless).

SOLID PRESSURE MODEL

The solid pressure models the particle dispersion due to collisions and friction between the solid particles. Details of the implemented models are described in Solid Pressure.

This section is available when **Solid particles** is selected as the **Dispersed phase** in The Euler-Euler Model Interfaces. Select a **Solid pressure model** ∇p_s—**No solid pressure** (the default), **Gidaspow-Ettehadieh**, **Gidaspow**, **Ettehadieh**, or **User defined**. For **User defined** enter values or expressions in the table for each component.

Initial Values

The **Initial Values** node adds initial values for the velocity fields for the continuous and dispersed phases, the pressure, and the volume fraction of the dispersed phase that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions in the tables for each component of:

- **Velocity field, continuous phase uc**
- **Velocity field, dispersed phase ud**

Enter initial values or expressions for:

- **Pressure** p

- **Volume fraction, dispersed phase** $phid$

For the The Euler-Euler Model, Turbulent Flow Interface, initial values are needed for the turbulence variables. When **Mixture** is selected as **Two-phase turbulence**, enter values or expressions for:

- **Turbulent kinetic energy, mixture** k

- **Turbulent dissipation rate, mixture** ep

When **Phase specific** is selected as **Two-phase turbulence**, enter values or expressions for:

- **Turbulent kinetic energy, continuous phase** kc

- **Turbulent dissipation rate, continuous phase** epc

- **Turbulent kinetic energy, dispersed phase** kd

- **Turbulent dissipation rate, dispersed phase** epd

Wall

The **Wall** node includes a set of boundary conditions to describe the flow conditions at a wall. The conditions for each phase are selected separately.

CONTINUOUS PHASE BOUNDARY CONDITION

Select a **Continuous Phase Condition** — **No slip** (laminar flow only), **Slip**, or **Wall functions** (turbulent flow only).

Slip
Slip prescribes the velocity component normal to the wall to zero $\mathbf{u} \cdot \mathbf{n} = 0$.

No Slip
No slip prescribes $\mathbf{u} = 0$, that is, the fluid at the wall is at rest. This is the default boundary condition for The Mixture Model, Laminar Flow Interface.

Wall Functions
Wall functions are used in the case of turbulent flow to model the thin region near solid (no slip) walls with high gradients in the flow variables. It is the default boundary condition for The Mixture Model, Turbulent Flow Interface.

Select a **Dispersed Phase Boundary Condition** — **No slip** (laminar flow only), **Slip**, or **Wall functions** (turbulent flow only). The conditions prescribed correspond to those described for the continuous phase above.

Dispersed Phase Boundary Condition

The **Dispersed Phase Boundary Condition** defines the condition at the wall for the volume fraction of the dispersed phase.

No dispersed phase flux prescribes a zero flux condition at the wall.

Dispersed phase concentration prescribes the dispersed phase volume fraction at the wall ϕ_{d0} (dimensionless).

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

Inlet

The **Inlet** node prescribes the flow and turbulence conditions (when applicable) at a boundary where one or both phases enter the adjacent domain.

TWO-PHASE INLET TYPE

Selecting **Mixture** as the **Two-Phase Inlet Type**, inlet conditions are prescribed for both phases. Selecting **Continuous phase** or **Dispersed phase,** inlet conditions are prescribed for the corresponding phase, while wall conditions are applied to the remaining phase.

CONTINUOUS PHASE

The options available in this section are based on the **Two-phase inlet type** selected.

When **Mixture** or **Continuous phase** is selected as the **Two-phase inlet typ** the **Velocity field, continuous phase** $\mathbf{u}_{c0}$ is prescribed.

When **Dispersed phase** is selected as the **Two-phase inlet type**, the conditions applied to the continuous phase are **No slip** ($\mathbf{u}_c = \mathbf{0}$) or **Slip** ($\mathbf{u}_c \cdot \mathbf{n} = 0$, and no viscous stresses in the tangential directions).

Using the Phase specific option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the continuous phase turbulence variables.

- **Specify turbulent length scale and intensity** defines the turbulence inlet conditions using the **Turbulent intensity** $I_{T,c}$ (dimensionless) and the **Turbulence length scale** $L_{T,c}$ (SI unit: m).

- **Specify turbulence variables** prescribes the **Turbulent kinetic energy** $k_{0,c}$ (SI unit: m^2/s^2) and the **Turbulent dissipation rate** $\varepsilon_{0,c}$ (SI unit: m^2/s^3) at the inlet.

DISPERSED PHASE

The options available in this section are based on the **Two-phase inlet type** selected.

When **Mixture** or **Dispersed phase** is selected as the **Two-phase inlet type**, the **Velocity field, dispersed phase** $\mathbf{u}_{d0}$ and the **Dispersed phase volume fraction**, ϕ_{d0}, at the inlet are defined.

When **Continuous phase** is selected as the **Two-phase inlet type**, the conditions applied to the dispersed phase are **No slip** ($\mathbf{u}_d = \mathbf{0}$) or **Slip** ($\mathbf{u}_d \cdot \mathbf{n} = 0$, and no viscous stresses in the tangential directions).

Using the Phase specific option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the dispersed phase turbulence variables.

- **Specify turbulent length scale and intensity** defines the turbulence inlet conditions using the **Turbulent intensity** $I_{T,d}$ (dimensionless) and the **Turbulence length scale** $L_{T,d}$ (SI unit: m).

- **Specify turbulence variables** prescribes the **Turbulent kinetic energy** $k_{0,d}$ (SI unit: m^2/s^2) and the **Turbulent dissipation rate** $\varepsilon_{0,d}$ (SI unit: m^2/s^3) at the inlet.

TURBULENCE CONDITIONS

Using the Mixture option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the mixture turbulence variables.

- **Specify turbulent length scale and intensity** defines the turbulence inlet conditions using the **Turbulent intensity** I_T (dimensionless) and the **Turbulence length scale** L_T (SI unit: m).

- **Specify turbulence variables** prescribes the **Turbulent kinetic energy** k_0 (SI unit: m^2/s^2) and the **Turbulent dissipation rate** ε_0 (SI unit: m^2/s^3) at the inlet.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**.

Outlet

This node is used to prescribe conditions at boundaries where the two-phase mixture exits the computational domain. The settings available in the node specifies conditions for the entire mixture, as opposed to the Inlet, Outlet and Wall nodes where the conditions for can be specified for each phase individually.

MIXTURE BOUNDARY CONDITION

Select **Mixture boundary conditions** — **Pressure, no viscous stress**, **Pressure**, **normal flow**, **Velocity**, **Degassing**, or **Filtration**.

Pressure Conditions

When **Pressure, no viscous stress** or **Pressure, normal flow** is selected as the **Mixture boundary condition**, specify the **Pressure** p_0 (SI unit: Pa) at the outlet. Note that the prescribed pressure should be consistent with the reference pressure level specified at the interface level as well as consistent with present volume forces (including gravity).

Velocity

Select **Velocity** to specify the **Velocity field, continuous phase** $\mathbf{u}_{c0}$ (SI unit: m/s) together with the **Velocity field, dispersed phase** $\mathbf{u}_d$ (SI unit: m/s) at the outlet.

Degassing and Filtration

Selecting **Degassing** allows the dispersed phase to exit the domain but prevents the continuous phase from exiting. This is achieved through a pressure (p_0), no viscous stress condition for the dispersed phase, in combination with a no penetration condition for the continuous phase.

Selecting **Filtration** on the other hand allows the continuous phase to exit the domain but prevents the continuous phase from exiting. This is achieved through a pressure (p_0), no viscous stress condition for the continuous phase, in combination with a no penetration condition for the dispersed phase.

📝	**Pressure, no viscous stress** is the least constraining option and allows the flow to exit the domain in non-normal directions.
	Pressure, normal flow restricts the flow to be completely normal to the outlet boundary. This option can influence the flow quite a bit upstream of the inlet.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**.

Gravity

The **Gravity** node adds the gravity force vector to the right-hand side of the momentum equations; $\rho_c \mathbf{g}$ for the continuous phase and $\rho_d \mathbf{g}$ for the dispersed phase.

Gravity nodes are mutually exclusive, that is, there can only be one active Gravity node per domain.

GRAVITY

Enter the components of the **Gravity vector**, $\mathbf{g}$ (SI unit: m/s^2). For 2D components the default Gravity vector is defined as (0,-g_const). Here g_const is a physical constant equal to 9.8066 m/s^2. For 3D and 2D axisymmetric components, the gravity acts in the negative z direction by default.

Volume Force

The **Volume Force** node specifies the volume forces on the right-hand side of the momentum equations; $\mathbf{F}_c$ for the continuous phase and $\mathbf{F}_d$ for the dispersed phase. It may for example be used to add user defined interaction forces (a part from the interphase drag force).

If several volume force nodes are added to the same domain, the sum of all contributions are added to the respective momentum equations.

Theory for the Two-Phase Flow Interfaces

The Two-Phase Flow, Level Set and Phase Field interfaces can be used to model the flow of two different, immiscible fluids, where the exact position of the interface between the two fluids is of interest. The fluid-fluid interface is tracked using an auxiliary function on a fixed mesh. These methods account for differences in the two fluids' densities and viscosities and include the effects of surface tension and gravity.

The Two-Phase Flow, Level Set and Phase Field Interfaces theory is described in this section:

- Level Set and Phase Field Equations
- Conservative and Nonconservative Formulations
- Phase Initialization
- Numerical Stabilization
- References for the Level Set and Phase Field Interfaces

Level Set and Phase Field Equations

By default, the Level Set and Phase Field interfaces use the incompressible formulation of the Navier-Stokes equations:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \mathbf{F}_g + \mathbf{F}_{st} + \mathbf{F}_{ext} + \mathbf{F} \qquad (5\text{-}7)$$

$$\nabla \cdot \mathbf{u} = 0 \qquad (5\text{-}8)$$

Note that Equation 5-7, and Equation 5-8 are solved in the contained interface, **Laminar Flow** or **Turbulent Flow** interface. Note that if the Laminar Flow and Turbulent Flow are added automatically when we add a Two-Phase Flow, Level Set and Phase Field multiphysics interface, these interfaces contain a **Multiphysics coupling option** property to control the form of the continuity equation. The **Multiphysics coupling option** is automatically set to **Level Set** or **Phase Field**. In this case, the continuity equation takes the form as in Equation 5-8. When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow InterfacesTheory for the single-phase flow.

USING THE LEVEL SET METHOD

If the level set method is used to track the interface, it adds the following equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{5-9}$$

where γ is the reinitialization parameter (set to 1 by default), and ε is the interface thickness controlling parameter (set to $h_{max}/2$ where h_{max} is the maximum element size in the component). The density is a function of the level set function defined as

$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$

and the dynamic viscosity is given by

$$\mu = \mu_1 + (\mu_2 - \mu_1)\phi$$

where ρ_1 and ρ_2 are the constant densities of Fluid 1 and Fluid 2, respectively, and μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively. Here, Fluid 1 corresponds to the domain where $\phi < 0.5$, and Fluid 2 corresponds to the domain where $\phi > 0.5$.

Further details of the theory for the level set method are in Ref. 1.

USING THE PHASE FIELD METHOD

If the phase field method is used to track the interface, it adds the following equations:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \frac{\gamma \lambda}{\varepsilon^2} \nabla \psi \tag{5-10}$$

$$\psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda} \right) \frac{\partial f_{ext}}{\partial \phi} \tag{5-11}$$

where the quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3} \frac{\lambda}{\varepsilon}$$

and γ is related to ε through $\gamma = \chi \varepsilon^2$ where χ is the mobility tuning parameter (set to 1 by default). The volume fraction of Fluid 2 is computed as

$$V_f = \min(\max([(1+\phi)/2], 0), 1)$$

where the `min` and `max` operators are used so that the volume fraction has a lower limit of 0 and an upper limit of 1. The density is then defined as

$$\rho = \rho_1 + (\rho_2 - \rho_1)V_f$$

and the dynamic viscosity according to

$$\mu = \mu_1 + (\mu_2 - \mu_1)V_f$$

where ρ_1 and ρ_2 are the densities and μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively.

The mean curvature (SI unit: $1/m$) can be computed by entering the following expression:

$$\kappa = 2(1 + \phi)(1 - \phi)\frac{G}{\sigma}$$

where G is the chemical potential defined as:

$$G = \lambda\left(-\nabla^2\phi + \frac{\phi(\phi^2 - 1)}{\varepsilon^2}\right) + \frac{\partial f}{\partial \phi}$$

Details of the theory for the phase field method are in Ref. 2.

FORCE TERMS

The four forces on the right-hand side of Equation 5-7 are due to gravity, surface tension, a force due to an external contribution to the free energy (using the phase field method only), and a user-defined volume force.

The Surface Tension Force for the Level Set Method

For the level set method, the surface tension force acting on the interface between the two fluids is $\mathbf{F}_{st} = \sigma\kappa\delta\mathbf{n}$ where σ is the surface tensions coefficient (SI unit: N/m), κ is the curvature, and $\mathbf{n}$ is the unit normal to the interface. δ (SI unit: $1/m$) is a Dirac delta function located at the interface. κ depends on second derivatives of the level set function ϕ. This can lead to poor accuracy of the surface tension force. Therefore, the following alternative formulation is used:

$$\mathbf{F}_{st} = \nabla \cdot (\sigma(\mathbf{I} - (\mathbf{nn}^T))\delta)$$

For a derivation of this formulation, see Appendix A in Ref. 3. In the weak formulation of the momentum equation, it is possible to move the divergence operator, using integration by parts, to the test functions for the velocity components.

The δ-function is approximated by a smooth function according to

$$\delta = 6|\nabla\phi||\phi(1-\phi)|$$

The Surface Tension Force for the Phase Field Method

The surface tension force for the phase field method is implemented as a body force

$$F_{st} = \left(G - \frac{\partial f}{\partial\phi}\right)\nabla\phi$$

where G is the chemical potential (SI unit: J/m^3) defined in The Equations for the Phase Field Method and $\partial f/\partial\phi$ is a user-defined source of free energy.

The Gravity Force

The gravity force is $\mathbf{F}_g = \rho\mathbf{g}$ where $\mathbf{g}$ is the gravity vector. Add this as a Gravity feature to the fluid domain.

The User Defined Volume Force

When using a Phase Field interface, a force arising due to a user-defined source of free energy is computed according to:

$$\mathbf{F}_{ext} = \left(\frac{\partial f}{\partial\phi}\right)\nabla\phi$$

This force is added when a ϕ-derivative of the external free energy has been defined in the External Free Energy section of the Fluid Properties feature.

Conservative and Nonconservative Formulations

When the velocity field is divergence free, you can use either the conservative or the nonconservative formulation of the level set or phase field equation. The conservative form perfectly conserves the mass of each fluid, but the computational time is generally longer.

Phase Initialization

If the study type Transient with Phase Initialization is used in the model, the level set or phase field variable is automatically initialized. For this study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface >, D_{wi}. The Time Dependent step then uses the initial condition for the level set function according to the following expression:

$$\phi_0 = \frac{1}{1 + e^{D_{wi}/\varepsilon}}$$

in domains initially filled with Fluid 1 and

$$\phi_0 = \frac{1}{1 + e^{-D_{wi}/\varepsilon}}$$

in domains initially filled with Fluid 2.

Correspondingly, for the phase field method the following expressions are used:

$$\phi_0 = -\tanh\left(\frac{D_{wi}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{wi}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 2. The initial condition for the help variable is $\psi_0 = 0$. These expressions are based on the analytical solution of the steady state solution of Equation 5-9, Equation 5-10, and Equation 5-11 for a straight, non-moving interface.

!	For the initialization to work it is crucial that there are two **Initial Values** nodes and one **Initial Interface** node. One of the Initial Values nodes should use **Domain Initially: Fluid 1(ϕ =0)** and the other **Fluid initially in domain: Fluid 2(ϕ =0)**. The **Initial Interface** node is not default but can be added which should have all interior boundaries where the interface is initially present as selection. If the selection of the **Initial Interface** node is empty, the initialization fails. Note that the default value of **Domain Initially** is **Specified level set function explicitly** allowing arbitrary user defined initial value. In this case, no **Initial Interface** node should be added, and Time-dependent study should be used instead of Transient with Phase Initialization.

?	• The Two-Phase Flow, Level Set and Phase Field Interfaces • Studies and Solvers and Transient with Phase Initialization in the *COMSOL Multiphysics Reference Manual*

Numerical Stabilization

Four types of stabilization methods are available for the flow (Navier-Stokes), turbulence, and interface (level set or phase field) equations. Two are consistent stabilization methods — Streamline diffusion and Crosswind diffusion — and two are inconsistent — Isotropic diffusion and Anisotropic diffusion.

To display this section, click the **Show** button ( ) and select **Stabilization**.

> - The Two-Phase Flow, Level Set and Phase Field Interfaces
> - Stabilization in the *COMSOL Multiphysics Reference Manual*

References for the Level Set and Phase Field Interfaces

1. E. Olsson and G. Kreiss, "A Conservative Level Set Method for Two Phase Flow", *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

2. P. Yue, J.J. Feng, C. Liu, and J. Shen, "A Diffuse-interface Method for Simulating Two-phase Flows of Complex Fluids", *J. Fluid Mech.*, vol. 515, pp. 293–317, 2004.

3. B. Lafaurie, C. Nardone, R. Scardovelli, S. Zaleski, and G. Zanetti "Modelling Merging and Fragmentation in Multiphase Flows with SURFER.", *J. Comput. Phys.*, vol. 113, no. 1, pp. 134–147, 1994.

Theory for the Three-Phase Flow Interface

The Three-Phase Flow, Phase Field interface can be used to model the flow and interaction of three different, immiscible fluids, when the exact positions of the interfaces separating the fluids are of interest. The fluid-fluid interfaces are tracked using a ternary phase field formulation which account for differences in the fluids' densities and viscosities and include the effects of surface tension.

The Three-Phase Flow, Phase Field Interface theory is described in the following sections:

• Governing Equations of the Three-Phase Flow, Phase Field Interface
• Reference for the Three-Phase Flow, Phase Field Interface

Governing Equations of the Three-Phase Flow, Phase Field Interface

LAMINAR FLOW EQUATIONS

The Three-Phase Flow, Phase Field interface is used to study the evolution of three immiscible fluid phases denoted by fluid A, fluid B, and fluid C. The interface solves the Navier-Stokes equations governing conservation of momentum and mass. The momentum equations solved correspond to

$$\rho\frac{\partial\mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u}+\nabla\mathbf{u}^{T}) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] + \mathbf{F}_{\mathrm{st}} + \mathbf{F} \qquad (5\text{-}12)$$

where $\mathbf{F}_{\mathrm{st}}$ is the surface tension force. The physics interface assumes that the density of each phase is constant. The density may however vary between the phases. In order to accurately handle systems where density of the phases are significantly different, as well as systems with phases of similar density, the following fully compressible continuity equation is solved by the interface

$$\frac{\partial\log\rho}{\partial t} + \nabla\cdot\mathbf{u} + \mathbf{u}\cdot\nabla\log\rho = 0 \qquad (5\text{-}13)$$

TERNARY PHASE FIELD EQUATIONS

In order to track the interfaces between three immiscible fluids, a ternary phase field model based on the work of Boyer and co-workers in Ref. 1 is used. The model solves the following Cahn-Hilliard equations

$$\frac{\partial \phi_i}{\partial t} + \nabla \cdot (\mathbf{u}\phi_i) = \nabla \cdot \left(\frac{M_0}{\Sigma_i}\nabla\eta_i\right)$$

$$\eta_i = \frac{4\Sigma_T}{\varepsilon}\sum_{j \neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial \phi_i} - \frac{\partial F}{\partial \phi_j}\right)\right) - \frac{3}{4}\varepsilon\Sigma_j\nabla^2\phi_i$$

(5-14)

governing the phase field variable, ϕ_i, and a generalized chemical potential, η_i, of each phase $i = A, B, C$. The phase field variables vary between 0 and 1 and are a measure of the concentration of each phase. The phase field variable for phase A is one in instances containing only this phase, and zero where there is no phase A. Since the fluids are immiscible, variations in the phase field variable occur, and define the interface separating two phases. At each point the phase field variables satisfy the following constraint

$$\sum_{i = A, B, C} \phi_i = 1$$

(5-15)

The density of each phase is assumed to be constant which implies that the phase field variable corresponds to the volume fraction of the phase in question. In order to satisfy Equation 5-15, two sets of the equations shown in Equation 5-14 are solved, namely those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 5-15.

The density and viscosity of the fluid mixture used in Equation 5-7 and 5-8 are defined as:

$$\rho = \rho_A\phi_A + \rho_B\phi_B + \rho_C\phi_C$$

$$\mu = \mu_A\phi_A + \mu_B\phi_B + \mu_C\phi_C$$

(5-16)

Free energy

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$F = \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 +$$

$$\phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2$$

(5-17)

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase i and j, and the capillary parameters Σ_i are defined for each phase in the manner of:

$$\Sigma_A = \sigma_{AB} + \sigma_{AC} - \sigma_{BC}$$
$$\Sigma_B = \sigma_{AB} + \sigma_{BC} - \sigma_{AC} \qquad (5\text{-}18)$$
$$\Sigma_C = \sigma_{BC} + \sigma_{AC} - \sigma_{AB}$$

Λ in the free energy is a function or parameter specifying the additional free bulk energy of the system. By default Λ is zero. In this case it can be seen that the free energy in Equation 5-17 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

Ternary Phase Field parameters
In Equation 5-14, ε (SI unit: $1/\mathrm{m}$) is a parameter controlling the interface thickness, M_0 (SI unit: m^3/s) is a molecular mobility parameter, and the parameter Σ_T is defined as

$$\frac{3}{\Sigma_T} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \qquad (5\text{-}19)$$

When using the interface it is recommended that the parameter ε is given a value in the same order as the elements in the regions passed by the fluid-fluid interfaces. The mobility determines the time scale of the Cahn-Hilliard diffusion and must be large enough to retain a constant interfacial thickness, but small enough to avoid damping the convective transport. In order to ensure that the mobility is in the correct range, it is recommended to a apply a mobility parameter such that the following holds approximately

$$M_0 = L_c U_c \varepsilon \cdot 10^{-2} \qquad (5\text{-}20)$$

where L_c and U_c are the characteristic length and velocity scales of the system at hand.

SURFACE TENSION
The surface tension force applied in the momentum equations (Equation 5-7) as a body force computed from the generalized chemical potentials:

$$\mathbf{F}_{st} = \sum_{i = A, B, C} \eta_i \nabla \phi_i \qquad (5\text{-}21)$$

Reference for the Three-Phase Flow, Phase Field Interface

1. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar and M. Quintard, "Cahn-hilliard/Navier-Stokes model for the simulation of three-phase flows", *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

Theory for the Bubbly Flow Interfaces

The Bubbly Flow interfaces are suitable for macroscopic modeling of mixtures of liquids and gas bubbles. These physics interfaces solve for the averaged volume fraction occupied by each of the two phases, rather than tracking each bubble in detail. Each phase has its own velocity field.

In this section:

- The Bubbly Flow Equations
- Turbulence Modeling in Bubbly Flow Applications
- References for the Bubbly Flow Interfaces

The Bubbly Flow Equations

The two-fluid Euler-Euler Model is a general, macroscopic model for two-phase fluid flow. It treats the two phases as interpenetrating media, tracking the averaged concentration of the phases. One velocity field is associated with each phase. A momentum balance equation and a continuity equation describe the dynamics of each of the phases. The *bubbly flow* model is a simplification of the two-fluid model, relying on the following assumptions:

- The gas density is negligible compared to the liquid density.
- The motion of the gas bubbles relative to the liquid is determined by a balance between viscous drag and pressure forces.
- The two phases share the same pressure field.

Based on these assumptions, the momentum and continuity equations for the two phases can be combined and a gas phase transport equation is kept in order to track the volume fraction of the bubbles. The momentum equation is

$$
\begin{aligned}
\phi_1 \rho_1 \frac{\partial \mathbf{u}_1}{\partial t} &+ \phi_1 \rho_1 \mathbf{u}_1 \cdot \nabla \mathbf{u}_1 = \\
&= -\nabla p + \nabla \cdot \left[\phi_1 (\mu_1 + \mu_T) \left(\nabla \mathbf{u}_1 + \nabla \mathbf{u}_1{}^T - \frac{2}{3} (\nabla \cdot \mathbf{u}_1) \mathbf{I} \right) \right] + \phi_1 \rho_1 \mathbf{g} + \mathbf{F}
\end{aligned}
\tag{5-22}
$$

In Equation 5-22, the variables are as follows:

- $\mathbf{u}_l$ is the velocity vector (SI unit: m/s)
- p is the pressure (SI unit: Pa)
- ϕ is the phase volume fraction (SI unit: m^3/m^3)
- ρ is the density (SI unit: kg/m^3)
- $\mathbf{g}$ is the gravity vector (SI unit: m/s^2)
- $\mathbf{F}$ is any additional volume force (SI unit: N/m^3)
- μ_l is the dynamic viscosity of the liquid (SI unit: Pa·s), and
- μ_T is the turbulent viscosity (SI unit: Pa·s)

The subscripts "l" and "g" denote quantities related to the liquid phase and the gas phase, respectively.

The continuity equation is

$$\frac{\partial}{\partial t}(\rho_l\phi_l + \rho_g\phi_g) + \nabla \cdot (\rho_l\phi_l\mathbf{u}_l + \rho_g\phi_g\mathbf{u}_g) = 0 \tag{5-23}$$

and the gas phase transport equation is

$$\frac{\partial \rho_g\phi_g}{\partial t} + \nabla \cdot (\phi_g\rho_g\mathbf{u}_g) = -m_{gl} \tag{5-24}$$

where m_{gl} is the mass transfer rate from the gas to the liquid (SI unit: $kg/(m^3 \cdot s)$).

For low gas volume fractions ($\phi_g \sim 0.01$), you can replace the momentum equations, Equation 5-22, and the continuity equation, Equation 5-23, by

$$\phi_l\rho_l\frac{\partial \mathbf{u}_l}{\partial t} + \phi_l\rho_l\mathbf{u}_l \cdot \nabla \mathbf{u}_l =$$
$$= -\nabla p + \nabla \cdot [\phi_l(\mu_l + \mu_T)(\nabla \mathbf{u}_l + \nabla \mathbf{u}_l^T)] + \phi_l\rho_l\mathbf{g} + \mathbf{F} \tag{5-25}$$

$$\rho_l\nabla \cdot \mathbf{u}_l = 0 \tag{5-26}$$

By default, the Laminar Bubbly Flow interface uses Equation 5-25 and 5-26. To switch to Equation 5-22 and 5-23, click to clear the **Low gas concentration** check box under the **Physical Model** section.

The physics interface solves for $\mathbf{u}_l, p$, and

$$\tilde{\rho}_g = \rho_g \phi_g$$

the effective gas density. The gas velocity $\mathbf{u}_g$ is the sum of the following velocities:

$$\mathbf{u}_g = \mathbf{u}_l + \mathbf{u}_{slip} + \mathbf{u}_{drift} \tag{5-27}$$

where $\mathbf{u}_{slip}$ is the relative velocity between the phases and $\mathbf{u}_{drift}$ is a drift velocity (see Turbulence Modeling in Bubbly Flow Applications). The physics interface calculates the gas density from the ideal gas law:

$$\rho_g = \frac{(p + p_{ref})M}{RT}$$

where M is the molecular weight of the gas (SI unit: kg/mol), R is the ideal gas constant (8.314472 J/(mol·K)), p_{ref} a reference pressure (SI unit: Pa), and T is temperature (SI unit: K). p_{ref} is a scalar variable, which by default is 1 atm (1 atmosphere or 101,325 Pa). The liquid volume fraction is calculated from

$$\phi_l = 1 - \phi_g$$

When there is a drift velocity, it has the form

$$\mathbf{u}_{drift} = -\frac{\tilde{\mu}}{\rho_l} \frac{\nabla \phi_g}{\phi_g} \tag{5-28}$$

Where $\tilde{\mu}$ is an effective viscosity causing the drift. Inserting Equation 5-28 and Equation 5-27 into Equation 5-24 gives

$$\frac{\partial \rho_g \phi_g}{\partial t} + \nabla \cdot (\phi_g \rho_g (\mathbf{u}_l + \mathbf{u}_{slip})) = \nabla \cdot \left(\frac{\tilde{\mu} \rho_g}{\rho_l} \nabla \phi_g \right) - m_{gl}$$

That is, the drift velocity introduces a diffusive term in the gas transport equation. This is how the equation for the transport of the volume fraction of gas is actually implemented in the physics interface.

The bubbly-flow equation formulation is relatively simple, but it can display some nonphysical behavior. One is artificial accumulation of bubbles, for example, beneath walls where the pressure gradient forces the bubbles upward, but the bubbles have no place to go and there is no term in the model to prevent the volume fraction of gas from growing. To prevent this from happening, $\tilde{\mu}$ is set to μ_l in the laminar case. The only apparent effect of this in most cases where the bubbly-flow equations are applicable is that nonphysical

accumulation of bubbles is reduced. The small effective viscosity in the transport equation for ϕ_g has beneficial effects on the numerical properties of the equation system.

MASS TRANSFER AND INTERFACIAL AREA

It is possible to account for mass transfer between the two phases by specifying an expression for the mass transfer rate from the gas to the liquid m_{gl} (SI unit: kg/(m^3·s)).

The mass transfer rate typically depends on the interfacial area between the two phases. An example is when gas dissolves into a liquid. In order to determine the interfacial area, it is necessary to solve for the bubble number density (that is, the number of bubbles per volume) in addition to the phase volume fraction. The Bubbly Flow interface assumes that the gas bubbles can expand or shrink but not completely vanish, merge, or split. The conservation of the number density n (SI unit: $1/m^3$) then gives

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}_g) = 0$$

The number density and the volume fraction of gas give the interfacial area per unit volume (SI unit: m^2/m^3):

$$a = (4n\pi)^{1/3}(3\phi_g)^{2/3}$$

SLIP MODEL

The simplest possible approximation for the slip velocity $\mathbf{u}_{slip}$ is to assume that the bubbles always follow the liquid phase; that is, $\mathbf{u}_{slip} = \mathbf{0}$. This is known as homogeneous flow.

A better model can be obtained from the momentum equation for the gas phase. Comparing size of different terms, it can be argued that the equation can be reduced to a balance between the viscous drag force, $\mathbf{f}_D$ and the pressure gradient (Ref. 3), a so called pressure-drag balance:

$$\phi_g \nabla p = \mathbf{f}_D \tag{5-29}$$

Here $\mathbf{f}_D$ can be written as

$$\mathbf{f}_D = -\phi_d C_d \frac{3}{4}\frac{\rho_l}{d_b}|\mathbf{u}_{slip}|\mathbf{u}_{slip} \tag{5-30}$$

where in turn d_b (SI unit: m) is the bubble diameter, and C_d (dimensionless) is the viscous drag coefficient. Given C_d and d_b, Equation 5-29 can be used to calculate the slip velocity.

Schwarz and Turner (Ref. 4) proposed a linearized version of Equation 5-30 appropriate for air bubbles of 1–10 mm mean diameter in water:

$$\mathbf{f}_D = -\phi_d C_W \mathbf{u}_{slip} \qquad C_W = 5 \cdot 10^4 \ \frac{kg}{m^3 s} \tag{5-31}$$

The Hadamard-Rybczynski model is appropriate for small spherical bubbles with diameter less than 2 mm. The model uses the following expression for the drag coefficient (Ref. 5):

$$C_d = \frac{16}{Re_b}, \qquad Re_b = \frac{d_b \rho_l |\mathbf{u}_{slip}|}{\mu_l}$$

For bubbles with diameter larger than 2 mm, the model suggested by Sokolichin, Eigenberger, and Lapin (Ref. 1) is a more appropriate choice:

$$C_d = \frac{0{,}622}{\dfrac{1}{E\ddot{o}} + 0{,}235}$$

where $E\ddot{o}$ is the Eötvös number

$$E\ddot{o} = \frac{g \rho_l d_b^2}{\sigma}$$

Here, g is the magnitude of the gravity vector and σ the surface tension coefficient.

Turbulence Modeling in Bubbly Flow Applications

For most *bubbly flow* applications the flow field is turbulent. In that case, use a turbulence model and solve for the averaged velocity field. For the Turbulent Bubbly Flow interface, the k-ε turbulence model is used. In addition to the options of the single-phase flow model, it is also possible to account for bubble-induced turbulence—that is, extra production of turbulence due to relative motion between the gas bubbles and the liquid.

The k-ε model solves two extra transport equations for two additional variables: the turbulent kinetic energy, k (SI unit: m^2/s^2) and the dissipation rate of turbulent energy, ε (SI unit: m/s^3). The turbulent viscosity is then

$$\mu_T = \rho_l C_\mu \frac{k^2}{\varepsilon}$$

where C_μ is a model constant.

The transport equation for the turbulent kinetic energy, k, is

$$\rho_1\frac{\partial k}{\partial t} + \rho_1\mathbf{u}_1 \cdot \nabla k = \nabla \cdot \left[\left(\mu_1 + \frac{\mu_T}{\sigma_k}\right)\nabla k\right] + P_k - \rho_1\varepsilon + S_k \tag{5-32}$$

where the production term is

$$P_k = \mu_T\left(\nabla\mathbf{u}_1:(\nabla\mathbf{u}_1 + (\nabla\mathbf{u}_1)^T) - \frac{2}{3}(\nabla\cdot\mathbf{u}_1)^2\right) - \frac{2}{3}\rho k\nabla\cdot\mathbf{u}_1$$

and the evolution of the turbulent energy's dissipation rate ε is given by:

$$\rho_1\frac{\partial\varepsilon}{\partial t} + \rho_1\mathbf{u}_1 \cdot \nabla\varepsilon = \nabla\cdot\left[\left(\mu_1 + \frac{\mu_T}{\sigma_\varepsilon}\right)\nabla\varepsilon\right] + C_{\varepsilon 1}\frac{\varepsilon}{k}C_{\varepsilon 1}P_k - \rho_1 C_{\varepsilon 2}\frac{\varepsilon^2}{k} + C_\varepsilon S_k\frac{\varepsilon}{k} \tag{5-33}$$

In all the previous equations, the velocity, $\mathbf{u}_1$, is the liquid phase averaged velocity field.

The standard k-ε turbulence model uses the following constants:

CONSTANT	VALUE
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3

The included source term S_k accounts for bubble-induced turbulence and is given by

$$S_k = -C_k\phi_g\nabla p \cdot \mathbf{u}_{slip}$$

Suitable values for the model parameters C_k and C_ε are not as well established as the parameters for single-phase flow. In the literature, values within the ranges $0.01 < C_k < 1$ and $1 < C_\varepsilon < 1.92$ have been suggested (Ref. 1). The turbulent viscosity appears in the momentum equation and when adding a drift term to the gas velocity:

$$\mathbf{u}_{drift} = -\frac{\mu_T}{\rho_1}\frac{\nabla\phi_g}{\phi_g}$$

Using the k-ε model together with a gas concentration that is not assumed to be low, the stress tensor contains an extra contribution, and the momentum equations becomes

$$\phi_1\rho_1\frac{\partial \mathbf{u}_1}{\partial t} + \phi_1\rho_1\mathbf{u}_1 \cdot \nabla \mathbf{u}_1 =$$

$$= -\nabla p + \nabla \cdot \left[\phi_1(\mu_1 + \mu_T)\left(\nabla \mathbf{u}_1 + \nabla \mathbf{u}_1^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_1)\mathbf{I}\right) - \frac{2}{3}\phi_1\rho_1 k \mathbf{I}\right] + \phi_1\rho_1\mathbf{g} + \mathbf{F} \tag{5-34}$$

References for the Bubbly Flow Interfaces

1. A. Sokolichin, G. Eigenberger, and A. Lapin, "Simulations of Buoyancy Driven Bubbly Flow: Established Simplifications and Open Questions," *AIChE Journal*, vol. 50, no. 1, pp. 24–49, 2004.

2. D. Kuzmin and S. Turek, *Efficient Numerical Techniques for Flow Simulation in Bubble Column Reactors,* Institute of Applied Mathematics, University of Dortmund, 2000.

3. D. Kuzmin, S. Turek, and H. Haario, *Finite Element Simulation of Turbulent Bubbly Flows in Gas-liquid Reactors*, Ergebnisberichte Angew, Math, 298, University of Dortmund, 2005.

4. M.P. Schwarz and W.J. Turner, "Applicability of the Standard k-ε Turbulence Model to Gas-stirred Baths," *Applied Mathematical Modelling*, vol. 12, pp. 273–279, 1988.

5. C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows with Droplets and Particles,* CRC Press, 1998.

Theory for the Mixture Model Interfaces

The mixture model is a macroscopic two-phase flow model, in many ways similar to the bubbly flow model. It tracks the averaged phase concentration, or volume fraction, and solves a single momentum equation for the mixture velocity. It is suitable for mixtures consisting of solid particles or liquid droplets immersed in a liquid.

The Mixture Model interface theory is described in this section:

- The Mixture Model Equations
- Dispersed Phase Boundary Conditions Equations
- Turbulence Modeling in Mixture Models
- Slip Velocity Models
- References for the Mixture Model Interfaces

The Mixture Model Equations

Just as for the Bubbly Flow interfaces, the Mixture Model interfaces are based on the two fluid Euler-Euler Model. The two phases consist of one dispersed phase and one continuous phase. The mixture model is valid if the continuous phase is a liquid, and the dispersed phase consists of solid particles, liquid droplets, or gas bubbles. For gas bubbles in a liquid, however, the bubbly flow model is preferable. The mixture model relies on the following assumptions.

- The density of each phase is approximately constant.
- Both phases share the same pressure field.
- The relative velocity between the two phases is essentially determined assuming a balance between the pressure gradient and viscous drag.

The momentum equation for the mixture is

$$\rho \mathbf{u}_t + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p - \nabla \cdot \boldsymbol{\tau}_{\mathrm{Gm}} + \rho \boldsymbol{g} + \mathbf{F}$$
$$-\nabla \cdot \left[\rho c_{\mathrm{d}} (1 - c_{\mathrm{d}}) \left(\mathbf{u}_{\mathrm{slip}} - \frac{D_{m\mathrm{d}}}{(1 - c_{\mathrm{d}}) \phi_{\mathrm{d}}} \nabla \phi_{\mathrm{d}} \right) \left(\mathbf{u}_{\mathrm{slip}} - \frac{D_{m\mathrm{d}}}{(1 - c_{\mathrm{d}}) \phi_{\mathrm{d}}} \nabla \phi_{\mathrm{d}} \right)^T \right]$$

where:

- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- ρ is the density (SI unit: kg/m^3)
- p is the pressure (SI unit: Pa)
- c_d is the mass fraction of the dispersed phase (SI unit: kg/kg)
- $\mathbf{u}_{slip}$ is the relative velocity vector between the two phases (SI unit: m/s)
- $\boldsymbol{\tau}_{Gm}$ is the sum of the viscous and turbulent stresses (SI unit: kg/(m·s^2))
- $\mathbf{g}$ is the gravity vector (SI unit: m/s^2), and
- $\mathbf{F}$ is any additional volume force (SI unit: N/m^3)

The velocity $\mathbf{u}$ used here is the mass-averaged mixture velocity (SI unit: m/s), defined as

$$\mathbf{u} = \frac{\phi_c \rho_c \mathbf{u}_c + \phi_d \rho_d \mathbf{u}_d}{\rho}$$

where

- ϕ_c and ϕ_d denote the volume fractions of the continuous phase and the dispersed phase (SI unit: m^3/m^3), respectively
- $\mathbf{u}_c$ is the continuous phase velocity vector (SI unit: m/s)
- $\mathbf{u}_d$ is the dispersed phase velocity vector (SI unit: m/s)
- ρ_c is the continuous phase density (SI unit: kg/m^3)
- ρ_d is the dispersed phase density (SI unit: kg/m^3), and
- ρ is the mixture density (SI unit: kg/m^3)

The relationship between the velocities of the two phases is defined by

$$\mathbf{u}_d - \mathbf{u}_c = \mathbf{u}_{cd} = \mathbf{u}_{slip} - \frac{D_{md}}{(1 - c_d)\phi_d}\nabla\phi_d \qquad (5\text{-}35)$$

Here, $\mathbf{u}_{slip}$ (SI unit: m/s) denotes the relative velocity between the two phases. For different available models for the slip velocity, see Slip Velocity Models. D_{md} is a turbulent dispersion coefficient (SI unit: m^2/s) (see Turbulence Modeling in Mixture Models), accounting for extra diffusion due to turbulent eddies. When a turbulence model is not used, D_{md} is zero.

The mixture density is given by

$$\rho = \phi_c \rho_c + \phi_d \rho_d$$

where ρ_c and ρ_d (SI units: kg/m^3) are the densities of the two phases. The mass fraction of the dispersed phase c_d is given by

$$c_d = \frac{\phi_d \rho_d}{\rho}$$

The sum of the viscous and turbulent stresses is

$$\boldsymbol{\tau}_{Gm} = (\mu + \mu_T)\left[(\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I}\right] \tag{5-36}$$

where μ (SI unit: Pa·s) is the mixture viscosity and μ_T (SI unit: Pa·s) the turbulent viscosity. If no turbulence model is used, μ_T equals zero.

The transport equation for ϕ_d, the dispersed phase volume fraction, is

$$\frac{\partial}{\partial t}(\phi_d \rho_d) + \nabla \cdot (\phi_d \rho_d \mathbf{u}_d) = -m_{dc} \tag{5-37}$$

where m_{dc} (SI unit: kg/(m^3·s)) is the mass transfer rate from the dispersed to the continuous phase and $\mathbf{u}_d$ (SI unit: m/s) is the dispersed phase velocity according to Equation 5-35. Assuming constant density for the dispersed phase, Equation 5-37 can be rewritten as

$$\frac{\partial}{\partial t}(\phi_d) + \nabla \cdot (\phi_d \mathbf{u}_d) = -\frac{m_{dc}}{\rho_d} \tag{5-38}$$

The continuous phase volume fraction ϕ_c is

$$\phi_c = 1 - \phi_d$$

The continuity equation for the mixture is

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{5-39}$$

In the Mixture Model interfaces it is assumed that the densities of both phases, ρ_c and ρ_d, are constant, and therefore the following alternative form of the continuity equation for the mixture is used

$$(\rho_c - \rho_d)\left[\nabla \cdot (\phi_d(1 - c_d)\mathbf{u}_{slip} - D_{md}\nabla \phi_d) + \frac{m_{dc}}{\rho_d}\right] + \rho_c(\nabla \cdot \mathbf{u}) = 0 \tag{5-40}$$

Equation 5-40 is derived from Equation 5-37 and Equation 5-39.

MASS TRANSFER AND INTERFACIAL AREA

It is possible to account for mass transfer between the two phases by specifying an expression for the mass transfer rate from the dispersed phase to the continuous m_{dc} (SI unit: $kg/(m^3 \cdot s)$).

The mass transfer rate typically depends on the interfacial area between the two phases. An example is when gas dissolves into a liquid. In order to determine the interfacial area, it is necessary to solve for the dispersed phase number density (that is, the number of particles per volume) in addition to the phase volume fraction. The Mixture Model interface assumes that the particles can increase or decrease in size but not completely vanish, merge, or split. The conservation of the number density n (SI unit: $1/m^3$) then gives

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{u}_d) = 0$$

The number density and the volume fraction dispersed particles give the interfacial area per unit volume (SI unit: m^2/m^3):

$$a = (4n\pi)^{1/3}(3\phi_d)^{2/3}$$

Dispersed Phase Boundary Conditions Equations

In addition to the boundary conditions for the mixture, specify boundary conditions for the dispersed phase on Wall, Inlet, and Outlet nodes. For these boundary types, the boundary condition's Settings window contains a Dispersed Phase Boundary Condition section.

DISPERSED PHASE CONCENTRATION

This is the default for the Inlet node. Specify the dispersed phase volume fraction:

$$\phi_d = \phi_{d0}$$

Enter the **Dispersed phase volume fraction** (dimensionless) in the ϕ_{d0} field.

DISPERSED PHASE OUTLET

This is the default for the Outlet node. This boundary condition is appropriate for boundaries where the dispersed phase leaves the domain with the dispersed phase velocity $\mathbf{u}_d$. No condition is imposed on the volume fractions at the boundary.

DISPERSED PHASE FLUX

Using this boundary condition, specify the dispersed phase flux through the boundary:

$$-\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = N_{\phi_d}$$

Enter the **Dispersed phase flux** (SI unit: m/s) in the N_{ϕ_d} field.

SYMMETRY

This boundary condition, which is useful on boundaries that represent a symmetry line for the dispersed phase, sets the dispersed phase flux through the boundary to zero:

$$\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = 0$$

NO DISPERSED FLUX

This is the default for the Wall node. This boundary condition represents boundaries where the dispersed phase flux through the boundary is zero:

$$\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = 0$$

Turbulence Modeling in Mixture Models

For turbulence modeling, use the k-ε turbulence model. Turbulence modeling is particularly relevant for dilute flows, that is, for flows with a low dispersed phase volume fraction. For dense flows, the mixture viscosity usually becomes high. In such cases, the flow is laminar and no turbulence modeling is necessary.

The k-ε turbulence model solves two extra transport equations for two additional variables: the turbulent kinetic energy, k (SI unit: m^2/s^2), and the dissipation rate of turbulent kinetic energy, ε (SI unit: m^2/s^3). The turbulent viscosity is given by

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon}$$

where C_μ is a model constant.

The transport equation for the turbulent kinetic energy k is

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon$$

where the production term is

$$P_k = \mu_T \left(\nabla \mathbf{u} : (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u})^2 \right) - \frac{2}{3} \rho k \nabla \cdot \mathbf{u}$$

The evolution of the dissipation rate of the turbulent kinetic energy, ε, is determined by

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k}$$

By default, the following variables are used for the dimensionless parameters:

CONSTANT	VALUE
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3

The turbulence must also be accounted for in the calculation of the dispersed phase volume fraction. This is accomplished by introducing a turbulent dispersion coefficient D_{md} (SI unit: m^2/s) in Equation 5-35 as

$$D_{md} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is the turbulent particle Schmidt number (dimensionless). The particle Schmidt number is usually suggested a value ranging from 0.35 to 0.7. In the physics interface the default value is 0.35. The so-called drift velocity is included in Equation 5-38 as a diffusion term

$$\frac{\partial}{\partial t}(\phi_d) + \nabla \cdot (\phi_d \beta_d) = \nabla \cdot (D_{md} \nabla \phi_d) - \frac{m_{dc}}{\rho_d}$$

where in turn

$$\beta_d = \mathbf{u} + \mathbf{u}_{slip}(1 - c_d)$$

Similarly, the number density equation (used to compute the interfacial area) for turbulent flow corresponds to

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \beta_d) = \nabla \cdot (D_{md} \nabla n)$$

Using the k-ε turbulence model, the viscous stress tensor contains an extra contribution and eq.Equation 5-36 is replaced by

$$\boldsymbol{\tau}_{\mathrm{G}m} \;=\; (\mu + \mu_{\mathrm{T}})\left[(\nabla\mathbf{u} + \nabla\mathbf{u}^{T}) - \frac{2}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right] - \frac{2}{3}\rho k\mathbf{I} \tag{5-41}$$

Slip Velocity Models

The Mixture Model interfaces contain three predefined models for the relative velocity between the two phases $\mathbf{u}_{\mathrm{slip}}$ (SI unit: m/s):

- The *Schiller-Naumann model*
- The *Haider-Levenspiel model*
- The *Hadamard-Rybczynski model*

All three models use the following relation for the slip velocity:

$$\frac{3}{4}\frac{C_{\mathrm{d}}}{d_{\mathrm{d}}}\rho_c\left|\mathbf{u}_{\mathrm{slip}}\right|\mathbf{u}_{\mathrm{slip}} \;=\; -\frac{(\rho - \rho_{\mathrm{d}})}{\rho}\left(-\mathbf{u}_t - (\mathbf{u}\cdot\nabla)\mathbf{u} + \mathbf{g} + \frac{\mathbf{F}}{\rho}\right) \tag{5-42}$$

where C_{d} (dimensionless) is the particle drag coefficient. Essentially, interpret the relation as a balance between viscous drag and buoyancy forces acting on the dispersed phase.

The Schiller-Naumann model models the drag coefficient according to

$$C_{\mathrm{d}} \;=\; \begin{cases} \dfrac{24}{\mathrm{Re}_{\mathrm{p}}}(1 + 0{,}15\,\mathrm{Re}_{\mathrm{p}}^{0{,}687}) & \mathrm{Re}_{\mathrm{p}} < 1000 \\[2mm] 0{,}44 & \mathrm{Re}_{\mathrm{p}} > 1000 \end{cases}$$

where Re_{p} is the particle Reynolds number

$$\mathrm{Re}_{\mathrm{p}} \;=\; \frac{d_{\mathrm{d}}\rho_c\left|\mathbf{u}_{\mathrm{slip}}\right|}{\mu}$$

Because the particle Reynolds number depends on the slip velocity, an implicit equation must be solved to obtain the slip velocity. Therefore, the Mixture Model interfaces add an additional equation for

$$\left|\mathbf{u}_{\mathrm{slip}}\right|^{2}$$

when the Schiller-Naumann slip model is used. The Schiller-Naumann model is particularly well-suited for solid particles in a liquid.

The Haider-Levenspiel model is applicable to non-spherical particles. It models the drag coefficient according to

$$C_d = \frac{24}{Re_p}\left(1 + A(S_p)Re_p^{B(S_p)}\right) + \frac{C(S_p)}{1 + D(S_p)/Re_p}$$

where A, B, C and D are empirical correlations of the particle sphericity. The sphericity is defined as the ratio of the surface area of a volume equivalent sphere to the surface area of the considered non-spherical particle

$$0 < S_p = \frac{A_{sphere}}{A_{particle}} \le 1$$

The correlation coefficients are given by

$$A(S_p) = e^{2.3288 - 6.4581 S_p + 2.4486 S_p^2}$$

$$B(S_p) = 0.0964 + 0.5565 S_p$$

$$C(S_p) = e^{4.905 - 13.8944 S_p + 18.4222 S_p^2 - 10.2599 S_p^3}$$

$$D(S_p) = e^{1.4681 + 12.2584 S_p - 20.7322 S_p^2 + 15.8855 S_p^3}$$

The diameter used in the particle Reynolds number is that of the volume equivalent sphere. The equation for the squared slip velocity is also added when the Haider-Levenspiel slip model is used.

The Hadamard-Rybczynski drag law is valid for particle Reynolds numbers less than 1, for particles, bubbles, and droplets. The drag coefficient for liquid droplets or bubbles is

$$C_d = \frac{24}{Re_p}\left(\frac{1 + \frac{2}{3}\frac{\mu_c}{\mu_d}}{1 + \frac{\mu_c}{\mu_d}}\right)$$

which yields the following explicit expression for the slip velocity

$$\mathbf{u}_{slip} = -\frac{(\rho - \rho_d)d_d^2}{18\rho\eta_c}\left(\frac{1 + \frac{\mu_c}{\mu_d}}{1 + \frac{2}{3}\frac{\mu_c}{\mu_d}}\right)\nabla p$$

For solid particles, the slip velocity is given by

$$\mathbf{u}_{\text{slip}} = -\frac{(\rho - \rho_d)d_d^2}{18\rho\mu_c}\nabla p$$

when $\text{Re}_p < 1$. For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

References for the Mixture Model Interfaces

1. M. Manninen, V. Taivassalo, and S. Kallio, *On the Mixture Model for Multiphase Flow,* VTT Publications, 288, VTT Energy, Nuclear Energy, Technical Research Center of Finland (VTT), 1996.

2. C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows with Droplets and Particles,* CRC Press, 1998.

Theory for the Euler-Euler Model Interfaces

The Euler-Euler Model interfaces are based on averaging the Navier-Stokes equations for each present phase over a volume that is small compared to the computational domain but large compared to the dispersed phase (particles, droplets, or bubbles). The two phases, the continuous and the dispersed phase, are assumed to behave as two continuous and interpenetrating fluids, and the physics interface solves one set of momentum equations for each phase.

In this section:

- The Euler-Euler Model Equations
- Turbulent Two-Phase Flow Modeling
- References for the Euler-Euler Model Interfaces

The Euler-Euler Model Equations

MASS BALANCE

Assuming that the mass transfer between the two phases is zero, the following continuity relations hold for the continuous and dispersed phases (Ref. 3):

$$\frac{\partial}{\partial t}(\rho_c \phi_c) + \nabla \cdot (\rho_c \phi_c \mathbf{u}_c) = 0 \tag{5-43}$$

$$\frac{\partial}{\partial t}(\rho_d \phi_d) + \nabla \cdot (\rho_d \phi_d \mathbf{u}_d) = 0 \tag{5-44}$$

Here ϕ (dimensionless) denotes the phase volume fraction, ρ (SI unit: kg/m^3) is the density, and $\mathbf{u}$ (SI unit: m/s) the velocity of each phase. The subscripts c and d denote quantities relating to the continuous and the dispersed and phase, respectively. The following relation between the volume fractions must hold

$$\phi_c = 1 - \phi_d$$

Both phases are considered to be incompressible, in which case Equation 5-43 and Equation 5-44 can be simplified as:

$$\frac{\partial \phi_d}{\partial t} + \nabla \cdot (\phi_d \mathbf{u}_d) = 0 \tag{5-45}$$

$$\frac{\partial \phi_c}{\partial t} + \nabla \cdot (\phi_c \mathbf{u}_c) = 0 \tag{5-46}$$

If Equation 5-45 and Equation 5-46 are added together, a continuity equation for the mixture is obtained:

$$\nabla \cdot (\phi_d \mathbf{u}_d + \mathbf{u}_c (1 - \phi_d)) = 0 \tag{5-47}$$

In order to control the mass balance of the two phases, the Euler-Euler Model interfaces solves Equation 5-45 together with Equation 5-47. Equation 5-45 is used to compute the volume fraction of the dispersed phase, and Equation 5-47 is used to compute the mixture pressure.

MOMENTUM BALANCE

The momentum equations for the continuous and dispersed phases, using the non-conservative forms of Ishii (Ref. 4), are:

$$\rho_c \phi_c \left[\frac{\partial}{\partial t}(\mathbf{u}_c) + \mathbf{u}_c \nabla \cdot (\mathbf{u}_c) \right] = -\phi_c \nabla p + \nabla \cdot (\phi_c \boldsymbol{\tau}_c) + \phi_c \rho_c \mathbf{g} + \mathbf{F}_{m,c} + \phi_c \mathbf{F}_c \tag{5-48}$$

$$\rho_d \phi_d \left[\frac{\partial}{\partial t}(\mathbf{u}_d) + \mathbf{u}_d \nabla \cdot (\mathbf{u}_d) \right] = -\phi_d \nabla p + \nabla \cdot (\phi_d \boldsymbol{\tau}_d) + \phi_d \rho_d \mathbf{g} + \mathbf{F}_{m,d} + \phi_d \mathbf{F}_d \tag{5-49}$$

Here p (SI unit: Pa) is the mixture pressure, which is assumed to be equal for the two phases. In the momentum equations the viscous stress tensor for each phase is denoted by $\boldsymbol{\tau}$ (SI unit: Pa), $\mathbf{g}$ (SI unit: m/s^2) is the vector of gravitational acceleration, $\mathbf{F}_m$ (SI unit: N/m^3) is the interphase momentum transfer term (that is, the volume force exerted on each phase by the other phase), and $\mathbf{F}$ (SI unit: N/m^3) is any other volume force term.

In these equations, the influence of surface tension in the case of liquid phases has been neglected, and the potential size distribution of the dispersed particles or droplets is not considered.

For fluid-solid mixtures, Equation 5-49 is modified in the manner of Enwald (Ref. 5)

$$\rho_d \phi_d \left[\frac{\partial}{\partial t}(\mathbf{u}_d) + \mathbf{u}_d \nabla \cdot (\mathbf{u}_d) \right] = \tag{5-50}$$
$$-\phi_d \nabla p + \nabla \cdot (\phi_d \boldsymbol{\tau}_d) - \nabla p_s + \phi_d \rho_d \mathbf{g} + \mathbf{F}_{m,d} + \phi_d \mathbf{F}_d$$

where p_s (SI unit: Pa) is the solid pressure.

The fluid phases in the above equations are assumed to be Newtonian and the viscous stress tensors are defined as

$$\boldsymbol{\tau}_c = \mu_C\left(\nabla\mathbf{u}_c + (\nabla\mathbf{u}_c)^T - \frac{2}{3}(\nabla\cdot\mathbf{u}_c)\mathbf{I}\right)$$

$$\boldsymbol{\tau}_d = \mu_D\left(\nabla\mathbf{u}_d + (\nabla\mathbf{u}_d)^T - \frac{2}{3}(\nabla\cdot\mathbf{u}_d)\mathbf{I}\right)$$

where μ (SI unit: Pa·s) is the dynamic viscosity of the respective phase.

In order to avoid singular solutions when the volume fractions tend to zero, the governing equations above are divided by the corresponding volume fraction. The implemented momentum equation for the continuous phase is:

$$\rho_c\frac{\partial}{\partial t}(\mathbf{u}_c) + \rho_c\mathbf{u}_c\nabla\cdot(\mathbf{u}_c) = -\nabla p + \nabla\cdot\boldsymbol{\tau}_c + \frac{\nabla\phi_c\boldsymbol{\tau}_c}{\phi_c} + \rho_c\mathbf{g} + \frac{\mathbf{F}_{m,c}}{\phi_c} + \mathbf{F}_c$$

The implemented momentum equations for the dispersed phase in the case of dispersed liquid droplets or bubbles is:

$$\rho_d\frac{\partial}{\partial t}(\mathbf{u}_d) + \rho_d\mathbf{u}_d\nabla\cdot(\mathbf{u}_d) = -\nabla p + \nabla\cdot\boldsymbol{\tau}_d + \frac{\nabla\phi_d\cdot\boldsymbol{\tau}_d}{\phi_d} + \rho_d\mathbf{g} + \frac{\mathbf{F}_{m,d}}{\phi_d} + \mathbf{F}_d \qquad \text{(5-51)}$$

and in the case of dispersed solid particles:

$$\rho_d\frac{\partial}{\partial t}(\mathbf{u}_d) + \rho_d\mathbf{u}_d\nabla\cdot(\mathbf{u}_d) =$$
$$-\nabla p + \nabla\cdot\boldsymbol{\tau}_d + \frac{\nabla\phi_d\cdot\boldsymbol{\tau}_d}{\phi_d} - \frac{\nabla p_s}{\phi_d} + \rho_d\mathbf{g} + \frac{\mathbf{F}_{m,d}}{\phi_d} + \mathbf{F}_d \qquad \text{(5-52)}$$

DISPERSED PHASE VISCOSITY

The Newtonian viscosities of interpenetrating media are not readily available. Instead empirical and analytical models for the dynamic viscosity of the two-phase mixture have been developed by various researchers, usually as a function of the dispersed volume fraction. Using an expression for the mixture viscosity, the default values for the dynamic viscosities of the two interpenetrating phases are taken to be:

$$\mu_C = \mu_D = \mu_{mix} \qquad \text{(5-53)}$$

A simple mixture viscosity covering the entire range of particle concentrations is the Krieger type model (Ref. 5):

$$\mu_{mix} = \mu_c\left(1 - \frac{\phi_d}{\phi_{d,max}}\right)^{-2.5\phi_{d,max}} \tag{5-54}$$

Here $\phi_{d,max}$ is the maximum packing limit, by default 0.62 for solid particles. Equation 5-54 can be applied when $\mu_c \ll \mu_d$. An extension of Equation 5-54 can be applied for liquid droplets/bubbles:

$$\mu_{mix} = \mu_c\left(1 - \frac{\phi_d}{\phi_{d,max}}\right)^{-2.5\phi_{d,max}\frac{\mu_d + 0.4\mu_c}{\mu_d + \mu_c}} \tag{5-55}$$

For liquid droplets/bubbles the default value of $\phi_{d,max}$ is 1.

INTERPHASE MOMENTUM TRANSFER

In all the equations, $\mathbf{F}_m$ denotes the interphase momentum transfer, that is the force imposed on one phase by the other phase. Considering a particle, droplet, or bubble in a fluid flow, it is affected by a number of forces, for example, the drag force, the added mass force, the Basset force, and the lift force. The most important force is usually the drag force, especially in fluids with a high concentration of dispersed solids, and hence this is the predefined force included in the Euler-Euler model. The drag force added to the momentum equation is defined as:

$$\mathbf{F}_{drag,c} = -\mathbf{F}_{drag,d} = \beta\mathbf{u}_{slip} \tag{5-56}$$

where β is a drag force coefficient and the slip velocity is defined as

$$\mathbf{u}_{slip} = \mathbf{u}_d - \mathbf{u}_c$$

🗐	The drag force on the dispersed phase is equal to the one on the continuous phase but is working in the opposite direction.

Dense Flows

For dense flows with a high concentration of the dispersed phase—for example, in fluidized bed models—the Gidaspow model (Ref. 6) for the drag coefficient can be used. It combines the Wen and Yu (Ref. 7) fluidized state expression:

For $\phi_c > 0.8$

$$\beta = \frac{3\phi_c\phi_d\rho_c C_d}{4d_d}|\mathbf{u}_{\text{slip}}|\phi_c^{-2.65} \tag{5-57}$$

with the Ergun (Ref. 8) packed bed expression:

For $\phi_c < 0.8$

$$\beta = 150\frac{\mu_c\phi_d^2}{\phi_c d_d^2} + 1.75\frac{\phi_d\rho_c}{d_d}|\mathbf{u}_{\text{slip}}| \tag{5-58}$$

In the above equations, d_d (SI unit: m) is the dispersed particle diameter, and C_d is the drag coefficient for a single dispersed particle. The drag coefficient is in general a function of the particle Reynolds number

$$\text{Re}_p = \frac{\phi_c d_d\rho_c|\mathbf{u}_{\text{slip}}|}{\mu_c}$$

No universally valid expression for the drag coefficient exists. Using the implemented Gidaspow model, C_d is computed using the Schiller-Naumann relation

$$C_d = \begin{cases} \dfrac{24}{\text{Re}_p}(1 + 0.15\,\text{Re}_p^{0.687}) & \text{Re}_p < 1000 \\ 0.44 & \text{Re}_p > 1000 \end{cases} \tag{5-59}$$

Dilute Flows

For dilute flows the drag force coefficient β can be modeled as:

$$\beta = \frac{3\phi_d\rho_c C_d}{4d_d}|\mathbf{u}_{\text{slip}}| \tag{5-60}$$

In this case the drag coefficient can be computed from the Schiller-Naumann model in Equation 5-59, the Haider-Levenspiel model, or by using the Hadamard-Rybczynski drag law. The Haider-Levenspiel model is applicable to nonspherical particles. It models the drag coefficient according to

$$C_d = \frac{24}{\text{Re}_p}\Big(1 + A(S_p)\text{Re}_p^{B(S_p)}\Big) + \frac{C(S_p)}{1 + D(S_p)/\text{Re}_p}$$

where $A, B, C,$ and D are empirical correlations of the particle sphericity (see Slip Velocity Models for further details). The Hadamard-Rybczynski drag law is valid for particle Reynolds number less than one for particles, bubbles, and droplets and is defined as:

$$C_d = \frac{24}{\mathrm{Re}_p} \left(\frac{1 + \frac{2}{3}\frac{\mu_c}{\mu_d}}{1 + \frac{\mu_c}{\mu_d}} \right)$$

for bubbles and droplets and as

$$C_d = \frac{24}{\mathrm{Re}_p}$$

for solid particles (the Stokes limit). For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

SOLID PRESSURE

For fluid-solid mixtures, a model for the solid pressure, p_s in Equation 5-52, is needed. The solid pressure models the particle interaction due to collisions and friction between the particles. The solid pressure model implemented uses a gradient diffusion based assumption:

$$\nabla p_s = -G(\phi_c)\nabla\phi_c$$

where the empirical function G is given by

$$G(\phi_c) = 10^{B_1\phi_c + B_2} \tag{5-61}$$

described in Ref. 5. The available predefined models (all defined in Ref. 5) are those of Gidaspow and Ettehadieh,

$$G(\phi_c) = 10^{-8.76\phi_c + 5.43} \tag{5-62}$$

Ettehadieh,

$$G(\phi_c) = 10^{-10.46\phi_c + 6.577} \tag{5-63}$$

and Gidaspow,

$$G(\phi_c) = 10^{-10.5\phi_c + 9.0} \tag{5-64}$$

There are several equations with potentially singular terms and expressions such as the term

$$\frac{\mathbf{F}_{m,d}}{\phi_d}$$

in Equation 5-51. Also, ϕ_d is a degree of freedom and can therefore, during computations, obtain nonphysical values in small areas. This can, in turn, lead to nonphysical values of material properties such as viscosity and density. To avoid these problems, the implementation uses the following regularizations:

- $1/\phi_k$, $k=c,d$ is replaced by $1/\phi_{k,pos}$ where

$$\phi_{k,\,pos} = 0.001 + 0.999 \cdot \text{flc1hs}(\phi_k - 5e^{-4}, 5e^{-4})$$

- $\nabla\phi_k/\phi_k$ is evaluated as $\nabla(\log(\phi_{k,\,pos}))$.

- The variable ϕ_d is only used directly in Equation 5-45. It is everywhere else replaced by

$$\phi_{d,\,reg} = \min(\max(\phi_d, 0), 1)$$

  Note that this includes the way ϕ_c is calculated; that is,

$$\phi_c = 1 - \phi_{d,\,reg}$$

- An extra diffusion term is added to the right-hand side of Equation 5-45 to minimize the occurrence of negative values of ϕ_d . The "barrier" viscosity is calculated as

$$\nu_b = (e^{\max(-\phi_d/0.0025,\,0)} - 1)\frac{\mu_k}{\rho_k}$$

  where the index k indicates that the viscosity and density are taken from the continuous phase if the dispersed phase is a solid and from the dispersed phase otherwise. Note that ν_b is only nonzero if ϕ_d is less than zero.

Turbulent Two-Phase Flow Modeling

When the characteristic Reynolds number of the two-phase mixture under investigation becomes high, the flow transitions and becomes turbulent. The influence of the turbulence on the flow characteristics (mixing, particle dispersion, pressure drop etc.) are usually significant and warrants the use of a turbulence model.

In order to model fluid flow turbulence, the Euler-Euler Model, Turbulent Flow interface uses the k-ε turbulence model. This is realized by solving transport equations for the kinetic energy k (SI unit: m^2/s^2) and the dissipation rate of turbulent kinetic energy ε (SI unit: m^2/s^3).

The interface includes the possibility to model the turbulent flow of the two-phase mixture, or to solve for turbulent flow of each phase separately. In the former case one set of k-ε equations are solved, while in the latter two sets of k-ε equations are solved for, one for each phase.

MIXTURE TURBULENCE

Mixture turbulence assumes that the turbulence effects on the both continuous and dispersed phase can be modeled by solving for the turbulence of the resulting two-phase mixture. Here this is done using a two-equation k-ε model where the transport of turbulence quantities is based on based on the mixture velocity

$$\mathbf{u}_m = \frac{\phi_c \rho_c \mathbf{u}_m + \phi_d \rho_d \mathbf{u}_m}{\rho},$$

and a volume averaged mixture viscosity

$$\mu_m = \phi_c \mu_C + \phi_d \mu_D$$

This implies that the model is appropriate for flows where the relaxation time of the dispersed particles (the time scale on which particles react to changes in the carrier fluid velocity) is not significantly different to the time scale of the turbulence. It is also appropriate for stratified flows, where the mixture mainly consists of one of the phases.

Setting the **Two-phase turbulence** interface property to **Mixture**, the turbulence of the two-phase flow is modeled by solving the following k and ε equations:

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u}_m \cdot \nabla k = \nabla \cdot \left(\left(\mu_m + \frac{\mu_T}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon \qquad (5\text{-}65)$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u}_m \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu_m + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} \qquad (5\text{-}66)$$

The equations correspond to the standard two-equation k-ε model including realizability constraints.

The production term is defined accordingly as

$$P_k = \mu_T \left(\nabla \mathbf{u}_m : (\nabla \mathbf{u}_m + (\nabla \mathbf{u}_m)^T) - \frac{2}{3}(\nabla \cdot \mathbf{u}_m)^2 \right) - \frac{2}{3}\rho k \nabla \cdot \mathbf{u}_m$$

and the resulting turbulent viscosity is defined as

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon}$$

where C_μ is a model constant. The viscous stress tensors for the phases are hence defined as

$$\boldsymbol{\tau}_c = (\mu_C + \mu_T)\left(\nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_c)\mathbf{I} \right) - \frac{2}{3}\rho_c k \mathbf{I},$$

$$\boldsymbol{\tau}_d = (\mu_D + \mu_T)\left(\nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_d)\mathbf{I} \right) - \frac{2}{3}\rho_d k \mathbf{I}.$$

Assuming mixture turbulence, the transport equation for the volume fraction is:

$$\frac{\partial}{\partial t}(\phi_d) + \nabla \cdot (\phi_d \mathbf{u}_d) = \nabla \cdot (D_{md} \nabla \phi_d) \qquad (5\text{-}67)$$

Here the dispersion of the particulate phase by the turbulent fluctuations is modeled using a gradient based hypothesis. The turbulent dispersion coefficient is defined from the turbulent viscosity of the two-phase mixture in the manner of

$$D_{md} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is a turbulent particle Schmidt number (dimensionless).

Th default values of the dimensionless parameters using the Mixture Two-phase turbulence model are:

CONSTANT	VALUE
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3
K_v	0.41

CONSTANT	VALUE
B	5.2
σ_T	0.35

PHASE SPECIFIC TURBULENCE

Phase specific Two-phase turbulence model assumes that the turbulent flow of the continuous and dispersed phase can be modeled by solving for the turbulence of each phase separately by a using two sets of k-ε equations. The model implies that the time scales of the turbulent flow of each phase can differ, but it is also computationally more expensive than assuming solving one set of k-ε equations for the mixture.

Setting the **Two-phase turbulence** interface property to **Phase specific**, the turbulent flow of the two phases is modeled by solving two sets of k and ε equations, one for each phase. For the continuous phase, the transport equations for k and ε are

$$\rho_c \frac{\partial k_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla k_c = \nabla \cdot \left(\left(\mu_C + \frac{\mu_{T,c}}{\sigma_{k,c}} \right) \nabla k_c \right) + P_{k,c} - \rho_c \varepsilon_c \tag{5-68}$$

$$\rho_c \frac{\partial \varepsilon_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla \varepsilon_c = \nabla \cdot \left(\left(\mu_C + \frac{\mu_{T,c}}{\sigma_{\varepsilon,c}} \right) \nabla \varepsilon_c \right) + C_{\varepsilon 1,c} \frac{\varepsilon_c}{k_c} P_{k,c} - C_{\varepsilon 2,c} \rho \frac{\varepsilon_d^2}{k_d} \tag{5-69}$$

while for the dispersed phase the corresponding equations are

$$\rho_d \frac{\partial k_d}{\partial t} + \rho_d \mathbf{u}_d \cdot \nabla k_d = \nabla \cdot \left(\left(\mu_D + \frac{\mu_{T,d}}{\sigma_{k,d}} \right) \nabla k_d \right) + P_{k,d} - \rho_d \varepsilon_d \tag{5-70}$$

$$\rho_d \frac{\partial \varepsilon_d}{\partial t} + \rho_d \mathbf{u}_d \cdot \nabla \varepsilon_d = \nabla \cdot \left(\left(\mu_D + \frac{\mu_{T,d}}{\sigma_{\varepsilon,d}} \right) \nabla \varepsilon_d \right) + C_{\varepsilon 1,d} \frac{\varepsilon_d}{k_d} P_{k,d} - C_{\varepsilon 2,d} \rho \frac{\varepsilon_d^2}{k_d} \tag{5-71}$$

The equations for each phase correspond to the standard two-equation k-ε model including realizability constraints.

The production terms are defined as

$$P_{k,c} = \mu_{T,c} \left(\nabla \mathbf{u}_c : (\nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_c)^2 \right) - \frac{2}{3} \rho_c k_d \nabla \cdot \mathbf{u}_c$$

$$P_{k,d} = \mu_{T,d} \left(\nabla \mathbf{u}_d : (\nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_d)^2 \right) - \frac{2}{3} \rho_d k_d \nabla \cdot \mathbf{u}_d$$

The resulting turbulent viscosity, applied individually in the momentum equations of the continuous and the dispersed phases, are

$$\mu_{T,\,c} = \rho_c C_{\mu,\,c} \frac{k_c^2}{\varepsilon_c}, \; \mu_{T,\,d} = \rho_d C_{\mu,\,d} \frac{k_d^2}{\varepsilon_d} \tag{5-72}$$

where $C_{\mu,c}$ and $C_{\mu,d}$ are model constants. The viscous stress tensors for the phases are hence defined as

$$\boldsymbol{\tau}_c = (\mu_C + \mu_{T,\,c})\left(\nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_c)\mathbf{I}\right) - \frac{2}{3}\rho_c k_c \mathbf{I},$$

$$\boldsymbol{\tau}_d = (\mu_D + \mu_{T,\,d})\left(\nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_d)\mathbf{I}\right) - \frac{2}{3}\rho_d k_d \mathbf{I}.$$

As in the case of mixture turbulence, the dispersion of the particulate phase by the turbulent fluctuations is modeled using a gradient based hypothesis (Equation 5-67). For phase specific turbulence the dispersion coefficient is modeled as a volume average of the respective turbulent diffusivity of each phase

$$D_{md} = \frac{1}{\sigma_{T,\,d}}\left(\phi_c \frac{\mu_{T,\,c}}{\rho_c} + \phi_d \frac{\mu_{T,\,d}}{\rho_d}\right)$$

using a turbulent particle Schmidt number $\sigma_{T,d}$ (dimensionless).

The default values of the turbulence model parameters for phase specific turbulence are

CONTINUOUS PHASE CONSTANTS	VALUE	DISPERSED PHASE CONSTANTS	VALUE
$C_{\mu,c}$	0.09	$C_{\mu,d}$	0.09
$C_{\varepsilon1,c}$	1.44	$C_{\varepsilon1,d}$	1.44
$C_{\varepsilon2,c}$	1.92	$C_{\varepsilon2,d}$	1.92
$\sigma_{k,c}$	1.0	$\sigma_{k,d}$	1.0
$\sigma_{\varepsilon,c}$	1.3	$\sigma_{\varepsilon,d}$	1.3
$K_{v,c}$	0.41	$K_{v,d}$	0.41
B_c	5.2	B_d	5.2
		$\sigma_{T,d}$	0.35

References for the Euler-Euler Model Interfaces

1. M.J.V. Goldschmidt, B.P.B. Hoomans, and J.A.M. Kuipers, "Recent Progress Towards Hydrodynamic Modelling of Dense Gas-Particle Flows," *Recent Research Developments in Chemical Engineering*, Transworld Research Network, India, pp. 273–292, 2000.

2. A. Soulaimani and M. Fortin, "Finite Element Solution of Compressible Viscous Flows Using Conservative Variables," *Computer Methods in Applied Mechanics and Engineering*, vol. 118, pp. 319–350, 1994.

3. C. Crowe, M. Sommerfeld, and Y Tsuji, *Multiphase Flows with Droplets and Particles*, CRC Press, Boca Raton, 1998.

4. B.G.M. van Wachem, J.C. Schouten, C.M. van den Bleek, R. Krishna, and J.L. Sinclair, "Comparative Analysis of CFD Models of Dense Gas-Solid Systems," *AIChE Journal*, vol. 47, no. 5, pp. 1035–1051, 2001.

5. H. Enwald, E. Peirano, and A.-E. Almstedt, "Eulerian Two-Phase Flow Theory Applied to Fluidization," *Int. J. Multiphase Flow*, vol. 22, pp. 21–66, 1996.

6. D. Gidaspow, *Multiphase Flow and Fluidization*, Academic Press, San Diego, 1994.

7. C.Y. Wen and Y.H. Yu, "Mechanics of Fluidization," *Chemical Engineering Progress Symposium Series*, vol. 62, pp. 100–110, 1966.

8. S. Ergun, "Fluid Flow Through Packed Columns," *Chemical Engineering Progress*, vol. 48, pp. 89–94, 1952.

6

High Mach Number Flow Interfaces

This chapter discusses physics interfaces found under the **Fluid Flow>High Mach Number Flow** branch ( ).

In this chapter:

- The High Mach Number Flow Interfaces
- Theory for the High Mach Number Flow Interfaces

The High Mach Number Flow Interfaces

There are three versions of the same predefined multiphysics interface (all with the name `hmnf`) that combine the heat equation with either the laminar or turbulent flow equations. The advantage of using the multiphysics interfaces—compared to adding the individual physics interfaces separately—is that a set of two-way couplings has been predefined. In particular, the physics interfaces use the same definition of the density, which can therefore be a function of both pressure and temperature. Solving this coupled system of equations usually requires numerical stabilization, which the predefined multiphysics interface also sets up.

These physics interfaces vary only by one or two default settings (see Table 6-1) or selections from check boxes or lists under the **Physical Model** section for the physics interface.

TABLE 6-1: THE HIGH MACH NUMBER FLOW PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	TURBULENCE MODEL TYPE	TURBULENCE MODEL	HEAT TRANSPORT TURBULENCE MODEL
High Mach Number Flow, Laminar	hmnf	None	N/A	N/A
High Mach Number Flow, k-ε	hmnf	RANS	k-ε	Kays-Crawford
High Mach Number Flow, Spalart- Allmaras	hmnf	RANS	Spalart-Allmaras	Kays-Crawford

📑 Most of the other physics nodes share the same setting options as described in this section and in Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces. See also The Heat Transfer in Solids Interface in the *Heat Transfer Module User's Guide* for details about the Heat Transfer in Solids physics node.

The High Mach Number Flow, Laminar Interface

The **High Mach Number Flow, Laminar (hmnf)** interface (▦), found under the **Fluid Flow>High Mach Number Flow** branch (▨) when adding a physics interface, is used to model gas flows at low and moderate Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, laminar flows in the transonic and supersonic range. This state is often connected to very low pressures.

The physics interface solves for conservation of energy, mass and momentum. The interface also supports heat transfer in solids as well as surface-to-surface radiation.

This physics interface is a predefined multiphysics coupling consisting of a Laminar Flow interface, applied to compressible flow, in combination with a Heat Transfer interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall, Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `hmnf`.

PHYSICAL MODEL

Define physics interface properties to control the overall type of model.

Turbulence Model Type

By definition, no turbulence model is needed when studying laminar flows. The default is **None**. See The High Mach Number Flow, k-e Interface or The High Mach Number Flow, Spalart-Allmaras Interface for the settings if **RANS** is chosen as the **Turbulence model type**.

SURFACE-TO-SURFACE RADIATION

This section requires an additional Heat Transfer Module license and displays when the **Surface-to-surface radiation** check box is selected. See the *Heat Transfer Module User's Guide* for details.

Select the **Surface-to-surface radiation** check box to enable the **Radiation Settings** section.

RADIATION SETTINGS

This section requires an additional Heat Transfer Module license and displays when the **Surface-to-surface radiation** check box is selected. See the *Heat Transfer Module User's Guide* for details.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). The names can be changed but the names of fields and dependent variables must be unique within a component.

ADVANCED SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression**—**Automatic** (the default) or **Manual**. **Automatic** calculates the local CFL number (from the Courant–Friedrichs– Lewy condition) from a built-in expression. For **Manual** enter a **Local CFL number** CFL_{loc}.

By default the **Enable conversions between material and spatial frames** check box is selected.

Q
- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
- The Heat Transfer Module Interfaces
- The High Mach Number Flow, k-e Interface
- The High Mach Number Flow, Spalart-Allmaras Interface

The High Mach Number Flow, k-ε Interface

The **High Mach Number Flow, k-ε (hmnf)** interface (▨), found under the **High Mach Number Flow>Turbulent Flow** branch (▨) when adding a physics interface, is used to model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow and heat transfer close to walls are modeled using wall functions. The physics interface also supports heat transfer in solids as well as surface-to-surface radiation.

This is a predefined multiphysics coupling consisting of a Turbulent Flow k-ε interface, applied to compressible flow, in combination with a heat transfer interface. As shown in Table 6-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default turbulence model selected — **k-ε** for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall, Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

SETTINGS
The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern

`<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `hmnf`.

PHYSICAL MODEL

The default **Turbulence model type** is **RANS**, the default **Turbulence model** is **k-ε**, and the default **Heat transport turbulence model** is **Kays-Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

TURBULENCE MODEL PARAMETERS

Edit the model parameters of the k-ε model as needed. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling and heat radiation, the **Turbulent kinetic energy** k (SI unit: m^2/s^2) and **Turbulent dissipation rate** ep (SI unit: m^2/s^3) variables are also available.

The names can be changed but the names of fields and dependent variables must be unique within a model.

- The Heat Transfer Module Interfaces in the H
- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
- The High Mach Number Flow, Laminar Interface
- The High Mach Number Flow, Spalart-Allmaras Interface

The High Mach Number Flow, Spalart-Allmaras Interface

The **High Mach Number Flow, Spalart-Allmaras (hmnf)** interface ( ), found under the **High Mach Number Flow>Turbulent Flow** branch ( ) when adding a physics interface, is used to model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the one-equation Spalart-Allmaras turbulence model. The Spalart-Allmaras model is a so-called low-Reynolds number model, which means that it resolves the velocity, pressure, and temperature fields all the way down to the wall. The Spalart-Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation. It also supports heat transfer in solids as well as surface-to-surface radiation.

This is a predefined multiphysics coupling consisting of a Turbulent Flow, Spalart-Allmaras interface, applied to compressible flow, in combination with a Heat Transfer interface. As shown in Table 6-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default Turbulence model selected—**Spalart-Allmaras** for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder**—**Fluid**, **Wall, Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

PHYSICAL MODEL

The default **Turbulence model type** is **RANS**, the default **Turbulence model** is **Spalart-Allmaras**., and the default **Heat transport turbulence model** is **Kays-Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling

and heat radiation, the **Reciprocal wall distance** G (SI unit: $1/m$) and **Undamped turbulent kinematic viscosity** $nutilde$ (SI unit: m^2/s) variables are also available.

ℚ	• The Heat Transfer Module Interfaces in the *Heat Transfer Module User's Guide* • Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces • The High Mach Number Flow, Laminar Interface • The High Mach Number Flow, k-e Interface

▥	*Transonic Flow in a Sajben Diffuser*: Application Library path **CFD_Module/High_Mach_Number_Flow/sajben_diffuser**

Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow Interfaces has these domain, boundary, edge, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

The following nodes are slightly different from those in the other physics interfaces and are described in this section (listed in alphabetical order):

• Fluid

• Initial Values

• Inlet

• Outlet

• Symmetry

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface:

- Pressure Point Constraint
- Volume Force
- Wall

For The High Mach Number Flow, k-e Interface, the same nodes are selected from the **Turbulent Flow, k-ε** submenus. For The High Mach Number Flow, Spalart-Allmaras Interface, the same nodes are selected from the **Turbulent Flow, Spalart-Allmaras** submenus.

The following physics nodes and subnodes (listed in alphabetical order) are described for the Heat Transfer interfaces in the *Heat Transfer Module User's Guide*. Additional features can also be available when you have additional licenses:

- Boundary Heat Source
- Heat Flux
- Heat Source
- Solid
- Line Heat Source
- Periodic Condition

- Point Heat Source
- Diffuse Surface
- Temperature
- Thermal Insulation
- Thin Layer

⚠	In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Initial Values

The **Initial Values** node adds initial values for the velocity field, the pressure and the temperature that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver. For turbulent flow there are also initial values for the turbulence model variables. The surface radiosity is only applicable for surface-to-surface radiation.

INITIAL VALUES

Enter values or expressions for the initial value of the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). The default values are 0 m/s for the velocity, 1 atm for the pressure, and 293.15 K for the temperature.

In a turbulent flow interface, initial values for the turbulence variables are also specified. By default these are specified using the predefined variables defined by the expressions described in Theory for the High Mach Number Flow Interfaces under Initial Values.

Fluid

The **Fluid** node adds the continuity, momentum and temperature equations for an ideal gas but omits volume forces and heat sources. Volume forces and heat sources can be added as separate physics features. Viscous heating and pressure work terms are added by default to the temperature equation.

When the turbulence model type is set to **RANS**, the Fluid node also adds the equations for k and ε, or the undamped turbulent kinematic viscosity, depending on the turbulence model used.

The thermal conductivity describes the relationship between the heat flux vector $\mathbf{q}$ and the temperature gradient ∇T as in $\mathbf{q} = -k\nabla T$, which is Fourier's law of heat conduction. Enter this quantity as power per length and temperature.

HEAT CONDUCTION

Select a **Thermal conductivity** k (SI unit: W/(m·K)) from the list—**Sutherland's Law** (the default), **From material**, or **User defined**. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the characteristics of the thermal conductivity and enter another value or expression in the field or matrix.

Sutherland's Law

For **Sutherland's Law** enter the following model parameters:

- **Conductivity at reference temperature** k_{ref} (SI unit: W/(m·K))
- **Reference temperature** $T_{\mathrm{k,ref}}$ (SI unit: K)
- **Sutherland constant** S_{k} (SI unit: K)

Sutherland's law describes the relationship between the thermal conductivity and the total temperature of an ideal fluid according to

$$k = k_{\mathrm{ref}}\left(\frac{T}{T_{k,\,\mathrm{ref}}}\right)^{3/2}\frac{T_{k,\,\mathrm{ref}} + S_k}{T + S_k}$$

THERMODYNAMICS

The High Mach Number Flow interface is applicable for ideal gases. Specify the thermodynamics properties by selecting a gas constant type and selecting between entering the heat capacity at constant pressure or the ratio of specific heats. For an ideal gas the density is defined as

$$\rho = \frac{M_n p_A}{RT} = \frac{p_A}{R_s T}$$

where p_A is the absolute pressure, and T is the temperature.

- Select a **Gas constant type**—**Specific gas constant** R_s (SI unit: J/(kg·K)) or **Mean molar mass** M_n (SI unit: kg/mol). The default setting is to use the property value **From material**. For **User defined** enter another value or expression for either material property. For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K), which is a built-in physical constant, is also used.

- From the **Specify Cp or γ** list, select **Heat capacity at constant pressure** C_p (SI unit: J/(kg·K)) or **Ratio of specific heats** γ (dimensionless). The default setting is to use the property value **From material**. For **User defined** enter another value or expression for either material property.

DYNAMIC VISCOSITY

The dynamic viscosity describes the relationship between the shear rate and the shear stresses in a fluid.

Select a **Dynamic viscosity** μ (SI unit: Pa·s) from the list—**Sutherland's Law** (the default), **From material**, or **User defined**.

Sutherland's Law
For **Sutherland's Law** enter the following model parameters:

- **Dynamic viscosity at reference temperature** μ_{ref} (SI unit: Pa·s)
- **Reference temperature** $T_{\mu,ref}$ (SI unit: K)
- **Sutherland constant** S_μ (SI unit: K)

Sutherland's law describes the relationship between the dynamic viscosity and the total temperature of an ideal fluid according to

$$\mu = \mu_{ref}\left(\frac{T}{T_{\mu,ref}}\right)^{3/2}\frac{T_{\mu,ref} + S_\mu}{T + S_\mu}$$

MIXING LENGTH LIMIT

This section is available for the **Turbulent Flow, k-ε** model.

The k-ε turbulence model needs an upper limit on the mixing length to be numerically robust. Select a **Mixing length limit** — **Automatic** (the default) or **Manual**.

- For **Automatic** this limit is automatically evaluated as:

$$l_{\text{mix}}^{\text{lim}} = 0.5 l_{bb} \tag{6-1}$$

  where l_{bb} is the shortest side of the geometry bounding box. If the geometry is a complicated system of very slender entities, for example, Equation 6-1 tends to give a result that is too large. In such cases, define $l_{\text{mix}}^{\text{lim}}$ manually.

- For **Manual** enter a value or expression for the **Mixing length limit** $l_{\text{mix}}^{\text{lim}}$ (SI unit: m).

DISTANCE EQUATION

This section is available for Turbulent Flow, Spalart-Allmaras since a Wall Distance interface is then included.

Select how the **Reference length scale** l_{ref} (SI unit: m) is defined—**Automatic** (default) or **Manual**:

- For **Automatic** the wall distance is automatically evaluated to one tenth of the shortest side of the geometry bounding box. This is usually quite accurate but it can sometimes give a too high value if the geometry consists of several slim entities. In such cases, define the reference length scale manually.

- For **Manual** it defines a different value or expression for the length scale. The default is 1 m.

l_{ref} controls the result of the distance equation. Objects that are much smaller than l_{ref} are effectively be diminished while the distance to objects much larger than l_{ref} are accurately represented.

Inlet

The **Inlet** node includes a set of boundary conditions describing the fluid flow and temperature conditions at an inlet. The applied conditions are controlled by the **Flow Condition**.

FLOW CONDITION

Select a **Flow condition** — **Characteristics based** (the default) or **Supersonic**.

For **Characteristics based** the current flow situation is analyzed using the inviscid flow characteristics at the inlet. This can be used to specify either a subsonic ($Ma < 1$) inlet or a supersonic inlet ($Ma > 1$).

For **Supersonic** the inlet flow is assumed to be supersonic.

FLOW PROPERTIES

Specify the flow properties at the inlet in terms of the static or total pressure, static or total temperature, Mach number, and flow direction. By default **Static** input variables are used.

Select an **Input state** — **Static** (the default) or **Total**. For either selection also enter values or expressions for the **Mach number** Ma_0 (dimensionless) at the inlet. The default is 1.5.

- For **Static** enter values or expressions for the **Static pressure** $p_{0,\text{stat}}$ (SI unit: Pa) and **Static temperature** $T_{0,\text{stat}}$ (SI unit: K).

- For **Total** enter values or expressions for the **Total pressure** $p_{0,\text{tot}}$ (SI unit: Pa) and **Total temperature** $T_{0,\text{tot}}$ (SI unit: K).

The relationships between the static and total states are:

$$\frac{p_{\text{tot}}}{p_{\text{stat}}} = \left(1 + \frac{\gamma - 1}{2} Ma^2\right)^{\frac{\gamma}{\gamma - 1}}$$

$$\frac{T_{\text{tot}}}{T_{\text{stat}}} = \left(1 + \frac{\gamma - 1}{2} Ma^2\right)$$

(6-2)

Select a **Flow direction**—**Normal inflow** (the default) or **User defined** to specify an arbitrary flow direction. Then enter the components of the direction normal n_M (dimensionless).

TURBULENCE PROPERTIES

This section displays when **RANS** is selected as **Turbulence model type**.

Using a turbulence model, specify the turbulence properties at an inlet. For the **Turbulent Flow, k-ε** model, specify turbulence quantities according to one of the following options:

- Select **Specify turbulence length scale and intensity** to enter values or expressions for the **Turbulent intensity** I_T (dimensionless) and **Turbulence length scale** L_T (SI unit: m). I_T and L_T values are related to the turbulence variables via

$$k = \frac{3}{2}(|\mathbf{U}|I_\mathrm{T})^2, \qquad \varepsilon = C_\mu^{3/4}\frac{k^{3/2}}{L_\mathrm{T}}$$

- For **Specify turbulence variables** enter values or expressions for the **Turbulent kinetic energy** k_0 (SI unit: m^2/s^2) and **Turbulent dissipation rate**, ε_0 (SI unit: m^2/s^3).

📋	For The High Mach Number Flow, Spalart-Allmaras Interface, enter a value or expression for the **Undamped turbulent kinematic viscosity** υ_0 (SI unit: m^2/s).

🔍	For background on the derivation and implementation of the conditions, see Theory for the High Mach Number Flow Interfaces.
	For recommendations of physically sound values see Inlet Values for the Turbulence Length Scale and Turbulent Intensity.

Outlet

The **Outlet** node includes a set of boundary conditions describing fluid flow and temperature conditions at an outlet. The applied conditions are controlled by the **Flow Condition**.

FLOW CONDITION

Select a **Flow condition** — **Hybrid** (the default), **Supersonic**, or **Subsonic**.

- Using a **Hybrid** condition, both subsonic ($Ma < 1$) and supersonic flow ($Ma > 1$) conditions at the outlet are supported.

- Select **Supersonic** when the flow at the outlet is known to be supersonic.

- Select **Subsonic** when the flow at the outlet is known to be subsonic.

FLOW PROPERTIES

This section displays when the **Hybrid** or **Subsonic** flow condition is selected.

Hybrid

For **Hybrid** an outlet pressure is specified. This pressure is enforced at the outlet when the flow is subsonic. Select an **Input state** — **Static** (the default) or **Total**. The relation

between the static and total pressure is defined in Equation 6-2.

- For **Static** enter a value or expression for the **Static pressure** $p_{0,\text{stat}}$ (SI unit: Pa). The default is 1 atm.

- For **Total** enter a value or expression for the **Total pressure** $p_{0,\text{tot}}$ (SI unit: Pa). The default is 1 atm.

Subsonic

For **Subsonic** select the **Boundary condition** —**Normal Stress** (the default) or **Pressure**. Then enter a value or expression for the **Normal stress** f_0 (SI unit: N/m^2) or **Pressure** p_0 (SI unit: Pa). The defaults are 1 atm for both.

Symmetry

The **Symmetry** boundary condition prescribes no heat flux, no penetration and vanishing shear stresses. The boundary condition is a combination of Dirichlet conditions and a Neumann condition.

$$\mathbf{q} \cdot \mathbf{n} = \mathbf{0}, \quad \mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \quad \left(\left(-p\mathbf{I} + \left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = \mathbf{0}\right)$$

🔍	These conditions correspond to the ones for the Single-Phase Flow, Laminar Flow interface. See Inlet and Outlet.
	For a background on the derivation and implementation of the conditions, see Theory for the High Mach Number Flow Interfaces.

💡	Selecting appropriate outlet conditions for the Navier-Stokes equations is not a trivial task. Generally, if there is something interesting happening at an outflow boundary, extend the computational domain to include this phenomenon.

Theory for the High Mach Number Flow Interfaces

In some industrial applications involving fluid flow, the flow velocity is large enough to introduce significant changes in the density and temperature of the fluid. This occurs because the thermodynamic properties of the fluid are coupled. Appreciable changes in the fluid properties are encountered as the flow velocity approaches, or exceeds, the speed of sound. As a rule of thumb, velocities greater than 0.3 times the speed of sound are considered to be *high Mach number* flows.

The High Mach Number Flow interface theory is described in this section:

- Compressible Flow for All Mach Numbers
- Sutherland's Law
- Consistent Inlet and Outlet Conditions
- Pseudo Time Stepping for High Mach Number Flow Models
- References for the High Mach Number Flow Interfaces

Compressible Flow for All Mach Numbers

The High Mach Number Flow interfaces solve the following equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{6-3}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} \tag{6-4}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = -(\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T} \bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla) p \right) + Q \tag{6-5}$$

where

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is the pressure (SI unit: Pa)
- τ is the viscous stress tensor (SI unit: Pa)

- **F** is the volume force vector (SI unit: N/m^3)
- C_p is the specific heat capacity at constant pressure (SI unit: $J/(kg \cdot K)$)
- T is the absolute temperature (SI unit: K)
- **q** is the heat flux vector (SI unit: W/m^2)
- Q contains the heat sources (SI unit: W/m^3)
- **S** is the strain-rate tensor:

$$\mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

These are the fully compressible Navier-Stokes equations for a simple compressible fluid. As can be seen, the same set of equations can be assembled using, for example, a Nonisothermal Flow interface or by manually coupling a Single-Phase Flow interface with a Heat Transfer interface. The difference is that the High Mach Number Flow interface can handle flow of any Mach numbers, while the other physics interfaces are subject to The Mach Number Limit. The Mach number is defined as

$$\mathrm{Ma} = \frac{|\mathbf{u}|}{a}$$

where a is the speed of sound. Equation 6-3 is hyperbolic whereas Equation 6-4 and Equation 6-5 are parabolic for time-dependent flow and elliptic for stationary flow. If diffusive effects can be neglected, as is usually the case for high-speed flows, the entire system of equations becomes hyperbolic. When the Mach number passes through unity, the direction of the characteristics associated with the hyperbolic system changes. This means that new phenomena not observed for incompressible flows, such as shock waves and expansion fans, can occur (Ref. 2). The stabilization and boundary conditions must be adapted to the change in direction of the characteristics.

Note that the diffusive effects do not disappear entirely unless these terms are explicitly excluded from the equations. Instead, they are confined to either boundary layers or to "shock-waves", which are really thin regions with steep gradients. In the High Mach Number Flow interfaces these thin regions are assumed to be underresolved, and the stabilization takes this into account. If the details of these regions are of physical interest they must be adequately resolved.

The physics interface assumes that the fluid is an ideal gas. This is necessary for the formulation of the Consistent Inlet and Outlet Conditions. The ideal gas law relates density and specific heats to the pressure and temperature. The viscosity and thermal conductivity of an ideal gas can be accurately approximated using Sutherland's Law,

which is included as an option in the High Mach Number Flow interface.

ⓠ | The Mach Number Limit

Sutherland's Law

Sutherland's law, or Sutherland's formula, is an approximation for how the viscosity of gases depends on the temperature. This law is based on an idealized intermolecular-force potential and reads (Ref. 5)

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S_\mu}{T + S_\mu} \tag{6-6}$$

where S_μ is an effective temperature called the Sutherland constant. Each gas has its own Sutherland constant. Equation 6-6 is strictly valid only for single-component gases at low pressure. It does, however, work well for air because air is mainly composed of nitrogen and oxygen, which have very similar properties. Parameter values for some common gases are given in Table 6-2 (Ref. 5).

TABLE 6-2: SUTHERLAND'S LAW PARAMETERS FOR DYNAMIC VISCOSITY

GAS	μ_0	T_0	S_μ
Air	$1.716 \cdot 10^{-5}$	273	111
Argon	$2.125 \cdot 10^{-5}$	273	114
CO_2	$1.370 \cdot 10^{-5}$	273	222
CO	$1.657 \cdot 10^{-5}$	273	136
N_2	$1.663 \cdot 10^{-5}$	273	107
O_2	$1.919 \cdot 10^{-5}$	273	139
H_2	$8.411 \cdot 10^{-5}$	273	97
Steam	$1.12 \cdot 10^{-5}$	350	1064

The SI unit for μ_0 in Table 6-2 is $N \cdot s/m^2$. The SI unit for T_0 and S_μ is Kelvin (K).

Sutherland's law can also be formulated for thermal conductivity (Ref. 5):

$$\frac{k}{k_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S_k}{T + S_k} \tag{6-7}$$

Values for k_0, T_0 and S_k for some common gases are given in Table 6-3(Ref. 5).

TABLE 6-3: SUTHERLAND'S LAW PARAMETERS FOR THERMAL CONDUCTIVITY

GAS	K_0	T_0	S_k
Air	0.0241	273 K	194
Argon	0.0163	273	170
CO_2	0.0146	273	1800
CO	0.0232	273	180
N_2	0.0242	273	150
O_2	0.0244	273	240
H_2	0.168	273	120
Steam	0.0181	300	2200

The unit for k_0 in Table 6-3 is W/(m·K). The unit for T_0 and S_k is Kelvin (K).

Consistent Inlet and Outlet Conditions

In order to provide consistent inlet and outlet conditions for high Mach number flow, the flow situation needs to be monitored at the boundary. Because all flow properties are coupled, the number and combinations of boundary conditions needed for *well posedness* depend on the flow state — that is, with which speeds the different flow quantities are propagated at the boundary. For a detailed specification on the number of physical boundary conditions needed for well posedness, see Ref. 1.

PLANE WAVE ANALYSIS OF INVISCID FLOW

On inlets a plane wave analysis of the inviscid part of the flow is used in order to apply a consistent number of boundary conditions. The method used here is described in Ref. 3.

Inviscid flow is governed by Euler's equations, which, provided that the solution is smooth and neglecting the gravity terms, can be written as

$$\frac{\partial Q}{\partial t} + \frac{\partial F_j}{\partial Q}\frac{\partial Q}{\partial x_j} = 0$$

Considering a small region close to a boundary, the Jacobian matrices can be regarded as constant, which leads to a system of linear equations

$$\frac{\partial Q}{\partial t} + \left(\frac{\partial F_j}{\partial Q}\right)_0\frac{\partial Q}{\partial x_j} = 0$$

where the subscript 0 denotes a reference state at the boundary. Assuming that the state at the boundary, described by a surface normal vector α_i (pointing out from the domain), is perturbed by a plane wave, the linear system of equations can be transformed to

$$\frac{\partial Q}{\partial t} + A_0 \frac{\partial Q}{\partial \xi} = 0$$

where

$$A_0 = \alpha_j \left(\frac{\partial F_j}{\partial Q}\right)_0$$

and ξ corresponds to the direction normal to the boundary. In the unsteady case, Euler's equations are known to be hyperbolic in all flow regimes: subsonic, sonic, and supersonic flow (Ref. 4). This implies that A_0 has real-valued eigenvalues and corresponding eigenvectors, and it can therefore be diagonalized according to

$$T A_0 T^{-1} = \Lambda, \quad \Lambda_{ii} = \{\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5\}$$

The matrix T contains the (left) eigenvectors, and the matrix Λ is a diagonal matrix containing the eigenvalues. The eigenvalues are given exactly by

$$\lambda_1 = \alpha_i u_i$$
$$\lambda_2 = \lambda_1$$
$$\lambda_3 = \lambda_1$$
$$\lambda_4 = \lambda_1 + c_s$$
$$\lambda_5 = \lambda_1 - c_s$$

where c_s is the speed of sound. Using the primitive variables

$$Q = \begin{bmatrix} \rho \\ u \\ v \\ w \\ p \end{bmatrix}$$

The characteristic variables on the boundary are

$$w_1 = \rho - \frac{p}{(c_s^A)^2}$$

$$w_2 = \frac{\alpha_1 v - \alpha_2 u}{\sqrt{\alpha_1 \alpha_1 + \alpha_2 \alpha_2}}$$

$$w_3 = \frac{1}{\sqrt{\alpha_i \alpha_i}}\left[(w\sqrt{\alpha_1 \alpha_1 + \alpha_2 \alpha_2}) - \alpha_3\left(\frac{\alpha_1 u + \alpha_2 v}{\sqrt{\alpha_1 \alpha_1 + \alpha_2 \alpha_2}} \right) \right] \qquad (6\text{-}8)$$

$$w_4 = \frac{1}{2}\left(\frac{\rho^A}{c_s^A} \frac{\alpha_i u_i}{\sqrt{\alpha_i \alpha_i}} + \frac{p}{(c_s^A)^2} \right)$$

$$w_5 = \frac{1}{2}\left(-\frac{\rho^A}{c_s^A} \frac{\alpha_i u_i}{\sqrt{\alpha_i \alpha_i}} + \frac{p}{(c_s^A)^2} \right)$$

Each characteristic can be interpreted to describe a wave transporting some quantity. The first one is an entropy wave while the next two correspond to vorticity waves. The fourth and fifth, in turn, are sound waves.

Evaluating the primitive variables in Equation 6-8, the values are taken from the outside (specified values) or from the inside (domain values) depending on the sign of the eigenvalue corresponding to that characteristic variable. At inlets, a negative eigenvalue implies that the characteristic is pointing into the domain and hence outside values are used. Correspondingly, for a positive eigenvalue the inside values are used.

Variables in Equation 6-8 with a superscript A are computed as averages of the inside and outside values.

The characteristic variables are then transformed to consistent face values of the primitive variables on the boundary in the manner of

$$\rho_b = w_1 + w_4 + w_5$$

$$u_{1,b} = -\frac{\alpha_2 w_2}{\sqrt{\alpha_1\alpha_1 + \alpha_2\alpha_2}} - \frac{\alpha_1}{\sqrt{\alpha_i\alpha_i}}\left(\frac{\alpha_3 w_3}{\sqrt{\alpha_1\alpha_1 + \alpha_2\alpha_2}} - \frac{c_s^A}{\rho^A}(w_4 - w_5)\right)$$

$$u_{2,b} = \frac{\alpha_1 w_2}{\sqrt{\alpha_1\alpha_1 + \alpha_2\alpha_2}} - \frac{\alpha_2}{\sqrt{\alpha_i\alpha_i}}\left(\frac{\alpha_3 w_3}{\sqrt{\alpha_1\alpha_1 + \alpha_2\alpha_2}} - \frac{c_s^A}{\rho^A}(w_4 - w_5)\right) \qquad (6\text{-}9)$$

$$u_{3,b} = \frac{1}{\sqrt{\alpha_i\alpha_i}}\left(w_3\sqrt{\alpha_1\alpha_1 + \alpha_2\alpha_2} + \alpha_3\frac{c_s^A}{\rho^A}(w_4 - w_5)\right)$$

$$p_b = (c_s^A)^2(w_4 + w_5)$$

Characteristics Based Inlets

Applying this condition implies using the plane wave analysis described in Consistent Inlet and Outlet Conditions. With this condition, a varying flow situation at the inlet can be handled. This means that changes due to prescribed variations at the boundary, due to upstream propagating sound waves or spurious conditions encountered during the nonlinear solution procedure, can be handled in a consistent manner. The full flow condition at the inlet is specified by the following properties

$$M_{in}, p_{in}, T_{in} \qquad (6\text{-}10)$$

from which the density is computed using the ideal gas law. The dependent variables defined in Equation 6-10 are applied as the outside values used in Equation 6-8, and the boundary values of the dependent variables are obtained from Equation 6-9.

Supersonic Inlets

Applying a supersonic inlet, the full flow at the inlet is specified using the inlet properties in Equation 6-10. Because the flow is supersonic, all characteristic at the inlet are known to be directed into the domain, and the boundary values of the dependent variables are computed directly from the inlet properties.

Hybrid Outlet

When building a model, it is recommended that it is constructed so that as little as possible happens at the outlet. In the high Mach number flow case this implies keeping the conditions either subsonic or supersonic at the outlet. This is, however, usually not possible. For example, often one boundary adjacent to the outlet consists of a no slip wall, in which case a boundary layer containing a subsonic region is present. The hybrid outlet feature adds the following weak expression:

$$\Gamma W_{NS} = \begin{cases} 0.5(-p - p_{out})\mathbf{n} \cdot \hat{\mathbf{u}} & Ma < 1 \\ (-p)\mathbf{n} \cdot \hat{\mathbf{u}} & \text{else} \end{cases}$$

where $\hat{\mathbf{u}}$ is the test function for the velocity vector. This corresponds to a pressure, no viscous stress condition in regions with subsonic flow and a no viscous stress condition in regions with supersonic flow. When the static pressure at the outlet is not known beforehand, it is recommended that it is set to the inlet pressure. When a converged solution has been reached, the solution can be analyzed to find the pressure level just outside the sonic point ($Ma = 1$) along the boundary. You can then apply this pressure level instead.

Supersonic Outlet
When the outlet condition is known to be fully supersonic, the viscous stress is specified in accordance with the equations and hence no physical condition is applied. This is done by prescribing the boundary stress using the full stress vector:

$$W_{NS} = \left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right](\mathbf{n} \cdot \hat{\mathbf{u}})$$

It is often possible to use the supersonic condition at outlets that are not strictly supersonic but mainly supersonic (the main part of the outlet boundary contains supersonic flow).

Pseudo Time Stepping for High Mach Number Flow Models

Pseudo time stepping is per default applied to all governing equations for stationary problems, for 2D component models as well as 3D component models. The momentum, continuity, energy and turbulence equations (when present) use the same expression for the pseudo time step symbol $\tilde{\Delta t}$.

For laminar models the automatic expression for CFL_{loc} is

$$1 +$$
$$\text{if(niterCMP} > 10, 1.2^{\min(\text{niterCMP} - 10, 12)}, 0) +$$
$$\text{if(niterCMP} > 32, 9 \cdot 1.3^{\min(\text{niterCMP} - 32, 9)}, 0) +$$
$$\text{if(niterCMP} > 60, 40 \cdot 1.3^{\min(\text{niterCMP} - 60, 9)}, 0)$$

while for models with turbulent flow it is

$$1 +$$
$$\text{if}(\text{niterCMP} > 10,\ 1.2^{\min(\text{niterCMP} - 10,\ 12)},\ 0) +$$
$$\text{if}(\text{niterCMP} > 120,\ 1.3^{\min(\text{niterCMP} - 120,\ 9)},\ 0) +$$
$$\text{if}(\text{niterCMP} > 220,\ 1.3^{\min(\text{niterCMP} - 220,\ 9)},\ 0)$$

- The Projection Method for the Navier-Stokes Equations
- Pseudo Time Stepping for Turbulent Flow Models

References for the High Mach Number Flow Interfaces

1. T. Poinsot and D. Veynante, *Theoretical and Numerical Combustion*, 2nd ed., Edwards, 2005.

2. J.D. Anderson, *Modern Compressible Flow*, 3rd ed., McGraw-Hill, 2003.

3. J. Larsson, *Numerical Simulation of Turbulent Flows for Turbine Blade Heat Transfer Applications*, Ph.D thesis, Chalmers University of Technology, 1998.

4. J.D. Tannehill, D.A. Anderson, and R.H. Pletcher, *Computational Fluid Mechanics and Heat Transfer*, 2nd ed., Taylor & Francis, 1997.

5. F.M. White, *Viscous Fluid Flow*, 3rd ed., McGraw-Hill, 2006.

7

Porous Media and Subsurface Flow Interfaces

This chapter discusses physics interfaces under the **Fluid Flow>Porous Media and Subsurface Flow** branch (🌐). The section Modeling Porous Media and Subsurface Flow helps you choose the best physics interface to start with.

In this chapter:

- The Darcy's Law Interface
- The Brinkman Equations Interface
- The Free and Porous Media Flow Interface
- The Two-Phase Darcy's Law Interface
- Theory for the Darcy's Law Interface
- Theory for the Brinkman Equations Interface
- Theory for the Free and Porous Media Flow Interface
- Theory for the Two-Phase Darcy's Law Interface

Modeling Porous Media and Subsurface Flow

In this section:

- Selecting the Right Physics Interface
- The Porous Media Flow Interface Options
- Coupling to Other Physics Interfaces

Selecting the Right Physics Interface

The **Porous Media and Subsurface Flow** branch ( ) included with the CFD Module has a number of subbranches to describe momentum transport. These can be added either singularly or in combination with other physics interfaces modeling mass and energy transfer, and even chemical reactions.

Different types of flow require different equations to describe them. If the flow type to model is known, then select it directly. However, when you are not certain of the flow type, or when it is difficult to obtain a solution, you can instead start with a simplified model and add complexity as you build the model. Then you can successively advance forward, comparing models and results. For porous media flow, the **Darcy's Law** interface is a good place to start if this is the case.

In other cases, you might know exactly how a fluid behaves and which equations, models, or physics interfaces best describe it, but because the model is so complex it is difficult to reach convergence. Simplifying assumptions can be made to solve the problem, and other physics interfaces can be better at fine-tuning the solution process for the more complex problem. The next section gives you an overview of each of the physics interfaces to help you choose.

TABLE 7-1: THE POROUS MEDIA FLOW DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM	PORE SIZE
Darcy's Law	dl	n/a	n/a	Low porosity and low permeability, slow flow
Two-Phase Darcy's law	tpdl	n/a	n/a	Low porosity and low permeability, slow flow

TABLE 7-1: THE POROUS MEDIA FLOW DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM	PORE SIZE
Brinkman Equations	br	Incompressible flow	Yes - Stokes-Brinkman	High permeability and porosity, faster flow
Free and Porous Media Flow	fp	Incompressible flow	Not selected	High permeability and porosity, fast flow

Figure 7-1 is an example of the **Settings** window for **Brinkman Equations** where you can select either Compressible or Incompressible flow, and either normal or Stokes Brinkman flow.

The Porous Media Flow Interface Options

DARCY'S LAW

The Darcy's Law Interface ( ) is used for modeling fluid movement through interstices in a porous medium by homogenizing the porous and fluid media into a single medium. Together with the continuity equation and equation of state for the pore fluid (or gas) this physics interface can be used to model low velocity flows, for which the pressure gradient is the major driving force. The penetration of reacting gases into a tight catalytic layer, such as a washcoat or membrane, is a classic example for the use of Darcy's Law.

Darcy's law can be used in porous media where the fluid is mostly influenced by the frictional resistance within the pores. It applies to very slow flows, or media where the pore size is very small.

BRINKMAN EQUATIONS

Where the size of the interstices are larger, and the fluid is also influenced by internal shear or shear stresses on boundaries, the viscous shear within the fluid must be considered. This is done in the Brinkman Equations interface. Fluid penetration of filters and packed beds are applications for this mode. The Brinkman Equations Interface ( ) is used to model compressible flow at speeds less than Mach 0.3, but you have to maintain control over the density and any of the mass balances that are deployed to accomplish this. You can also choose to model incompressible flow, and simplify the equations to be solved. Furthermore, you can select the Stokes-Brinkman flow feature to reduce the influence of inertial effects (see Figure 7-1).
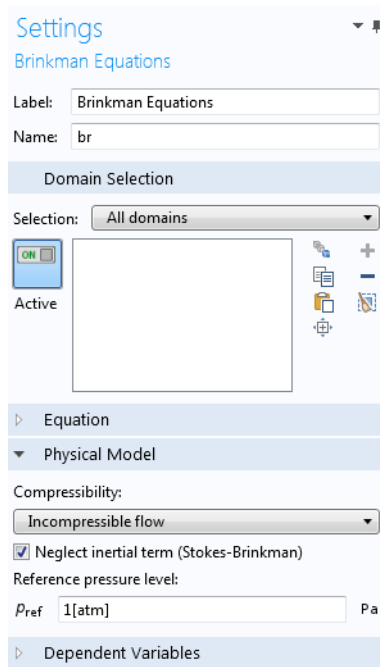
Figure 7-1: The Settings window for the Brinkman Equations interface. You can model compressible or incompressible flow as well as Stokes-Brinkman flow. Combinations are also possible.

The *Brinkman equations* extend Darcy's law to describe the dissipation of momentum by viscous shear, similar to the Navier-Stokes equation. Consequently, they are well suited to model transitions between slow flow in porous media, governed by Darcy's law, and fast flow in channels described by the Navier-Stokes equations.

The Brinkman Equations interface also includes the possibility to add a Forchheimer drag term, which is a viscous drag on the porous matrix proportional to the square of the flow velocity. This term accounts for an inertial turbulent drag effect that comes into play for fast flows through large pores. Adding the Forchheimer term takes into account all drag contributions that the Ergun equation covers.

FREE AND POROUS MEDIA FLOW

The Free and Porous Media Flow Interface ( ) is useful for modeling equipment that contains domains with both free flow and porous media flow, such as packed-bed reactors and catalytic converters. It should be noted that if the porous medium is large

in comparison with the free channel, and you are not primarily interested in results in the vicinity of the interface, you can always couple a Fluid Flow interface to a Darcy's Law interface, to make your overall model computationally cheaper.

The Free and Porous Media Flow interface is used on at least two different domains; a free channel and a porous medium. The physics interface adds functionality that allows the equations to be optimized according to the definitions of the material properties of the relevant domain. For example, you can select the Stokes-Brinkman flow feature to reduce the dependence on inertial effects in the porous domain, or just the Stoke's flow feature to reduce the dependence on inertial effects in the free channel.

Compressible flow is also possible to model in this physics interface at speeds less than Mach 0.3, but you have to maintain control over the density and any of the mass balances that are deployed to accomplish this. You can also choose to model incompressible flow, and simplify the equations to be solved.

As always, the physics interface gives you provides you with options to define, either by constants or expressions, the material properties that describe the porous media flow. This includes the density, dynamic viscosity, permeability, porosity, and matrix properties.

TWO-PHASE DARCY'S LAW

The Two-Phase Darcy's Law Interface ( ) has the equations and boundary conditions for modeling two-phase fluid movement through interstices in a porous medium using Darcy's law. The two fluids are considered immiscible, and in general, have different densities and viscosities.

As for the single phase Darcy's Law, the total velocity field is determined by the total pressure gradient and the structure of the porous medium, but the average viscosity and average density are calculated from the saturation of each immiscible phase and their fluid properties. An extra equation is computed—the fluid content of one phase—in order to calculate the saturation transport.

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple fluid flow in porous or subsurface media to another type of phenomenon described in another physics interface. This can include chemical reactions and mass transport, as described in Chemical Species Transport Interfaces, or energy transport in porous media described in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of modeling chemical reactions and mass transport are found in the Chemical Reaction Engineering Module. Furthermore, some applications that involve electrochemical reactions and porous electrodes, particularly in electrochemical power source applications, are supported in the Batteries & Fuel Cells Module.

Fluid flow is an important phenomenon for cooling in electromagnetic applications, such as heat created through induction and microwave heating, which are simulated in the AC/DC Module and RF Module, respectively. Other applications can involve the effect of fluid-imposed momentum on structural applications; poroelasticity. The Structural Mechanics Module and Subsurface Flow Module have interfaces specifically for these multiphysics applications.

The following sections list all the physics interfaces and the features associated with them under the Porous Media Subsurface Flow branch. The descriptions follow a structured order as defined by the order in the branch. Because many of the physics interfaces are integrated with each other, some features described also cross reference to other physics interfaces. At the end of this section is a summary of the theory for the physics interfaces under the Porous Media Subsurface Flow branch.

The Darcy's Law Interface

The **Darcy's Law (dl)** interface (🔹), found under the **Porous Media and Subsurface Flow** branch (🔹) when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. Set up multiple **Darcy's Law** interfaces to model multiphase flows involving more than one mobile phase. The Darcy's Law interface can be used for stationary and time-dependent analyses.

The main feature is the Fluid and Matrix Properties node, which provides an interface for defining the fluid material along with the porous medium properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder**— **Fluid and Matrix Properties**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Darcy's Law** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `dl`.

PHYSICAL MODEL

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure**. The name can be changed but the names of fields and dependent variables must be unique within a model.

DISCRETIZATION

To display this section, click the **Show** button (👁) and select **Discretization.**

The **Compute boundary fluxes** check box is not activated by default. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the check box is cleared, COMSOL instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results, but does not create extra dependent variables on the boundaries for the fluxes.

Also the **Apply smoothing to boundary fluxes** check box is available if the previous check box is checked. The smoothing can provide a better behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the COMSOL Multiphysics Reference Manual.

The **Value type when using splitting of complex variables** setting should in most pure mass transport problems be set to **Real** which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the COMSOL Multiphysics Reference Manual.

🔍	• Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface
	• Theory for the Darcy's Law Interface
	• Physical Constants in the *COMSOL Multiphysics Reference Manual*

Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface

The Darcy's Law Interface has the following domain, boundary, edge, point, and pair nodes, These nodes available from the **Physics** ribbon toolbar (Windows users), **Physics**

context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

	For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

	In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

DOMAIN

- Fluid and Matrix Properties
- Initial Values
- Mass Source

BOUNDARY, EDGE, AND POINT

The following nodes (listed in alphabetical order) are available on exterior boundaries:

The relevant physics interface condition at interior boundaries is continuity:

$$\mathbf{n} \cdot (\rho_1 \mathbf{u}_1 - \rho_2 \mathbf{u}_2) = 0$$

The continuity boundary condition ensures that the pressure and mass flux are continuous. In addition, the Pressure boundary condition is available on interior boundaries.

Fluid and Matrix Properties

The **Fluid and Matrix Properties** node adds the equations for Darcy's law, Equation 7-1 and Equation 7-2(excluding any mass sources), and contains settings for the fluid properties and the porous matrix properties such as the effective porosity.

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho\mathbf{u}) = Q_\mathrm{m} \tag{7-1}$$

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{7-2}$$

FLUID PROPERTIES

Select the **Fluid material** to use for the fluid properties. Select **Domain material** (the default) to use the material defined for the domain. Select another material to use that material's properties for the fluid.

Density
The default **Density** ρ (SI unit: kg/m^3) uses values **From material** based on the **Fluid material** selection.

- For **User defined** enter another value or expression. The default is 0 kg/m^3.

- For **Ideal gas** it uses the ideal gas law to describe the fluid. In this case, specify the thermodynamics properties. Select a **Gas constant type**—**Specific gas constant** R_s (the default) or **Mean molar mass** M_n (SI unit: J/(mol·K)). For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K) is used as the built-in physical constant. For both properties, the defaults use values **From material**. For **User defined** enter another value or expression.

Dynamic Viscosity
Select a **Dynamic viscosity** μ (SI unit: Pa·s). The default uses values **From material** as defined by the **Fluid material** selected. For **User defined** the default is 0 Pa·s.

MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** from the **Porous material** list (the default) to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From material**, defined by the **Porous material** selected. For **User defined** the default is 0.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material** selected. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to define a tensor value and enter another value or expression in the field or matrix.

Mass Source

The **Mass Source** node adds a mass source Q_m, which appears on the right-hand side of the Darcy's Law equation (Equation 7-3, the equation for porosity).

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho\mathbf{u}) = Q_m \qquad (7\text{-}3)$$

MASS SOURCE

Enter a value or expression for the **Mass source** Q_m (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

Initial Values

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa.

Pressure

Use the **Pressure** node to specify the pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example.

PRESSURE

Enter a value or expression for the **Pressure** p_0 (SI unit: Pa). Enter a relative pressure value in p_0 (SI unit: Pa).

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**.

Mass Flux

Use the **Mass Flux** node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0. A positive value of N_0 represents an inward mass flux whereas a negative value represents an outward mass flux. The units are based on the geometric entity: **Boundaries**: (SI unit: $kg/(m^2 \cdot s)$), **Edges** (SI unit: $kg/(m \cdot s)$, and **Points** (SI unit: kg/s)).

Inlet

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = \rho U_0$$

where U_0 is a value or expression for the specified inward (or outward) Darcy velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas a negative value represents an outflow.

INLET

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity. A negative value represents an outflow velocity.

Symmetry

The **Symmetry** node describes a symmetry boundary. The following condition implements the symmetry condition on an axis or a flow divide:

$$\mathbf{n} \cdot \frac{\kappa}{\mu} \nabla p = 0$$

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

No Flow

The **No Flow** node is the default boundary condition stating that there is no flow across impervious boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = 0$$

where $\mathbf{n}$ is the vector normal to the boundary.

Flux Discontinuity

Use the **Flux Discontinuity** node to specify a mass flux discontinuity through an interior boundary. The condition is represented by the following equation:

$$-\mathbf{n} \cdot (\rho \mathbf{u}_1 - \rho \mathbf{u}_2) = N_0$$

In this equation, $\mathbf{n}$ is the vector normal (perpendicular) to the interior boundary, ρ is the fluid density, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the Darcy's velocities in the adjacent domains (as defined in Equation 7-4) and N_0 is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \qquad (7\text{-}4)$$

For this boundary condition, a positive value of N_0 corresponds to a flow discontinuity in the opposite direction to the normal vector of the interior boundary.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: kg/(m^2·s)). A positive value of N_0 represents a mass flux discontinuity in the opposite direction to the normal vector of the interior boundary.

Outlet

The **Outlet** node adds a boundary condition for the outflow (or inflow) perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = \rho U_0$$

where U_0 is a specified value or expression for the outward (or inward) Darcy velocity. A positive value of the velocity U_0 corresponds to flow out of the model domain whereas a negative value represents an inflow.

OUTLET

Enter a value or expression for the **Normal outflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an outflow velocity whereas a negative value represents an inflow velocity.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an internal boundary. It allows discontinuities of velocity and pressure across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

Thin Barrier

The **Thin Barrier** boundary condition models interior permeable walls, membranes, geotextiles, or perforated plates as thin permeable barriers. The **Thin Barrier** boundary condition can only be applied on interior boundaries.

WALL

Enter a value or expression for the **Thickness** d_b (SI unit: m, the default is 0.1 m) and for the **Permeability** κ_b (SI unit: m^2, the default is 0 m^2).

The Brinkman Equations Interface

The **Brinkman Equations (br)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. The physics interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. To simplify the equations, select the Stokes-Brinkman flow feature to reduce the dependence on inertial effects when the Reynolds number is significantly less than 1. The physics interface can be used for stationary and time-dependent analyses.

The main node is the Fluid and Matrix Properties feature, which adds the Brinkman equations and provides an interface for defining the fluid material and the porous matrix.

When this physics interface is added, the following default nodes are also added in the **Model Builder**—**Fluid and Matrix Properties**, **Wall** (the default boundary type, using **No slip** as the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Brinkman Equations** to select physics features from the context menu.

The boundary conditions are essentially the same as for the Laminar Flow interface. Differences exist for the following boundary types: Outlet, Symmetry, Open Boundary, and Boundary Stress where the viscous part of the stress is divided by the porosity to appear as

$$\frac{1}{\varepsilon_p}\left\{\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}$$

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections such as **Discretization**, **Consistent Stabilization**, and **Inconsistent Stabilization**, and **Advanced Settings** sections, all accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is br.

PHYSICAL MODEL

This node specifies the properties of the Brinkman Equations interface, which describe the overall type of fluid flow model.

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Brinkman equations to model constant density flow. Alternatively, select **Compressible flow (Ma<0.3)** from the **Compressibility** list if there are small variations in the density, typically dependent on the temperature (non-isothermal flow). For compressible flow modeled with the Brinkman Equations interface, the Mach number must be below 0.3.

Neglect Inertial Term (Stokes-Brinkman Flow)

The **Neglect inertial term (Stokes-Brinkman)** check box is selected by default to model flow at very low Reynolds numbers for which the inertial term can be neglected in the Brinkman equations. This results in the linear Stokes-Brinkman equations.

Enable porous media domains

The **Enable porous media domains** check box is selected by default to solve Brinkman equations in porous domains.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm].

Swirl Flow

For 2D axisymmetric models, select the **Swirl flow** check box to include the swirl velocity component, that is the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction.

The following dependent variables (fields) are defined for this physics interface—the **Velocity field u** (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

ADVANCED SETTINGS

To display this section, click the **Show** button (⬚) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. When selected, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

Q
- Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface
- Theory for the Brinkman Equations Interface
- Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Discontinuous Galerkin Formulation

Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface

The Brinkman Equations Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡
In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

These nodes are described in this section:

- Fluid and Matrix Properties
- Forchheimer Drag
- Initial Values

- Mass Source
- Volume Force
- Fluid Properties

The following nodes(listed in alphabetical order) are described for the Laminar Flow interface :

- Flow Continuity
- Inlet
- Line Mass Source
- Boundary Stress
- Outlet
- Open Boundary

- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Wall

> In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid and Matrix Properties

The **Fluid and Matrix Properties** node adds the Brinkman equations: Equation 7-5 and Equation 7-6 (excluding any mass sources), and provides an interface for defining the properties of the fluid material and the porous matrix The Forchheimer Drag subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

Both the default **Density** ρ (SI unit: kg/m^3) and **Dynamic viscosity** μ (SI unit: Pa·s) use values **From material** based on the **Fluid material** selection. For **User defined** enter

another value or expression. In this case, the default is 0 kg/m^3 for the density and 0 Pa·s for the dynamic viscosity. The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. Non-Newtonian fluids have a viscosity that is shear-rate dependent. Examples of non-Newtonian fluids include yoghurt, paper pulp, and polymer suspensions.

POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** (the material defined for the domain) for the porous matrix. Select another material as needed.

Both the default **Porosity** ε_p (a dimensionless number between 0 and 1) and **Permeability** κ (SI unit: m^2) use values **From material** as defined by the **Porous material** selection. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the characteristics of the permeability, and enter another value or expression. The components of a permeability in the case that it is a tensor (κ_{xx}, κ_{yy}, and so on, representing an anisotropic permeability) are available as `br.kappaxx`, `br.kappayy`, and so on (using the default name `br`).

Forchheimer Drag

The **Forchheimer Drag** subnode is available from the context menu (right-click the Fluid and Matrix Properties parent node) or from the **Physics** toolbar, **Attributes** menu. While the drag of the fluid on the porous matrix in the basic Brinkman equations is proportional to the flow velocity, (Darcy's law drag), the Forchheimer drag is proportional to the square of the fluid velocity. The latter term accounts for an inertial turbulent drag effect that comes into play for fast flows through large pores. Adding the Forchheimer term takes into account all drag contributions that the Ergun equation covers.

FORCHHEIMER DRAG

Enter a value for the **Forchheimer coefficient** β_F (SI unit: kg/m^4). The default is 0 kg/m^4.

Mass Source

The **Mass Source** node adds a mass source (or mass sink) Q_{br} to the right-hand side of the continuity equation: Equation 7-5. This term accounts for mass deposit and/or

mass creation in porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{br} \qquad (7\text{-}5)$$

DOMAIN SELECTION

Only Porous Matrix domains are available.

MASS SOURCE

Enter a value or expression for the **Source term** Q_{br} (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

Volume Force

Use the **Volume Force** node to specify the force $\mathbf{F}$ on the right-hand side of Equation 7-6. It then acts on each fluid element in the specified domains. A common application is to include gravity effects.

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) =$$

$$-\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_{br}}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F} \qquad (7\text{-}6)$$

VOLUME FORCE

Enter the components of **Volume force** $\mathbf{F}$ (SI unit: N/m^3).

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field u** (SI unit: m/s) and the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations to solve for free flow in non-porous domains. The node also provides an interface for defining the material properties of the fluid.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables or by selecting a material. For the latter option, additional inputs, for example temperature and/or pressure, may be required to define these properties.

Temperature

By default, the single-phase flow interfaces are set to model isothermal flow. Hence, the **Temperature** is **User defined** and defaults to 293.15 K. If a Heat Transfer interface is included in the component, the temperature may alternatively be selected from this physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p+p_{ref}$ where p is the dependent pressure variable from the Navier-Stokes equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is non zero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

FLUID PROPERTIES

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible.

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

The Free and Porous Media Flow Interface

The **Free and Porous Media Flow (fp)** interface (🔲), found under the **Porous Media and Subsurface Flow** branch (🔷) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow where free flow is connected to porous media. The Free and Porous Media Flow interface is used over at least two different domains: a free channel and a porous medium. The physics interface is well suited for transitions between slow flow in porous media, governed by the Brinkman equations, and fast flow in channels described by the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. The physics interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder**— **Fluid Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add a **Porous Matrix Properties** node to be used on the domain selection corresponding to the porous media, or add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Free and Porous Media Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `fp`.

PHYSICAL MODEL

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Navier-Stokes and Brinkman equations to model constant density flow. If required, select **Compressible flow (Ma<0.3)** from the **Compressibility** list, to account for small

variations in the density, typically dependent on the temperature (non-isothermal flow). For compressible flow modeled with this physics interface, the Mach number must be below 0.3.

Neglect Inertial Term

Select the **Neglect inertial term in free flow (Stokes flow)** check box if the inertial forces are small compared to the viscous forces. This is typical for creeping flow, where $\mathrm{Re} \ll 1$.

Select the **Neglect inertial term in porous media flow (Stokes-Brinkman)** check box to model flow at very low Reynolds numbers in the porous media, for which the inertial term in the Brinkman equations can be neglected. The physics interface then solves the linear Stokes-Brinkman equations.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

Swirl Flow

For 2D axisymmetric components, select the **Swirl flow** check box to include the swirl velocity component, that is the velocity component u_{φ} in the azimuthal direction. While u_{φ} can be nonzero, there can be no gradients in the φ direction.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface—the **Velocity field u** (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

⊘	• Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow Interface • Theory for the Free and Porous Media Flow Interface

---

Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow Interface

The Free and Porous Media Flow Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon

toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

> In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid Properties
- Forchheimer Drag
- Initial Values
- Mass Source

- Microfluidic Wall Conditions
- Porous Matrix Properties
- Volume Force
- Wall

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface:

- No Viscous Stress
- Flow Continuity
- Inlet
- Line Mass Source
- Outlet
- Open Boundary

- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry

> In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

Use the **Fluid Properties** node to define the fluid material, density, and dynamic viscosity.

FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

The default **Density** ρ (SI unit: kg/m^3) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 kg/m^3.

The **Dynamic viscosity** μ (SI unit: Pa·s) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

Porous Matrix Properties

Use the **Porous Matrix Properties** node to define which domains contain porous material and to define the porous matrix properties, such as the porosity and permeability in these domains. The Forchheimer Drag subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

DOMAIN SELECTION

Choose domains from the **Selection** list, to solve for porous media flow governed by the Brinkman equations. In the domains not selected, the Free and Porous Media Flow interface solves for laminar flow governed by the Navier-Stokes (or Stokes) equations.

POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** (the material defined for the domain) for the porous matrix. Select another material as needed.

Porosity
The default **Porosity** ε_{p} (a dimensionless number between 0 and 1) uses values **From material** as defined by the **Porous material** selection. For **User defined** enter another value or expression. The default is 0.

Permeability
The default **Permeability** κ_{br} (SI unit: m^2) uses values **From material** as defined by the **Porous material** selection. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** from the list and then enter other values or expressions. The components of a permeability in the case that it is a tensor (κ_{xx}, κ_{yy}, and so on, representing an anisotropic permeability) are available as `fp.kappaxx`, `fp.kappayy`, and so on (using the default name `fp`). The defaults is 0 m^2.

Source Term

Enter a value or expression for an optional mass source (or sink) **Source term** Q_{br} (SI unit: kg/(m^3·s)). This term accounts for mass deposit and mass creation within domains. The physics interface assumes that the mass exchange occurs at zero velocity.

Effective Mass Transport Parameters

A correction factor (**Bruggeman**, **No Correction**, or **User defined**) to the mass transport parameters (defined in the **Transport Properties** node) can be applied for the porous domain. Species diffusivities and mobilities are automatically adjusted by the porous media corrections. For **User defined** enter a value or expression for the **Conversion factor** f_{eff}. The default is 1. Species diffusivities and mobilities are automatically adjusted by the porous media corrections.

Volume Force

The **Volume Force** node specifies the force $\mathbf{F}$ on the right-hand side of the Navier-Stokes or Brinkman equations, depending on whether the Porous Matrix Properties node is active for the domain. Use it, for example, to incorporate the effects of gravity in a model.

VOLUME FORCE

Enter the components of the **Volume force F** (SI unit: N/m^3).

Forchheimer Drag

The **Forchheimer Drag** subnode is available from the context menu (right-click the Porous Matrix Properties parent node) or from the **Physics** toolbar, **Attributes** menu. It can be used on the domain selection that corresponds to the porous medium. For the Brinkman equations the drag of the fluid on the porous matrix is proportional to the flow velocity, in the same way as for Darcy's law. Add a Forchheimer drag, proportional to the square of the fluid velocity, as needed.

FORCHHEIMER DRAG

Enter a value for the **Forchheimer coefficient** β_F (SI unit: kg/m^4).

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field u** (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Microfluidic Wall Conditions

Use the **Microfluidic Wall Conditions** node to add boundary conditions to the moving wall and specify whether to use viscous slip or thermal creep.

BOUNDARY CONDITION

The default **Boundary condition** for the wall is **Slip velocity**. Enter values or expressions for the components of the **Velocity of moving wall u_w** (SI unit: m/s).

Use Viscous Slip

Select the **Use viscous slip** check box to define the slip length:

- The default is **User defined**. Enter a value for L_s (SI unit: m). The default is 1e-7 m.

- Select **Maxwell's model** to calculate it from:

$$L_s = \left(\frac{2 - \alpha_v}{\alpha_v} \right) \lambda$$

- Then enter values or expressions for the **Tangential momentum accommodation coefficient** (TMAC) a_v (dimensionless) (the default is 0.9) and the **Mean free path** λ (SI unit: m) (the default is 1e-6 m).

Use Thermal Creep

Select the **Use thermal creep** check box to activate the thermal creep component of the boundary condition. Enter the fluid's **Temperature** T (SI unit: K) and the **Thermal slip coefficient** σ_T. The default temperature is 293.15 K and the default thermal slip coefficient is 0.75.

If you also have a license for the MEMS Module, an additional **Boundary condition** option **Electroosmotic velocity** is available. This is described in the *MEMS Module User's Guide*.

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls.

BOUNDARY CONDITION

Select a **Boundary condition** for the wall.

- No Slip[1]
- Slip
- Sliding Wall
- Moving Wall
- Leaking Wall

No Slip

No slip is the default boundary condition for a stationary solid wall for laminar flow (and SST, Low Re k-ε, Algebraic yPlus, L-VEL, and Spalart-Allmaras turbulence models). The condition prescribes $\mathbf{u} = 0$; that is, the fluid at the wall is not moving.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Sliding Wall

The **Sliding wall** boundary condition is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall $\mathbf{u}_w$** should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.

- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.

- For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the **Velocity of moving wall, φ component** v_w may also be specified.

Moving Wall

For an arbitrary wall movement, the condition $\mathbf{u} = \mathbf{u}_w$ may be prescribed. In this case, the components of the **Velocity of moving wall $\mathbf{u}_w$** should be specified.

Specifying this boundary condition does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_l$ through a perforated wall. The components of the **Fluid velocity $\mathbf{u}_l$** on the leaking wall should be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (![icon]( )) and selecting **Advanced Physics Options**.

![magnifier]	• Theory for the Wall Boundary Condition
	• Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

The Two-Phase Darcy's Law Interface

The **Two-Phase Darcy's Law (tpdl)** interface (🔹), found under the **Porous Media and Subsurface Flow** branch (🔹) when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It solves Darcy's law for the total pressure and the transport of the fluid content for one fluid phase. The physics interface can be used to model low velocity flows or media where the permeability and porosity are very small, for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. The physics interface can be used for stationary and time-dependent analyses.

The main feature is the Fluids and Matrix Properties node, which provides an interface for defining the two immiscible fluids properties along with the porous medium properties. The physics interface is available in 2D, 2D axisymmetric, and 3D.

When this physics interface is added, the following default nodes are also added in the **Model Builder**— **Fluids and Matrix Properties**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Two-Phase Darcy's Law** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tpdl`.

PHYSICAL MODEL

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Pressure** and **Fluid content 1**. The name can be changed but the names of fields and dependent variables must be unique within a component.

To display this section, click the **Show** button (🔄) and select **Stabilization**.

There are two consistent stabilization methods available —**Streamline diffusion** and **Crosswind diffusion**. **Streamline diffusion** is active by default. The **Residual** setting applies to both the consistent stabilization methods. **Approximate residual** is the default setting and it means that derivatives of the capillary diffusion tensor components are neglected. This setting is usually accurate enough and computationally faster. If required, select **Full residual** instead.

DISCRETIZATION

To display this section, click the **Show** button (🔄) and select **Discretization**.

⊙
- Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface
- Theory for the Two-Phase Darcy's Law Interface

Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law Interface has these domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡
In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid and Matrix Properties
- Inlet
- Initial Values
- Interior Wall

- Mass Flux
- No Flux
- Outlet
- Pressure and Saturation

For axisymmetric models, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Fluid and Matrix Properties

The **Fluids and Matrix Properties** node adds Equation 7-7 and Equation 7-8 and defines properties including density, dynamic viscosity, relative permeability, and porosity.

$$\frac{\partial}{\partial t}(\rho \varepsilon_p) + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{7-7}$$

$$\frac{\partial}{\partial t}(c_1 \varepsilon_p) + \nabla \cdot (c_1 \mathbf{u}) = \nabla \cdot D_c \nabla c_1 \tag{7-8}$$

CAPILLARY MODEL

The list defaults to **Capillary diffusion** or choose **Capillary pressure**.

For **Capillary diffusion**, choose **Isotropic** to define a scalar or **Diagonal**, **Symmetric**, or **Anisotropic** to enter a tensor, and then enter values or expressions in the D_c (SI unit: m^2/s) field or fields.

For **Capillary pressure**, select a **Pressure model**—**van Genuchten** (the default), **Brooks and Corey**, or **User defined**.

- For **van Genuchten**, enter an **Entry capillary pressure** p_{ec} (SI unit: Pa), the **Constitutive relations constant** m_{vG} (dimensionless), and **Constitutive relations constant** I_{vG} (dimensionless).
- For **Brooks and Corey**, enter an **Entry capillary pressure** p_{ec} (SI unit: Pa) and the **Pore size distribution index** λ_p (dimensionless).
- For **User defined**, enter a **Capillary pressure** p_c (SI unit: Pa).

FLUID 1 PROPERTIES

Select the material to use for **Fluid 1**. Select **Domain material** (the default value) to use the material defined for the domain. Select another material to use that material's properties.

Define the properties for **Fluid 1**:

The default **Density** ρ_1 (SI unit: kg/m^3) uses values **From material** based on the **Fluid 1** selection. For **User defined** enter another value or expression. The default is 0 kg/m^3.

Select a **Dynamic viscosity** μ_1 (SI unit: Pa·s). The default uses values **From material** as defined by the **Fluid 1** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

Select the **Relative permeability** κ_{r1} (a dimensionless number between 0 and 1) for fluid 1. The default is 1.

FLUID 2 PROPERTIES

The settings to define the properties for **Fluid 2** are similar as for **Fluid 1**.

MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** (the default) from the **Porous material** list to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From material**, defined by the **Porous material** selection. For **User defined** enter another value or expression The default is 0.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material** selection. For **User defined** select **Isotropic** to define a scalar or **Diagonal**, **Symmetric** or **Anisotropic** to enter a tensor and enter other values or expressions in the field or matrix.

Initial Values

The **Initial Values** node adds initial values for the pressure and the saturation of fluid 1 (that is, the fraction of that fluid inside the pore space) that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa. Enter a value or expression for the initial value of the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1). The default value is 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

No Flux

The **No Flux** node is the default boundary condition stating that there is no flow across impervious boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \mathbf{u} = 0$$

where $\mathbf{n}$ is the vector normal to the boundary.

Also, the No Flux boundary enforces a zero gradient condition for the fluid content across the selected boundary

$$\mathbf{n} \cdot \nabla c_1 = 0$$

Pressure and Saturation

Use the **Pressure and Saturation** node to specify the pressure and fluid volume fractions on a boundary. In many cases the distribution of pressure and saturation are known as numbers, distributions, or expressions involving time, t, for example.

PRESSURE AND SATURATION

Enter a value or expression for the **Pressure** p (SI unit: Pa), and for the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1). The default values are 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

Mass Flux

Use the **Mass Flux** node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain

$$-\mathbf{n} \cdot \rho \mathbf{u} = N_0$$

where N_0 is a value or expression for the inward (or outward) Darcy's flux that is specified.

MASS FLUX AND SATURATION

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: kg/(m$^2 \cdot$s)). A positive value of N_0 represents an inward mass flux, whereas a negative value represents an outward mass flux.

Enter a value or expression for the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1) in the mass flux. The default value is 0.

Inlet

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot \rho\mathbf{u} = (s_1\rho_1 + s_2\rho_1)U_0$$

where U_0 is a specified value or expression for the inward (or outward) Darcy's velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas a negative value represents an outflow.

INLET

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity, whereas a negative value represents an outward velocity.

Enter a value or expression for the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1). The default value is 0.

Outlet

The **Outlet** node adds a boundary condition for the outflow perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot D_c \nabla c_1 = 0$$

where D_c is the capillary diffusion (SI unit: m^2/s) and $c_1 = s_1\rho_1$ is the fluid 1 content (SI unit: kg/m^3). This means that the normal gradient of fluid saturation does not change through this boundary.

PRESSURE

Enter a value or expression for the **Pressure** p. The default value is 0. If the reference pressure p_{ref}, defined at the physics interface level is 0, enter the absolute pressure. Otherwise, enter the relative pressure.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an internal boundary. It allows discontinuities of velocity and

pressure across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

Theory for the Darcy's Law Interface

The Darcy's Law Interface theory is described in this section.

In a porous medium, the global transport of momentum by shear stresses in the fluid is often negligible: the pore walls impede momentum transport between fluid occupying different pores. In most applications, a detailed description of the resolution of every pore is not practical. A homogenization of the porous and fluid media into a single medium is a common alternative approach. Darcy's law, together with the continuity equation and equation of state for the pore fluid provides a complete mathematical model suitable for a variety of applications involving porous media flows when the pressure gradient is the major driving force.

Darcy's Law—Equation Formulation

Darcy's law states that the velocity field is determined by the pressure gradient, the fluid viscosity, and the structure of the porous medium:

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{7-9}$$

In this equation, κ (SI unit: m^2) denotes the permeability of the porous medium, μ (SI unit: kg/(m·s)) the dynamic viscosity of the fluid, p (SI unit: Pa) the pressure, and $\mathbf{u}$ (SI unit: m/s) the Darcy velocity. The Darcy's Law interface combines Darcy's law with the continuity equation:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho\mathbf{u}) = Q_m \tag{7-10}$$

In the above equation, ρ (SI unit: kg/m^3) is the density of the fluid, ε (dimensionless) is the porosity, and Q_m (SI unit: kg/(m^3·s)) is a mass source term. Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

If the Darcy's Law interface is coupled to an energy balance, then the fluid density can be a function of the temperature, pressure, and composition (for mixture flows). For gas flows in porous media, the relation is given by the ideal gas law:

$$\rho = \frac{pM}{RT} \tag{7-11}$$

where $R = 8.314$ J/(mol·K) is the universal gas constant, M (SI unit: kg/mol) is the molecular weight of the gas, and T (SI unit: K) is the temperature.

Theory for the Brinkman Equations Interface

The Brinkman Equations Interface theory is described in this section:

- About the Brinkman Equations
- Brinkman Equations Theory
- References for the Brinkman Equations Interface

About the Brinkman Equations

The *Brinkman equations* describe fluids in porous media for which the momentum transport within the fluid due to shear stresses is of importance. This mathematical model extends Darcy's law to include a term that accounts for the viscous transport in the momentum balance, and it treats both the pressure and the flow velocity vector as independent variables. Use the Free and Porous Media Flow interface to model combinations of porous media and free flow domains. These types of problems are often encountered in applications such as monolithic reactors and fuel cells.

🔍	The Free and Porous Media Flow Interface

In porous domains, the flow variables and fluid properties are defined at any point inside the medium by means of averaging of the actual variables and properties over a certain volume surrounding the point. This control volume must be small compared to the typical macroscopic dimensions of the problem, but it must be large enough to contain many pores and solid matrix elements.

Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

The physical properties of the fluid, such as density and viscosity, are defined as *intrinsic volume averages* that correspond to a unit volume of the pores. Defined this way, they present the relevant physical parameters that can be measured experimentally, and they are assumed to be continuous with the corresponding parameters in the adjacent free flow.

The flow velocity is defined as a *superficial volume average*, and it corresponds to a unit volume of the medium including both the pores and the matrix. It is sometimes called the Darcy velocity, defined as the volume flow rate per unit cross section of the medium. Such a definition makes the velocity field continuous across the boundaries between porous regions and regions of free flow.

Brinkman Equations Theory

The dependent variables in the Brinkman equations are the Darcy velocity and the pressure. The flow in porous media is governed by a combination of the continuity equation and the momentum equation, which together form the Brinkman equations:

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{br} \tag{7-12}$$

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) =$$

$$\tag{7-13}$$

$$-\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_{br}}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F}$$

In these equations:

- μ (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- $\mathbf{u}$ (SI unit: m/s) is the velocity vector
- ρ (SI unit: kg/m^3) is the density of the fluid
- p (SI unit: Pa) is the pressure
- ε_p is the porosity
- κ (SI unit: m^2) is the permeability tensor of the porous medium, and
- Q_{br} (SI unit: kg/(m^3·s)) is a mass source or mass sink

Influence of gravity and other volume forces can be accounted for via the force term $\mathbf{F}$ (SI unit: kg/(m^2·s^2)).

When the Neglect inertial term (Stokes-Brinkman) check box is selected, the term $(\mathbf{u} \cdot \nabla)(\mathbf{u}/\varepsilon_p)$ on the left-hand side of Equation 7-6 is disabled.

The mass source, Q_{br}, accounts for mass deposit and mass creation within the domains. The mass exchange is assumed to occur at zero velocity.

The Forchheimer drag option, β_F (SI unit: kg/m^4), adds a viscous force proportional to the square of the fluid velocity, $\mathbf{F}_F = -\beta_F|\mathbf{u}|\mathbf{u}$, to the right-hand side of Equation 7-6.

In case of a flow with variable density, Equation 7-5 and Equation 7-6 must be solved together with the equation of state that relates the density to the temperature and pressure (for instance the ideal gas law).

For incompressible flow, the density stays constant in any fluid particle, which can be expressed as

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \mathbf{u} \cdot \nabla \rho = 0$$

and the continuity equation (Equation 7-5) reduces to

$$\rho \nabla \cdot \mathbf{u} = Q_{\text{br}}$$

References for the Brinkman Equations Interface

1. D. Nield and A. Bejan, *Convection in Porous Media,* 3rd ed., Springer, 2006.

2. M. Le Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. of Fluid Mechanics,* vol. 550, pp. 149–173, 2006.

Theory for the Free and Porous Media Flow Interface

The Free and Porous Media Flow Interface uses the Navier-Stokes equations to describe the flow in open regions, and the Brinkman equations to describe the flow in porous regions.

The same fields, $\mathbf{u}$ and p, are solved for in both the free flow domains and in the porous domains. This means that the pressure in the free fluid and the pressure in the pores is continuous over the interface between a free flow domain and a porous domain. It also means that continuity is enforced between the fluid velocity in the free flow and the Darcy velocity in the porous domain. This treatment is one of several possible models for the physics at the interface. Examples of other models can be found in Ref. 1.

The continuity in $\mathbf{u}$ and p implies a stress discontinuity at the interface between a free-flow domain and a porous domain. The difference corresponds to the stress absorbed by the rigid porous matrix, which is a consequence implicit in the formulations of the Navier-Stokes and Brinkman equations.

Reference for the Free and Porous Media Flow Interface

1. M.L. Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

Theory for the Two-Phase Darcy's Law Interface

Darcy's Law

Darcy's law states that the velocity field is determined by the pressure gradient, the fluid viscosity, and the permeability of the porous medium. According to Darcy's law, the velocity field is given by

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \qquad (7\text{-}14)$$

In this equation:

- $\mathbf{u}$ (SI unit: m/s) is the Darcy velocity vector
- κ (SI unit: m^2) is the permeability of the porous medium
- μ (SI unit: Pa·s) is the fluid's dynamic viscosity, and
- p (SI unit: Pa) is the fluid's pressure

The permeability, κ, represents the resistance to flow over a representative volume consisting of solid grains and pores.

In the presence of two fluid phases, the average density ρ and average viscosity μ are calculated from the saturation and fluid property of each phase

$$1 = s_1 + s_2 \qquad (7\text{-}15)$$

$$\rho = s_1\rho_1 + s_2\rho_2 \qquad (7\text{-}16)$$

$$\frac{1}{\mu} = s_1\frac{\kappa_{r1}}{\mu_1} + s_2\frac{\kappa_{r2}}{\mu_2} \qquad (7\text{-}17)$$

here, s_1 and s_2 represent the saturation of each phase, ρ_1 and ρ_2 the densities, and κ_{r1} and κ_{r2} the relative permeabilities.

The Two-Phase Darcy's Law interface combines Darcy's law (Equation 7-14) with the continuity equation for the average density ρ

$$\frac{\partial}{\partial t}(\rho\varepsilon_p) + \nabla \cdot (\rho\mathbf{u}) = 0 \qquad (7\text{-}18)$$

here, ε_p is the porosity, defined as the fraction of the control volume that is occupied by pores. Inserting Darcy's law (Equation 7-14) into the continuity equation (Equation 7-18) produces the governing equation

$$\frac{\partial}{\partial t}(\rho \varepsilon_p) + \nabla \cdot \rho\left[-\frac{\kappa}{\mu}\nabla p\right] = 0 \tag{7-19}$$

When either of the fluids is compressible, its density can be related to the pressure (for instance using the ideal gas law).

Capillary Pressure

Beside the continuity equation for the mixture (Equation 7-19), the Two-Phase Darcy's Law interface also solves the transport equation for the fluid content of one of the phases, $c_1 = s_1\rho_1$

$$\frac{\partial}{\partial t}(\varepsilon_p c_1) + \nabla \cdot (c_1\mathbf{u}) = \nabla \cdot D_c \nabla c_1 \tag{7-20}$$

here, D_c (SI unit: m^2/s) is the capillary diffusion coefficient, which can be directly specified, or it can be derived from a capillary pressure expression. Normally, the fluid content c_1 will be the concentration of the wetting phase.

When *capillary pressure* is selected as capillary model, the capillary diffusion coefficient is computed from the saturation of one of the phases and the capillary pressure

$$D_c = \frac{\kappa_{r1}}{\mu_1}\kappa(s_1 - 1)\frac{\partial p_c}{\partial s_1} \tag{7-21}$$

The capillary pressure is defined as the pressure difference between the phases, and it can be defined as a function of saturation, $p_c(s_1)$. The capillary pressure can be a user defined expression, or it can be derived from van Genuchten or Brooks and Corey models.

For van Genuchten model, the expression for the capillary pressure as a function of saturation follows the curve

$$p_c = p_{ec}\left(\frac{1}{s_1^{1/m}} - 1\right)^{1-m} \tag{7-22}$$

where p_{ec} is the entry capillary pressure and m is a constitutive exponent.

For the Brooks and Corey model, the capillary pressure curve depends on saturation as

$$p_c = p_{ec} \frac{1}{s_1^{1/\lambda}}$$

(7-23)

where λ is the pore distribution index.

8

Chemical Species Transport Interfaces

The physics interfaces under the **Chemical Species Transport** branch ( ) accommodate all types of material transport that can occur through diffusion and convection. The section Modeling Chemical Species Transport helps you choose the best physics interface to start with.

In this chapter:

- The Transport of Diluted Species Interface
- The Transport of Concentrated Species Interface
- The Reacting Flow Multiphysics Interfaces
- The Reacting Flow in Porous Media Interfaces
- Theory for the Transport of Diluted Species Interface
- Theory for the Transport of Concentrated Species Interface
- Theory for the Reacting Flow Interfaces

Modeling Chemical Species Transport

In this section:

- Selecting the Right Physics Interface
- Coupling to Other Physics Interfaces
- Adding a Chemical Species Transport Interface

Selecting the Right Physics Interface

The behavior of chemical reactions in real environments is often not adequately described by the assumptions of perfectly mixed or controlled environments. This means that the transport of material through both time and space need to be considered. Physics interfaces in the **Chemical Species Transport** branch accommodate all types of material transport that can occur through diffusion and convection—either alone or in combination with one another. The branch includes physics interfaces solving equations for diluted as well as concentrated mixtures, where the species propagation can occur in solids, free flowing fluids, or through porous media.

The Transport of Diluted Species Interface ( ) is applicable for solutions (either fluid or solid) where the transported species have concentrations at least one order of magnitude less than the solvent. The settings for this physics interface can be chosen to simulate chemical species transport through diffusion (Fick's law) and convection (when coupled to fluid flow).

The Transport of Concentrated Species Interface ( ) is used for modeling transport within mixtures where no single component is clearly dominant. Often the concentrations of the participating species are of the same order of magnitude, and the molecular effects of the respective species on each other need to be considered. This physics interface supports transport through Fickean diffusion, a mixture average diffusion model, and as described by the Maxwell-Stefan equations.

REACTING FLOW

The Reacting Flow Multiphysics Interfaces ( ) combines the functionality of the Laminar Flow and Transport of Concentrated Species interfaces. Using this physics interface the mass and momentum transport in a reacting fluid can be modeled, with the couplings between the velocity field and the mixture density set up automatically. This physics interface is applicable for fluid flow in the laminar regime.

The Reacting Turbulent Flow, k-e Interface ($\approx$) combines the functionality of the Turbulent Flow, k-ε and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the standard k-ε model, solving for the turbulent kinetic energy k and the rate of dissipation of turbulent kinetic energy ε.

The Reacting Turbulent Flow, k-w Interface ($\approx$) combines the functionality of the Turbulent Flow, k-ω and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the Wilcox revised k-ω model, solving for the turbulent kinetic energy k and the rate of specific dissipation of turbulent kinetic energy ω.

The Reacting Turbulent Flow, SST Interface ($\approx$) combines the functionality of the Turbulent Flow, SST and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the Menter SST model, solving for the turbulent kinetic energy k and the rate of specific dissipation of turbulent kinetic energy ω. The physics interface also includes a wall distance equation that solves for the reciprocal wall distance.

The Reacting Turbulent Flow, Low Re k-e Interface ($\approx$) combines the functionality of the Turbulent Flow, Low Re k-ε and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the AKN low-Reynolds number k-ε model, solving for the turbulent kinetic energy k and the rate of dissipation of turbulent kinetic energy ε. The physics interface also includes a wall distance equation that solves for the reciprocal wall distance.

The Reacting Flow in Porous Media, Transport of Diluted Species Interface ( ),
merges the functionality of the Transport of Diluted Species and the Free and Porous
Media Flow interfaces into a multiphysics interface. This way, coupled mass and
momentum transport in free and porous media can be modeled from a single physics
interface, with the component coupling for the velocity field set up automatically. In
addition, the effective transport coefficients in a porous matrix domain can be derived
based on the corresponding values in for a non-porous domain.

The Reacting Flow in Porous Media, Transport of Concentrated Species Interface
( ), combines the Transport of Concentrated Species and the Free and Porous
Media Flow interfaces. This means that mass and momentum transport can be
modeled from a single physics interface, with the couplings between the velocity field
and the mixture density set up automatically. Also, the effective transport coefficients
in a porous matrix domain are derived based on the corresponding values for a
non-porous domain. This physics interface is applicable for fluid flow in the laminar
regime.

Coupling to Other Physics Interfaces

When you are simulating applications that can be described by the material transport
interfaces in the **Chemical Species Transport** branch, there is often a need to couple the
material transport to other physics interfaces. Convection is often the cause of the
material transport, so couplings to Fluid Flow interfaces is required. The CFD Module
includes physics interfaces for Laminar Flow and Porous Media Flow as well as more
advanced descriptions of fluid flow, such as turbulent and Multiphase Flow.

Moreover, most chemical reactions or other types of material processing, such as
casting, either require or produce heat, which in turn affects both the reaction and
other physical processes connected to the system. This module includes physics
interfaces for heat transfer through conduction and convection as well as through
porous media. More extensive description of heat transfer, such as surface-to-surface
radiation, can be found in the Heat Transfer Module.

Finally, COMSOL Multiphysics supports simulations of electrostatics or DC-based
physical phenomena, even when the conductivity is nonlinear. If the electric field is
AC/DC in nature, or if your system is affected by electromagnetic waves, then the
AC/DC Module and RF Module include appropriate physics interfaces for such
phenomena. Furthermore, some applications of electrochemical reactions, particularly

in electrochemical power source applications, are better handled by the Batteries & Fuel Cells Module.

Adding a Chemical Species Transport Interface

A chemical species transport interface can be added when first creating a new model, or at any time during the modeling process.

Q	Creating a New Model in the *COMSOL Multiphysics Reference Manual*

1 To add a physics interface:

- Select **New** to open the **Model Wizard**, after selecting a space dimension, go to the **Select Physics** page.

- From the **Home** toolbar, click **Add Physics** (🜨). Or right-click the **Component** node in the **Model Builder** and select **Add Physics**. Go to the **Add Physics** window.

2 Under **Chemical Species Transport**, navigate to the physics interface to add and double-click it.

There are other ways to add a physics interface depending on whether you are in the Model Builder or Add Physics window:

- In the **Model Wizard**, click **Add** or right-click and select **Add Physics** (➕). The physics interface displays under **Added physics interfaces**.

- In the **Add Physics** window, click **Add to Component** (➕) or right-click and select **Add to Component**.

3 Specify the number of species (concentrations or mass fractions) and the names:

- In the **Model Wizard**, on the **Review Physics Interface** page under **Dependent Variables**.

- In the **Add Physics** window, click to expand the **Dependent Variables** section.

- After adding the physics interface, you can also edit this information—click the node in the **Model Builder**, then, on the **Settings** window under **Dependent Variables**, specify the information.

4 Continue by adding more interfaces and specifying the number of species (concentrations or mass fractions) that are to be simulated in a mass transport physics interface when adding that interface.

5 In the **Dependent Variables** section, enter the **Number of species**. To add a single species, click the **Add Concentration** button (➕) underneath the table or enter a value into the **Number of species** field. Click the **Remove Concentration** button (▤ₓ) underneath the table if required.

The **Transport of Concentrated Species** interface needs to contain at least two species (the default). Also edit the strings or names directly in the table. The names must be unique for all species (and all other dependent variables) in the model.

The Transport of Diluted Species Interface

The **Transport of Diluted Species (tds)** interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid, or solid can be handled with this interface. The driving forces for transport can be diffusion by Fick's law, convection when coupled to a flow field, and migration, when coupled to an electric field.

The interface supports simulation of transport by convection and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, c_i, of each species i.

> Some features are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit http://www.comsol.com/products/specifications/

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tds`.

DOMAIN SELECTION

If any part of the model geometry should not partake in the mass transfer model, remove that part from the selection list.

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the check boxes available under **Additional transport mechanisms** to control other transport mechanisms.

Note: Not all additional transport mechanisms listed below are available in all products. For details see http://www.comsol.com/products/specifications/.

- By default, the **Convection** check box is selected. Clear the check box to disable convective transport.

- Select the **Migration in electric field** check box to activate the migration transport of ionic species. See further the theory section Adding Transport Through Migration.

Mass Transport in Porous Media

The **Mass transport in porous media** check box activates functionality specific to species transport in porous media. When selected, the following transport mechanisms are available:

- Select the **Dispersion in porous media** check box to activate the dispersion mechanism in porous media. See further Dispersion in the theory chapter.

- Select the **Volatilization in partially saturated porous media** check box to model volatilization in partially saturated domains. Theory for the Transport of Diluted Species Interface

The following features are also enabled when selecting the **Mass transport in porous media** check box:

- Adsorption
- Porous Media Transport Properties

CONSISTENT STABILIZATION

To display this sections, click the **Show** button ( ) and select **Stabilization**.

- When the **Crosswind diffusion** check box is selected, a weak term that reduces spurious oscillations is added to the transport equation. The resulting equation system is always nonlinear. There are two options for the **Crosswind diffusion type**:

  - **Do Carmo and Galeão** — the default option. This type of crosswind diffusion reduces undershoots and overshoots to a minimum but can in rare cases give equation systems that are difficult to fully converge.

  - **Codina**. This option is less diffusive compared to the Do Carmo and Galeão option but can result in more undershoots and overshoots. It is also less effective for anisotropic meshes. The Codina option activates a text field for the **Lower**

gradient limit g_{lim}. It defaults to `0.1[mol/m^3]/tds.helem`, where `tds.helem` is the local element size.

- For both consistent stabilization methods, select an **Equation residual**. **Approximate residual** is the default and means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is computationally faster. If required, select **Full residual** instead.

INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**. By default, the **Isotropic diffusion** check box is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for under-resolved problems.

ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed. Select a **Convective term**— **Non-conservative form** (the default) or **Conservative form**. The conservative formulation should be used for compressible flow. See Convective Term Formulation for more information.

DISCRETIZATION

To display this section, click the **Show** button ( ) and select **Discretization**.

The **Compute boundary fluxes** check box is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option is checked, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the check box is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

The flux variables affected in the interface are:

- ndflux_*c* (where *c* is the dependent variable for the concentration). This is the normal diffusive flux and corresponds to the boundary flux when diffusion is the only contribution to the flux term.

- ntflux_*c* (where *c* is the dependent variable for the concentration). This is the normal total flux and corresponds to the boundary flux plus additional transport terms, for example, the convective flux when you use the non-conservative form.

Also the **Apply smoothing to boundary fluxes** check box is available if the previous check box is checked. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the *COMSOL Multiphysics Reference Manual*.

The **Value type when using splitting of complex variables** setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variable name is **Concentration** c by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the **Number of species**. Use the **Add concentration** (➕) and **Remove concentration** (▤✗) buttons as needed.

- Theory for the Transport of Diluted Species Interface
- Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*.
- Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface
- In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

- *Effective Diffusivity in Porous Materials*: Application Library path **COMSOL_Multiphysics/Diffusion/effective_diffusivity**
- *Thin-Layer Diffusion*: Application Library path **COMSOL_Multiphysics/ Diffusion/thin_layer_diffusion**

The Transport of Diluted Species in Porous Media Interface

This interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the species concentration and transport in free and porous media. The interface is the same as the *Transport of Diluted Species* interface but it uses other defaults: The Mass Transport in Porous Media property is selected, and a Porous Media Transport Properties node is added by default. The interface includes reaction rate expressions and solute sources for modeling of species transport and reaction in porous media.

This interface is dedicated to modeling transport in porous media, including immobile and mobile phases, where the chemical species may be subjected to diffusion, convection, migration, dispersion, adsorption, and volatilization in porous media. It supports cases where either the solid phase substrate is exclusively immobile, or when a gas-filling medium is also assumed to be immobile.

It applies to one or more diluted species or solutes that move primarily within a fluid that fills (saturated) or partially fills (unsaturated) the voids in a solid porous medium. The pore space not filled with fluid contains an immobile gas phase. Models including a combination of porous media types can be studied.

The main feature nodes are the **Porous Media Transport Properties** and **Partially Saturated Porous Media** nodes, which add the equations for the species concentrations and provide an interface for defining the properties of the porous media, as well as additional properties governing adsorption, volatilization, dispersion and diffusion, migration, and the velocity field to model convection.

The physics interface can be used for stationary and time-dependent analysis.

When this physics interface is added, these default nodes are also added to the **Model Builder**—**Porous Media Transport Properties**, **No Flux** (the default boundary condition), and . Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, reaction rate expressions, and species sources. You can also right-click **Transport of Diluted Species in Porous Media** to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as The Transport of Diluted Species Interface.

FURTHER READING

ℚ	• Theory for the Transport of Diluted Species Interface • Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

▥	• *Variably Saturated Flow and Transport—Sorbing Solute*: Application Library path **Subsurface_Flow_Module/Solute_Transport/ sorbing_solute** Web link: http://www.comsol.com/model/ variably-saturated-flow-and-transport-sorbing-solute-490

Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface has the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar

(Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

> To add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Adsorption
- Concentration
- Flux
- Flux Discontinuity
- InflowInitial Values
- Initial Values
- Line Mass Source
- No Flux
- Open Boundary

- Outflow
- Periodic Condition
- Point Mass Source
- Reactions
- Symmetry
- Thin Diffusion Barrier
- Thin Impermeable Barrier
- Transport Properties
- Turbulent Mixing

Some features may require certain add-on modules. See details http://www.comsol.com/products/specifications/

> For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on boundaries representing the symmetry axis.

> In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Transport Properties

The settings in this node are dependent on the check boxes selected under Transport Mechanisms on the Settings window for the Transport of Diluted Species interface. It

includes only the sections required by the activated transport mechanisms. It has all the equations defining transport of diluted species as well as inputs for the material properties.

When the **Convection** check box is selected, the Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu. Note that this feature is only available in some COMSOL products. See details: http://www.comsol.com/products/specifications/.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Select an option from the **Material** list. This selection list can only be used if a material has been added in the Materials node and if that material has a diffusion coefficient defined. Else, you need to type in the diffusivity in the **User Defined** edit field.

Enter the **Diffusion coefficient** D_c for each species. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type —**Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: http://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

- Enter a value or expression for the **Electric potential** V, which is **User defined**; this input option is always available.

- Select the electric potential solved by an AC/DC-based interface that has also been added to the model.

- Select the electric potential defined or solved by Electrochemistry interface that has been added to the component.

By default the **Mobility** is set to be calculated based on the species diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, and under **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** — and type in the value of expression of the mobility $u_{m,c}$.

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based on the Nernst-Einstein relation) is taken from **Model Inputs** section.

Note that the migration in electric fields feature is only available in some COMSOL products. See details: http://www.comsol.com/products/specifications/.

EXAMPLE MODELS

▦	*Separation Through Dialysis*: Application Library path **Chemical_Reaction_Engineering_Module/Separation_Processes/dialysis** Web link: http://www.comsol.com/model/separation-through-dialysis-258

Transport in an Electrokinetic Valve: Application Library path
Microfluidics_Module/Fluid_Flow/electrokinetic_valve

Web link:
http://www.comsol.com/model/electrokinetic-valve-603

Turbulent Mixing

Note that the Turbulent Mixing node is only available for some product add-ons. See details: http://www.comsol.com/products/specifications/.

This subnode is available from the context menu (right-click the Transport Properties parent node) as well as from the **Physics** toolbar, **Attributes** menu, if **Convection** is selected as a transport mechanism. Use this node to account for the turbulent mixing caused by the eddy diffusivity. An example is when the specified velocity field corresponds to a RANS solution.

TURBULENT MIXING PARAMETERS

Some physics interfaces provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** ν_T list. The list always contains the **User defined** option where any value or expression can be entered.

The default **Turbulent Schmidt number** Sc_T is 0.71 (dimensionless).

FURTHER READING

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

Turbulent Mixing of a Trace Species: Application Library path
CFD_Module/Single-Phase_Tutorials/turbulent_mixing

Web link:
http://www.comsol.com/model/
turbulent-mixing-of-a-trace-species-12727

Initial Values

The **Initial Values** node specifies the initial values for the concentration of each species. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

INITIAL VALUES

Enter a value or expression for the initial value of the **Concentration** or concentrations, c_i. This also serves as a starting guess for stationary problems.

Mass-Based Concentrations

Use the **Mass-Based Concentrations** node to add postprocessing variables for mass-based concentrations (SI unit: kg/m^3) and mass fractions (dimensionless) for all species.

MIXTURE PROPERTIES

The default **Solvent density** ρ_{solvent} is taken **From material**. For **User defined,** enter a value or expression manually. Define the **Molar mass** of each species, which is needed to calculate the mass-based concentration.

Reactions

Use the **Reactions** node to account for the consumption or production of species through chemical reactions. Define the rate expressions as required.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

REACTION RATES

Add a rate expression R_i (SI unit: mol/(m^3·s)) for species i. Enter a value or expression in the field. Note that if you have the *Chemistry* interface available, provided with the

Chemical Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down menu. For an example, see the application *Fine Chemical Production in a Plate Reactor* as linked below.

REACTING VOLUME

This section is only available when the Mass Transport in Porous Media property is available and selected. See http://www.comsol.com/products/specifications/ for more details on availability.

When specifying reaction rates for a species in porous media, the specified reaction rate may have the basis of the total volume, the pore volume, or the volume of a particular phase.

- For **Total volume**, the reaction expressions in mol/(m^3·s) are specified per unit volume of the model domain (multiplied by unity).

- For **Pore volume**, the reaction expressions in mol/(m^3·s) are specified per unit volume of total pore space. The reaction expressions will be multiplied by the domain porosity, ε_p. (ε_p equals unity for nonporous domains.)

- For **Liquid phase**, the reaction expressions in mol/(m^3·s) are specified per unit volume of liquid in the pore space. The expressions will be multiplied by the liquid volume fraction θ. (θ equals ε_p for Saturated Porous Media domains).

- For **Gas phase**, the expressions are multiplied by the gas volume fraction $a_v = \varepsilon_p - \theta$. a_v equals 0 for Saturated Porous Media domains.

FURTHER READING

See the theory chapter on chemical species transport, starting with the section *Mass Balance Equation*.

	- *Fine Chemical Production in a Plate Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/ Reactors_with_Mass_and_Heat_Transfer/plate_reactor** Web link: http://www.comsol.com/model/ fine-chemical-production-in-a-plate-reactor-8589

No Flux

This node is the default boundary condition on exterior boundaries. It represents boundaries where no mass flows in or out of the boundaries. Hence, the total flux is zero.

Inflow

Use this node to specify all species concentrations at an inlet boundary.

If you want to specify the concentration of a subset of the partaking species, this can be done by using the Concentration node instead.

For the **Electroanalysis** interface, this node is available when you select the **Convection** check box on the physics interface **Settings** window.

CONCENTRATION
For the concentration of each species $c_{0,c}$ (SI unit: mol/m^3), enter a value or expression.

BOUNDARY CONDITION TYPE
This section in the settings is only available for some products. Search for "Inflow" on the page: http://www.comsol.com/products/specifications/ for more details on availability.

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints. The other option, **Flux (Danckwerts)** can be more stable and fast to solve when high reaction rates are anticipated in the vicinity of the inlet. Oscillations on the solutions can also be avoided in such cases. The latter condition uses a flux boundary condition based on the velocity across the boundary and the concentration values. See further details in the theory section.

CONSTRAINT SETTINGS
To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms.

FURTHER READING
See the theory chapter in the section .

Outflow

This node is not available if **Diffusion** only is included in the model.

Set this condition at outlets where species are transported out of the model domain by fluid motion. It is assumed that convection is the dominating transport mechanism across outflow boundaries, and therefore that diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D\nabla c) = 0$$

Concentration

This condition node adds a boundary condition for the species concentration. For example, a $c = c_0$ condition specifies the concentration of species c.

CONCENTRATION

Individually specify the concentration for each species. Select the check box for the **Species** to specify the concentration, and then enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the check box for the concentration of that species.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms.

Flux

This node can be used to specify the total species flux across a boundary. The total flux of species c is defined accordingly:

$$-\mathbf{n} \cdot (c\mathbf{u} - D\nabla c) = N_0$$

where N_0 is an arbitrary user-specified flux expression (SI unit: mol/(m^2·s)). For example, N_0 can represent a flux from or into a much larger surrounding environment, a phase change, or a flux due to chemical reactions. N_0 can also be a function of the concentration and the electric potential (if the mass transport includes migration of ionic species).

When diffusion is the only transport mechanism present, the flux condition is extended to include a mass transfer term to describe flux into a surrounding environment:

$$-\mathbf{n} \cdot (-D\nabla c) = N_0 + k_c(c_b - c)$$

where k_c is a mass transfer coefficient (SI unit: m/s), and c_b is the concentration (SI unit: mol/m^3) in the surroundings of the modeled system (the bulk concentration). The mass transfer coefficient (to be specified) is often given by boundary-layer theory.

INWARD FLUX

This is used to individually specify the flux of each species. To use another boundary condition for a specific species, click to clear the check box for the mass fraction of that species.

Note: Use a minus sign when specifying a flux leaving the system.

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric, that is, where there is no mass flux in the normal direction across the boundary.

This boundary condition is identical to that of the No Flux node, but applies to all species and cannot be applied to individual species.

Flux Discontinuity

This node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n} \cdot (\mathbf{N}_d - \mathbf{N}_u) = N_0 \qquad \mathbf{N} = (c\mathbf{u} - D\nabla c)$$

where the value N_0 (SI unit: mol/(m^2·s)) specifies the jump in flux at the boundary. This can be used to model a boundary source, for example a surface reaction, adsorption or desorption.

FLUX DISCONTINUITY

In this section the jump in species flux (or surface source) is specified.

Select the Species check box for the species to specify and enter a value or expression for the material flux jump in the corresponding field. To use a different boundary

condition for a specific species, click to clear the check box for the flux discontinuity of that species.

Periodic Condition

The **Periodic Condition** node can be used to define periodicity or antiperiodicity between two boundaries. The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that can each consist of several connected boundaries. For more complex geometries, it might be necessary to add the **Destination Selection** subnode, which is available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

With this subnode, the boundaries that constitute the source and destination surfaces can be manually specified.

FURTHER READING

For an example of using a periodic condition, see this application example:

	The KdV Equation and Solitons: Application Library path **COMSOL_Multiphysics/Equation_Based/kdv_equation**

Line Mass Source

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

The **Line Mass Source** feature models mass flow originating from a tube or line region with an infinitely small radius.

For the "Reacting Flow in Porous Media, Diluted Species" interface, which is available in some add-on products, the **Line Mass Source** node is available in two versions, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the symmetry axis and the symmetry axis
3D	Edges

SPECIES SOURCE

Enter the source strength, $\dot{q}_{l,c}$, for each species (SI unit: mol/(m·s)). A positive value results in species injection from the line into the computational domain, and a negative value means that the species is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Point Mass Source

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

The **Point Mass Source** feature models mass flow originating from an infinitely small domain around a point.

For the "Reacting Flow in Porous Media, Diluted Species" interface, which is available in some add-on products, the **Point Mass Source** node is available in two versions, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

SPECIES SOURCE

Enter the source strength, $\dot{q}_{p,c}$, for each species (SI unit: mol/s). A positive value results in species injection from the point into the computational domain, and a negative value means that the species is removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.

See the section Mass Sources for Species Transport.

Open Boundary

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to set up mass transport across boundaries where both convective inflow and outflow can occur. Use this boundary condition to specify an exterior species concentration on parts of the boundary where fluid flows into the domain. A condition equivalent to the **Outflow** node applies to the parts of the boundary where fluid flows out of the domain.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Transport of Diluted Species interface.

EXTERIOR CONCENTRATION

Enter a value or expression for the **Exterior concentration**.

Thin Diffusion Barrier

Use this boundary condition to model a thin layer through which mass is transported by diffusion only. To set up the node, specify the layer thickness and a diffusion coefficient for each transported species.

THIN DIFFUSION BARRIER

Enter a **Layer thickness** d_s (SI unit: m). The default is 0.005 m (5 mm). Enter a **Diffusion coefficient** $D_{s,c}$ (SI unit: m^2/s). The default is 0.

Thin Impermeable Barrier

This feature models a thin mass transfer barrier. The feature is available on interior boundaries and introduces a discontinuity in the concentration across the boundary. On each side of the boundary, a no-flux condition is prescribed for the mass transport. The Thin Impermeable Barrier boundary feature can be used to avoid meshing thin structures.

Solving a model involving coupled fluid flow and mass transfer, the Thin Impermeable Barrier feature can be combined with an Interior Wall or Rotating Interior Wall feature in order to model a thin solid wall.

Equilibrium Reaction

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model an equilibrium reaction in a domain. This feature is available with two species or more.

The equilibrium reaction is defined by the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition) and the stoichiometry of the reaction.

The node solves for an additional degree of freedom (the reaction rate) to fulfill the equilibrium condition at all times in all space coordinates.

If the **Apply equilibrium condition on inflow boundaries** check box is selected, the specified inflow concentration values in all active **Inflow** boundary nodes for the physics interface are modified to comply with the equilibrium condition.

EQUILIBRIUM CONDITION

The list defaults to **Equilibrium constant** or select **User defined**. For either option, the **Apply equilibrium condition on inflow boundaries** check box is selected by default.

For **Equilibrium constant**, enter an **Equilibrium constant** K_{eq} (dimensionless). The default is 1. Enter a value or expression for the **Unit activity concentration** C_{a0} (SI unit: mol/m^3). The default is $1 \cdot 10^{-3}$ mol/m^3. **Equilibrium constant** creates an equilibrium condition based on the stoichiometric coefficients, the species activities, and the law of mass action.

For **User defined**, enter an **Equilibrium expression** E_{eq} (dimensionless).

STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient ν_c (dimensionless). The default is 0. Use negative values for reactants and positive values for products in the modeled reaction.

Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium Reaction** node.

Surface Equilibrium Reaction

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model an equilibrium reaction on a boundary (surface). The settings for this node are similar to Equilibrium Reaction.

Porous Electrode Coupling

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to add a molar source in a domain that is coupled to one or multiple Porous Electrode Reaction nodes of an Electrochemistry Interface.

The molar source is calculated from the number of electrons, stoichiometric coefficients, and volumetric current densities of the coupled porous electrode reactions specified in the **Reaction Coefficients** subnodes.

In the Transport of Concentrated Species interface, the molar sources (or sinks) are multiplied by the species molar masses to obtain the corresponding mass sources.

Additional Reaction Coefficients subnodes are available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Note that if you are also modeling the momentum transport and expect a non-negligible total mass source or sink, which is often the case in gas diffusion electrodes, you need to also add a corresponding Porous Electrode Coupling node in the Fluid Flow interface.

Reaction Coefficients

Add this node to the Electrode Surface Coupling and Porous Electrode Coupling features to define molar fluxes and sources based on electrode current densities in an **Electrochemistry** interface.

The molar flux or source is proportional to the stoichiometric coefficients and the current density according to Faraday's law.

Current densities from **Electrode Reaction** (i_{loc}, SI unit: A/m^2) or **Porous Electrode Reaction** nodes (i_v, SI unit: A/m^3) of any **Electrochemistry** interface in the model are

available for selection as the **Coupled reaction**, and user-defined expressions are also supported.

Enter the **Number of participating electrons** n_m (dimensionless) and the **Stoichiometric coefficient** v_c (dimensionless) as explained in the theory section linked below.

Use multiple subnodes to couple to multiple reactions.

Electrode Surface Coupling

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to define a flux boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flux is proportional to the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficients subnodes.

In the Transport of Concentrated Species interface, the molar fluxes are multiplied by the species molar masses to obtain the corresponding mass fluxes.

Note that if you are also modeling the momentum transport and expect a non-negligible total mass flux over the boundary, which is often the case for gas diffusion electrodes, you need to also add a corresponding Electrode Surface Coupling node in the Fluid Flow interface.

Porous Media Transport Properties

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model the concentration of diluted species transported through interstices in porous media. A part form convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and reaction.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

MATRIX PROPERTIES

Select an option from the **Porous material** list. The default is **Domain material**.

By default the **Porosity,** ε_p (dimensionless) is taken **From material**. For **User defined**, enter a different value. The default is 0.3.

When the **Mass transport in porous media** check box is selected in the **Settings** window of the physics interface, a setting for the **Density** ρ of the porous media is available. By default it is set to be taken **From material**.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Select a **Fluid material** (when available and applicable).

Specify the **Fluid diffusion coefficient** $D_{F,i}$ (SI unit: m^2/s). Enter a value or expression for each of the species in the corresponding input field. The default is 1×10^{-9} m^2/s.

Select the **Effective diffusivity model**: **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{F,i}$ (dimensionless). The default is 1.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

• Enter a value or expression for the **Electric potential** V, which is **User defined**; this input option is always available.

- Select the electric potential solved by an AC/DC-based interface that has also been added to the model.

- Select the electric potential defined or solved by Electrochemistry interface that has been added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, and under **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** — and type in the value of expression of the effective mobility $u_{\mathrm{me,c}}$.

Enter the **Charge number** z_c for each species.

DISPERSION

This section is available when the **Dispersion in porous media** check box is selected on the **Settings** window for the physics interface.

Select the **Specify dispersion for each species individually** check box to specify the dispersion tensor D_D (SI unit: m^2/s) for each species separately. The default is to use the same dispersion tensor D_D for all species.

Select an option from the **Dispersion tensor** list—**User defined** (the default) or **Dispersivity**. For **User defined**, use it to specify the dispersion components as user-defined constants or expressions. Select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the properties of the dispersion tensor.

Select **Dispersivity** when **Convection** has been added as the transport mechanism. Specify the dispersivities (SI unit: m) to define the dispersion tensor D_D (SI unit: m^2/s) together with the velocity field **u**. Select an option from the **Dispersivity model** list: **Isotropic** (the default) or **Transverse isotropic** based on the properties of the porous media. For isotropic porous media, specify the longitudinal and transverse dispersivities. For transverse isotropic porous media, specify the longitudinal, horizontal transverse, and vertical transverse dispersivities.

Adsorption

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model adsorption of the fluid phase species onto the porous media surface. It is available as a subnode to the Porous Media Transport Properties and the Partially Saturated Porous Media nodes.

Select a **Sorption type** — **Langmuir** (the default), **Freundlich**, or **User defined** to specify how to compute c_P, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

- For **Langmuir**:

  Enter a **Langmuir constant** $k_{L,c}$ (SI unit: m^3/mol) and an **Adsorption maximum** $c_{p,max,c}$ (SI unit: mol/kg):

- For **Freundlich**:

  Enter a **Freundlich constant** $k_{F,c}$ (SI unit: mol/kg), a **Freundlich exponent** $N_{F,c}$ (dimensionless), and a **Reference concentration** $c_{ref,c}$ (SI unit: mol/m^3).

- For **User defined**:

  Enter an **Adsorption isotherm** $k_{P,c}$ (SI unit: m^3/kg).

For more information, see Adsorption in the theory section.

FURTHER READING

See the theory chapter in the section .

Partially Saturated Porous Media

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model the concentration of diluted species transported by a liquid through in partially filled porous media. The interstices of the porous media contains the liquid carrier phase and gas pockets. A part form convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, reaction, and volatilization.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

SATURATION

Select **Saturation** or **Liquid volume fraction** from the list.

For **Saturation**, enter a value for s (dimensionless) between 0 and 1. The liquid volume fraction is then computed from the saturation and porosity as $\theta = s\varepsilon_p$.

For **Liquid volume fraction**, enter a value for θ (dimensionless) between 0 and the value of porosity. The saturation is then computed from the porosity and the liquid volume fraction as $s = \theta\varepsilon_p$.

Select a **Fluid fraction time change**: **Fluid fraction constant in time** (the default), **Time change in fluid fraction**, or **Time change in pressure head**.

- For **Time change in fluid fraction**, enter $d\theta/dt$ (SI unit: 1/s).

- For **Time change in pressure head**, enter dH_p/dt (SI unit: m/s) and a **Specific moisture capacity** C_m (SI unit: 1/m).

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Select a **Liquid material** from the list.

Specify the **Liquid diffusion coefficient** $D_{L,c}$ (SI unit: m^2/s). Enter a value or expression for each of the species in the corresponding input field. The default is 1 x 10^{-9} m^2/s.

Select the **Effective diffusivity model, liquid**: **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined**. For **Tortuosity model**, enter a value for $\tau_{L,c}$ (dimensionless). The default is 1.

When the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface, also define the **Gas material**, **Gas diffusion coefficient**, and **Effective diffusivity model, gas**.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. It is similar to that in **Porous Media Transport Properties** feature. Select the source of electric field from the **Electric potential** list. The default selection to **Mobility** is the **Nernst-Einstein relation**.

DISPERSION

This section is available when the **Dispersion in porous media** check box is selected on the **Settings** window for the physics interface. The settings are the same as for Porous Media Transport Properties.

VOLATILIZATION

This section is available when the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface.

Enter a value for the **Volatilization** $k_{G,c}$ (dimensionless) for each species.

Volatilization

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

This feature is available when the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface.

Use the boundary condition to model a thin layer through which mass is transported by volatilization only. To set up the node, specify the layer thickness and the atmospheric concentration of each species in the thin layer for each transported species.

VOLATILIZATION

Enter a **Layer thickness** d_s and the atmospheric concentration for each species. The **Gas diffusion coefficient** $D_{G,c}$ (SI unit: m^2/s) and the **Volatilization** coefficient $k_{G,c}$ (dimensionless) for each species are taken from the adjacent **Partially Saturated Porous Media** domain.

Reactive Pellet Bed

This feature is only available if you are licensed to use the Chemical Reaction Engineering Module. See details: http://www.comsol.com/products/specifications.

Use this feature to model packed bed reactors with catalytic pellets. For details, see the section Theory for the Reactive Pellet Bed in the *Chemical Reaction Engineering Module User's Guide*. By default, subnodes for Reactions and Initial Values are added.

BED PARAMETERS

Here you can specify the bed porosity, which is the void fraction in the packed bed structure. Select **From densities** to calculate the porosity from the bed density and the individual pellet density. Select **User defined** to specify the porosity directly.

PELLET SHAPE AND SIZE

The default shape is spherical. Cylinders, flakes, and user-defined shapes can also be selected. A uniform pellet size or a discrete size distribution can be selected. Select a **Pellet size distribution** — **Uniform size** (the default), **Two sizes**, **Three sizes**, **Four sizes**, or **Five sizes** to select up to five different particle sizes.

Depending on the shape selection, equivalent radii or volumes and surface areas will be required as input. If a size distribution is selected, the volume percentage of each size is required as input.

Note that different chemical reactions can be specified for each pellet size if a distribution is specified.

SURFACE SPECIES

In order to add surface species, click the **Add** button and enter the species name in the **Surface species** table. Added surface species are be available inside all pellet types defined in the **Pellet Shape and Size** section, but not in the bulk fluid.

For each pellet type, specify the **Reactive specific surface area**, $S_{b,reac}$ (SI unit: $1/m$), corresponding to the surface area, per volume, available for surface reactions.

PELLET PARAMETERS

Enter a **Pellet porosity** ε_{pe} (dimensionless) to specify the porosity of the pellet internals.

Select **Diffusion model**—**Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined** to describe the effective correction of the diffusion coefficient in the pellet. In the case of the **Tortuosity model**, a value for the tortuosity τ_{pe} within the pellet is required.

Enter also the **Diffusion coefficient** $D_{pe,c}$ (SI unit: m^2/s). If a **User defined** diffusion model is selected, an **Effective diffusion coefficient** $D_{peff,c}$ (SI unit: m^2/s) is entered. The default value is $1 \cdot 10^{-9}$ m^2/s in both cases.

PELLET-FLUID SURFACE

For the coupling of concentration between the pellet internals and the surrounding fluid, two **Coupling type** options are available:

- **Continuous concentration**, assuming that all resistance to mass transfer to/from the pellet is within the pellet and no resistance to pellet-fluid mass transfer is on the bulk fluid side. The concentration in the fluid will thus be equal to that in the pellet pore just at the pellet surface: $c_{pe,i} = c_i$. This constraint also automatically ensures flux continuity between the internal pellet domain and the free fluid domain through so-called reaction forces in the finite element formulation.

- **Film resistance (mass flux)**: The flux of mass across the pellet-fluid interface into the pellet is possibly rate determined on the bulk fluid side, by film resistance. The resistance is expressed in terms of a film mass transfer coefficient, h_{Di}, such that:

$$N_{i,\text{inward}} = h_{D,i}(c_i - c_{pe,i}) \, .$$

The **Film resistance (mass flux)** option computes the inward surface flux, $N_{i,\text{inward}} = h_{Di}(c_i - c_{pe,i})$. h_{Di} is the mass transfer coefficient (SI unit: m/s) and is calculated with the default **Automatic** setting from a dimensionless **Sherwood number expression** or with **User defined** mass transfer coefficients.

The **Active specific surface area** (SI unit: m^{-1}) is required to couple the mass transfer between the pellets and the bed fluid. Select either the **Automatic** setting that calculates the specific surface area from the shape information given above. User defined is also available for explicit surface area specification.

The **Sherwood number expression** can be computed from three available expressions: **Frössling**, **Rosner**, and **Garner and Keey**. The Frössling equation is the default and probably the most commonly used for packed spheres. All of these are based on the dimensionless Reynolds, Re, and Schmidt, Sc, numbers, which are computed from **Density** and **Dynamic viscosity**. Select these to be taken either **From material** or choose the **User defined** alternative.

PELLET DISCRETIZATION

The extra dimension in the pellet needs to be discretized into elements. Select a **Distribution** — **Cubic root sequence** (the default), **Linear**, or **Square root sequence**. Enter the **Number of elements** N_{elem}.

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**. See the details about the different constraint settings in the section Constraint Reaction Terms.

FURTHER READING

Theory for the Reactive Pellet Bed in the *Chemical Reaction Engineering Module User's Guide*.

For an application using the Reactive Pellet Bed feature, see

▥	*A Multiscale 3D Packed Bed Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/ packed_bed_reactor_3d** • Web link: http://www.comsol.com/model/ a-multiscale-3d-packed-bed-reactor-17019

Reactions

The Reactions subfeature to the Reactive Pellet Bed is used to define reaction terms to the transport within the reactive pellets. The feature also defines the corresponding averaged heat sources to be applied to heat transport in the bulk fluid.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern source terms in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

REACTION RATES

Add a rate expression R_i (SI unit: mol/(m^3·s)) for species i using a value or an expression. One reaction rate per species and pellet type can be entered.

Note that if you have the *Chemistry* interface available, provided with the *Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down menu. For an example, see the application *Fine Chemical Production in a Plate Reactor* as linked below.

SURFACE REACTION RATES

The section is available when one or more surface species have been added in the **Surface Species** section of the Reactive Pellet Bed feature.

Specify the rate expression $R_{\text{surf},i}$ (SI unit: mol/(m^2·s)) corresponding to the surface reaction rate of each volumetric species i participating in the surface reaction. Furthermore, specify the surface reaction rates for the participating surface species in the corresponding table.

If several pellet types have been defined, one set of surface reaction rates per pellet type can be defined.

Note that if you have the *Chemistry* interface available, provided with the *Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down menu.

HEAT SOURCE

Specify the heat source originating from the heat of reaction of the chemical reactions inside the pellet can be specified. Both heat sources from reactions in the fluid, and heat sources resulting from surface reactions can be defined. When using several pellet types, heat sources for each type can be added.

The heat sources are most conveniently picked up from a Chemistry feature that defines the reaction rate and the heat of reactions. In that case, the Rate expression can be selected from the drop-down menu. Else it can be set to User Defined.

The defined heat source can be used by a Heat Source feature in any of the heat transfer interfaces.

Species Source

In order to account for consumption or production of species in porous domains, the **Species Source** node adds source terms expressions S_i to the right-hand side of the species transport equations.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

If there are several types of domains, with subsequent and different reactions occurring within them, it might be necessary to remove some domains from the selection. These are then defined in an additional **Species Source** node.

SPECIES SOURCE

Add a source term S_i (SI unit: mol/(m^3·s)) for each of the species solved for. Enter a value or expression in the field of the corresponding species.

Hygroscopic Swelling

The **Hygroscopic Swelling** multiphysics coupling node (◢) is used for moisture concentration coupling between the Solid Mechanics interface and either the Transport of Diluted Species or Transport of Diluted Species in Porous Media interfaces.

Hygroscopic swelling is an effect of internal strain caused by changes in moisture content. This strain can be written as

$$\varepsilon_{hs} = \beta_h (c_{mo} - c_{mo,ref})$$

where β_h is the coefficient of hygroscopic swelling, c_{mo} is the moisture concentration, and $c_{mo,ref}$ is the strain-free reference concentration.

It requires a license of either the MEMS Module or the Structural Mechanics Module. The multiphysics feature will appear automatically if both the Transport of Diluted Species and the Solid Mechanics interfaces are added to the same component. For the most current information about licensing, please see See http://www.comsol.com/products/specifications/.

FURTHER READING

More information about how to use hygroscopic swelling can be found in Hygroscopic Swelling Coupling section in the *Structural Mechanics Module User's Guide*.

More information about multiphysics coupling nodes can be found in the section The Multiphysics Node.

Fracture

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model mass transport along thin fractures in porous media. The node assumes that the transport in the tangential direction along the fracture is dominant, as a result of lower flow resistance.

FRACTURE PROPERTIES

Specify a value for the **Fracture thickness** d_{fr}.

POROUS MATERIAL

Select an option from the **Porous material** list. The default is **Domain material**.

By default the **Porosity,** ε_p (dimensionless) is taken **From material**. Select **User defined** to enter a different value or expression.

CONVECTION

Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use a Fracture Flow feature in a Darcy's Law interface to compute the fluid flow velocity in the fracture.

For **User defined**, enter values or expressions for the velocity components in the table shown.

The settings for the **Diffusion**, and **Dispersion** sections are the same as for Porous Media Transport Properties.

The Transport of Concentrated Species Interface

The **Transport of Concentrated Species (tcs)** interface ( ), found under the **Chemical Species Transport** branch ( ) when adding a physics interface, is used to study gaseous and liquid mixtures where the species concentrations are of the same order of magnitude and none of the species can be identified as a solvent. In this case, properties of the mixture depend on the composition, and the molecular and ionic interactions between all species need to be considered. The physics interface includes models for multicomponent diffusion, where the diffusive driving force of each species depends on the mixture composition, temperature, and pressure.

The physics interface solves for the mass fractions of all participating species. Transport through convection, diffusion, and migration in an electric field can be included.

It supports simulations of transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The physics interface defines the equations for the species mass fractions, including a diffusion model (Mixture-averaged, Maxwell-Stefan, or Fick's law).

The available transport mechanisms and diffusion models differs between various COMSOL products (see http://www.comsol.com/products/specifications/).

Some examples of what can be studied with this physics interface include:

• The evolution of chemical species transported by convection and diffusion.

• The migration in an electric field in the case of ionic species, in mixtures and solutions that cannot be deemed as being diluted.

• Concentrated solutions or gas mixtures, where the concentration of all participating species are of the same order of magnitude, and their molecular and ionic interaction with each other therefore must be considered. This implies that the diffusive transport of a single species is dependent on the mixture composition, and possibly on the temperature, the electric potential, the pressure, or any combination.

When this physics interface is added, the following default nodes are also added in the **Model Builder**— **Transport Properties**, **No Flux**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and reactions. You can also right-click **Transport of Concentrated Species** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tcs`.

EQUATION

The basic equation for an individual species i is:

$$\frac{\partial}{\partial t}(\rho \omega_i) + \nabla \cdot (\rho \omega_i \mathbf{u}) = -\nabla \cdot \mathbf{j}_i + R_i \tag{8-1}$$

The displayed formulation changes depending on the active transport mechanisms and the selected diffusion model.

TRANSPORT MECHANISMS

The Transport of Concentrated Species interface always accounts for transport due to diffusion.

The available diffusion models and the additional transport mechanisms differs between various COMSOL products (see http://www.comsol.com/products/specifications/).

Diffusion Model

- The **Maxwell-Stefan** option employs the most detailed diffusion model, but is also the most computationally expensive. The model is intended for diffusion dominated models, and requires that the multicomponent Maxwell-Stefan diffusivities of all component pairs are known. No stabilization is available when selecting this model.

- The **Mixture-averaged** option is less computationally expensive than the Maxwell-Stefan model. It is a simpler model that can be used when variations in the partial pressures and temperature can be assumed to not affect the multicomponent diffusion. The model includes stabilization but requires the multicomponent Maxwell-Stefan diffusivities of all component pairs.

- The **Fick's law** model is a general model that should be used when the diffusion is assumed Fickian, or when no multicomponent diffusivities are available. Also, when molecular diffusion is not the dominating transport mechanism and a robust but

low order model is wanted, the Fick's law options should be used. The model includes stabilization.

Additional Transport Mechanisms

Under **Additional transport mechanisms**, click to select or clear any combination of check boxes as needed. The **Convection** check box is selected by default. The second term on the left-hand side of Equation 8-1 represents mass transport by convection.

Migration in Electric Field

Select the **Migration in electric field** check box to activate migration of ionic species due to an electric field. The resulting migration term is part of the relative mass flux vector.

Mass Transport in Porous Media

The **Mass transport in porous media** check box activates functionality specific to species transport in porous media. When selected the following features are enabled:

- Porous Media Transport Properties
- Porous Electrode Coupling

Knudsen Diffusion

For **Mixture-averaged** and **Fick's law**, it is possible to include **Knudsen diffusion**. This mechanism accounts for species collisions with the surrounding media, for example, the pore walls the species pass through. It is also an important component when setting up a Dusty gas model.

Mixture-Averaged Diffusion Model

When using the **Mixture-averaged** diffusion model the relative mass flux vector is

$$\mathbf{j}_i = -\left(\rho D_i^m \nabla \omega_i + \rho \omega_i D_i^m \frac{\nabla M}{M} + D_i^T \frac{\nabla T}{T}\right)$$

where the last term on the right-hand side is the migratory flux, which is added by selecting the **Migration in electric field** check box.

The mixture-averaged diffusion coefficient D_i^m is computed as

$$D_i^m = \frac{1 - \omega_i}{\sum_{k \neq i}^{N} \frac{x_k}{D_{ik}}}$$

where D_{ik} (SI unit: m^2/s) is the multicomponent Maxwell-Stefan diffusivities, which are supplied as inputs to the model.

Maxwell-Stefan Diffusion Model

When using the **Maxwell-Stefan** diffusion model the relative mass flux vector is

$$\mathbf{j}_i = -\rho \omega_i \sum_{k=1}^{Q} \tilde{D}_{ik} \mathbf{d}_k - \frac{D_i^T}{T} \nabla T$$

where $\tilde{D}_{ik}$ (SI unit: m^2/s) are the multicomponent Fick diffusivities, $\mathbf{d}_k$ (SI unit: 1/m) is the diffusional driving force, T (SI unit: K) is the temperature, and D_i^T (SI unit: kg/(m·s)) is the thermal diffusion coefficient.

The diffusional driving force is defined as

$$\mathbf{d}_k = \nabla x_k + \frac{1}{p} \left[(x_k - \omega_k) \nabla p - \rho \omega_k \mathbf{g}_k + \omega_k \sum_{l=1}^{Q} \rho \omega_l \mathbf{g}_l \right] \qquad (8\text{-}2)$$

where $\mathbf{g}_k$ is an external force (per unit mass) acting on species k. In the case of an ionic species, the external force due to the electric field, which is added by selecting the **Migration in electric field** check box, is

$$\mathbf{g}_k = -\frac{z_k F}{M_k} \nabla \phi \qquad (8\text{-}3)$$

where z_k is the species charge number, F (SI unit: A·s/mol) is Faraday's constant and ϕ (SI unit: V) is the electric potential.

Fick's Law Diffusion Model

When using the **Fick's law** diffusion model the relative mass flux vector is

$$\mathbf{j}_i = -\left(\rho D_i^F \nabla \omega_i + \rho \omega_i D_i^F \frac{\nabla M}{M} + D_i^T \frac{\nabla T}{T} \right)$$

where D_i^F (SI unit: m^2/s) is a user-defined diffusion coefficient (isotropic, diagonal, or symmetric). The last term on the right-hand side is the migratory flux, which is added by selecting the **Migration in electric field** check box.

SPECIES

Select the species that this physics interface solves for using the mass constraint in Equation 8-4 (that is, its value comes from the fact that the sum of all mass fractions must equal 1). In the **From mass constraint** list, select the preferred species. To

minimize the impact of any numerical errors, use the species with the highest concentration. By default, the first species is used.

$$\omega_1 = 1 - \sum_{i=2}^{Q} \omega_i \qquad (8\text{-}4)$$

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**.

• There are two consistent stabilization methods available when using the Mixture-Averaged Diffusion Model or Fick's Law Diffusion Model—**Streamline diffusion** and **Crosswind diffusion**. Both are active by default.

  The **Residual** setting applies to both the consistent stabilization methods. **Approximate residual** is the default setting and it means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and computationally faster. If required, select **Full residual** instead.

• There is one inconsistent stabilization method, **Isotropic diffusion**, which is available when using the Mixture-Averaged Diffusion Model or Fick's Law Diffusion Model.

ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Regularization
From the **Regularization** list, select **On** (the default) or **Off**. When turned **On**, regularized mass fractions are calculated such that

$$0 \le w_{i,\text{reg}} \le 1$$

Regularized mass fractions are used for the calculation of composition-dependent material properties, such as the density.

Pseudo time stepping
The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary** equation form is used in order to speed up convergence. When selected, a CFL number expression should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator. For more information, see Pseudo Time Stepping for Mass Transport.

DISCRETIZATION

To display this section, click the **Show** button (⊕) and select **Discretization**. For more information about these settings, see the Discretization section in the The Transport of Diluted Species Interface documentation.

⚠	In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

⊙	• Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface • Theory for the Transport of Concentrated Species Interface

▥	*Species Transport in the Gas Diffusion Layers of a PEM*: Application Library path **Batteries_and_Fuel_Cells_Module/Fuel_Cells/ pem_gdl_species_transport_2d** Web link: http://www.comsol.com/model/ species-transport-in-the-gas-diffusion-layers-of-a-pem-260

DEPENDENT VARIABLES

Add or remove species in the model and also change the names of the dependent variables that represent the species concentrations.

Specify the **Number of species**. There must be at least two species. To add a single species, click the **Add concentration** button (➕) under the table. To remove a species, select it in the list and click the **Remove concentration** button (▤) under the table. Edit the names of the species directly in the table.

⚠	The species are dependent variables, and their names must be unique with respect to all other dependent variables in the component.

⊙	Adding a Chemical Species Transport Interface

Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface

The Transport of Concentrated Species Interface has these domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

❗	In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

	For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.

These nodes are described in this section or as indicated:

- Flux
- Flux Discontinuity
- Inflow
- Initial Values
- Mass Fraction
- No Flux
- Open Boundary
- Outflow
- Porous Media Transport Properties
- Reaction
- Reaction Sources
- Symmetry
- Thin Impermeable Barrier[1]
- Turbulent Mixing
- Transport Properties

[1] The node is described for the Transport of Diluted Species interface.

Transport Properties

The **Transport Properties** is the main node used to model mass transfer in a fluid mixture with the Transport of Concentrates species interface. The node adds the equations governing the mass fractions of all present species, and provides inputs for the transport mechanisms and for the material properties of the fluid mixture.

The settings in this node are dependent on the check boxes selected under Transport Mechanisms in the Settings window of the Transport of Concentrated Species interface.

When the **Convection** check box is selected, the Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu.

The options available in this feature differs between COMSOL products. (See http://www.comsol.com/products/specifications/).

MODEL INPUTS

Specify the temperature and pressure to be used in the physics interface. The temperature model input is used when calculating the density from the ideal gas law, but also when thermal diffusion is accounted for by supplying thermal diffusion coefficients. The pressure model input is used in the diffusional driving force in Equation 8-2 (that is, when a Maxwell-Stefan Diffusion Model is used) and when calculating the density from the ideal gas law.

Temperature

Select the source of the **Temperature** field T:

• Select **User defined** to enter a value or an expression for the temperature (SI unit: K). This input is always available.

• If required, select a temperature defined by a Heat Transfer interface present in the model (if any). For example, select **Temperature (ht)** to use the temperature defined by the Heat Transfer in Fluids interface with the ht name.

Absolute Pressure

Select the source of the **Absolute pressure** p:

• Select **User defined** to enter a value or an expression for the absolute pressure (SI unit: Pa). This input is always available.

• In addition, select a pressure defined by a Fluid Flow interface present in the model (if any). For example, select **Absolute pressure (spf)** to use the pressure defined in a Laminar Flow interface with spf as the Name.

DENSITY

Define the density of the mixture and the molar masses of the participating species.

Mixture Density

Select a way to define the density from the **Mixture density** list—**Ideal gas** or **User defined**:

- For **Ideal gas**, the density is computed from the ideal gas law in the manner of:

$$\rho = \frac{pM}{R_g T}$$

  Here M is the mean molar mass of the mixture and R_g is the universal gas constant. The absolute pressure, p, and temperature, T, used corresponds to the ones defined in the Model Inputs section.

- For **User defined** enter a value or expression for the **Mixture density** ρ.

Molar Mass

Enter a value or expression for the **Molar mass** M_w for each species. The default value is 0.032 kg/mol, which is the molar mass of O_2 gas.

CONVECTION

This section is available when the **Convection** check box is selected.

Select the source of the **Velocity field u**:

- Select **User defined** to enter manually defined values or expressions for the velocity components. This input is always available.

- Select a velocity field defined by a Fluid Flow interface present in the model (if any). For example, select **Velocity field (spf)** to use the velocity field defined by the **Fluid Properties** node fp1 in a Single-Phase Flow, Laminar Flow interface with spf as the Name.

DIFFUSION

Specify the molecular and thermal diffusivities of the present species based on the selected **Diffusion model**.

When using a Maxwell-Stefan Diffusion Model or a Mixture-Averaged Diffusion Model, specify the **Maxwell-Stefan diffusivity matrix** D_{ik} and the **Thermal diffusion coefficients** D_w^T.

When using a Fick's Law Diffusion Model, specify the **Diffusion coefficient** D_w^F and the **Thermal diffusion coefficients** D_w^T for each of the species.

Maxwell-Stefan Diffusivity Matrix

Using a Maxwell-Stefan Diffusion Model or a Mixture-Averaged Diffusion Model, the **Maxwell-Stefan diffusivity matrix** D_{ik} (SI unit: m^2/s) can be specified. For a simulation involving Q species the Maxwell-Stefan diffusivity matrix is a Q-by-Q symmetric matrix, where the diagonal components are 1. Enter values for the upper triangular components, D_{ij}, which describe the inter-diffusion between species i and j. The numbering of the species corresponds to the order, from top to bottom, used for all the input fields for species properties (see for example the molar mass fields in the Density section).

Diffusion Coefficient

Using a Fick's Law Diffusion Model, the diffusion is by default assumed to be isotropic and governed by one **Diffusion coefficient** D_w^F (SI unit: m^2/s) for each species. To allow for a general representation, it is also possible to use diffusion matrices (diagonal, symmetric, or anisotropic).

Thermal Diffusion Coefficient

To model thermal diffusion, prescribe the **Thermal diffusion coefficients** D_i^T (SI unit: kg/m·s), by entering one thermal diffusion coefficient for each species in the corresponding field. In a multicomponent mixture, the sum of the thermal diffusion coefficients is zero. The default value for all thermal diffusion coefficients is 0.

Specify the molecular and thermal diffusivities of the present species based on the selected **Diffusion model**.

KNUDSEN DIFFUSION

The Knudsen diffusion transport mechanism accounts for the interaction of the species with the surroundings (inter-species collisions excluded), for example the pore wall when a species passes through porous media.

Depending on which **Diffusion model** is selected, either the **Fick's law** or the **Mixture-averaged** diffusion coefficient D_i^M is corrected with the **Knudsen diffusion** coefficient D_i^K in the following way

$$D_i^{MK} = \left(\frac{1}{D_i^M} + \frac{1}{D_i^K} \right)^{-1}$$

For gases, the **Kinetic gas theory** is often valid and requires the **Mean path length** λ_{path} (SI unit: m). Typically, for transport in porous media, the pore diameter can be entered here. For other cases, choose **User defined**.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected for the Transport of Concentrated Species interface.

Electric Potential

- Select **User defined** to enter a value or expression for the electric potential . This input is always available.
- If required, select an electric potential defined by an AC/DC interface that is present in the model (if any). For example, select **Electric potential (ec)** to use the electric field defined by the Current Conservation node cucn1 in an Electric Currents interface ec.

Settings for the mobilities are used for the **Mixture-averaged** and **Fick's law** transport models. By default the mobility is set to be calculated based on the species diffusivities and the temperature using the **Nernst-Einstein relation**. To manually specify the mobilities, select **User defined** for the mobility $u_{m,c}$ (SI unit: s·mol/kg) and enter one value for each species.

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based on the Nernst-Einstein relation) is taken from the **Model Inputs** section.

Porous Media Transport Properties

The **Porous Media Transport Properties** node is used to model mass transfer in porous media using the Transport of Concentrated Species interface. The node adds the equations governing the mass fractions of all present species, and provides inputs for the transport mechanisms and for the material properties of the fluid mixture.

The settings in this node are dependent on the check boxes selected under Transport Mechanisms in the Settings window of the Transport of Concentrated Species interface.

The options available in this feature differs between COMSOL products. (See http://www.comsol.com/products/specifications/).

MODEL INPUTS

Specify the temperature and pressure to be used in the physics interface. The temperature model input is used when calculating the density from the ideal gas law,

but also when thermal diffusion is accounted for by supplying thermal diffusion coefficients. The pressure model input is used in the diffusional driving force in Equation 8-2 (that is, when a Maxwell-Stefan Diffusion Model is used) and when calculating the density from the ideal gas law.

Temperature
Select the source of the **Temperature** field T:

- Select **User defined** to enter a value or an expression for the temperature (SI unit: K). This input is always available.

- If required, select a temperature defined by a Heat Transfer interface present in the model (if any). For example, select **Temperature (ht)** to use the temperature defined by the Heat Transfer in Fluids interface with the ht name.

Absolute Pressure
Select the source of the **Absolute pressure** p:

- Select **User defined** to enter a value or an expression for the absolute pressure (SI unit: Pa). This input is always available.

- In addition, select a pressure defined by a Fluid Flow interface present in the model (if any). For example, select **Absolute pressure (spf)** to use the pressure defined in a Laminar Flow interface with spf as the Name.

MATRIX PROPERTIES

Enter a value or expression for the **Porosity,** ε_p (dimensionless), of the porous media.

In order use a porosity defined in a material; specify the material using the **Porous material** list, and select **From material** from the **Porosity** list.

DENSITY

Use this section to define the mixture density, and to specify the molar masses of the participating species.

Mixture Density
Select a way to define the density from the **Mixture density** list—**Ideal gas** or **User defined**:

- For **Ideal gas**, the density is computed from the ideal gas law in the manner of:

$$\rho = \frac{pM}{R_g T}$$

Here M is the mean molar mass of the mixture and R_g is the universal gas constant. The absolute pressure, p, and temperature, T, used corresponds to the ones defined in the Model Inputs section.

- For **User defined** enter a value or expression for the **Mixture density** ρ.

Molar Mass

Enter a value or expression for the **Molar mass** M_w for each species. The default value is 0.032 kg/mol, which is the molar mass of O_2 gas.

CONVECTION

This section is available when the **Convection** check box is selected.

Select the source of the **Velocity field u**:

- Select **User defined** to enter values or expressions for the velocity components. This input is always available.
- Select a velocity field defined by a Fluid Flow interface present in the model (if any). For example, select **Velocity field (spf)** to use the velocity field defined by the **Fluid Properties** node fp1 in a Single-Phase Flow, Laminar Flow interface with spf as the Name.

DIFFUSION

Specify the species molecular and thermal diffusivities in nonporous media in the manner described for the Transport Properties node.

To account for the effect of porosity in the diffusivities, select an **Effective diffusivity model** — **Millington and Quirk model**, **Bruggeman model**, **Tortuosity model**, or **No correction.** Using one of the first four models, the effective transport factor, f_e, is defined from the porosity and the fluid tortuosity factor in the manner of:

$$f_e = \frac{\varepsilon_p}{\tau_F} \tag{8-5}$$

For **No correction**, the effective transport factor is set to one.

- For the **Millington and Quirk model,** the effective transport factor is $\tau_F = \varepsilon_p^{-1/3}$.
- For the **Bruggeman model,** the effective transport factor is $\tau_F = \varepsilon_p^{-1/2}$.
- For the **Tortuosity model,** specify the tortuosity factor is τ_F.

The species diffusivities and mobilities are automatically adjusted for porous media transport using the effective transport factor.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected in the Transport Mechanisms section of the interface, select the source of the **Electric potential** V:

- Select **User defined** to enter a value or expression for the electric potential. This input is always available.

- If required, select an electric potential defined by an AC/DC interface that is present in the model (if any). For example, select **Electric potential (ec)** to use the electric field defined by the Current Conservation node cucn1 in an Electric Currents interface ec.

Settings for the mobilities are needed for the **Mixture-averaged** and **Fick's law** diffusion models. By default the mobility is set to be calculated based on the species diffusivities (adjusted by the **Effective diffusivity model** in the **Diffusion** section) using the **Nernst-Einstein relation**. To manually specify the mobilities, select **User defined** for the mobility $u_{m,w}$ (SI unit: s·mol/kg) and enter one value for each species.

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based or the Nernst-Einstein relation) is taken from the **Model Inputs** section.

Turbulent Mixing

Use this node to account for the turbulent mixing caused by the eddy diffusivity. An example is when the specified velocity field corresponds to a RANS solution.

The **Turbulent Mixing** subnode is available from the context menu (right-click the Transport Properties parent node) or from the **Physics** toolbar, **Attributes** menu. The node defines the turbulent kinematic viscosity using a turbulent Schmidt number.

This feature is available if **Convection** is selected as a transport mechanism and if the **Diffusion model** is **Mixture-averaged** or **Fick's law**.

TURBULENT MIXING

Some physics interfaces provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** ν_T (SI unit: m^2/s) list. The list always contains the **User defined** option that makes it possible to enter any value or expression.

The default **Turbulent Schmidt number** Sc_T is 0.71 (dimensionless).

Q | About Turbulent Mixing

Reaction

Use the **Reaction** node to define species source terms resulting from a single chemical reaction. For turbulent flow, the Reaction node includes the Eddy-dissipation turbulent-reactions model.

REACTION RATE

Select a **Reaction rate** — **Automatic** (the default), or **User defined**. Selecting **Automatic** the laminar flow reaction rate is computed using the mass action law.

For **User defined**, input a custom expression or constants for the **Reaction rate** r.

Specify the reaction stoichiometry by entering values for the stoichiometric coefficients (dimensionless) of each species. Enter negative values for reactants and positive values for products.

RATE CONSTANTS

When the **Use Arrhenius expressions** check box is not selected, input custom expressions or constants for the **Forward rate constant** k^f and **Reverse rate constant** k^r.

When the **Use Arrhenius expressions** check box is selected, enter values for the following parameters of the forward and reverse reactions:

- **Forward frequency factor** A^f and **Reverse frequency factor** A^r (dimensionless)
- **Forward activation energy** E^f and **Reverse activation energy** E^r
- **Forward temperature exponent** n^f and **Reverse temperature exponent** n^r (dimensionless)

TURBULENT FLOW

Note this section is only available when then licensed to the CFD Module (see http:/ /www.comsol.com/products/specifications/).

When the **Turbulent-reaction model** is set to **None**, laminar flow is assumed and the reaction source terms are defined from the reaction stoichiometry and reaction rates prescribed.

When the **Turbulent-reaction model** is set to **Eddy-dissipation**, turbulent flow will be accounted for in the reaction mass sources in the manner described in The Reaction Source Term for Turbulent Flow. In this case, enter values for the **Turbulent reaction model parameters** α_{ED} and β_{ED} (dimensionless).

The **Eddy-dissipation** model also requires an estimation of the turbulent mixing time of the fluid flow turbulence. When a Fluid Flow interface defining it is present in the model, it can be selected from the **Turbulence time scale** list. For example, select **Turbulence time scale (spf/fp1)** to use the time scale defined by the **Fluid Properties** node fp1 in a Turbulent Flow, k-ε interface with the **Name** set to spf.

REGULARIZATION

Select **Rate expression** in order to regularize the individual rate expressions that are added to each species. If the mass fraction for a reactant species ω_i becomes smaller than its **damping limit**, ω_i^{dl}, the rate expression added to species ω_i is reduced linearly. If $\omega_i \leq 0$ for a reactant species, the reaction rate contribution to that species is completely removed. Similarly, the if the mass fraction for a product species ω_j becomes larger than $1-\omega_j^{dl}$, the rate expression added to that species is damped linearly. If $\omega_j \geq 1$ for a product species, the reaction rate contribution to that species is completely removed.

The default value for the **damping limit**, ω_i^{dl}, is $1e^{-6}$, which is appropriate for most applications, but can require adjustment when working with for example catalytic trace species.

Regularization of the rate expressions adds considerable stability to the reaction expressions, but should optimally only be used as a mean to reach convergence. If the regularization is active in too large parts of the domain, the mass balance can become affected since the regularization acts on the contributions to each individual species, not the reaction as a whole.

Reaction Sources

In order to account for consumption or production of species due to one or more reactions, the **Reaction Sources** node adds source terms to the right-hand side of the species transport equations.

REACTIONS

Add an expression for the reaction mass source, R_i, for each individual species present, except for the one computed from the mass constraint (see Species). Enter a value or expression in the field for the corresponding species.

Select the **Mass transport to other phases** check box if mass is leaving or entering the fluid as a result of the reactions, for instance due to condensation or vaporization in a porous matrix. In this case the mass source for the species calculated from the mass constraint can also be specified. The net mass transfer corresponds to the sum of the mass sources for all species.

REACTING VOLUME

When specifying reaction sources for a species in porous media, the specified mass source may have the basis of the total volume, or the pore volume. For nonporous domains, the **Reacting Volume** setting has no impact.

- For **Total volume**, the reaction mass source expressions are specified per unit volume of the model domain.

- For **Pore volume**, the reaction mass source expressions are specified per unit volume pore space. In this case the reaction mass sources will be multiplied by the domain porosity ε_p (ε_p equals unity for nonporous domains).

Initial Values

The **Initial Values** node adds initial values for the mass fractions that can serve as an initial condition for a transient simulation, or as an initial guess for a nonlinear solver. If required, add additional **Initial Values** nodes from the **Physics** toolbar.

INITIAL VALUES

The initial mass fractions can be specified using a number of quantities. Select the type of input from the **Mixture specification** list. Select:

- **Mass fractions** (the default) to enter mass fractions ($\omega_{0,\,\omega 1}$ for example)
- **Mole fractions** to enter mole fractions ($x_{0,\,\omega 1}$ for example)

- **Molar concentrations** (SI unit: mol/m^3) to enter molar concentrations ($c_{0,\omega1}$ for example)

- **Number densities** (SI unit: $1/m^3$) to enter number densities ($n_{0,\omega1}$ for example)

- **Densities** (SI unit: kg/m^3) to enter densities ($\rho_{0,\omega1}$ for example)

Enter a value or expression in the field for each species except for the one computed from the mass constraint.

INITIAL MIXTURE DENSITY

When the selecting **Molar concentrations**, **Number densities**, or **Densities** are selected from the **Mixture specification** list, the should also be specified. Select **Ideal gas** or **User defined** from the **Initial mixture density** list.

- For **Ideal gas**, also specify the **Initial pressure** p_0 and the **Initial Temperature** T_0. Note that dependent variables solved for are evaluated to zero for initial values. When solving for pressure or temperature together with the mass fractions, apply the initial values from the corresponding interfaces here as well.

- For **User defined**, input a custom for the **Initial mixture density** ρ_{m0}.

Mass Fraction

The **Mass Fraction** node adds boundary conditions for the species mass fractions. For example, the following condition specifies the mass fraction of species i: $\omega_i = \omega_{i,0}$.

Set the mass fractions of all species except the one computed from the mass constraint. This ensures that the sum of the mass fractions is equal to one (see Species). This node is available for exterior and interior boundaries.

MASS FRACTION

Specify the mass fraction for each species individually. Select the check box for the species to specify the mass fraction, and enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the check box for the mass fraction of that species.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**.

Flux

The **Flux** node can be used to specify the total mass flux across a boundary. The total inward flux is defined in the manner of:

$$-\mathbf{n} \cdot (\rho \omega_i \mathbf{u} + \mathbf{j}_i) = N_{0,i} \tag{8-6}$$

In Equation 8-6, $N_{0,i}$ (SI unit: Pa·s/m) is an arbitrary flux expression for species i and can be a function of ω_i, temperature, pressure or even electric potential. Set the mass flux of all species except the one computed from the mass constraint. This ensures that the sum of the mass fractions is equal to one (see Species). This node is available for exterior boundaries. The Flux node can, for example, be used to describe a *heterogeneous reaction* or a separation process occurring at the boundary.

INWARD FLUX

Specify the **Inward flux** for each species individually. Select the check box for the species to prescribe a flux and enter a value or expression for the flux in the corresponding field. To use another boundary condition for a specific species, click to clear the check box for the flux of that species. Use a positive value for an inward flux.

Inflow

The **Inflow** node adds a boundary condition for an inflow boundary where one condition for each species is specified. It is available for exterior boundaries. The condition can be specified using the following quantities:

- The mass fraction: $\omega = \omega_0$
- The mole fraction: $x = x_0$
- The molar concentration: $c = c_0$
- The number density, which describes the number of particles per volume: $n = n_0$
- The density: $\rho = \rho_0$

A concentration quantity other than the mass fractions can only be used when all species are defined, as in this boundary condition. The other quantities are composition dependent and therefore unambiguous only when all species are defined. For this reason the Mass Fraction node, which allows some species to use a different boundary condition, only includes inputs for the mass fractions.

Select a **Mixture specification**:

- **Mass fractions** (the default) to enter mass fractions ($\omega_{0, \omega 1}$ for example)

- **Mole fractions** to enter mole fractions ($x_{0, \omega 1}$ for example)

- **Molar concentrations** (SI unit: mol/m^3) to enter molar concentrations ($c_{0, \omega 1}$ for example)

- **Number densities** (SI unit: $1/\text{m}^3$) to enter number densities ($n_{0, \omega 1}$ for example)

- **Densities** (SI unit: kg/m^3) to enter densities ($\rho_{0, \omega 1}$ for example)

Enter a value or expression in the field for each species except for the one computed from the mass constraint.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (👁) and select **Advanced Physics Options**.

No Flux

The **No Flux** node, which is the default boundary condition available for exterior boundaries, represents boundaries where no mass flows in or out; that is, the total flux is zero:

$$-\mathbf{n} \cdot \mathbf{N} = -\mathbf{n} \cdot (\rho \omega_i \mathbf{u} + \mathbf{j}_i) = 0$$

NO FLUX

Select **Apply for all species** to specify no flux for all species. Select **Apply for** to specify no flux for each species individually. To use another boundary condition for a specific species, click to clear the check box for that species.

Outflow

The **Outflow** node is the preferred boundary condition at outlets where the species are to be transported out of the model domain. It is useful, for example, in mass transport models where it is assumed that convection is the dominating effect driving the mass flow through the outflow boundary. This node is available for exterior boundaries. The boundary condition is applied to all species and corresponds to one of the following equations depending on the selected diffusion model:

- For the Mixture-Averaged Diffusion Model:

$$-\mathbf{n} \cdot \rho D_i^m \nabla \omega_i = 0$$

- For the Fick's Law Diffusion Model:

$$-\mathbf{n} \cdot \rho D_i^f \nabla \omega_i = 0$$

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric; that is, there is no mass flux in the normal direction across the boundary:

$$-\mathbf{n} \cdot \mathbf{N} = -\mathbf{n} \cdot (\rho \omega_i \mathbf{u} + \mathbf{j}_i) = 0$$

This boundary condition is identical to the No Flux node, but applies to all species and cannot be applied to individual species. The Symmetry node is available for exterior boundaries.

Flux Discontinuity

The **Flux Discontinuity** node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n} \cdot (\mathbf{N}_d - \mathbf{N}_u) = N_0 \qquad \mathbf{N} = (\rho \omega_i \mathbf{u} + \mathbf{j}_i)$$

where the value of N_0 specifies the size of the flux jump evaluated from the down to the upside of the boundary.

FLUX DISCONTINUITY

Specify the jump in species mass flux. Use a positive value for increasing flux when going from the downside to the upside of the boundary. The boundary normal points in the direction from the downside to the upside of an interior boundary and can be plotted for visualization.

Select the **Species** check boxes to specify a flux discontinuity, and enter a value or expression for the **Flux discontinuity** N_0 (SI unit: kg/(m^2·s)) in the corresponding field, $N_{0,\,\text{w1}}$ for example. To use a different boundary condition for a specific species, click to clear the check box for the flux discontinuity of that species.

Open Boundary

Use the **Open Boundary** node to set up mass transport across boundaries where both convective inflow and outflow can occur. Use the node to specify an exterior species composition on parts of the boundary where fluid flows into the domain. A condition equivalent to the Outflow node applies to the parts of the boundary where fluid flows out of the domain. The direction of the flow across the boundary is typically calculated by a Fluid Flow interface and is entered as Model Inputs.

EXTERIOR COMPOSITION

Enter a value or expression for the species composition. Select:

- **Mass fractions** (the default) to enter mass fractions ($\omega_{0,\omega 1}$, for example)
- **Mole fractions** to enter mole fractions ($x_{0,\omega 1}$, for example)
- **Molar concentrations** (SI unit: mol/m^3) to enter molar concentrations ($c_{0,\omega 1}$, for example)
- **Number densities** (SI unit: $1/m^3$) to enter number densities ($n_{0,\omega 1}$, for example) and to describe the number of particles per volume $n = n_0$
- **Densities** (SI unit: kg/m^3) to enter densities ($\rho_{0,\omega 1}$, for example)

💡	A concentration quantity other than the mass fractions can only be used when all species are defined.

The Reacting Flow Multiphysics Interfaces

The CFD Module includes predefined multiphysics interfaces that couples fluid with mass transport and reactions.

Selecting a multiphysics interface under the **Chemical Species Transport>Reacting Flow** branch of the **Model Wizard** or **Add Physics** windows, one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) and a **Transport of Concentrated Species** interface are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature **Reacting Flow**. The **Reacting Flow** feature predefines and controls the couplings between the separate interfaces in order to facilitate easy set up of models.

In this section:

- The Reacting Laminar Flow Interface
- The Reacting Turbulent Flow, k-e Interface
- The Reacting Turbulent Flow, k-w Interface
- The Reacting Turbulent Flow, SST Interface
- The Reacting Turbulent Flow, Low Re k-e Interface
- The Reacting Flow Coupling Feature
- Physics Interface Features

The Reacting Laminar Flow Interface

The **Reacting Laminar Flow** multiphysics interface is used to simulate laminar flow coupled to species transport in a gas or liquid.

It combines the **Laminar Flow**, and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport. The fluid flow can either be free flow, or flow in a porous medium. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The equations solved by the **Laminar Flow** interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. A **Fluid Properties** feature is active by default on the entire interface selection. A **Fluid and Matrix Properties** feature can be added in order to model flow in porous media by solving the Brinkman equations.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The Reacting Turbulent Flow, k-ε Interface

The **Reacting Turbulent Flow, k**-ε multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow, k**-ε and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples the fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, k**-ε interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation k-e model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions, and reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, k-ω Interface

The **Reacting Turbulent Flow k-ω** multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow k-ω** and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow k-ω** interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the Wilcox revised k-ω model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions, and reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, SST Interface

The **Reacting Turbulent Flow, SST** multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow, SST** and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, SST** interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the SST model. The SST model is a low-Reynolds number model which means that it resolves the velocity, pressure, and mass fractions all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The SST model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, Low Re k-ε Interface

The **Reacting Turbulent Flow, Low Re k-ε** multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow, Low Re k-ε** and **Transport of Concentrated Species** interfaces. **The Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, Low Re k-ε** interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the AKN low-Reynolds number k-e model. The low-Reynolds number model resolves the velocity, pressure, and mass fractions all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The AKN model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and,

optionally, migration in an electric field. Reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Flow Coupling Feature

Use the **Reacting Flow** (⬙) multiphysics coupling to simulate mass transport and reactions in a gas or liquid mixture where the fluid flow can be dependent on the mixture composition.

DOMAIN LEVEL SYNCHRONIZATION

The **Reacting Flow** coupling synchronizes the features from a Single-Phase Flow, or Brinkman Equations, interface and a Transport of Concentrated Species interface. When added, the density in the Single-Phase Flow interface is automatically synchronized to the one defined by the Transport of Concentrated Species interface. Conversely, the velocity field used by the latter interface is synchronized to the one computed in the former interface.

THE STEFAN VELOCITY

The **Reacting Flow** coupling feature automatically couples mass transfer on boundaries and applies a corresponding velocity contribution for the flow. Prescribing a net mass boundary flux in the **Transport of Concentrated Species** interface, either using a **Flux** or **Mass Fraction** feature, the **Reacting Flow** feature computes the The Stefan Velocity, and applies this in **Wall** features using the same selection.

MASS TRANSFER TO OTHER PHASES IN POROUS MEDIA

When coupled to the **Brinkman Equations** interface, the **Reacting Flow** node automatically computes the net mass source or sink in a **Reactions** (when **Mass transfer to other phases is enabled**) node in the **Transport of Concentrated Species** interface and adds the corresponding source/sink to the momentum equations of the **Fluid and Matrix Properties** domains.

TURBULENT MASS TRANSFER

When a turbulence model is used, the **Reacting Flow** coupling applies turbulence modeling for the mass transport in the following manners:

• Turbulent mass transport is added, defined from the turbulent viscosity and a turbulent Schmidt number (for more information, see Turbulent Mass Transport Models).

- Mass transport wall functions. When a turbulence model using wall functions is used for the fluid flow, the Reacting Flow coupling automatically adds wall functions for the mass transport on the same boundaries (for more information, see Mass Transport Wall Functions).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is rf1.

DOMAIN SELECTION

The **Reacting Flow** coupling is automatically defined on the intersection of the selections for the coupled interfaces.

The **Selection** list displays the domains where the coupling feature is active.

TURBULENCE

When the flow interface uses a turbulence model, select an option from the **Mass transport turbulence model** list—**Kays-Crawford**, **High Schmidt Number**, or **User-defined turbulent Schmidt number**.

For **User-defined turbulent Schmidt number**, enter a **Turbulent Schmidt number** Sc_T (dimensionless).

The turbulent mass transfer added to the mass fraction equations is defined as

$$N_{i, T} = -\frac{\mu_T}{Sc_T}\nabla\omega_i$$

where μ_T is the turbulent viscosity defined by the flow interface, and the turbulent Schmidt number, Sc_T, depends on the **Mass transport turbulence model** used.

Note, since the **Reacting Flow** coupling feature adds the turbulent mass transport, it should not be combined with a **Turbulent Mixing** feature (subfeature to **Transport Properties** in the **Transport of Concentrated Species interface**).

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Species transport** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.

- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Laminar Flow** is deleted, then the **Species transport** list defaults to **None** as there is nothing to couple to.

📑	If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Species transport** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Approaches in the *COMSOL Multiphysics Reference Manual*.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

LAMINAR FLOW

The available physics features for The Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow in the *COMSOL Multiphysics Reference Manual*.

TURBULENT FLOW, k-ε

The available physics features for The Turbulent Flow, k-ε interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ω

The available physics features for The Turbulent Flow, k-ω interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE k-ε

The available physics features for The Turbulent Flow, Low Re k-ε interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for The Transport of Concentrated Species interface are listed in the section Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface.

The Reacting Flow in Porous Media Interfaces

The CFD Module includes two predefined multiphysics interface that couples fluid flow in porous media with mass transport and reactions in porous media.

Selecting a multiphysics interface under the **Chemical Species Transport>Reacting Flow in Porous Media** branch of the **Model Wizard** or **Add Physics** windows, a **Brinkman Equations** interface combined with either the **Transport of Diluted Species in Porous Media** interface or the **Transport of Concentrated Species** interfaces are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature. The multiphysics coupling feature controls the coupling between the separate interfaces in order to facilitate easy set up of models.

In this section:

The Reacting Flow in Porous Media, Transport of Diluted Species Interface

The **Reacting Flow in Porous Media, Transport of Diluted Species** interface ( ) is used to study the flow and chemical composition of a gas or liquid moving through the interstices of a porous medium.

It combines the **Brinkman Equations**, and **Transport of Diluted Species in Porous Media** interfaces. The **Flow coupling** multiphysics coupling feature, which is added automatically, couples the fluid flow and mass transport.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The **Brinkman Equations** interface computes the fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. A **Fluid and Matrix Properties** feature is active by default on the entire interface selection.

The **Transport of Diluted Species in Porous Media** interface computes the species concentration in free and porous media, assuming that the species are of solutes, dissolved in a solvent of significantly higher concentration. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The Reacting Flow in Porous Media, Transport of Concentrated Species Interface

The **Reacting Flow in Porous Media, Transport of Concentrated Species** interface ( ) is used to study the flow and chemical composition of a gas or liquid moving through the interstices of a porous medium. The fluid can consist of a mixture of species where the individual concentrations are of comparable order of magnitude.

It combines the **Brinkman Equations**, and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling feature, which is added automatically, couples the fluid flow and mass transport.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The **Brinkman Equations** interface computes the fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. A **Fluid and Matrix Properties** feature is active by default on the entire interface selection.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions in free and porous media. In the current multiphysics interface a **Porous Media Transport Properties** feature is active by default on the entire interface selection.

The Flow Coupling Feature

For the settings of this feature see Flow Coupling in the *Heat Transfer Module User's Guide*.

The Reacting Flow Coupling Feature

For the settings of this feature see The Reacting Flow Coupling Feature in the *Chemical Reaction Engineering Module User's Guide*.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

BRINKMAN EQUATIONS

The available physics features for The Brinkman Equations interface are listed in the Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface section in the *CFD Module User's Guide*.

TRANSPORT OF DILUTED SPECIES

The available physics features for The Transport of Diluted Species interface are listed in the Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface section.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for The Transport of Concentrated Species interface are listed in the Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface section.

Theory for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution of chemical species transported by diffusion and convection. The physics interface assumes that all species present are dilute; that is, that their concentration is small compared to a solvent fluid or solid. As a rule of thumb, a mixture containing several species can be considered dilute when the concentration of the solvent is more than 90 mol%. Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent.

When studying mixtures that are not dilute, the mixture and transport properties depend on the composition, and a different physics interface is recommended. See The Transport of Concentrated Species Interface for more information.

Fick's law governs the diffusion of the solutes, dilute mixtures, or solutions, while the phenomenon of ionic migration is sometimes referred to as *electrokinetic flow*. The Transport of Diluted Species interface supports the simulations of chemical species transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D.

In this section:

- Convective Term Formulation
- Crosswind Diffusion
- Danckwerts Inflow Boundary Condition
- Mass Balance Equation
- Mass Sources for Species Transport
- Solving a Diffusion Equation Only
- References

Mass Balance Equation

The default node attributed to the Transport of Diluted Species interface models chemical species transport through diffusion and convection and solves the mass conservation equation for one or more chemical species i:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \tag{8-7}$$

Equation 8-7 in its form above includes the transport mechanisms diffusion and convection. If *Migration in Electric Field* is activated (only available in some add-on products), the migration mechanism will be added to the equation as well. See more details in the section Adding Transport Through Migration.

- c_i is the concentration of the species (SI unit: mol/m^3)
- D_i denotes the diffusion coefficient (SI unit: m^2/s)
- R_i is a reaction rate expression for the species (SI unit: mol/(m^3·s))
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)

The flux vector $\mathbf{N}$ (SI unit: mol/(m^2·s)) is associated with the mass balance equation above and used in boundary conditions and flux computations. For the case where the diffusion and convection are the only transport mechanisms, the flux vector is defined as

$$\mathbf{N}_i = -D \nabla c + \mathbf{u} c \tag{8-8}$$

If *Migration in Electric Fields* is activated, the flux vector is amended with the migration term as shown in the section Adding Transport Through Migration.

The first term on the left side of Equation 8-7 corresponds to the accumulation (or indeed consumption) of the species.

The second term accounts for the diffusive transport, accounting for the interaction between the dilute species and the solvent. An input field for the diffusion coefficient is available. Anisotropic diffusion coefficient tensor input is supported.

The third term on the left side of Equation 8-7 describes the convective transport due to a velocity field $\mathbf{u}$. This field can be expressed analytically or obtained from coupling this physics interface to one that computes fluid flow, such as *Laminar Flow*.

On the right-hand side of the mass balance equation (Equation 8-7), R_i represents a source or sink term, typically due to a chemical reaction or desorption on a porous matrix. To specify R_i, another node must be added to the Transport of Diluted Species interface—the **Reaction** node, which has a field for specifying a reaction equation using the variable names of all participating species.

Equilibrium Reaction Theory

The feature Equilibrium Reaction is described in this section. A chemical equilibrium reaction system is defined by the stoichiometry of the reaction and the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition).

The kinetics of the reaction is so fast that the equilibrium condition is fulfilled at all times in all space coordinates.

The equilibrium condition is commonly based on the stoichiometric coefficients, ν_i (dimensionless), of the reaction; the species activities of the reacting species a_i (dimensionless); and an equilibrium constant, K_{eq} (1) according to:

$$K_{eq} = \frac{\prod\limits_{i \in \text{ products}} a_i^{\nu_i}}{\prod\limits_{i \in \text{ reactants}} a_i^{-\nu_i}}$$

where the species activities are defined as

$$a_i = \gamma_{c,i} \frac{c_i}{c_{a0}}$$

where c_{a0} (SI unit: mol/m^3) is the standard molarity, and $\gamma_{c,i}$ (dimensionless) an activity coefficient.

Defining the stoichiometric coefficients positive for products and negative for reactants, the above equilibrium condition can also be written:

$$K_{eq} = \prod_i a_i^{\nu_i}$$

> $\gamma_{c,i}$ is set to unity when the Equilibrium constant is selected on the Settings window. For nonunity activity coefficients, a user defined equilibrium condition can be used.

EQUILIBRIUM REACTIONS AND INFLOW BOUNDARY CONDITIONS

Contradictory constraints arise if the boundary conditions for concentrations or activities are set so that the domain equilibrium condition is not fulfilled. Special treatment is therefore needed at Inflow boundaries, where the concentrations are set for all species in the mass transport interfaces.

One way of avoiding competing constraints on an inflow boundary is to add an additional reaction coordinate degree of freedom, solved for to create a set of modified inflow concentrations that fulfill the domain equilibrium condition. The reaction coordinate gives rise to a concentration shift, which is the offset to the inflow concentrations provided by the user. The shift for each species obeys the stoichiometry of the reaction and the equilibrium expression. The modified inflow concentrations are then used in the boundary conditions for the domain mass transport equations. The resulting modified inflow concentrations can be seen as the stationary solution for a batch reactor with the user inflow concentrations as initial concentrations. In addition, the domain reaction rate degree of freedom of the equilibrium reaction is constrained to zero on all Inflow boundaries.

EQUILIBRIUM REACTIONS AND CONCENTRATION BOUNDARY CONDITIONS

No special treatment is made with regards to input concentration values of the Concentration boundary node. Using this feature, you can explicitly set one or a set of concentrations, and the equilibrium condition acts on the rest of the concentrations. However, there is no solution to the problem if more concentrations than the number of species minus the number of equilibrium reactions are set using this feature.

EQUILIBRIUM REACTIONS AND TIME-DEPENDENT SIMULATIONS

Spurious oscillations may occur in a time-dependent problem if the initial conditions do not fulfill the equilibrium condition. Since equilibrium reactions are assumed to be infinitely fast, the solution is to initialize the problem using an additional study step, solving for a stationary problem with all non-equilibrium reaction rates set to zero. Manual scaling of the reaction rate dependent variables is needed in this study step.

Convective Term Formulation

The default node attributed to The Transport of Diluted Species Interface assumes chemical species transport through diffusion and convection and implements the mass balance equation in Equation 8-7.

There are two ways to present a mass balance where chemical species transport occurs through diffusion and convection. These are the non-conservative and conservative formulations of the convective term:

$$\text{non-conservative: } \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot (D \nabla c) + R \tag{8-9}$$

$$\text{conservative: } \frac{\partial c}{\partial t} + \nabla \cdot (c \mathbf{u}) = \nabla \cdot (D \nabla c) + R \tag{8-10}$$

and each is treated slightly differently by the solver algorithms. In these equations D (SI unit: m^2/s) is the diffusion coefficient, R (SI unit: $mol/(m^3 \cdot s)$) is a production or consumption rate expression, and $\mathbf{u}$ (SI unit: m/s) is the solvent velocity field. The diffusion process can be anisotropic, in which case D is a tensor.

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c \nabla \cdot \mathbf{u}$, would equal zero for an incompressible fluid and would result in the non-conservative formulation above. This is in fact the default formulation in this physics interface and ensures that nonphysical source terms do not emerge from a solution for the flow field. To switch between the two formulations, click the **Show** button (👁) and select **Advanced Physics Options**.

Solving a Diffusion Equation Only

Remove the convection term from Equation 8-9 and Equation 8-10 by clearing the Convection check box in the Transport Mechanisms section for The Transport of Diluted Species Interface. The equation then becomes

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) + R$$

Mass Sources for Species Transport

There are two types of mass sources in the Transport of Diluted Species interface: point sources and line sources.

Note: The features below are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit http://www.comsol.com/products/specifications/

POINT SOURCE

A point source is theoretically formed by assuming a mass injection/ejection, $\dot{Q}_c$ (SI unit: mol/(m^3·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_{p,c}$ (SI unit: mol/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q}_c = \dot{q}_{p,c} \tag{8-11}$$

An alternative way to form a point source is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant results in the same point source. For this alternative approach, effects resulting from the physical object's volume need to be neglected.

The weak contribution

$$\dot{q}_{p,c} \text{test}(c)$$

is added at a point in the geometry. As can be seen from Equation 8-11, $\dot{Q}_c$ must tend to plus or minus infinity as δV tends to zero. This means that in theory the concentration also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 8-11 corresponds to a finite concentration at a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region but also a more extreme concentration value. It is important not to mesh too finely around a point source since this can result in unphysical concentration values. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}_{l,c}$ (SI unit: mol/(m^3·s)), located within a tube with cross section δS and then letting δS tend to zero while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_{l,c}$ (SI unit: mol/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q}_{l,c} = \dot{q}_{l,c} \qquad (8\text{-}12)$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects resulting from the physical object's volume are neglected.

The weak contribution

$$\dot{q}_{l,c} \text{test}(c)$$

is added on lines in 3D or at points in 2D (which represent cut-through views of lines). Line sources can also be added on the axisymmetry line in 2D axisymmetry components. It cannot, however, be added on geometrical lines in 2D since those represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

🔍	For feature node information, see Line Mass Source and Point Mass Source in the *COMSOL Multiphysics Reference Manual*.

❗	For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Batteries & Fuel Cells Module, these shared physics nodes are renamed as follows: • The **Line Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**). • The **Point Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

Adding Transport Through Migration

Note: Migration is only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit
http://www.comsol.com/products/specifications/

In addition to transport due to convection and diffusion, the Transport of Diluted Species interface supports ionic species transport by *migration*. This is done by selecting the Migration in Electric Field check box under the Transport Mechanisms section for the physics interface. The mass balance then becomes:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (- D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V + c_i \mathbf{u}) = R_i \tag{8-13}$$

where

- c_i (SI unit: mol/ m^3) denotes the concentration of species i
- D_i (SI unit: m^2/s) is the diffusion coefficient of species i
- $\mathbf{u}$ (SI unit: m/s) is the fluid velocity
- F (SI unit: A·s/mol) refers to Faraday's constant
- V (SI unit: V) denotes the electric potential
- z_i (dimensionless) is the charge number of the ionic species, and
- $u_{m,i}$ (SI unit: mol·s/kg) is its ionic mobility

The velocity, $\mathbf{u}$, can be a computed fluid velocity field from a Fluid Flow interface or a specified function of the spatial variables x, y, and z. The potential can be provided by an expression or by coupling the system of equations to a current balance, such as the Electrostatics interface. Sometimes it is assumed to be a supporting electrolyte present, which simplifies the transport equations. In that case, the modeled charged species concentration is very low compared to other ions dissolved in the solution. Thus, the species concentration does not influence the solution's conductivity and the net charge within the fluid.

The Nernst-Einstein relation can in many cases be used for relating the species mobility to the species diffusivity according to

$$u_{m,i} = \frac{D_i}{RT}$$

where R (SI unit: J/(mol·K)) is the molar gas constant and T (SI unit: K) is the temperature.

Note: In the *Nernst-Planck Equations* interface, the ionic species contribute to the charge transfer in the solution. It includes an *electroneutrality condition* and also computes the electric potential field in the electrolyte. For more information, see Theory for the Nernst-Planck Equations Interface. This interface is included in the Chemical Reaction Engineering Module.

Supporting Electrolytes

In *electrolyte* solutions, a salt can be added to provide a high electrolyte conductivity and decrease the ohmic losses in a cell. These solutions are often called *supporting electrolytes*, buffer solutions, or carrier electrolytes. The added species, a negative and a positive ion pair, predominates over all other species. Therefore, the supporting electrolyte species can be assumed to dominate the current transport in the solution. In addition, the predominant supporting ions are usually selected so that they do not react at the electrode surfaces since the high conductivity should be kept through the process, that is, they should not be electro-active species. This also means that the concentration gradients of the predominant species in a supporting electrolyte are usually negligible.

Modeling and solving for a supporting electrolyte in the *Electrostatics* or *Secondary Current Distribution* interfaces will give a potential distribution that drives the migration in the Transport of Diluted Species Interface.

The current density vector is proportional to the sum of all species fluxes as expressed by Faraday's law:

$$\mathbf{i} = F\sum_i z_i \mathbf{N}_i$$

The electroneutrality condition ensures that there is always a zero net charge at any position in a dilute solution. Intuitively, this means that it is impossible to create a current by manually pumping positive ions in one direction and negative ions in the other. Therefore, the convective term is canceled out to yield the following expression for the electrolyte current density, where j denotes the supporting species:

$$\mathbf{i} = F\sum_j -z_j^2 u_{\mathrm{m},j} F c_j \nabla \phi \qquad (8\text{-}14)$$

Equation 8-14 is simply Ohm's law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa \nabla \phi \tag{8-15}$$

where κ is the conductivity of the supporting electrolyte. A current balance gives the current and potential density in the cell

$$\nabla \cdot \mathbf{i} = 0$$

which, in combination with Equation 8-15, yields:

$$\nabla \cdot (-\kappa \nabla \phi) = 0 \tag{8-16}$$

Equation 8-16 can be easily solved using the Electrostatics or Secondary Current Distribution interface and, when coupled to the Transport in Diluted Species interface, the potential distribution shows up in the migration term.

Crosswind Diffusion

Transport of diluted species applications can often result in models with a very high cell Péclèt number—that is, systems where convection or migration dominates over diffusion. Streamline diffusion and crosswind diffusion are of paramount importance to obtain physically reasonable results. The Transport of Diluted Species interface provides two crosswind diffusion options using different formulations. Observe that crosswind diffusion makes the equation system nonlinear even if the transport equation is linear.

DO CARMO AND GALEÃO

This is the formulation described in Numerical Stabilization. The method reduces over- and undershoots to a minimum, even for anisotropic meshes.

In some cases, the resulting nonlinear equation system can be difficult to converge. This can happen when the cell Péclèt number is very high and the model contains many thin layers, such as contact discontinuities. You then have three options:

• Refine the mesh, especially in regions with thin layers.

• Use a nonlinear solver with a constant damping factor less than one.

• Switch to the Codina crosswind formulation.

CODINA

The Codina formulation is described in Ref. 1. It adds diffusion strictly in the direction orthogonal to the streamline direction. Compared to the do Carmo and Galeão

formulation, the Codina formulation adds less diffusion but is not as efficient at reducing over- and undershoots. It also does not work as well for anisotropic meshes. The advantage is that the resulting nonlinear system is easier to converge and that under-resolved gradients are less smeared out.

Danckwerts Inflow Boundary Condition

Constraining the composition to fixed values at an inlet to a reactor may sometimes result in issues with unreasonably high reaction rates or singularities at the inlet boundary. These problems may many times be mitigated by using a flux boundary condition instead, based on the inlet concentrations and the fluid velocity. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet concentrations to domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an inlet concentration $c_{i,0}$, the Danckwerts inflow boundary condition reads

$$\mathbf{n} \cdot \mathbf{N}_i = \mathbf{n} \cdot (\mathbf{u} \, c_{i,0})$$

References

1. R. Codina, "A discontinuity-capturing crosswind-dissipation for the finite element solution of the convection-diffusion equation", *Computer Methods in Applied Mechanics and Engineering*, vol. 110, pp. 325–342, 1993.

2. P.V. Danckwerts, "Continuous flow systems: Distribution of residence times", *Chem. Eng. Sci.*, vol. 2, no. 1, 1953.

3. J.M. Coulson and J.F. Richardson, *Chemical Engineering, vol. 2*, 4th ed., Pergamon Press, Oxford, U.K., 1991.

4. J.M. Coulson and J.F. Richardson, *Chemical Engineering, vol. 1*, 4th ed., Pergamon Press, Oxford, U.K., 1991.

5. D.E Rosner, *Transport Processes in Chemically Reacting Flow Systems*, ISBN-13: 978-1483130262, Butterworth-Heinemann, 1986

6. D.M. Mackay, D.L. Freyberg, P.V. Roberts, and J.A. Cherry, "A Natural Gradient Experiment on Solute Transport in a Sand Aquifer: 1. Approach and Overview of Plume Movement", *Water Resourc. Res.*, vol. 22, no. 13, pp. 2017–2030, 1986.

7. C.W. Fetter, *Contaminant Hydrogeology*, Prentice Hall, 1999.

8. J. Bear and A. Verruijt, *Modeling Groundwater Flow and Pollution*, D. Reidel Publishing, 1994.

9. J. Bear, *Hydraulics of Groundwater*, McGraw-Hill, 1979.

10. R.D. Burnett and E.O. Frind, "An Alternating Direction Galerkin Technique for Simulation of Groundwater Contaminant Transport in Three Dimensions: 2. Dimensionality Effects", *Water Resour. Res.*, vol. 23, no. 4, pp. 695–705, 1987.

11. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing, 1972.

12. R.J. Millington and J.M. Quirk, "Permeability of Porous Solids", *Trans. Faraday Soc.*, vol. 57, pp. 1200–1207, 1961.

13. I. Langmuir, "Chemical Reactions at Low Temperatures", *J. Amer. Chem. Soc.*, vol. 37, 1915.

14. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, Inc., 2007.

About Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The **Transport of Diluted Species** interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis which adds the following contribution to the diffusion coefficient tensor:

$$\frac{\nu_T}{Sc_T}\mathbf{I} \tag{8-17}$$

where ν_T is the turbulent kinematic viscosity, Sc_T is the turbulent Schmidt number and $\mathbf{I}$ is the unit matrix. While having the form of a diffusive contribution, Equation 8-17 really models a convective phenomenon and it can therefore only be applied along with convection.

The Schmidt number is typically given a value between 0.7 and 0.72, but it can range between 0.3 and 1.3 (at least) depending on the application.

Theory for the Transport of Concentrated Species Interface

The Transport of Concentrated Species Interface theory is described in this section:

- Multicomponent Mass Transport
- Multicomponent Diffusion: Mixture-Average Approximation
- Multispecies Diffusion: Fick's Law Approximation
- Multicomponent Thermal Diffusion
- Turbulent Mixing
- Regularization of Reaction Rate Expression
- References for the Transport of Concentrated Species Interface

Multicomponent Mass Transport

Suppose a reacting flow consists of a mixture with $i = 1, \dots, Q$ species and $j = 1, \dots, N$ reactions. Equation 8-1 then describes the mass transport for an individual species:

$$\frac{\partial}{\partial t}(\rho \omega_i) + \nabla \cdot (\rho \omega_i \mathbf{u}) = -\nabla \cdot \mathbf{j}_i + R_i \tag{8-18}$$

where, ρ (SI unit: kg/m^3) denotes the mixture density and $\mathbf{u}$ (SI unit: m/s) the mass averaged velocity of the mixture. The remaining variables are specific for each of the species, i, being described by the mass transfer equation:

- ω_i is the mass fraction (1)
- $\mathbf{j}_i$ (SI unit: kg/(m^2·s)) is the mass flux relative to the mass averaged velocity, and
- R_i (SI unit: kg/ (m^3·s)) is the rate expression describing its production or consumption.

The relative mass flux vector $\mathbf{j}_i$ can include contributions due to molecular diffusion and thermal diffusion.

Summation of the transport equations over all present species gives Equation 8-19 for the conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{8-19}$$

assuming that

$$\sum_{i=1}^{Q} \omega_i = 1, \; \sum_{i=1}^{Q} \mathbf{j}_i = 0, \; \sum_{i=1}^{Q} R_i = 0$$

Using the mass conservation equation, the species transport for an individual species, i, is given by:

$$\rho \frac{\partial}{\partial t}(\omega_i) + \rho(\mathbf{u} \cdot \nabla)\omega_i = -\nabla \cdot \mathbf{j}_i + R_i \tag{8-20}$$

$Q - 1$ of the species equations are independent and possible to solve for using Equation 8-20. To compute the mass fraction of the remaining species, COMSOL Multiphysics uses the fact that the sum of the mass fractions is equal to 1:

$$\omega_1 = 1 - \sum_{i=2}^{Q} \omega_i \tag{8-21}$$

Multicomponent Diffusion: Mixture-Average Approximation

The mixture-averaged diffusion model assumes that the relative mass flux due to molecular diffusion is governed by a Fick's law type expression

$$\mathbf{j}_{\mathrm{md},\,i} = -\rho_i D_i^m \frac{\nabla x_i}{x_i} \tag{8-22}$$

where ρ_i is the density and x_i the mole fraction of species i. The diffusion hence depends on a single concentration gradient and is proportional to a diffusion coefficient D_i^m. The diffusion coefficient describes the diffusion of species i relative to the remaining mixture and is referred to as the mixture-averaged diffusion coefficient. Equation 8-22 can be expressed in terms of mass fractions as

$$\mathbf{j}_{\mathrm{md},\,i} = -\left(\rho D_i^m \nabla \omega_i + \rho \frac{\omega_i}{M} D_i^m \nabla M \right)$$

using the definition of the species density and mole fraction

$$\rho_i = \rho\omega_i \,, \; x_i = \frac{\omega_i}{M_i}M$$

Assuming isobaric and isothermal conditions, the following expression for the mixture-averaged diffusion coefficient can be derived from the Maxwell-Stefan equations (Ref. 3):

$$D_i^m = \frac{1-\omega_i}{\displaystyle\sum_{k \neq i}^{N} \frac{x_k}{D_{ik}}}$$

The mixture-averaged diffusivities are explicitly given by be the multicomponent Maxwell-Stefan diffusivities D_{ik}. For low-density gas mixtures, the D_{ik} components can be replaced by the binary diffusivities for the species pairs present.

When using the mixture-averaged diffusion model, the species mass transport equations are

$$\rho\frac{\partial}{\partial t}(\omega_i) + \rho(\mathbf{u} \cdot \nabla)\omega_i =$$

$$\nabla \cdot \left(\rho D_i^m \nabla\omega_i + \rho\omega_i D_i^m \frac{\nabla M}{M} + D_i^T \frac{\nabla T}{T} \right) + R_i$$

Apart from molecular diffusion, transport due to thermal diffusion is accounted for through the third term within the parenthesis on the right-hand side. Here D_i^T (SI unit: kg/(m·s)) is the thermal diffusion coefficient.

Multispecies Diffusion: Fick's Law Approximation

Using a *Fick's law approximation*, the relative mass flux due to molecular diffusion is assumed to be governed by

$$\mathbf{j}_{\mathrm{md},\,i} = -\rho_i D_{i,\,kl}^F \frac{\nabla x_i}{x_i} \tag{8-23}$$

where $D_{i,\,kl}^F$ represents a general diffusion matrix (SI unit: m^2/s) describing the diffusion of species i into the mixture. This form makes it possible to use any diffusion coefficient, matrix, or empirical model based on Fick's law. For example, in situations when the mass transport is not dominated by diffusion, an alternative is to use the diffusion coefficients at infinite dilution,

$$D^F_{i,kk} = D^0_i$$

These coefficients are typically more readily available compared to the binary diffusion diffusivities, especially for liquid mixtures.

When using multicomponent diffusivities based on Fick's law, as described above, or when using mixture-averaged coefficients, the sum of the relative mass fluxes is not strictly constrained to zero. To reduce the relative error it is preferable to choose the species with the highest mass fraction as the species that is not solved for, and which is instead computed from the mass conservation constraint in Equation 8-4. It is not always necessary to know in advance which species has the highest mass fraction—it is possible to change the species solved for by the mass conservation constraint in Equation 8-4.

When using the Fick's law approximation for the diffusion model, the species mass transport equations are:

$$\rho \frac{\partial}{\partial t}(\omega_i) + \rho(\mathbf{u} \cdot \nabla)\omega_i =$$

$$\nabla \cdot \left(\rho D^F_i \nabla \omega_i + \rho \omega_i D^F_i \frac{\nabla M}{M} + D^T_i \frac{\nabla T}{T} \right) + R_i$$

Apart from molecular diffusion, transport due to thermal diffusion is accounted for through the third term within the parenthesis on the right-hand side. Here D^T_i is the thermal diffusion coefficient (SI unit: kg/(m·s)).

Multicomponent Thermal Diffusion

Mass diffusion in multicomponent mixtures due to temperature gradients is referred to as the *Soret effect*. This occurs in mixtures with high temperature gradients and large variations in molecular weight (or size) of the species. Typically species with high molecular weight accumulate in lower temperature regions while the diffusion due to the Soret effect transports species with low molecular weight to higher temperature regions. In COMSOL Multiphysics, thermal diffusion is included by prescribing the thermal diffusion coefficients D^T_i. In a multicomponent mixture, the sum of the thermal diffusion coefficients is zero:

$$\sum_{i=1}^{Q} D^T_i = 0$$

Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The Transport of Concentrated Species Interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis. In the case of mixture-averaged diffusion, it adds the following contribution to the diffusion coefficient for each species:

$$\frac{\nu_T}{Sc_T} \tag{8-24}$$

while for Fick's law diffusion, it adds the following contribution to the diffusion coefficient tensor:

$$\frac{\nu_T}{Sc_T}\mathbf{I} \tag{8-25}$$

Here, ν_T is the turbulent kinematic viscosity, Sc_T is the turbulent Schmidt number and $\mathbf{I}$ is the unit matrix. While having the form of diffusive contributions, Equation 8-24 and Equation 8-25 really model a convective phenomenon and they can therefore only be applied along with convection.

The Schmidt number is typically given a value between 0.7 and 0.72, but it can range between 0.3 and 1.3 (at least) depending on the application.

Regularization of Reaction Rate Expression

The flexibility of COMSOL means that a reaction can result in nearly any reaction rate contribution $R_i^{\mathbf{c}}$ to a mass fraction ω_i. But a reactant, ω_r, can physically only be consumed if $\omega_r > 0$ and a product, ω_k, can only be formed if $\omega_k < 1$. The Reaction feature in Transport of Concentrated Species Interface contains a way to regularize make the rate expression contributions comply to these restrictions.

When selected the "core", or unregularized reaction rate contribution, $R_i^{\mathbf{c}}$, to a mass fraction ω_i is replaced by

$$R_i = \frac{1}{2}\frac{R_i^c - \left|R_i^c\right|}{\max(\omega_i, \omega_i^{dl})}\max(\omega_i, 0) + \frac{1}{2}\frac{R_i^c + \left|R_i^c\right|}{\max(1 - \omega_i, \omega_i^{dl})}\max(1 - \omega_i, 0) \tag{8-26}$$

The first term on the right hand side of Equation 8-26 is active if $R_i^c < 0$, that is if ω_i is a reactant. The reaction rate contribution, R_i, is equal to the "core" reaction rate, R_i^c, as long as $\omega_i > \omega_i^{dl}$. As ω_i approaches zero, the regularization damps out negative R_i^c and for $\omega_i < 0$, R_i for reactant ω_i is equal to zero.

The second term on the right hand side of Equation 8-26 is active if $R_i^c > 0$, that is if ω_i is a product. The reaction rate contribution, R_i, is equal to the "core" reaction rate, R_i^c, as long as $\omega_i < 1 - \omega_i^{dl}$. As ω_i approaches one, the regularization damps out positive R_i^c and for $\omega_i > 1$, R_i for product ω_i is equal to zero.

The damping limits, ω_i^{dl}, should be in an order of magnitude that can be considered numerical noise for species i. The damping limits are per default set to $1e^{-6}$, which is appropriate for most applications. It can be advantageous to lower some limits when working with for example catalytic trace species and the limits can sometimes be raised to gain additional robustness.

References for the Transport of Concentrated Species Interface

1. C.F. Curtiss and R.B. Bird, "Multicomponent Diffusion," *Ind. Chem. Res.*, vol. 38 pp. 2515–2522, 1999.

2. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, 2005.

3. R.J. Kee, M.E. Coltrin, and P. Glarborg, *Chemically Reacting Flow*, John Wiley & Sons, 2003.

4. A. Soulaïmani and M. Fortin, "Finite Element Solution of Compressible Viscous Flows Using Conservative Variables," *Computer Methods in Applied Mechanics and Engineering*, vol. 118, pp. 319–350, 1994.

Theory for the Reacting Flow Interfaces

The following sections describe theory applicable for the Reacting Flow interfaces:

- Pseudo Time Stepping for Mass Transport
- The Stefan Velocity
- The Chemical Reaction Rate
- Turbulent Mass Transport Models
- Mass Transport Wall Functions
- Turbulent Reactions
- The Reaction Source Term for Turbulent Flow
- References for the Reacting Flow Interfaces

Pseudo Time Stepping for Mass Transport

In order to improve the solution robustness, pseudo time stepping can be used for the Transport of Concentrated Species interface when solving a stationary model. Using pseudo time stepping, a fictitious time derivative term:

$$\rho \frac{\omega_i - \mathrm{nojac}(\omega_i)}{\Delta \tilde{t}}$$

is added to the left-hand side of the mass fraction equations. Here ρ is the fluid mixture density, ω_i is the mass fraction (dimensionless) of species i, and $\Delta \tilde{t}$ is the *pseudo time step*. Since $\omega_i - \mathrm{nojac}(\omega_i)$ is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a time step of size $\Delta \tilde{t}$.

📄	For a description of the pseudo time step term for the Navier-Stokes equations and the pseudo time step see Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*.

The Stefan Velocity

Heterogeneous reactions on fluid-solid surfaces can affect the mass, momentum, and energy balances at the interface separating the fluid and the solid. On the reacting surface, the production or destruction rate, $r_{s,i}$ (SI unit: mol/(m^2·s)), of a fluid phase species is balanced by the total mass flux of the species. The mass balance for species i on a boundary representing a fluid-solid interface is given by:

$$\mathbf{n} \cdot [\rho\omega_i(\mathbf{u} + \mathbf{u}_{d,i})] = r_{s,i}M_i \tag{8-27}$$

Here, $\mathbf{n}$ is the unit normal pointing out of the fluid domain, $\mathbf{u}$ is the mass averaged velocity of the fluid mixture (SI unit: m/s), $\mathbf{u}_{d,i}$ denotes the diffusion velocity (SI unit: m/s), the velocity of species i relative to the mixture, and M_i is the species molar mass (SI unit: kg/mol). Summing the mass balances at the surface, over all species, results in an effective mixture velocity:

$$\mathbf{n} \cdot \rho\mathbf{u}_s = \sum_{i=1}^{N} r_{s,i}M_i \tag{8-28}$$

referred to as the Stefan velocity, here denoted $\mathbf{u}_s$. To reach Equation 8-28 the fact that the sum of all mass fractions is one, and that the sum of all relative diffusive fluxes is zero, was used.

Equation 8-28 implies that surface reactions result in a net flux between the surface and the domain. A net flux in turn corresponds to an effective convective velocity at the domain boundary; the Stefan velocity. It should be noted here that when solving for mass transport inside a fluid domain, an outer boundary of the domain corresponds to a position just outside of the a actual physical wall (on the fluid side). The domain boundary does not coincide with the physical wall.

In most reacting flow models, the species mass fractions in the fluid domain are solved for, without including the surface concentrations (mol per area) on exterior walls is not included in the model. One reason for this is that the surface reaction rates are often not known. In this case, surface reactions can be modeled either by applying a mass flux or prescribing the mass fraction, or a combination of both, on fluid boundaries adjacent to the reacting surface. The Stefan velocity on a fluid domain boundary is then defined as the net mass flux resulting from the boundary conditions applied:

$$\mathbf{n} \cdot \rho \mathbf{u}_s = \sum_{i=1}^{n_D} \mathbf{n} \cdot (\rho \omega_i \mathbf{u}_s + \mathbf{N}_{i,d}) + \sum_{j=1}^{n_N} \mathbf{n} \cdot \mathbf{N}_{j,tot} \qquad (8\text{-}29)$$

Here, the first sum contains flux contributions resulting from boundary conditions prescribing the mass fractions, and the second sum contains contributions from flux conditions. The resulting Stefan velocity based on mass transport boundary conditions is computed as:

$$\mathbf{n} \cdot \mathbf{u}_s = \frac{\left(\displaystyle\sum_{i=1}^{n_D} \mathbf{n} \cdot \mathbf{N}_{i,d} + \sum_{i=1}^{n_N} \mathbf{n} \cdot \mathbf{N}_{i,tot} \right)}{\rho \left(1 - \displaystyle\sum_i \omega_i \right)} \qquad (8\text{-}30)$$

Using a Reacting Flow interface, the Stefan velocity, defined in the manner of Equation 8-30, is automatically computed and applied on boundaries corresponding to walls by the Reacting Flow coupling feature. When a Mass Fraction or Flux feature (in the Transport of Concentrated Species interface) is applied on a selection shared by a Wall feature (in the Single-Phase Flow interface), the Stefan velocity is prescribed in the wall normal direction on the shared selection.

The Chemical Reaction Rate

For laminar flow, or when the **Turbulent-reaction model** is set to **None** in a Reaction feature (in Transport of Concentrated Species), the default (Automatic) reaction rate used by the Reaction feature is based on the mass action law. Consider a general reaction belonging to a set of j reactions and involving i species:

$$(8\text{-}31)$$
$$aA + bB + \cdots \; \underset{k_j^r}{\overset{k_j^f}{\rightleftharpoons}} \; xX + yY + \cdots$$
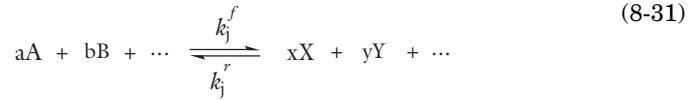
For such a reaction set, the reaction rates r_j (SI unit: mol/(m^3·s)), can be described by the mass action law:

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}} - k_j^r \prod_{i \in \text{prod}} c_i^{\nu_{ij}} \qquad (8\text{-}32)$$

Here, k_j^f and k_j^r denote the forward and reverse rate constants, respectively. The concentration of species i is denoted c_i (SI unit: mol/m^3). The stoichiometric coefficients are denoted ν_{ij}, and are defined to be negative for reactants and positive for products. In practice, a reaction seldom involves more than two species colliding in a reacting step, which means that a kinetic expression is usually of order 2 or less (with respect to the involved concentrations).

In addition to the concentration dependence, the temperature dependence can be included by using the predefined Arrhenius expressions for the rate constants:

$$k = AT^n \exp\left(-\frac{E}{R_g T}\right)$$

Here, A denotes the frequency factor, n the temperature exponent, E the activation energy (SI unit: J/mol) and R_g the gas constant, 8.314 J/(mol·K). The pre-exponential factor, including the frequency factor A and the temperature factor T^n, is given the units (m^3/mol)$^{\alpha-1}$/s, where α is the order of the reaction (with respect to the concentrations).

Turbulent Mass Transport Models

The RANS turbulence models included in the Reacting Flow interfaces are based on averaging of the fluid flow equations. Applying a corresponding decomposition of the fluctuating mass fraction, into mean and fluctuating parts, and averaging the mass transport equations, additional unclosed terms are introduced in the equations. These terms need to be modeled in order to close the set of equations. The most important terms, containing the correlations of the velocity and mass fraction fluctuations, referred to as the turbulent mass transport fluxes, are given by:

$$\frac{\partial(\overline{\rho u_i'' \omega''})}{\partial x_i}$$

Here the double primes denote Favre (density-based) fluctuations. In the case of varying density flow, Favre averaging is favored over Reynolds averaging since it reduces the number of unclosed terms and renders the equation on the same form as the incompressible RANS equations. For more background on averaging, see Turbulence Modeling.

The most common way to model this term is to use a gradient based assumption, where the additional turbulent transport is related to the turbulent viscosity through a turbulent Schmidt number Sc_T:

$$\overline{\rho u_i'' \omega''} = -\frac{\mu_T}{Sc_T}\frac{\partial \tilde{\omega}}{\partial x_i} = -\rho D_T \frac{\partial \tilde{\omega}}{\partial x_i} \qquad (8\text{-}33)$$

Here $\tilde{\omega}$ denotes the Favre averaged mass fraction which is the quantity solved for.

Using a RANS turbulence model, the turbulent mass flux is defined from Equation 8-33, and the equation solved for each species is:

$$\bar{\rho}\frac{\partial}{\partial t}(\tilde{\omega}_i) + \bar{\rho}(\tilde{\mathbf{u}} \cdot \nabla)\tilde{\omega}_i =$$

$$\nabla \cdot \left(\bar{\rho}\left(D_i + \frac{\nu_T}{Sc_T}\right)\nabla\tilde{\omega}_i + \bar{\rho}\tilde{\omega}_i D_i \frac{\nabla M}{M} + \bar{D}_i^T \frac{\nabla T}{T} + \bar{\rho}\tilde{\omega}_i z_i u_{m,i} F\nabla V \right) + \bar{R}_i$$

where the molecular diffusion coefficient, D_i, is given by the diffusion model (Mixture-Average or Fick's Law).

KAYS-CRAWFORD

Assuming that the turbulent transport mechanisms of heat and mass processes are analogous, the turbulent Schmidt number is defined by (Ref. 1):

$$Sc_T = \left(\frac{1}{2Sc_{T\infty}} + \frac{0.3 Pe_T}{\sqrt{Sc_{T\infty}}} - (0.3 Pe_T)^2 [1 - e^{-1/(0.3 Pe_T \sqrt{Sc_{T\infty}})}] \right)^{-1}$$

where the Schmidt number at infinity is $Sc_{T\infty} = 0.85$, and the turbulent Peclet number is defined as the ratio of the turbulent to molecular viscosity times the Schmidt number:

$$Pe_T = \frac{\nu_T}{\nu}Sc$$

HIGH SCHMIDT NUMBER MODEL

In the case of high Schmidt numbers, which is typical for mass transport in liquids, the mass transfer near walls can be significantly different than that for Schmidt numbers of order unity. A diffusion layer near a solid wall, due to, for example, a reaction on the wall, does not have the same properties as the (momentum) boundary layer. Most importantly the diffusion layer thickness is significantly smaller than the boundary layer thickness for high Schmidt numbers. In order to correctly capture the mass flux at the wall, the wall resolution required is dictated by the diffusion layer rather than by the boundary layer.

The High Schmidt number model is based on the model by Kubacki and Dick (Ref. 2) and is available when using the Low-Reynolds k-ε turbulence model or the SST turbulence model. In this case the fluid flow is resolved all the way to the physical wall and consequently, and species boundary equations are applied directly on the wall (without using wall functions).

In the near wall region, where the species transport is limited by diffusion, the mass diffusivity is modeled using an analytical function of the non-dimensional wall distance due to Na and Hanratty (Ref. 3):

$$\frac{D_{T,w}}{v} = b(l^*)^m$$

The non-dimensional wall distance applied, l^*, corresponds to that defined by the turbulence model. The value of the constants b and m are given in Table 8-1.

TABLE 8-1: NA AND HANRATTY PARAMETERS

SCHMIDT NUMBER	b	m
0.1 < Sc < 5	$7.3 \cdot 10^{-4}$	3
5 < Sc < 50	$5.3 \cdot 10^{-4}$	3
Sc > 50	$4.63 \cdot 10^{-4}$	3.38

Further out from the wall, where the mass transport is governed by the turbulent transport, the transport is modeled using a turbulent Schmidt number of the form (Ref. 2):

$$Sc_{T,c} = \left(0.5882 + 0.228\left(\frac{v_T}{v}\right) - 0.0441\left(\frac{v_T}{v}\right)^3 [1 - e^{-5.165/(v_T/v)}] \right)^{-1}$$

In order to combine the two descriptions, the blending function by Kader (Ref. 4) is used:

$$D_T = \frac{v_T}{Sc_{T,c}}e^{(-\Gamma)} + D_{T,w}e^{(-1/\Gamma)}$$

where

$$\Gamma = \frac{0.01(l^*)^4}{(1 + 5l^*)}$$

Mass Transport Wall Functions

Analogous to the single-phase flow wall functions (see Wall Functions applied for the Wall boundary condition), there is a theoretical gap between the solid wall and the computational domain of the fluid. This gap is often ignored when the computational geometry is drawn.

Assuming that the turbulent heat and mass transfer in the near-wall region are analogous, the same type of wall functions used for the temperature (Ref. 8) is also applicable for the mass transport. The mass transfer wall function is formulated as a function of the molecular and turbulent Schmidt numbers of each species, instead of the corresponding Prandtl numbers.

Assume that there is a mass fraction $\omega_{i,w}$ just outside the wall and that it is in equilibrium with the surface chemistry. The mass flux, for species i, between the wall and a fluid with a mass fraction of $\omega_{i,f}$ at the lift-off position is:

$$m_{wf} = \frac{\rho C_\mu^{1/4} k^{1/2}(\omega_{i,w} - \omega_{i,f})}{\omega_i^+}$$

where ρ is the fluid density, C_μ is a turbulence modeling constant, and k is the turbulent kinetic energy. ω_i^+ is the dimensionless mass fraction given by (Ref. 8):

$$\omega_i^+ = \begin{cases} Sc\,\delta_w^+ & \text{for } \delta_w^+ < \delta_{w1}^+ \\ \left(15 Sc^{2/3} - \dfrac{500}{\delta_w^{+2}}\right) & \text{for } \delta_{w1}^+ \leq \delta_w^+ < \delta_{w2}^+ \\ \dfrac{Sc_T}{\kappa}\ln\delta_w^+ + \beta & \text{for } \delta_{w2}^+ \leq \delta_w^+ \end{cases}$$

where in turn

$$\delta_w^+ = \frac{\delta_w \rho \sqrt{C_\mu^{1/2} k}}{\mu} \qquad\qquad \delta_{w1}^+ = \frac{10}{Sc^{1/3}}$$

$$\delta_{w2}^+ = 10\sqrt{10\frac{\kappa}{Sc_T}} \qquad\qquad Sc = \frac{\mu}{\rho D_{i,m}}$$

$$\beta = 15 Sc^{2/3} - \frac{Sc_T}{2\kappa_v}\left(1 + \ln\left(1000\frac{\kappa}{Sc_T}\right)\right)$$

κ_v is the von Karman constant, and $D_{i,m}$ the mean species diffusion coefficient. The latter corresponds directly to the mixture-averaged diffusion coefficient when using

the Mixture-average diffusion model. Using the Fick's law diffusion model, the mean diffusion coefficient is computed as $1/N \cdot \mathrm{tr}(D_i)$, where D_i is the diffusion tensor and N is the dimension of the model.

The computational result should be checked so that the distance between the computational fluid domain and the wall, δ_w, is almost everywhere small compared to any geometrical quantity of interest. The distance δ_w is available as a post processing variable (`delta_w`) on boundaries.

Turbulent Reactions

In turbulent flow the reaction rate is significantly affected by the turbulence. Turbulent fluctuations can increase the reaction rate due to the increased mixing, but it can also quench it through removal of species or the heat required for ignition. The interaction between the flow and the reactions can be quantified through the Damköhler number Da:

$$Da = \frac{\tau_T}{\tau_c}$$

which compares the time scale of the largest turbulent flow structures (the integral time scale), to the chemical time scale. In the limit of large Damköhler numbers Da >> 1, the reactive time scale is significantly smaller than that of the turbulence. In this regime the inner structure of a reaction zone is thin enough not to be affected by turbulence. The reacting regions are, however, convected and wrinkled by the turbulence. In this case the global reaction rate is proportional to the chemical reaction rate times the surface of the reacting regions. In the limit of small Damköhler numbers Da << 1, the chemical time scale is much larger than that of the turbulent flow. In this case the global reaction rate is controlled by the chemistry, while the turbulence acts by continuously mixing the species. This regime is referred to as a "perfectly stirred reactor".

MEAN VALUE CLOSURE

A mean turbulent production rate can be obtained by directly applying the mean concentrations and temperature in the kinetic reaction rate expressions:

$$R_i = \nu_i M_i r_{\mathrm{MVC},i}$$

where ν_i denotes the species stoichiometric coefficient, M_i the molar mass (SI unit: kg/mol), and $r_{MVC,i}$ is the reaction rate from Equation 8-32 using mean quantities.

This is referred to as mean value closure of the turbulent reaction rate, and corresponds to keeping the first term in a Taylor series expansion of the turbulent reaction rate following a Reynolds decomposition of the fluctuating variables (Ref. 5). The mean value closure is directly applicable in the perfectly-stirred-reactor limit ($Da \ll 1$). In this case the turbulence is able to mix the species in the sense of changing the mean concentration, but the turbulent fluctuations do not affect the chemical reaction rate. The mean value closure is also applicable in the limit of low turbulence levels since the turbulent fluctuations tend to zero as the laminar flow regime is approached.

EDDY DISSIPATION MODEL

The eddy-dissipation model for the mean reaction rate originally developed by Magnusson and Hjertager (Ref. 6) for non-premixed combustion. Using this reaction model, the mean production rate of species i is defined as:

$$R_i = \nu_i M_i \frac{\alpha}{\tau_T} \rho \cdot \min \left[\min \left(\frac{\omega_r}{\nu_r M_r} \right), \beta \sum_p \left(\frac{\omega_p}{\nu_p M_p} \right) \right] = \nu_i M_i r_{ED,i}$$

The model assumes that both the Reynolds and Damköhler numbers are sufficiently high for the reaction rate to be limited by the turbulent mixing time-scale τ_T. The reaction can hence at most progress at the rate at which fresh reactants are mixed, at the molecular level, by the turbulence present. Furthermore the reaction rate is limited by the deficient reactant; the reactant with the lowest local concentration. When the model parameter β is finite, the existence of product species is also required for reaction, modeling the activation energy required for reaction (ignition). For gaseous non-premixed combustion the model parameters have been found to correspond to (Ref. 6):

$$\alpha = 4 \, , \, \beta = 0.5$$

For liquid reactions it is recommended that the model parameters are calibrated against experimental or simulation data. Using a mix of the mean value closure and a modified version of the eddy-dissipation model Bakker and Fasano (Ref. 7) found the following parameter values

$$\alpha_2 = 0.08 \, , \, \alpha_1 = \beta_1 = \beta_2 = \infty$$

to give good results for a competitive reaction pair when compared with experimental results.

A common approximation for the turbulence mixing time-scale τ_T is $\tau_T \approx k/\varepsilon$ (Ref. 5). Due to realizability constraints, a more accurate approximation is however

$$\tau_T = \min\left(\frac{k}{\varepsilon}, \frac{1}{C_\mu 3\lambda_{max}}\right) \tag{8-34}$$

where in turn

$$\lambda_{max} = \frac{1}{2}\sqrt{S_{ij}S_{ij}}$$

for 2D and

$$\lambda_{max} = \sqrt{\frac{2S_{ij}S_{ij}}{3}}$$

for 3D and 2D axisymmetry. Equation 8-34 is directly applicable to the k-ε model. For the k-ω and SST turbulence models, Equation 8-34 reads

$$\tau_T = \min\left(\frac{1}{\beta^* \omega}, \frac{1}{\beta^* 3\lambda_{max}}\right)$$

Equation 8-34 is used also for the low-Reynolds k-ε model even though k/ε is not actually the turbulence mixing time scale. To obtain a consistent turbulence mixing time scale for low-Reynolds k-ε, k/ε needs to be multiplied by a damping function that goes to zero at solid walls. Ref. 5 does however notice that τ_T is not a relevant time scale close to walls since it is too small. The damping function is therefore neglected in the eddy-dissipation model.

The Reaction Source Term for Turbulent Flow

For turbulent flow, or when the **Turbulent-reaction model** is set to **Eddy-dissipation** in the Reaction feature (in Transport of Concentrated Species), the reaction source term is computed as the minimum of the mean value closure and that from the eddy dissipation model:

$$R_i = \nu_i M_i \cdot \min\left[r_{MVC,i}, r_{EDC,i}\right]$$

This approach combines the regimes of the separate models. For fast reactions the reaction rate is limited by the turbulent mixing. At the same time, in regions with low turbulence levels, or low kinetic reactions rates, the latter limits the production rate.

References for the Reacting Flow Interfaces

1. W.M. Kays, "Turbulent Prandtl Number—Where Are We?" *ASME Journal of Heat Transfer*, vol. 116, pp. 284–295, 1994.

2. S. Kubacki and E. Dick, "Simulation of Impinging Mass Transfer at High Schmidt Number with Algebraic Models," *Progress in Computational Fluid Dynamics*, vol. 11, no. 1, pp. 30–41, 2011.

3. Y. Na and T.J. Hanratty, "Limiting Behavior of Turbulent Scalar Transport Close to the Wall", *Int. J. Heat Mass Transfer*, vol. 43, pp. 1749–1758, 2000.

4. B.A. Kader, "Temperature and Concentration Profiles in Fully Turbulent Boundary Layers", *Int. J. of Heat and Mass Transfer*, vol. 24, pp. 1541–1544, 1981.

5. T. Poinsot and D. Veynante, *Theoretical and Numerical Combustion*, 2nd. ed., R.T. Edwards, Philadelphia, 2005.

6. B.F. Magnussen and B.H. Hjertager, "On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion," *16th Symp. (Int.) on Combustion*. Comb. Inst., Pittsburg, Pennsylvania, pp.719–729, 1976.

7. A. Bakker and J.B. Fasano, "Time Dependent, Turbulent Mixing and Chemical Reactions in Stirred Tank," *AIChE Symposium Series 299*, vol. 90, pp. 71–78, 1993.

8. D. Lacasse, È. Turgeon, and D. Pelletier, "On the Judicious Use of the k—ε Model, Wall Functions and Adaptivity," *Int.J. of Thermal Sciences,* vol. 43, pp. 925–938, 2004.

9

Thin-Film Flow Interfaces

The physics interfaces described in this section are found under the **Thin-Film Flow** branch (📘).

In this chapter

- The Thin-Film Flow Interfaces
- Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow Interfaces

In this section:

- The Thin-Film Flow, Shell Interface
- The Thin-Film Flow, Domain Interface
- The Thin-Film Flow, Edge Interface
- Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces

The physics interfaces found under the **Thin-Film Flow** branch ( ) when adding a physics interface describe momentum transport. These physics interfaces can be added either singularly or in combination with other physics interfaces describing mass and energy transfer. The thin-film flow interfaces are shown in Table 9-1.

TABLE 9-1: THE THIN-FILM FLOW INTERFACES DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	SPACE DIMENSION	GEOMETRIC ENTITY LEVEL
Thin-Film Flow, Shell	tffs	3D	Boundaries
Thin-Film Flow, Edge	tffs	2D, 2D axisymmetric	Boundaries
Thin-Film Flow, Domain	tff	2D	Domains

Each of the physics interfaces can be configured to solve either the standard **Reynolds Equation** (with a material or user-defined density specified at the absolute pressure), or to solve the **Modified Reynolds Equation**, which should be used for gas flows. The **Modified Reynolds Equation** assumes the ideal gas law and applies when gas pressure changes in the flow itself result in significant density changes.

> 🔍   Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow, Shell Interface

The **Thin-Film Flow, Shell (tffs)** interface ( ), found under the **Thin-Film Flow** branch ( ) when adding a physics interface, is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by a surface within the geometry. It is used for lubrication, elastohydrodynamics, or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the

Modified Reynolds equation to apply. The physics interface is available for 3D geometries.

This physics interface is defined in a boundary mode, which means that the boundary level is the highest level for which this physics interface has equations and features; it does not have any features or equations on the domain level. The boundary level represents a reference surface on which the flow is solved. On one side of the boundary level there is a wall and on the other a base surface, neither of which is represented in the geometry. The wall and base surfaces are orientated with respect to the reference surface normal as shown in Figure 9-1. Fluid flows in the gap between the wall and the base.
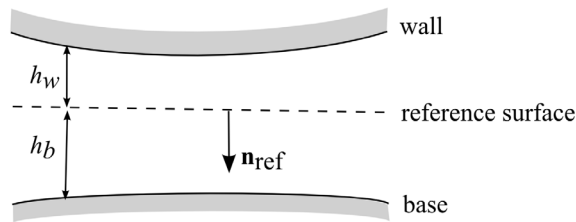
Figure 9-1: Diagram illustrating the orientation of the wall and the base surfaces with respect to the reference surface in the Thin-Film Flow interfaces. A vector from the reference surface to the corresponding point on the wall always points in the $-\mathbf{n}_{ref}$ direction, where $\mathbf{n}_{ref}$ is the reference surface normal. Similarly a vector from the reference surface to the corresponding point on the base points in the $+\mathbf{n}_{ref}$ direction. The height of the wall above the reference surface (h_w) and the height of the base below the reference surface (h_b) are also shown in the figure.

Using equations on the reference surface, the physics interface computes the pressure in a narrow gap between the wall and the base. When modeling the flow, it is assumed that the total gap height, $h = h_w + h_b$, is much smaller than the typical lateral dimension L of the reference surface. The physics interface is used to model laminar flow in thin gaps or channels. A lubricating oil between two rotating cylinders is an example of this.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid-Film Properties**, **Border**, and **Initial Values**. Then, from the **Physics** toolbar, you can add other nodes that implement, for example, boundary conditions. You can also right-click **Thin-Film Flow, Shell** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is tffs.

REFERENCE PRESSURE

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm]. This pressure represents the ambient pressure and fluid loads are computed without accounting for this pressure.

CAVITATION

To display this section, click the **Show** button (🔻) and select **Show Advanced Physics Options**. Select the **Cavitation** check box to use when modeling bearings, for example. Then enter a **Cavitation transition width** (SI unit: Pa). The default is 1 MPa.

Under normal operating conditions, the gases dissolved in the lubricant cause cavitation in the diverging clearance between the journal and the bearing. This happens because the pressure in the lubricant drops below the saturation pressure.

See theory for Cavitation for more information.

Note: Cavitation is only available in the **Thin-Film Flow, Shell** physics interface with a CFD Module license. It is not available for the **Thin-Film Damping** boundary condition, which can be added to the physics interfaces in the Structural Mechanics area.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure** p_f. The name can be changed but the names of fields and dependent variables must be unique within a component.

To display this section, click the **Show** button (👁) and select **Discretization**.

🔍
- [Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces](#)
- [Theory for the Thin-Film Flow Interfaces](#)

▥
- *Journal Bearing*: Application Library path **CFD_Module/Thin-Film_Flow/ journal_bearing**
- *Tilted Pad Thrust Bearing*: Application Library path **CFD_Module/ Thin-Film_Flow/tilted_pad_bearing**

The Thin-Film Flow, Domain Interface

The **Thin-Film Flow, Domain (tffs)** interface (📄), found under the **Thin-Film Flow** branch (📄) when adding a physics interface, is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by a domain within the geometry. It is used for lubrication or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the Modified Reynolds equation to apply. The physics interface is available for 2D geometries.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid-Film Properties**, **Border** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Thin-Film Flow, Domain** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tff`.

The rest of the settings are the same as for The Thin-Film Flow, Shell Interface.

ℚ	• Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces
	• Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow, Edge Interface

The **Thin-Film Flow, Edge (tff)** interface (⊞) is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by an edge within the geometry. It is used for lubrication, elastohydrodynamics, or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the Modified Reynolds equation to apply. The physics interface is for 2D and 2D axisymmetric components.

The rest of the settings are the same as for The Thin-Film Flow, Shell Interface.

ℚ	• Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces
	• Theory for the Thin-Film Flow Interfaces

Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces

For the physics interfaces under the Thin-Film Flow branch, the following domain, boundary, edge, point, and pair nodes (listed in alphabetical order) are described in this section:

- Border
- Fluid-Film Properties
- Initial Values
- Inlet
- Perforations
- Outlet
- Symmetry
- Wall

> **!** In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid-Film Properties

Use the **Fluid-Film Properties** node to set the wall properties, base properties, fluid properties, and the film flow model.

REFERENCE SURFACE PROPERTIES

In the **Thin-Film Flow, Shell (tffs)** and **Thin-Film Flow, Edge (tffs)** interfaces, the **Reference normal orientation** setting allows you to reverse the direction of the reference surface normal used by the physics interface. By default this is set to **Same direction as geometry normal**. To reverse the direction, select **Opposite direction to geometry normal**.

In the **Thin-Film Flow, Domain (tff)** interface, the **Reference surface normal orientation** setting allows you to set the direction of the reference normal so that it either points out of or into the plane of the domain. By default this is set to **Reference surface normal points out of plane**, such that the reference surface normal is given by {0,0,1}. Selecting **Reference surface normal points into plane** sets the reference surface normal to {0,0,-1}.

WALL PROPERTIES

Enter a value or expression for the **Height of wall above reference plane** h_{w1} (SI unit: m). The default is 10 μm.

By default the **Additional wall displacement** is **User defined**. Enter values or expressions for $\mathbf{u}_w$ (SI unit: m). The defaults are 0 m. Alternatively select a feature input (defined by a separate physics interface) or **None** from the list.

When using a feature input to define an additional displacement based on the movement of a structure, refer to Figure 9-1 to decide whether the additional displacement should be added to the wall or the base.

- If the reference normal points out of the structure for which the displacement is provided, the structure should be considered to be the wall, and its displacement should be added to the additional wall displacement.

If the reference normal points into the structure for which the displacement is provided, the structure is the base and its displacement should be added to the additional base displacement. To determine the reference normal orientation before fully solving the model, click **Show Default Solver** ( ) on the **Study** toolbar (or right-click the **Study 1** node and select **Show Default Solver**). Then expand the **Study 1>Solver Configurations>Solver 1** node, right-click the **Dependent variables** sub-node and select **Compute to Selected**.
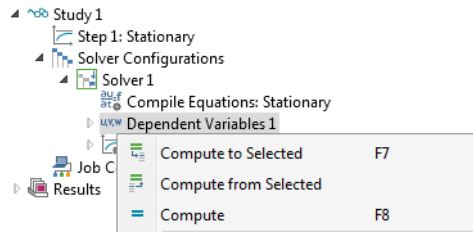
You can then add a 2D or 3D plot group with an **Arrow Surface** plot (in 3D) ( ) or **Arrow Line** plot (in 2D) ( ), and use the **Replace Expression** ( ) button to plot the **Reference surface normal**.

Note that the orientation of the reference surface normal can be changed using the **Reference normal orientation** setting in the Reference Surface Properties section.

Select a **Wall velocity** $\mathbf{v}_w$ (SI unit: m/s) — **None** (the default), **Calculate from wall displacement**, or **User defined**. For **User defined** enter values or expressions for the components of $\mathbf{v}_w$ (SI unit: m/s). The defaults are 0 m/s.

BASE PROPERTIES

See Wall Properties above for details to help you decide whether the additional displacement should be added to the wall or the base.

Enter a value or expression for the **Height of base below reference plane** h_{b1} (SI unit: m). The default is 0 m.

By default **Additional base displacement** is **User defined**. Enter values or expressions for $\mathbf{u}_b$ (SI unit: m). The defaults are 0 m. Or select **None** from the list.

Select a **Base velocity** $\mathbf{v}_b$ (SI unit: m/s) — **None** (the default), **Calculate from base displacement**, or **User defined**. For **User defined** enter values or expressions for the components of $\mathbf{v}_b$ (SI unit: m/s). The defaults are 0 m/s.

FLUID PROPERTIES

The default **Dynamic viscosity** μ (SI unit: Pa·s) is taken **From material**. For **User defined** enter a different value or expression. The default is 0 Pa·s.

With the default options, the **Density** ρ (SI unit: kg/m^3) is taken **From material**. For **User defined** enter a different value or expression. The default is 0 kg/m^3. If the **Modified Reynolds Equation** is being solved, the density is determined automatically by the ideal gas law. If cavitation is enabled, the density is assumed to take the form $\rho = \rho_c \exp(\beta p_f)$ where p_f is the fluid pressure, ρ_c is the density at the cavitation pressure, and β is the compressibility. (SI unit: 1/Pa). In this case enter the values for the **Density at cavitation pressure** ρ_c (SI unit: Pa) and the **Compressibility** β (SI unit: 1/Pa).

FILM FLOW MODEL

Select a **Film flow model** — **No-slip walls** (the default), **Slip at walls**, **User defined-relative flow function**, or **User defined-general**. The film flow model is used to compute the mean fluid velocity as a function of the pressure gradient, the wall velocity, and the base velocity. Within the gap the fluid velocity profile is a linear combination of the Poiseuille and Couette velocity profiles.

Non Slip Walls

This flow model assumes no slip at both the wall and base surfaces. Thus the average fluid velocity is computed by assuming that the fluid velocity at the wall and base is equal to the wall and base velocity, respectively.

Slip at Walls

Use **Slip at walls** when slip occurs at the wall and/or the base. In this case the difference between the wall or base velocity and the fluid velocity is proportional to the tangential part of the of the normal stress tensor component. The slip length divided by the fluid viscosity is the constant of proportionality in this relationship. The mean fluid velocity is computed using this assumption, given the pressure gradient and the wall and base velocities.

Enter a **Slip length, wall** L_{sw} (SI unit: m). The default is 0.1 μm. Select the **Use different slip length for base** check box to enter a **Slip length, base** L_{sb} (SI unit: m). The default is 0.1 μm.

For the **Modified Reynolds Equation** it is possible to use the gas mean free path to specify the slip length. Change the **Type of Slip** setting (which defaults to **Slip Length** with the settings described above) to **Mean free path and same accommodation coefficients** or to **Mean free path and different accommodation coefficients**.

- For **Mean free path and same accommodation coefficients** enter a value for the **Wall and base accommodation coefficient** α (dimensionless). The default is 0.9.

- For **Mean free path and different accommodation coefficients** enter values for the **Wall accommodation coefficient** α_w (dimensionless, default 0.9) and the **Base accommodation coefficient** α_b (dimensionless, default 0.9).

Select an option to define the **Mean free path**—**Compute from material properties** (the default), **User defined expression**, or **User defined with reference pressure**.

- For **User defined expression** enter an expression for the **Mean free path** λ (SI unit: m). The default expression is `((70[nm])´(1[atm]))/(tffs.ptot)`.

- For **User defined with reference pressure** enter values for the **Mean free path at reference pressure** λ_0 (SI unit: m; the default is 70 nm), and for the **Mean free path reference pressure** $p_{\lambda 0}$ (SI unit: Pa; the default is 1 atm).

Rarefied-Total Accommodation (Modified Reynolds Equation Only)

The **Rarefied-total accommodation** option provides a rarefied gas model that assumes total accommodation at the wall and the base. This model is accurate to within 5% over the range 0<Kn<880 (here Kn is the Knudsen number, which is the ratio of the film thickness to the mean free path). An empirical function, fitted to stationary solutions of the Boltzmann equation, is used to define the Poiseuille component of the flow.

Select an option to define the **Mean free path**—**Compute from material properties** (the default), **User defined expression**, or **User defined with reference pressure**.

- For **User defined expression** enter an expression for the **Mean free path** λ (SI unit: m). The default expression is `((70[nm])´(1[atm]))/(tffs.ptot)`.

- For **User defined with reference pressure** enter values for the **Mean free path at reference pressure** λ_0 (SI unit: m; the default is 70 nm) and for the **Mean free path reference pressure** $p_{\lambda 0}$ (SI unit: Pa; the default is 1 atm).

Select a **Force model**. Select:

- **Normal-pressure forces only** (the default) to include only the normal pressure forces in the model.
- **Couette (slide film) forces only** to include only the shear forces generated from an empirical model of the rarefied flow developed for pure Couette flows.
- **Shear and normal forces** to include both the shear and pressure forces, combining the other two force models.

Rarefied-General Accommodation (Modified Reynolds Equation Only)
The **Rarefied-general accommodation** option provides a rarefied gas model that assumes the same accommodation coefficient, α, at the wall and the base. This model is accurate to within 1% over the ranges 0.7<α<1 and 0.01<Kn<100 (here Kn is the Knudsen number, which is the ratio of the film thickness to the mean free path). An empirical function, fitted to stationary solutions of the Boltzmann equation, is used to define the Poiseuille component of the flow.

Select an option to define the **Mean free path**—**Compute from material properties** (the default), **User defined expression**, or **User defined with reference pressure**.

- For **User defined expression** enter an expression for the **Mean free path** λ (SI unit: m). The default expression is `70[nm]*1[atm]/tffs.ptot`.
- For **User defined with reference pressure** enter values for the **Mean free path at reference pressure** λ_0 (SI unit: m, the default is 70 nm) and for the **Mean free path reference pressure** $p_{\lambda 0}$ (SI unit: Pa, the default is 1 atm).

Select a **Force model**. Select:

- **Normal-pressure forces only** (the default) to include only the normal pressure forces in the model.
- **Couette (slide film) forces only** to include only the shear forces generated from an empirical model of the rarefied flow developed for pure Couette flows.
- **Shear and normal forces** to include both the shear and pressure forces, combining the other two force models.

User Defined-relative Flow Function
The **User defined-relative flow function** option enables user-defined models in which an effective fluid viscosity is employed. The fluid viscosity is divided by an additional factor Q_{ch}, which can be defined as an arbitrary expression in the GUI. It is also possible to define the expressions for the fluid forces on the wall and on the base (these are included as feature inputs in other physics interfaces).

Enter values or expressions for:

- **Relative flow rate function** Q_{ch} (dimensionless). The default is 0.
- **Fluid load on wall** $\mathbf{f}_w$ (SI unit: N/m^2). The defaults are 0 N/m^2.
- **Fluid load on base** $\mathbf{f}_b$ (SI unit: N/m^2). The defaults are 0 N/m^2.

User Defined - General

The **User defined-general** option allows for arbitrary flow models to be defined. Both the Poiseuille and Couette terms in the mean velocity can be defined arbitrarily. It is also possible to define the expressions for the fluid forces on the wall and on the base, (these are included as feature inputs in other physics interfaces).

Enter values or expressions for:

- **Poiseuille mean fluid velocity coefficient** $v_{\mathrm{ave},P}$ (SI unit: m^3·s/kg). The default is 0 m^3·s/kg.
- **Couette mean fluid velocity component** $\mathbf{v}_{\mathrm{ave},C}$ (SI unit: m/s). The defaults are 0 m/s.
- **Fluid load on wall** $\mathbf{f}_w$ (SI unit: N/m^2). The defaults are 0 N/m^2.
- **Fluid load on base** $\mathbf{f}_b$ (SI unit: N/m^2). The defaults are 0 N/m^2.

🔍	Arrow Line and Arrow Surface in the *COMSOL Multiphysics Reference Manual*

Border

Use the **Border** node to set a pressure condition at the border and the border flow type.

The **Border flow** condition is used to account for the pressure drop caused by the flow converging into the gap, outside the thin layer. The acoustic elongation options does this by adding additional thickness to the thin layer beyond the edge of the geometry (assuming a pressure gradient in this layer equal to that at the boundary). The Out-of-plane motion calculates the pressure gradient due to circulation of the fluid caused by motion of the wall or base surfaces using a predefined model. Alternatively the pressure gradient at the boundary can be specified using an arbitrary expression, which allows for more sophisticated, user-defined models.

BORDER SETTINGS

Select a **Border condition** — **Zero pressure** (the default), **Pressure**, or **Border flow**.

When the Cavitation check box is selected for the physics interface, **Starvation** is available.

For **Pressure** enter a **Pressure** p_{f0} (SI unit: Pa) to define $p_f = p_{f0}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure p_{ref}, defined at the physics interface level is 0, p_{f0} is the absolute pressure. Otherwise, p_{f0} is the relative pressure.

For **Border flow** select a **Border flow type** — **Acoustic boundary condition-absolute elongation**, **Acoustic boundary condition-relative elongation**, **Out-of-plane motion**, or **User defined**.

- For **Acoustic Boundary condition-absolute elongation** enter a **Border elongation** ΔL (SI unit: m). The default is 0.1 µm.
- For **Acoustic boundary condition-relative elongation** enter a **Relative border elongation** ΔL_r (dimensionless). The default is 0.7.
- For **Out-of-plane motion** enter the **Model coefficients** η, ζ, χ with defaults 0, 0, 1, respectively. Also enter the **Slip length**, Λ (SI unit: m). The default slip length uses an `if` condition to set the slip length equal to that defined in the **Fluid-Film Properties** node if a suitable **Film flow model** is selected. If the Slip length is not defined in the Fluid-Film Properties node, it defaults to 0.1µm.

Note that the coefficients can be specified according to the results given in the paper by Gallis and Torczynski (M. A. Gallis and J. R. Torczynski, "An Improved Reynolds-Equation Model for Gas Damping of Microbeam Motion", Journal of Microelectromechanical Systems, vol. 13, pp. 653–659, 2004). The following values are recommended:

$$\chi = \frac{1 + 8{,}834\left(\frac{\Lambda}{h}\right)}{1 + 5{,}118\left(\frac{\Lambda}{h}\right)}$$

$$\eta = \frac{0{,}634 + 1{,}572\left(\frac{\Lambda}{h}\right)}{1 + 0{,}537\left(\frac{\Lambda}{h}\right)}$$

$$\zeta = \frac{0{,}445 + 11{,}20\left(\frac{\Lambda}{h}\right)}{1 + 5{,}510\left(\frac{\Lambda}{h}\right)}$$

where h is the gap height. The above equations are valid in the range $0 \leq \Lambda/h \leq 1$.

- For **User defined** enter a **Normal pressure gradient** (SI unit: N/m^3). The default is $p_f/(0.1 \, \mu\text{m})$ N/m^3.

- For **Starvation** enter a value for the **Fluid fraction** θ_0 (dimensionless). The default is 0.6.

Perforations

Use the **Perforations** node for applications in MEMS devices, where the phenomenon of squeezed film damping is important. A free-hanging thin plate or the substrate often has an array of etch holes that allow the gas in-between to escape. The perforations feature acts as a sink for gas that is proportional to both the ambient pressure and to the pressure difference with respect to the ambient on the other side of the perforated surface. The constant of proportionality is known as the admittance, Y, and can either be defined directly or determined from the model due to Bao (M. Bao and H. Yang "Squeeze film air damping in MEMS", Sensors and Actuators A: Physical, vol. 136, no. 1, pp. 3–27, 2014). The ambient pressure (defined at the level of the parent physics interface or Thin-Film Damping feature) is assumed to be the reference pressure specified at the physics interface level.

Note that this feature applies only when the walls do not have tangential movement.

PERFORATIONS

Select a **Perforation admittance** — **User defined** (the default) or **Bao model**.

For **User defined**, enter a value or expression for Y (SI unit: m^2·s/kg).

For **Bao model**, choose a **Perforation shape** — **Square** (the default) or **Circular**. Then enter the following as applicable:

- **Side length** s_h (SI unit: m).

- **Hole radius** r_h (SI unit: m).

- **Hole length** l_h (SI unit: m).

- **Hole density** n_h (SI unit: 1/m^2).

Initial Values

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver. If more than one set of initial values is required, add additional **Initial Values** nodes from the **Physics** toolbar.

Enter a value or an expression for the initial value of the **Pressure** p_f (SI unit: Pa).

Inlet

Use the **Inlet** node to define an edge or point where fluid enters the gap.

INLET SETTINGS

Select an **Inlet condition** — **Zero pressure** (the default), **Pressure**, or **Normal inflow velocity**.

When the **Cavitation** check box is selected for the physics interface (see Cavitation), **Starvation** is also available.

- For **Zero pressure** $p_f = 0$ applies on the boundary, edge, or point.

- For **Pressure** enter a **Pressure** p_{f0} (SI unit: Pa) to impose $p_f = p_{f0}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure p_{ref}, defined at the physics interface level is 0, p_{f0} is the absolute pressure. Otherwise, p_{f0} is the relative pressure.

- For **Normal inflow velocity** enter a **Normal inflow velocity** U_0 (SI unit: m/s). The default is 0 m/s.

- For **Starvation** enter a value for the **Fluid fraction** θ_0 (dimensionless). The default is 0.6.

Outlet

The **Outlet** node defines an edge or point where fluid leaves the gap.

OUTLET SETTINGS

Select an **Outlet condition** — **Zero pressure** (the default), **Pressure**, or **Normal outflow velocity**.

When the **Cavitation** check box is selected for the physics interface (see Cavitation), **Starvation** is also available.

- For **Zero pressure**, $p_f = 0$ applies on the boundary, edge, or point.

- For **Pressure**, enter a **Pressure** p_{f0} (SI unit: Pa) to impose $p_f = p_{f0}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure p_{ref}, defined at the physics interface level is 0, p_{f0} is the absolute pressure. Otherwise, p_{f0} is the relative pressure.

- For **Normal outflow velocity**, enter a **Normal outflow velocity** U_0 (SI unit: m/s). The default is 0 m/s.

- For **Starvation**, enter a value for the **Fluid fraction** θ_0 (dimensionless). The default is 0.6.

Wall

The **Wall** node prevents fluid flow in the direction perpendicular to the boundary.

Symmetry

The **Symmetry** node sets the perpendicular component of the average velocity in the gap to zero.

Theory for the Thin-Film Flow Interfaces

The theory for the different versions of the Thin-Film Flow interfaces are described in this section:

- Thin-Film Flow
- The Reynolds Equation
- Flow Models
- The Modified Reynolds Equation — Gas Flows
- Flow Models for Rarefied Gases
- Frequency-Domain Formulation
- Boundary Conditions
- Cavitation
- References for the Thin-Film Flow Interfaces

Thin-Film Flow

Figure 9-2 shows a typical configuration for the flow of fluid in a thin layer. The upper boundary is referred to as the wall, and the lower boundary is referred to as the base. Damping or lubrication forces operate on both surfaces.

In many cases the gap is sufficiently small for the flow in the thin film to be isothermal. Usually the gap thickness, h, is much smaller than the lateral dimensions of the geometry, L. If this is the case it is possible to neglect inertial effects in the fluid in comparison to viscous effects (for MEMS devices this assumption is reasonable below MHz frequencies). Additionally, the curvature of the reference surface can be ignored when $h/L \ll 1$. Under these assumptions the *Reynolds equation* applies. For gas flows under the same conditions it is possible to derive a modified form of the Reynolds Equation, which uses the ideal gas law to eliminate the density from the equation system. Such a *modified Reynolds equation* can even be adapted to model the flow of rarefied gases.

Different terminology is used for thin-film flow in different fields of physics. In tribology the term *lubrication* is frequently used, especially when the fluid is a liquid. In resonant MEMS devices, flow in the thin layer of gas separating a device from the

substrate on which it is fabricated often provides significant *damping*. In this case there is usually a distinction between *squeezed-film damping*, when the direction of motion of the structure is predominantly perpendicular to the reference plane, and *slide-film damping* for motion predominantly parallel to the reference plane.
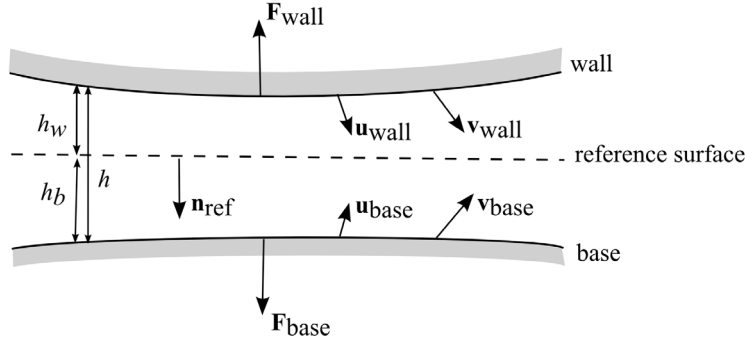
Figure 9-2: An example illustrating a typical configuration for thin-film flow. A reference surface with normal $\mathbf{n}_{ref}$ sits in a narrow gap between a wall and base. In COMSOL the vector $\mathbf{n}_{ref}$ points into the base and out of the wall. The wall moves with a displacement $\mathbf{u}_{wall}$ and velocity $\mathbf{v}_{wall}$ from its initial position. Similarly the base moves from its initial position with displacement $\mathbf{u}_{base}$ and velocity $\mathbf{v}_{base}$. The compression of the fluid results in an excess pressure, p_f, above the reference pressure, p_{ref}, and a fluid velocity in the gap. At a point on the reference surface the average value of the fluid velocity along a line perpendicular to the surface is given by the in plane vector $\mathbf{v}_{ave}$. The motion of the fluid results in forces on the wall ($\mathbf{F}_{wall}$) and on the base ($\mathbf{F}_{base}$). The distance to the wall above the reference surface is h_w while the base resides a distance h_b below the reference surface. The total size of the gap is $h=h_w+h_b$. At a given time $h_w=h_{w1}-\mathbf{n}_{ref}\cdot\mathbf{u}_{wall}$ and $h_b=h_{b1}-\mathbf{n}_{ref}\cdot\mathbf{u}_{wall}$ where h_{w1} and h_{b1} are the initial distances to the wall and base, respectively.

The Reynolds Equation

The equations of fluid flow in thin films are usually formulated on a reference surface in the Eulerian frame. Consider a cylinder, fixed with respect to a stationary reference surface, as shown in Figure 9-3.
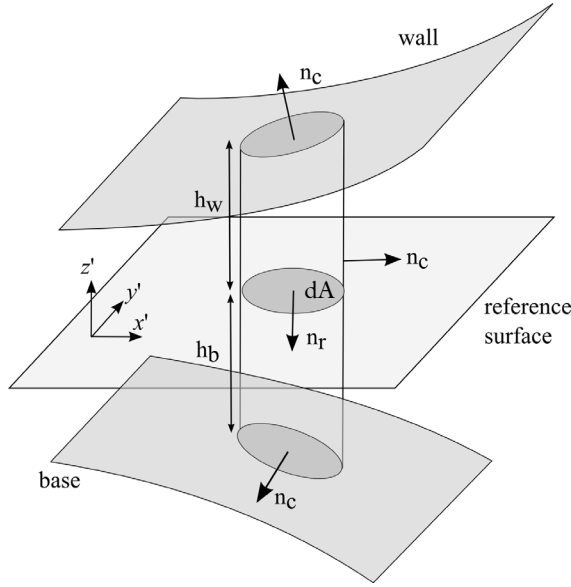
Figure 9-3: Reference cylinder, fixed with respect to the stationary reference surface, in a small gap between two surfaces (the wall and the base). The cylinder has outward normal, $\mathbf{n}_c$. Its area, projected onto the reference surface, is dA.

The cylinder is fixed with respect to the reference surface, but its height can change due to changes in the position of the base and the wall. Considering the flow in the reference plane, the rate at which mass accumulates within the reference cylinder is determined by the divergence of the mass flow field in the reference plane:

$$\frac{d}{dt}(\rho h) = -\nabla_t \cdot (\rho h \mathbf{v}_{av}) \tag{9-1}$$

where $h = h_w + h_b$ and the tangential velocity, $\mathbf{v}_{av}$ represents the mean velocity of the flow in the reference plane. Particular care must be taken with respect to the definition of h. The above equation applies if h is measured with respect to a fixed point on the reference surface as a function of time. The reference surface itself must be fixed in space and obviously cannot deform as time progresses. Equations represented on the reference surface are described as Eulerian, that is they are defined in a frame that is fixed with respect to the motion of the fluid or of the body. Fluid flow problems are usually formulated in the Eulerian frame, and COMSOL Multiphysics adopts this convention in most of its fluid flow interfaces. It is useful to note that the Eulerian

frame is usually called the spatial frame within the COMSOL Multiphysics interface. When a structure deforms in COMSOL Multiphysics, the spatial frame changes shape.

The wall and the base can, and often do, move with respect to the reference surface. The wall and base are usually the surfaces of mechanical components which are deforming as a result of the pressure building up within the region of fluid flow. When describing the physics of a deforming solid, it is often convenient to work in the Lagrangian frame, which is fixed with respect to a small control volume of the solid. As the solid deforms, the Lagrangian frame moves along with the material contained within the control volume. Using the Lagrangian frame for describing structural deformation means that changes in the local density and material orientation as a result of the distortion of the control volume do not need to be accounted for by complicated transformations. In COMSOL Multiphysics, the Lagrangian frame, usually referred to as the material frame, is used for describing structural deformations. When a structure deforms in COMSOL Multiphysics, the material frame remains in the original configuration of the structure, and the deformation is accounted for by the underlying equations.

Because of the mixed Eulerian-Lagrangian approach adopted within COMSOL Multiphysics, particular care must be taken with the formulation of the Reynolds equations. Typically it is not desirable to represent the geometry of the thin film itself directly, because it is often much smaller than the other components in the model. The equations apply on a single surface in the model, the reference surface. Since we do not wish the reference surface to deform, the equations are added on the material frame (even though this frame is normally used in a Lagrangian approach) and manual transformations are added to the system to account for the fact that the structural equations also exist on the material frame, and employ a truly Lagrangian approach.

The situation encountered when both the wall and the base undergo a displacement is depicted in Figure 9-4. The Eulerian wall height changes from an initial value h_{w1} to a final value h_w. Similarly the base height changes from an initial value h_{b1} to h_b.
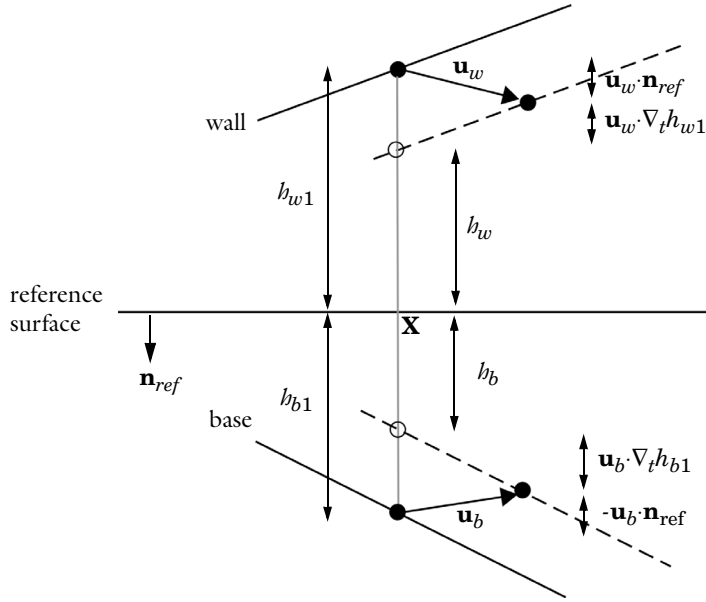
Figure 9-4: Diagram showing the displacement of the wall and the base with respect to the reference surface, and the corresponding change in the height of the channel.

From the figure it is clear that:

$$
\begin{aligned}
h_w &= h_{w1} - \mathbf{u}_w \cdot \mathbf{n}_{ref} - \mathbf{u}_w \cdot \nabla_t h_{w1} \\
h_b &= h_{b1} + \mathbf{u}_b \cdot \mathbf{n}_{ref} - \mathbf{u}_b \cdot \nabla_t h_{b1} \\
h &= h_w + h_b
\end{aligned}
\tag{9-2}
$$

It should be noted that similar corrections should be applied to the velocity of the wall, if it is computed from the structural displacement. That is the velocity should be modified by a term proportional to its spatial gradient. This correction term, is however, a second order term, and consequently it is usually negligible in practical circumstances. It is neglected in the thin film flow interface.

Consequently, provided that the definitions of the wall and base height from Equation 9-2 are used, the Reynolds equation takes the form:

$$
\frac{\partial}{\partial t}(\rho h) + \nabla_t \cdot (h \rho \mathbf{v}_{av}) = 0
\tag{9-3}
$$

The definition of the average flow velocity, $\mathbf{v}_{av}$, together with the forces that act on the structure, remain to be specified.

Flow Models

The Navier stokes equations can be nondimensionalized for a domain whose width (h_0) is much smaller than its lateral dimension(s) (l_0) (see Ref. 1 for a detailed discussion). When $\mathrm{Re}(h_0/l_0)^2 \ll 1$, and terms of order $(h_0/l_0)^2$ are neglected, the Navier-Stokes equations reduce to a modified form of the Stokes equation, which must be considered in conjunction with the continuity relation.
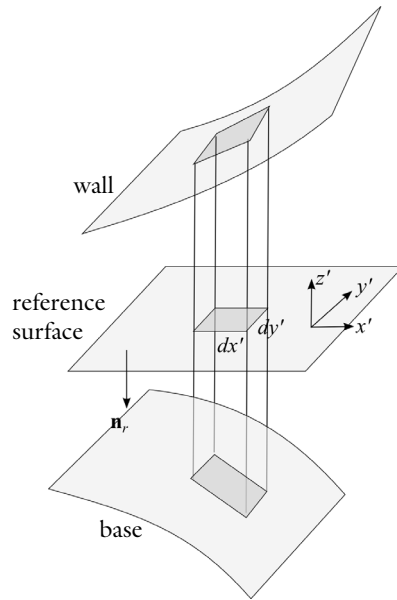
Figure 9-5: The coordinate system employed for the derivation of the average flow velocity.

The equations are most conveniently expressed by considering a local coordinate system in which x' and y' are tangent to the plane of the reference surface, and z' is perpendicular to the surface, as illustrated in Figure 9-5. Using this coordinate system:

$$\frac{\partial p_f}{\partial x'} = \frac{\partial}{\partial z'}\left(\mu\frac{\partial v_{x'}}{\partial z'}\right)$$

$$\frac{\partial p_f}{\partial y'} = \frac{\partial}{\partial z'}\left(\mu\frac{\partial v_{y'}}{\partial z'}\right)$$

$$\frac{\partial p}{\partial z'} = 0$$

Here p_f is the pressure resulting from the fluid flow, μ is the fluid viscosity, and $(v_{x'}, v_{y'})$ is the fluid velocity in the reference plane (which varies in the z' direction).

These equations can be integrated directly, yielding the in-plane velocity distributions, by making the assumption that the viscosity represents the mean viscosity through the film thickness. The following equations are derived:

$$\frac{\partial v_{x'}}{\partial z'} = \frac{z'\partial p_f}{\mu\partial x'} + \frac{C_{1x'}}{\mu} \qquad \frac{\partial v_{y'}}{\partial z'} = \frac{z'\partial p_f}{\mu\partial y'} + \frac{C_{1y'}}{\mu} \tag{9-4}$$

$$v_{x'} = \frac{z^2}{2\mu}\frac{\partial p_f}{\partial x'} + \frac{C_{1x'}z'}{\mu} + C_{2x'} \qquad v_{y'} = \frac{z^2}{2\mu}\frac{\partial p_f}{\partial y'} + \frac{C_{1y'}z'}{\mu} + C_{2y'} \tag{9-5}$$

The constants $C_{1x'}$, $C_{2x'}$, $C_{1y'}$, and $C_{2y'}$ are determined by the boundary conditions. Equation 9-4 shows that the flow is a linear combination of laminar Poiseuille and Couette flows. The velocity profile is quadratic in form, as shown in Equation 9-5.

The average flow rate in the reference plane, $\mathbf{v}_{av}$, is given by:

$$\mathbf{v}_{av} = \begin{bmatrix} \frac{1}{h}\int\limits_{-h_b}^{h_w} v_{x'}dz' \\ \frac{1}{h}\int\limits_{-h_b}^{h_w} v_{y'}dz' \end{bmatrix} = \frac{1}{h}\begin{bmatrix} \dfrac{(h_w^2 - h_w h_b + h_b^2)\partial p_f}{6\mu}\dfrac{}{\partial x'} + \dfrac{h_w - h_b}{2\mu}C_{1x'} + C_{2x'} \\ \dfrac{(h_w^2 - h_w h_b + h_b^2)\partial p_f}{6\mu}\dfrac{}{\partial y'} + \dfrac{h_w - h_b}{2\mu}C_{1y'} + C_{2y'} \end{bmatrix}$$

The forces acting on the walls are determined by the normal component of the viscous stress tensor, τ, at the walls ($\tau\mathbf{n}$ - where $\mathbf{n}$ is the normal that points out of the fluid domain). The viscous stress tensor takes the form:

$$\tau = \mu(\nabla\mathbf{v} + (\nabla\mathbf{v}^T)) - p\mathbf{I} = \begin{bmatrix} -p_f + 2\mu\dfrac{\partial v_{x'}}{\partial x'} & \mu\left(\dfrac{\partial v_{y'}}{\partial x'} + \dfrac{\partial v_{x'}}{\partial y'}\right) & \mu\left(\dfrac{\partial v_{z'}}{\partial x'} + \dfrac{\partial v_{x'}}{\partial z'}\right) \\ \mu\left(\dfrac{\partial v_{x'}}{\partial y'} + \dfrac{\partial v_{y'}}{\partial x'}\right) & -p_f + 2\mu\dfrac{\partial v_{y'}}{\partial y'} & \mu\left(\dfrac{\partial v_{z}}{\partial y'} + \dfrac{\partial v_{y'}}{\partial z'}\right) \\ \mu\left(\dfrac{\partial v_{x'}}{\partial z'} + \dfrac{\partial v_{z'}}{\partial x'}\right) & \mu\left(\dfrac{\partial v_{y'}}{\partial z'} + \dfrac{\partial v_{z}}{\partial y'}\right) & -p_f + 2\mu\dfrac{\partial v_{z'}}{\partial z'} \end{bmatrix}$$

Neglecting the gradient terms, which are of order h_0/l_0, results in the following form for the stress tensor:

$$\tau \approx \begin{bmatrix} -p_f & 0 & \mu\dfrac{\partial v_{x'}}{\partial z'} \\ 0 & -p_f & \mu\dfrac{\partial v_{y'}}{\partial z'} \\ \mu\dfrac{\partial v_{x'}}{\partial z'} & \mu\dfrac{\partial v_{y'}}{\partial z'} & -p_f \end{bmatrix} \tag{9-6}$$

The components of the stress tensor can be expressed in terms of the velocity and pressure gradients using Equation 9-4. Note that the normals to both the wall and the base are parallel to the z' direction, to zeroth order in h_0/l_0. The forces acting on the base and the wall are therefore given by:

$$f_w = \begin{bmatrix} \dfrac{h_w}{\mu}\dfrac{\partial p_f}{\partial x'} + \dfrac{C_{1x'}}{\mu} \\ \dfrac{h_w}{\mu}\dfrac{\partial p_f}{\partial y'} + \dfrac{C_{1y'}}{\mu} \\ p_f \end{bmatrix} \qquad f_b = \begin{bmatrix} \dfrac{h_b}{\mu}\dfrac{\partial p_f}{\partial x'} + \dfrac{C_{1x'}}{\mu} \\ \dfrac{h_b}{\mu}\dfrac{\partial p_f}{\partial y'} + \dfrac{C_{1y'}}{\mu} \\ -p_f \end{bmatrix}$$

GENERAL SLIP BOUNDARY CONDITION

Assuming a slip length of L_{sw} at the wall and a slip length of L_{sb} at the base, the general slip boundary conditions are given by:

$$v_{x'}(z' = -h_b) - v_{x'}^b = \frac{L_{sb}}{\mu}\tau_{z'x'}(z' = -h_b) = L_{sb}\frac{\partial v_{x'}}{\partial z'}(z' = -h_b)$$

$$v_{y'}(z' = -h_b) - v_{y'}^b = \frac{L_{sb}}{\mu}\tau_{z'y'}(z' = -h_b) = L_{sb}\frac{\partial v_{y'}}{\partial z'}(z' = -h_b)$$

$$v_{x'}(z' = h_w) - v_{x'}^w = -\frac{L_{sw}}{\mu}\tau_{z'x'}(z' = h_w) = -L_{sw}\frac{\partial v_{x'}}{\partial z'}(z' = h_w)$$

$$v_{y'}(z' = h_w) - v_{y'}^w = -\frac{L_{sw}}{\mu}\tau_{z'y'}(z' = h_w) = -L_{sw}\frac{\partial v_{y'}}{\partial z'}(z' = h_w)$$

For non-identical slip lengths the constants $C_{1x'}$, $C_{2x'}$, $C_{1y'}$, and $C_{2y'}$ take the following values:

$$C_{1x'} = \frac{\mu(v_{x'}^w - v_{x'}^b)}{h + L_{sw} + L_{sb}} - \frac{h_b^2 - h_w^2 - 2L_{sw}h_w + 2L_{sb}h_b}{2(h + L_{sb} + L_{sw})}\frac{\partial p_f}{\partial x'}$$

$$C_{2x'} = \frac{v_{x'}^w(h_b + L_{sb}) + v_{x'}^b(h_w + L_{sw})}{h + L_{sw} + L_{sb}}$$
$$-\frac{h_w^2(h_b + L_{sb}) + h_b^2(h_w + L_{sw}) + 2h_w h_b(L_{sw} + L_{sb}) + 2hL_{sw}L_{sb}}{2(h + L_{sw} + L_{sb})\mu}\frac{\partial p_f}{\partial x'}$$

$$C_{1y'} = \frac{\mu(v_{y'}^w - v_{y'}^b)}{h + L_{sw} + L_{sb}} - \frac{h_b^2 - h_w^2 - 2L_{sw}h_w + 2L_{sb}h_b}{2(h + L_{sw} + L_{sb})}\frac{\partial p_f}{\partial y'}$$

$$C_{2y'} = \frac{v_{y'}^w(h_b + L_{sb}) + v_{y'}^b(h_w + L_{sw})}{h + L_{sw} + L_{sb}}$$
$$-\frac{h_w^2(h_b + L_{sb}) + h_b^2(h_w + L_{sw}) + 2h_w h_b(L_{sw} + L_{sb}) + 2hL_{sw}L_{sb}}{2(h + L_{sw} + L_{sb})\mu}\frac{\partial p_f}{\partial y'}$$

The average flow rate becomes:

$$\mathbf{v}_{av} = \begin{bmatrix} \dfrac{h(v_{x'}^w + v_{x'}^b) + 2(L_{sw}v_{x'}^w + L_{sb}v_{x'}^b)}{2(h + L_{sw} + L_{sb})} - \dfrac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})}\dfrac{\partial p_f}{\partial x'} \\[4mm] \dfrac{h(v_{y'}^w + v_{y'}^b) + 2(L_{sw}v_{y'}^w + L_{sb}v_{y'}^b)}{2(h + L_{sw} + L_{sb})} - \dfrac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})}\dfrac{\partial p_f}{\partial y'} \end{bmatrix}$$

which can be expressed in vector notation as:

$$\mathbf{v}_{\text{av}} = \frac{1}{2(h + L_{sw} + L_{sb})}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r{}^T)((h + 2L_{sw})\mathbf{v}_w + (h + 2L_{sb})\mathbf{v}_b)$$

$$-\frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})}\nabla_t p_f$$

The above equation can be written on the form:

$$\mathbf{v}_{\text{av}} = \mathbf{v}_{av,c} - v_{av,p}\nabla_t p_f \tag{9-7}$$

where $\mathbf{v}_{av,c}$ is a term associated with Couette flow, and $v_{av,p}$ is a coefficient associated with Poiseuille flow (see Table 9-2 below).

The forces acting on the two boundaries are given by:

$$\mathbf{f}_w = \begin{bmatrix} -\dfrac{h(h + 2L_{sb})}{2(h + L_{sw} + L_{sb})}\dfrac{\partial p_f}{\partial x'} + \dfrac{(v_{x'}^b - v_{x'}^w)\mu}{(h + L_{sw} + L_{sb})} \\[2mm] -\dfrac{h(h + 2L_{sb})}{2(h + L_{sw} + L_{sb})}\dfrac{\partial p_f}{\partial y'} + \dfrac{(v_{y'}^b - v_{y'}^w)\mu}{(h + L_{sw} + L_{sb})} \\[2mm] p_f \end{bmatrix}$$

$$\mathbf{f}_b = \begin{bmatrix} -\dfrac{h(h + 2L_{sw})}{2(h + L_{sw} + L_{sb})}\dfrac{\partial p_f}{\partial x'} + \dfrac{(v_{x'}^w - v_{x'}^b)\mu}{(h + L_{sw} + L_{sb})} \\[2mm] -\dfrac{h(h + 2L_{sw})}{2(h + L_{sw} + L_{sb})}\dfrac{\partial p_f}{\partial y'} + \dfrac{(v_{y'}^w - v_{y'}^b)\mu}{(h + L_{sw} + L_{sb})} \\[2mm] -p_f \end{bmatrix} \tag{9-8}$$

Note that the z' direction corresponds to the $-\mathbf{n}_r$ direction. The x' and y' directions correspond to the two tangent vectors in the plane. Using vector notation the forces become:

$$\mathbf{f}_w = -\frac{h(h + 2L_{sb})}{2(h + L_{sw} + L_{sb})}\nabla_t p_f + \frac{\mu}{h + L_{sw} + L_{sb}}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^b - \mathbf{v}^w) + p_f\mathbf{n}_w$$

$$\mathbf{f}_b = -\frac{h(h + 2L_{sw})}{2(h + L_{sw} + L_{sb})}\nabla_t p_f + \frac{\mu}{h + L_{sw} + L_{sb}}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^w - \mathbf{v}^b) + p_f\mathbf{n}_b$$

In Equation 9-8 it is assumed that $\mathbf{n}_w = -\mathbf{n}_r$ and $\mathbf{n}_b = \mathbf{n}_r$. In COMSOL Multiphysics the accuracy of the force terms is improved slightly over the usual approximation (which

neglects the slope of the wall and base as it is of order h_0/l_0) by using the following equations for $\mathbf{n}_w$ and $\mathbf{n}_b$:

$$\mathbf{n}_w = (-\mathbf{n}_r - \nabla_t h_w)$$

$$\mathbf{n}_b = (\mathbf{n}_r - \nabla_t h_w)$$

These definitions are derived from Equation 9-4 and Equation 9-5 and include the additional area that the pressure acts on as a result of the wall slope.

Once again, the force terms can be written on the form:

$$\begin{aligned} \mathbf{f}_w &= -f_{w,p}\nabla_t p_f + \mathbf{f}_{w,c} \\ \mathbf{f}_b &= -f_{b,p}\nabla_t p_f + \mathbf{f}_{b,c} \end{aligned} \tag{9-9}$$

where $f_{w,p}$ is the Poiseuille coefficient for the force on the wall, and $\mathbf{f}_{w,c}$ incorporates the Couette and normal forces (due to the pressure) on the wall. Similarly, $f_{b,p}$ is the Poiseuille coefficient for the force on the base, and $\mathbf{f}_{b,c}$ incorporates the Couette and normal forces (due to the pressure) on the base.

The cases of identical slip length and non-slip are limiting cases of the formulas derived above. The main results are summarized in Table 9-2, where the constants defined in Equation 9-7 and Equation 9-9 are used.

TABLE 9-2: EQUATION VARIABLES FOR VARIOUS FLOW MODELS

VARIABLE	DEFINITION
General Slip Flow Model	
$\mathbf{v}_{\mathrm{av},c}$	$\dfrac{1}{2(h+L_{sw}+L_{sb})}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r{}^T)((h+2L_{sb})\mathbf{v}_w+(h+2L_{sw})\mathbf{v}_b)$
$v_{\mathrm{av},p}$	$\dfrac{h(h^2+4h(L_{sw}+L_{sb})+12L_{sb}L_{sw})}{12\mu(h+L_{sw}+L_{sb})}$
$\mathbf{f}_{w,c}$	$\dfrac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^b-\mathbf{v}^w)+p_f\mathbf{n}_w$
$f_{w,p}$	$\dfrac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})}$
$\mathbf{f}_{b,c}$	$\dfrac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^w-\mathbf{v}^b)+p_f\mathbf{n}_b$
$f_{b,p}$	$\dfrac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})}$
Equal Slip Lengths Flow Model Lsw=Lsb=L	
$\mathbf{v}_{\mathrm{av},c}$	$\dfrac{1}{2}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}_w+\mathbf{v}_b)$
$v_{\mathrm{av},p}$	$(h^2+6L_sh)/(12\mu)$
$\mathbf{f}_{w,c}$	$\dfrac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^b-\mathbf{v}^w)+p_f\mathbf{n}_w$
$f_{w,p}$	$h/2$
$\mathbf{f}_{b,c}$	$\dfrac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^w-\mathbf{v}^b)+p_f\mathbf{n}_b$
$f_{b,p}$	$h/2$

TABLE 9-2: EQUATION VARIABLES FOR VARIOUS FLOW MODELS

VARIABLE	DEFINITION
Non-Slip Flow Model Lsw=Lsb=0	
$\mathbf{v}_{\mathrm{av},c}$	$\frac{1}{2}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}_w + \mathbf{v}_b)$
$v_{\mathrm{av},p}$	$h^2/(12\mu)$
$\mathbf{f}_{w,c}$	$\frac{\mu}{h}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^b - \mathbf{v}^w) + p_f\mathbf{n}_w$
$f_{w,p}$	$h/2$
$\mathbf{f}_{b,c}$	$\frac{\mu}{h}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r{}^T)(\mathbf{v}^w - \mathbf{v}^b) + p_f\mathbf{n}_b$
$f_{b,p}$	$h/2$

The Modified Reynolds Equation — Gas Flows

Thin-film gas flows are often isothermal, and in many cases the ideal gas law can be assumed. Under these circumstances, the ideal gas law can be written on the form:

$$p_A = \frac{RT_0}{M_n}\rho$$

where T_0 is the (constant) temperature of the gas, M_n is the molar mass of the gas, and R is the universal gas constant. Here the total gas pressure, $p_A = p_{\mathrm{ref}} + p_f$, where p_A is the absolute pressure and p_f is the pressure developed as a result of the flow. Substituting this relation into Equation 9-3 and dividing through by the constant M_n/RT_0 results in a modified form of the Reynolds equation:

$$\frac{\partial}{\partial t}(p_A h) + \nabla_t \cdot (h p_A \mathbf{v}_{\mathrm{av}}) = 0 \tag{9-10}$$

This equation can be used to model isothermal flows of ideal gases. The average flow rate and the forces acting on the bearings are computed in the same manner as for the standard Reynolds equation.

SLIP BOUNDARY CONDITIONS FOR GASES

For a gas, the slip length is often expressed using the mean free path, λ, and a tangential momentum accommodation coefficient, α. For compatibility with the existing

literature on thin-film gas flow the following definition of the mean free path is used by COMSOL Multiphysics in the Thin-Film Flow interfaces:

$$\lambda = \frac{\mu}{p}\left(\frac{2RT}{M_n}\right)^{\frac{1}{2}}$$

The slip length is then defined as:

$$L_s = \frac{\sqrt{\pi}}{2}\lambda\left(\frac{2-\alpha}{\alpha}\right)$$

Values for the tangential-momentum-accommodation coefficients for various gas surface combinations are given in Ref. 2.

Flow Models for Rarefied Gases

For gases at low pressure, the ratio of the gas mean free path, λ, to the gap size (known as the Knudsen number: $Kn=\lambda/h$) grows. For Knudsen numbers greater than 0.1, the gas cannot be treated using the continuum Navier-Stokes equations and the Boltzmann equation must be solved instead.

At steady state, the solutions to the linearized Boltzmann equation for isothermal flow in a narrow gap between parallel plates can be expressed as a combination of Poiseuille and Couette flows. This is analogous to the solutions of the Navier-Stokes equations in the limit of small h_0/l_0. Provided that the surfaces of the wall and base are identical (which is normally the case in many practical applications), the Couette contribution to the bulk fluid velocity is unchanged (it remains the mean of the wall and base velocities for identical surfaces). The Poiseuille contribution to the flow is more complicated for a rarefied gas. A practical approach, pioneered by Fukui and Kaneko (Ref. 3) is to solve the linearized Boltzmann BGK equation over a range of Knudsen numbers and to provide an empirical fit to the flow. This results in the following form for the average velocity of the flow:

$$\mathbf{v}_{\mathrm{av}} = \frac{1}{2}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}_w + \mathbf{v}_b) - \frac{h^2}{12\mu_{\mathrm{eff}}}\nabla_t p$$

$$\mu_{\mathrm{eff}} = \frac{\mu}{Q(\mathrm{Kn}, \alpha_w, \alpha_b)}$$

(9-11)

where $Q(\mathrm{Kn}, \alpha_w, \alpha_b)$ is a nondimensional function of the Knudsen number (Kn) and the tangential momentum accommodation coefficient at the wall (α_w) and base (α_b).

$Q(\mathrm{Kn}, \alpha_w, \alpha_b)$ is obtained by solving the linearized Boltzmann BGK equation for steady Poiseuille flow with a range of Knudsen numbers and slip coefficients. This approach assumes that stationary solutions of the Boltzmann equation apply inside the gap, that is, that the flow can be treated as quasi-static.

Fukui and Kaneko provided data on $Q(\mathrm{Kn}, \alpha_w, \alpha_b)$ for the case where $\alpha_w = \alpha_b$ (Ref. 4), which was subsequently fitted to different empirical formulas by Veijola and others (Ref. 5). Note also that additional, more accurate, data is available in Ref. 6. Veijola provided two empirical formulas, which apply under different circumstances with various degrees of accuracy:

- $\alpha_w = \alpha_b = 1$ (available as the option Rarefied-Total Accommodation in COMSOL Multiphysics):

$$Q(Kn, 1, 1) = 1 + 9{,}638 Kn^{1,159}$$

(accurate to within 5% in the range $0 < Kn < 880$)

- $\alpha_w = \alpha_b = \alpha$ (available as the option Rarefied-General Accommodation in COMSOL Multiphysics):

$$Q(\mathrm{Kn}, \alpha, \alpha) = \frac{6\tilde{Q}(D, \alpha)}{D} \qquad D = \frac{\sqrt{\pi}}{2\mathrm{Kn}}$$

$$\tilde{Q}(D, \alpha) = \frac{D}{6} + \frac{1}{\alpha^{1.34}\sqrt{\pi}}\ln\left(\frac{1}{D} + 4.1\right) + \frac{\alpha}{6.4D} + \frac{1.3(1-\alpha)}{D + 0.08D^{1.83}} + \frac{0.64\alpha D^{0.17}}{1 + 1.12 D^{0.72}}$$

(accurate to within 1% in the ranges $D > 0.01$, $0.7 < \alpha < 1$ and $0.01 < \mathrm{Kn} < 100$).

Both of these empirical models are available as flow models with the options listed. Additionally, a user-defined relative flow rate function can be defined (which could, for example, be based on an interpolation function derived from the original data in Ref. 6). Data on the tangential momentum accommodation coefficients for various gas-surface combinations is available in Ref. 2.

Various definitions of the mean free path are used in the literature, frequently without explanation. For compatibility with the existing literature on thin-film flow, COMSOL Multiphysics uses the same mean free path definition as Veijola and others.

In this definition the mean free path and Knudsen number are defined as:

$$\lambda = \frac{\mu}{p}\left(\frac{2RT}{M_n}\right)^{\frac{1}{2}} \qquad \mathrm{Kn} = \frac{\mu}{ph}\left(\frac{2RT}{M_n}\right)^{\frac{1}{2}} \tag{9-12}$$

where μ is the gas viscosity, p is the gas pressure, R is the molar gas constant, T is the temperature, and M_n is the molar mass of the gas. Ref. 2 also employs this definition of the mean free path.

In many applications the forces acting on the wall and base are important. The pressure in the gas can be computed correctly by solving Equations 9-10 and 9-11. However, this approach provides only the normal component of the traction acting on the wall and base. To obtain the shear forces, the approach adopted by Torczynski and Gallis (Ref. 7) is used. They produced an empirical expression for the shear force that has the correct behavior in the free molecular flow and continuum limits as well as in the limits for the accommodation coefficient. Torczynski and Gallis solve the problem of pure Couette flow and derive an empirical function for the slip length that predicts the correct forces for the flow in the gap in several limiting cases. Their empirical expression for the slip length is given by:

$$L_s = \frac{2-\alpha}{\alpha}\frac{2\lambda}{\sqrt{\pi}\mu}\left(1 + \frac{d_1\alpha}{1 + (2d_2\mathrm{Kn})/\sqrt{\pi}}\right) \tag{9-13}$$

where $d_1 \approx 0.15$ and $d_2 \approx 0.59$. In principle d_1 and d_2 are variables themselves, but they were found to be constant to within the accuracy of the DSMC experiments used to derive their values.

📋 The slip length in Equation 9-13 (which is used in COMSOL Multiphysics) differs slightly from the equivalent expression in Ref. 7 as a result of a different definition of the mean free path (Torczynski and Gallis' mean free path is different from Equation 9-12 by a factor of $\sqrt{\pi}/2$).

Equation 9-7 gives the following expressions for the shear forces on the wall and base for pure Couette flow:

$$\mathbf{f}_w^{shear} = \frac{\mu}{h + 2L_s}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b - \mathbf{v}^w)$$

$$\mathbf{f}_b^{shear} = \frac{\mu}{h + 2L_s}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w - \mathbf{v}^b)$$

where L_s is taken from Equation 9-13.

A general flow incorporates both Poiseuille and Couette terms. Assuming that the Poiseuille and Couette flows can be superposed, the forces become:

$$\mathbf{f}_w = -\frac{h}{2}\nabla_t p + \frac{\mu}{h + 2L_s}(\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T)(\mathbf{v}^b - \mathbf{v}^w) - p\mathbf{n}_r$$

$$\mathbf{f}_b = -\frac{h}{2}\nabla_t p + \frac{\mu}{h + 2L_s}(\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T)(\mathbf{v}^w - \mathbf{v}^b) + p\mathbf{n}_r$$

(9-14)

here L_s is derived from Equation 9-13 and p is obtained by solving Equation 9-10 with Equation 9-11. Strictly speaking, Torczynski and Gallis' result applies for Couette flow only and was derived for a more general variable-soft-sphere gas rather than for the linearized BGK equations, using numerical simulations. From a practical perspective, it seems likely that solutions of the linearized BGK equations would also be fitted by these expressions, and in that case it should be possible to combine the forces using superposition. In the absence of a detailed proof Equation 9-14 is not the default option for the force model, but is available as an additional option.

> Both Veijola and others (Ref. 5) and Cercignani and others (Ref. 5) provided data for the relative flow rate $Q(\text{Kn}, \sigma_{sw}, \sigma_{sb})$ in specific cases where the wall and base have different accommodation coefficients. Since no details on how to compute the forces acting on the walls for highly rarefied gases were published, these models are not currently supported in COMSOL Multiphysics.

Frequency-Domain Formulation

In the frequency domain it is necessary to make additional simplifications to the equation system to produce a fully linearized equation set. In the general case, the physical quantities in the Reynolds and flow equations take the form:

$$h_w = h_{w1} + \tilde{h}_w \qquad h_b = h_{b1} + \tilde{h}_b \qquad h = h_{w1} + h_{b1} + \tilde{h}_w + \tilde{h}_b = h_1 + \tilde{h}$$

$$p_f = \tilde{p}_f \qquad p_A = p_{ref} + \tilde{p}_f$$

$$\mathbf{v}_w = \tilde{\mathbf{v}}_w \qquad \mathbf{v}_b = \tilde{\mathbf{v}}_b$$

Here the tilde denotes a harmonically varying component. The components marked with the subscript 1 are static offsets to the harmonic terms. In order to linearize the

equation system, it is necessary to assume that the offsets are much larger than the harmonic components. Practically speaking this means that the harmonically varying pressures induced by the flow should be significantly smaller than the ambient pressure, and the harmonic changes in the gap size due to the wall and base displacements should be significantly less than the gap height itself. Given these assumptions, the average fluid velocity can also be written on the form:

$$\mathbf{v}_{av} = \tilde{\mathbf{v}}_{av}$$

since in general both the Couette and Poiseuille terms vary harmonically to first-order accuracy.

Substituting these terms into the Reynolds equation gives:

$$\frac{\partial}{\partial t}(\rho(h_1 + \tilde{h})) + \nabla_t \cdot (\rho(h_1 + \tilde{h})\tilde{\mathbf{v}}_{av}) = 0$$

In the frequency domain, the total absolute pressure p_A is set to the reference pressure p_{ref} because the deviation from the reference pressure p_f in this case represents an oscillating component and cannot be added to the pressure in a straightforward manner. ρ is defined as a function of p_A and so contains no small harmonic component. The products of small harmonic terms result in second-order effects (at double the frequency of interest) and can be neglected provided the harmonic terms are much smaller than the static terms. The Reynolds equation therefore reduces to:

$$\rho\frac{\partial}{\partial t}(\tilde{h}) + \nabla_t \cdot (\rho h_1 \tilde{\mathbf{v}}_{av}) = 0$$

Note that:

$$\frac{\partial}{\partial t}(\tilde{h}) = \tilde{\mathbf{v}}_b \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_w \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_b \cdot \nabla_t h_{b1} - \tilde{\mathbf{v}}_w \cdot \nabla_t h_{w1} \qquad (9\text{-}15)$$

So the following result holds:

$$\rho(\tilde{\mathbf{v}}_b \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_w \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_b \cdot \nabla_t h_{b1} - \tilde{\mathbf{v}}_w \cdot \nabla_t h_{w1}) + \nabla_t \cdot (\rho h_1 \tilde{\mathbf{v}}_{av}) = 0 \quad (9\text{-}16)$$

Dropping the tildes leads to the form of the equation shown in the equation display:

$$\rho(\mathbf{v}_b \cdot \mathbf{n}_{ref} - \mathbf{v}_w \cdot \mathbf{n}_{ref} - \mathbf{v}_w \cdot \nabla_t h_{w1} - \mathbf{v}_b \cdot \nabla_t h_{b1}) + \nabla_t \cdot (\rho h_1 \mathbf{v}_{av}) = 0$$

The modified Reynolds Equation takes the following form:

$$\frac{\partial}{\partial t}((p_{ref}+\tilde{p}_f)(h_1+\tilde{h}))+\nabla_t\cdot((p_{ref}+\tilde{p}_f)(h_1+\tilde{h})\tilde{\mathbf{v}}_{av}) = 0 \qquad (9\text{-}17)$$

Linearizing Equation 9-17 gives:

$$p_{ref}\frac{\partial}{\partial t}\tilde{h}+h_1\frac{\partial}{\partial t}\tilde{p}_f+\nabla_t\cdot(p_{ref}h_1\tilde{\mathbf{v}}_{av}) = 0$$

Equation 9-15 can be used to substitute for the time derivative of the harmonic component of h in the above equation, yielding:

$$p_{ref}(\tilde{\mathbf{v}}_b\cdot\mathbf{n}_{ref}-\tilde{\mathbf{v}}_w\cdot\mathbf{n}_{ref}-\tilde{\mathbf{v}}_b\cdot\nabla_t h_{b1}-\tilde{\mathbf{v}}_w\cdot\nabla_t h_{w1})$$
$$+h_1\frac{\partial}{\partial t}(\tilde{p}_f)+\nabla_t\cdot(p_{ref}h_1\tilde{\mathbf{v}}_{av}) = 0 \qquad (9\text{-}18)$$

Dropping the tildes and using complex notation to express the time derivative of p_f gives:

$$p_{ref}(\mathbf{v}_b\cdot\mathbf{n}_{ref}-\mathbf{v}_w\cdot\mathbf{n}_{ref}-\mathbf{v}_w\cdot\nabla_t h_{w1}-\mathbf{v}_b\cdot\nabla_t h_{b1})$$
$$+i\omega h_1 p_f+\nabla_t\cdot(p_{ref}h_1\mathbf{v}_{av}) = 0$$

Equation 9-16 and Equation 9-18 are used as the basis for the frequency domain formulation in the Thin-Film Flow interfaces. It is important to note that these equations are independent of the harmonic components of the displacement, since those terms lead to second-order contributions to the frequency-domain response (that is, they produce a response proportional to the square of the harmonic term, which results in a signal at twice the driving frequency).

> Since the frequency domain results do not depend on the variation in the displacement, the additional displacement setting has no effect on the solution in a frequency-domain problem (unless the velocity is computed from it by selecting **Calculate from wall displacement** or **Calculate from base displacement** in the wall and base velocity settings, respectively). This is reflected in the equations given above (and in the equation display in the physics interface) but can be nonintuitive, particularly when setting up a model that is coupled with a structural analysis. If the velocity of both the wall and the base is set to zero, then in the frequency domain there is no response.

Boundary Conditions

Most of the boundary conditions either constrain the flow into the system by prescribing a fluid velocity or constrain the pressure at the boundary. The border flow condition is slightly more complex, requiring the gradient of the pressure to be set by specifying the value of the gradient of the pressure in the anti-normal direction such that:

$$-\mathbf{n} \cdot \nabla p = \Gamma$$

The **Border flow type** selection list enables four ways that the value of Γ can be specified:

• The **User defined** option allows the value of Γ to be directly entered as an expression in a text field. This allows for arbitrary normal pressure gradients.

• The two **Acoustic elongation** options assume a linear gradient in the pressure outside the domain away from the boundary. The pressure gradient is calculated by dividing the pressure at the boundary, p_f, by an elongation length, ΔL. The elongation length can either be specified as an absolute length or as a fraction of the domain width, such that:

$$-\mathbf{n} \cdot \nabla p = \frac{p_f}{\Delta L}$$

• The **Out-of-plane motion** option calculates the pressure gradient at the boundary using a model detailed in Ref. 8. This model is suitable for including the effects of gas damping when fluid in a thin gap is subjected to out-of-plane motion of the walls or base (for example, when a microbeam is oscillating above an extended surface). When this option is selected, text fields are provided to specify the required coefficients (ζ, η, χ) and the pressure gradient is defined according to

$$-\mathbf{n} \cdot \nabla p = \zeta \frac{12\mu U}{\eta h^2}\left(1 + \chi\frac{6\Lambda}{h}\right)^{-1} + \frac{p - p_\infty}{\eta h^2}$$

where U is the out-of-plane velocity, Λ is the slip length at the walls, and p_∞ is the ambient pressure far from the boundary away from the domain.

Cavitation

Several types of cavitation can occur in thin film flow. When the flow pressure drops below the ambient pressure, the air and other gases dissolved within the fluid are released. This phenomenon, characteristic of loaded bearings, is known as cavitation

or gaseous cavitation. In some cases involving high frequency varying loads, as in internal combustion engines, the pressure might drop below the fluid vapor pressure, which is lower than the ambient pressure. In this case, bubbles are formed by rapid evaporation or boiling of the fluid. This phenomenon is known as vapor cavitation. The cavitation feature in COMSOL Multiphysics is designed to address gaseous cavitation.

The implementation of the cavitation feature is based on a modified version of the Elrod's algorithm (Ref. 9 and Ref. 10). This algorithm automatically predicts film rupture and reformation in bearings and offers a reasonable compromise between accuracy and practicality. It is applicable to heavily and moderately loaded bearings but it is not suitable when surface tension plays an important role.

Elrod and Adam's algorithm is based on the JFO cavitation theory, a widely accepted and adopted theory developed by Jakobson (Ref. 11), Floberg (Ref. 12 and Ref. 13), and Olsson (Ref. 14). The JFO theory divides the flow in two regions:

• A full film region where the pressure varies but is limited from below by the cavitation pressure.
• A cavitation region where only part of the volume is occupied by the fluid. Because of the presence of the gas in the void fraction, the pressure in this region is assumed to be constant and equal to the cavitation pressure.

Elrod and Adams derived a general form of the Reynolds equation, Equation 9-1, by introducing a switch function, g, equal to 1 in the full film region and 0 in the cavitation region. This switch function allows for solving a single equation for both the full film and the cavitation region and leads to a modified version of Equation 9-7:

$$\mathbf{v}_{av} = \mathbf{v}_{av,c} - g v_{av,p} \nabla_t p_f$$

where the second and third terms on the left-hand side correspond to the average Couette and average Poiseuille velocities, respectively. This switch function sets the average Poiseuille velocity to zero in the cavitation region.

> ⚠️
>
> Because the average Poiseuille velocity is set to zero in the cavitation region, the density needs to be a function of the pressure variable and is defined as
>
> $$\rho = \rho_c e^{\beta p_f}$$
>
> where β is the compressibility, and ρ_c is the density at the cavitation pressure. A density that is not pressure dependent would lead to empty equations in the cavitation region since the pressure variable p_f would no longer present in the governing equations.

A variable θ can be defined, given by:

$$\theta = \frac{\rho}{\rho_c}$$

In the cavitation region ($\theta < 1$) θ represents the fractional film content.

NOTE ABOUT RESULTS POSTPROCESSING

While the pressure is constant and equal to the cavitation pressure in the cavitation region, the computed pressure is negative in this region. The value of this negative pressure can be physically be interpreted as the volume fraction of fluid in the cavitation region. The actual or physical pressure, available in the postprocessing section as `tffs.p`, is equal to the computed pressure in the full film region ($\theta \geq 1$) and equal to the cavitation pressure in the cavitation region ($\theta < 1$).

References for the Thin-Film Flow Interfaces

1. B.J. Hamrock, S.R. Schmid and B.O. Jacobson, *Fundamentals of Fluid Film Lubrication*, Marcel Dekker, 2004.

2. F. Sharipov, "Data on the Velocity Slip and Temperature Jump on a Gas-Solid Interface", *J. Phys. Chem. Ref. Data*, vol. 40, no. 2, 023101, 2011.

3. S. Fukui and R. Kaneko, "Analysis of Ultra-Thin Gas Film Lubrication Based on Linearized Boltzmann Equation: First Report — Derivation of a Generalized

Lubrication Equation Including Thermal Creep Flow", *J. Tribology*, vol. 110, no. 2, pp. 253–261, 1988.

4. S. Fukui and R. Kaneko, "A Database for Interpolation of Poiseuille Flow Rates for High Knudsen Number Lubrication", *Transactions of the ASME*, vol. 112, pp. 78–83, 1990.

5. T. Veijola, H. Kuisma, and J. Lahdenperä, "The Influence of Gas-surface Interaction on Gas Film Damping in a Silicon Accelerometer", *Sensors and Actuators*, vol. A 66, pp. 83–92, 1998.

6. C. Cercignani, Maria Lampis, and Silvia Lorenzani "Variational Approach to Gas Flows in Microchannels", *Physics of Fluids*, vol. 16, no. 9, 2004.

7. J.R. Torczynski and M.A. Gallis, "DSMC-Based Shear-Stress/Velocity-Slip Boundary Condition for Navier-Stokes Couette-Flow Simulations", 27th International Symposium on Rarefied Gas Dynamics (2010), *AIP Conf. Proc.* vol. 1333, pp. 802–807, 2011.

8. M. A. Gallis and J. R. Torczynski, "An Improved Reynolds-Equation Model for Gas Damping of Microbeam Motion", Journal of Microelectromechanical Systems, vol. 13, pp. 653–659, 2004.

9. H. G.Elrod, "A Cavitation Algorithm", *J. Lubrication Technology*, vol. 103, no. 3, pp. 350–354, 1981.

10. H. G. Elrod and M. L. Adams, "A computer program for cavitation and starvation problems", *Cavitation and related phenomena in lubrication, Proceedings of the 1st Leeds–Lyon Symposium on Tribology*, University of Leeds, UK, 1974.

11. B. Jacobson and L. Floberg, "The finite journal bearing considering vaporization", *Transactions of Chalmers University Technology*, Göteborg, Sweden, vol. 190, pp. 1–119, 1957.

12. L. Floberg, "On journal bearing lubrication considering the tensile strength of the liquid lubricant", *Transactions of the Machine Elements Division*, Lund Technical University, Lund, Sweden, pp. 1–26, 1973.

13. L. Floberg, "Cavitation boundary conditions with regard to the number of streamers and tensile strength of the liquid", *Cavitation and related phenomena in lubrication, Proceedings of the 1st Leeds–Lyon Symposium on Tribology*, University of Leeds, UK, pp. 31–36 (Mechanical Engineering Publications Ltd, London, UK), 1974.

14. K.O. Olsson, "Cavitation in dynamically loaded bearings", *Transactions of Chalmers University Technology*, Göteborg, Sweden, vol. 308, 1965.

10

Mathematics, Moving Interface Branch

The Level Set and Phase Field Moving interfaces are available under the
Mathematics>Moving Interface branch (▨). Also see Modeling Multiphase Flow to
help you choose the best interface to start with.

In this chapter:

- The Level Set Interface
- The Phase Field Interface
- The Ternary Phase Field Interface
- Theory for the Level Set Interface
- Theory for the Phase Field Interface
- Theory for the Ternary Phase Field Interface

The Level Set Interface

The **Level Set (ls)** interface (〴〴〴), found under the **Mathematics>Moving Interface** branch (▮) when adding an interface, is used to track moving interfaces in fluid-flow models by solving a transport equation for the level set function. Simulations using the **Level Set** interface are always time dependent since the position of an interface almost always depends on its history.

The main node is the Level Set Model feature, which adds the level set equation and provides an interface for defining the level set properties and the velocity field.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Level Set Model**, **No Flow** (the default boundary condition) and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Level Set** to select physics features from the context menu.

S E T T I N G S

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `ls`.

The dependent variable (field variable) is the **Level set variable** phi. The name can be changed but the names of fields and dependent variables must be unique within a model.

🔍
- Conservative and Non-Conservative Form
- Domain, Boundary, and Pair Nodes for the Level Set Interface
- Theory for the Level Set Interface
- Theory for the Two-Phase Flow Interfaces

Domain, Boundary, and Pair Nodes for the Level Set Interface

The Level Set Interface has the following domain, boundary and pair nodes described.

- Initial Interface
- Initial Values
- Inlet
- Level Set Model
- No Flow

- Outlet[1]
- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Symmetry[1]

[1] Described for the Laminar Flow interface.

Boundary conditions for axial symmetry boundaries are not required. For the symmetry axis at $r = 0$, the software automatically provides a suitable boundary condition and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Level Set Model

The **Level Set Model** node adds the following transport equation governing a level set function ϕ

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi (1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$

and provides the options to define the associated level set parameters and the velocity field.

LEVEL SET PARAMETERS

Enter a value or expression for the **Reinitialization parameter** γ (SI unit: m/s). The default is 1 m/s.

Enter a value or expression for the **Parameter controlling interface thickness** e_{ls} (SI unit: m). The default expression is `ls.hmax/2`, which means that the value is half of the maximum mesh element size in the region through which the interface passes.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field u** (SI unit: m/s). The applied velocity field transports the level set function through convection.

Initial Values

Use the **Initial Values** node to define the initial values of the level set variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the separating interface, can be specified in two ways. The level set function can be specified explicitly, using any type of variable or expression. Alternatively the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the level set function across the fluid-fluid interface.

Specify **Domain Initially** as one of the following:

• **Specify level set function explicitly**

- **Fluid 1 ($\phi = 0$)**
- **Fluid 2 ($\phi = 1$)**

	If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two Initial Values nodes and one Initial Interface node. The Initial Values nodes should specify the **Domain Intially** as **Fluid 1** and **Fluid 2** respectively. The Initial Interface node should include all interior boundaries that defines the initial position of the fluid-fluid interface.. If the selection of the **Initial interface** node is empty, the initialization fails.
	See Initializing the Level Set Function.

Inlet

The **Inlet** node adds a boundary condition for inlets (inflow boundaries).

SETTINGS

Specify **Level Set Condition** as one of the following:

- **Fluid 1 ($\phi = 0$)**
- **Fluid 2 ($\phi = 1$)**
- **Specify level set function explicitly**

When choose specify level set function explicitly, a value of the level set function ϕ must be specified. The value must be in the range from 0 to 1, and the default is 0.

Initial Interface

The **Initial Interface** node defines the boundary as the initial position of the interface
$\phi = 0$.

	If the **Transient with Initialization** ( ) study is being used, for the initialization to work it is crucial that there are two Initial Values nodes and one Initial Interface node. One of the Initial Values nodes should use **Domain initially: Inside interface** and the other **Domain initially: Outside interface**. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the **Initial interface** node is empty, the initialization fails.
	See Initializing the Level Set Function.

No Flow

The **No Flow** node adds a boundary condition that represents boundaries where there
is no flow across the boundary. This is the default boundary condition.

The Phase Field Interface

The **Phase Field (pf)** interface (▨), found under the **Mathematics>Moving Interface** branch (▨) when adding a physics interface, is used to track moving interfaces by solving two transport equations, one for the phase field variable, ϕ, and one for the mixing energy density, ψ. The position of the interface is determined by minimizing the free energy.

The main node is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Phase Field Model**, **Wetted Wall** (the default boundary condition) and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Phase Field** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `pf`.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields) **Phase field variable** ϕ and **Phase field help variable** ψ. If required, edit the name, but dependent variables must be unique within a model.

Q
- Conservative and Non-Conservative Forms
- Domain, Boundary, and Pair Nodes for the Phase Field Interface
- Theory for the Phase Field Interface

⊞	*Phase Separation*: Application Library path **CFD_Module/Multiphase_Tutorials/phase_separation**

Domain, Boundary, and Pair Nodes for the Phase Field Interface

The Phase Field Interface includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

💡	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Initial Interface
- Initial Values
- Inlet
- Outlet[1]

- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Phase Field Model
- Symmetry[1]
- Wetted Wall

[1] Described for the Laminar Flow interface.

❗	In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Phase Field Model

The **Phase Field Model** node adds the equations described in The Equations for the Phase Field Method. The node defines the associated phase field parameters including surface tension and interface thickness.

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- **Surface tension coefficient** σ (SI unit: N/m).

- **Parameter controlling interface thickness** e_{pf} (SI unit: m). The default expression is pf.hmax/2, which means that the value is half of the maximum mesh element size in the region through which the interface passes.

- **Mobility tuning parameter** χ (SI unit: m·s/kg). The default is 1 m·s/kg, which is a good starting point for most models. This parameter determines the time scale of the Cahn-Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface.

> 💡 Keep the χ parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets.

EXTERNAL FREE ENERGY

Add a source of external free energy to the phase field equations. This modifies the last term on the right-hand side of the equation:

$$\psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial \phi}$$

The external free energy f (SI unit: J/m^3) is a user-defined free energy. In most cases, the external free energy can be set to zero. Manually differentiate the expression for the external free energy with respect to ϕ and then enter it into the ϕ **-derivative of external free energy** field $\partial f/\partial \phi$.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** u (SI unit: m/s). The applied velocity field transports the phase field variables through convection.

> 🔍 Additional Sources of Free Energy

Initial Values

Use the **Initial Values** node to define the initial values of the phase field variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the fluid-fluid interface, can be specified in two ways. The phase field variable can be specified explicitly, using any type of variable or expression. Alternatively the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the phase field function across the fluid-fluid interface.

Specify **Domain Initially** as one of the following:

- **Specify phase field function explicitly**
- **Fluid 1 (ϕ = -1)**
- **Fluid 2 (ϕ = 1)**

> ⚠ If the **Phase Initialization** (![icon]) study step is being used, for the initialization to work it is crucial that there are two Initial Values nodes and one Initial Interface node. The Initial Values nodes should specify the **Domain Initially** as **Fluid 1** and **Fluid 2** respectively. The Initial Interface node should include all interior boundaries that defines the initial position of the fluid-fluid interface. If the selection of the **Initial interface** node is empty, the initialization fails.

Inlet

The **Inlet** feature node adds a boundary condition for inlets (inflow boundaries).

SETTINGS

Specify **Phase field Condition** as one of the following:

- **Fluid 1 (ϕ = -1)**
- **Fluid 2 (ϕ = 1)**
- **Specify phase field function explicitly**

When choose specify phase field function explicitly, a value of the phase field function ϕ must be specified. The value must be in the range from -1 to 1, and the default is 1.

Initial Interface

The **Initial Interface** node defines the boundary as the initial position of the interface $\phi = 0$.

	If the **Transient with Phase Initialization** ( ) study is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes and one **Initial Interface** node. One of the Initial Values nodes is set to phipf = 1 and the other to phipf = −1. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the Initial Interface node is empty, the initialization fails.

Wetted Wall

The **Wetted Wall** node is the default boundary condition representing wetted walls. Along a wetted wall the contact angle for the fluid, θ_w, is specified, and across it, the mass flow is zero. This is prescribed by

$$\mathbf{n} \cdot \varepsilon^2 \nabla \phi = \varepsilon^2 \cos(\theta_w) |\nabla \phi|$$

in combination with

$$\mathbf{n} \cdot \frac{\gamma \lambda}{\varepsilon^2} \nabla \psi = 0$$

WETTED WALL

Enter a value or expression for the **Contact angle** θ_w. The default value is $\pi/2$ rad.

The Ternary Phase Field Interface

The **Ternary Phase Field (terpf)** interface (▨), found under the **Mathematics>Moving Interface** branch (▨) when adding a physics interface, is used to track moving interfaces separating three different phases. The interface solves four transport equations: two equations governing phase field variables, ϕ_A and ϕ_B, and two equations for the corresponding generalized chemical potentials, η_A and η_B. The position of the interfaces are determined by minimization of the free energy.

The phase field variables are defined such that they represent the volume fraction of the respective phase. The volume fraction of the third phase not solved for, but computed from the natural constraint that the sum of the volume fractions of all phases is one.

The main node of the interface is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties such as surface tensions and parameters controlling the interface thickness.

When this physics interface is added, the following default nodes are also added in the **Model Builder**—**Mixture Properties**, **Wetted Wall** and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Ternary Phase Field** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `terpf`.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields):

- **Phase field variable, fluid A** `phiA`
- **Phase field variable, fluid B** `phiB`

- **Generalized chemical potential of fluid A** etaA

- **Generalized chemical potential of fluid B** etaB

If required, edit the any of the names, but dependent variables must be unique within a model.

<table>
<tr><td>Q</td><td>• Theory for the Ternary Phase Field Interface</td></tr>
</table>

Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface

The Ternary Phase Field Interface includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking the interface node to access the context menu (all users).

- Initial Values
- Inlet
- Outlet

- Phase Field Model
- Symmetry
- Wetted Wall

Mixture Properties

The **Mixture Properties** node adds the equations described in The Equations of the Ternary Phase Field Method. The node defines the associated phase field parameters, including the surface tension coefficients and parameters controlling the thickness of the interfaces.

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- **Parameter controlling interface thickness** ε. The default expression applied is terpf.hmax*sqrt(2), which means that the thickness is related to the maximum mesh element size in the domain. If the element size in the regions passed by the interfaces is known beforehand, it is recommended to apply a value of ε in that order.

- **Mobility tuning parameter** M_0. This parameter determines the time scale of the Cahn-Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Keep the mobility tuning parameter value large enough to maintain a constant interface thickness, but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets. By default M_0 is set to $1 \cdot 10^{-4}$ m^3·s/kg, which is a good starting point for most models.

- **Additional free bulk energy** Λ. When needed add an a user defined expression of the additional bulk energy.

SURFACE TENSION

Specify the surface tension coefficients for the three types of interfaces present.

- To use a predefined expression, select **Library coefficient, liquid/gas interface**, or **Library coefficient, liquid/liquid interface.** Then select an option from the list that displays below (for example, **Water/Air**, **Glycerol/Air**, and so forth).

- For **User defined**, enter a value or expression for the surface tension coefficient

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** u. The applied velocity field transports the phase field variables through convection.

Initial Values

The **Initial Values** node adds initial values for the phase field variables that can serve as initial conditions for a transient simulation.

INITIAL VALUES

Enter initial values or expressions for **Phase field variable A** and the **Phase field variable B** corresponding to the mass fraction of the respective phase. The value must be in the range from 0 to 1.

Inlet

This condition should be used on boundaries for which there is a net convective flow of the phases into the adjacent domain.

Specify phase field variables, corresponding to the volume fractions, of phase A and phase B. The value must be in the range from 0 to 1. The volume fraction of phase C will be evaluated such that the sum of all mass fractions equals one.

Mathematically this boundary condition imposes

$$\phi_i = \phi_{i,0}, \ \mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Outlet

This condition should be used on boundaries for which there is a net convective outflow from the domain.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Symmetry

This condition should be used on boundaries which represent a geometrical symmetry line across which the flow of the fluid phases is zero.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Wetted Wall

Use this node to represent a solid wall along which the contact angles between the separating interfaces and the wall should be prescribed.

WETTED WALL

Enter values or expressions for the contact angles for the three interfaces types:

- The **Contact angle of interface from phase A to phase C** θ_α.
- The **Contact angle of interface from phase B to phase C** θ_β.
- The **Contact angle of interface from phase A to phase B** θ_γ.

The definition of the contact angles with respect to the wall are shown in the figure below
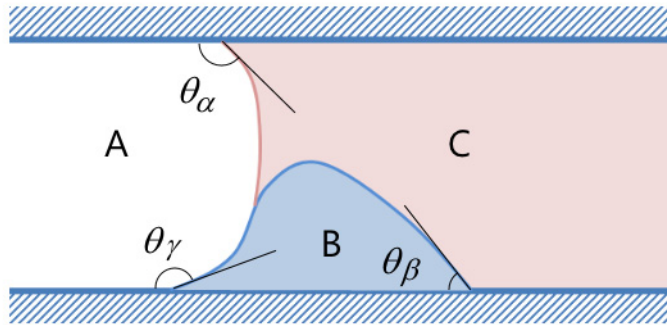
Figure 10-1: Definitions of the contact angels in the Wetted Wall feature of the Ternary Phase Field interface.

Theory for the Level Set Interface

Fluid flow with moving interfaces or boundaries occur in a number of different applications, such as *fluid-structure interaction*, multiphase flows, and flexible membranes moving in a liquid. One way to track moving interfaces is to use a level set method. A certain contour line of the globally defined function, the level set function, then represents the interface between the phases. For The Level Set Interface the fluid-fluid interface can be advected with an arbitrary velocity field.

In this section:

- The Level Set Method
- Conservative and Non-Conservative Form
- Initializing the Level Set Function
- Variables For Geometric Properties of the Interface
- Reference for the Level Set Interface

The Level Set Method

The *level set method* is a technique to represent moving interfaces or boundaries using a fixed mesh. It is useful for problems where the computational domain can be divided into two domains separated by an interface. Each of the two domains can consist of several parts. Figure 10-2 shows an example where one of the domains consists of two separated parts. The interface is represented by a certain level set or isocontour of a globally defined function, the level set function ϕ. In COMSOL Multiphysics, ϕ is a smooth step function that equals zero (0) in one domain and one (1) in the other. Across the interface, there is a smooth transition from zero to one. The interface is defined by the 0.5 isocontour, or level set, of ϕ. Figure 10-3 shows the level set

representation of the interface in Figure 10-2.
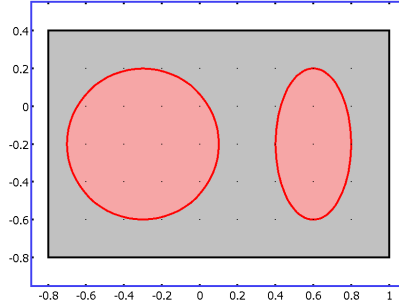
Figure 10-2: An example of two domains divided by an interface. In this case, one of the domains consists of two parts. Figure 10-3 shows the corresponding level set representation.
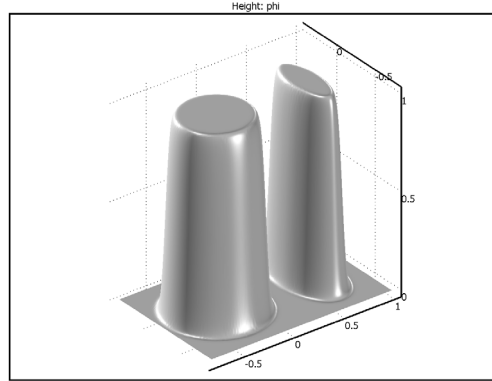
Figure 10-3: A surface plot of the level set function corresponding to Figure 10-2.

The physics interface solves Equation 10-1 in order to move the interface with the velocity field **u**:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|} \right) \qquad (10\text{-}1)$$

The terms on the left-hand side give the correct motion of the interface, while those on the right-hand side are necessary for numerical stability. The parameter, ε, determines the thickness of the region where ϕ varies smoothly from zero to one and is typically of the same order as the size of the elements of the mesh. By default, ε is constant within each domain and equals the largest value of the mesh size, h, within

the domain. The parameter γ determines the amount of reinitialization or stabilization of the level set function. It needs to be tuned for each specific problem. If γ is too small, the thickness of the interface might not remain constant and oscillations in ϕ can appear because of numerical instabilities. On the other hand, if γ is too large the interface moves incorrectly. A suitable value for γ is the maximum magnitude of the velocity field $\mathbf{u}$.

Conservative and Non-Conservative Form

If the velocity is divergence free, that is, if

$$\nabla \cdot \mathbf{u} = 0 \tag{10-2}$$

the volume (area for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the boundaries. To obtain exact numerical conservation, switch to the conservative form

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|} \right) \tag{10-3}$$

in Settings window for The Level Set Interface.

Using the conservative level set form, exact numerical conservation of the integral of ϕ is obtained. However, the non-conservative form is better suited for numerical calculations and usually converges more easily. The non-conservative form, which is the default form, only conserves the integral of the level set function approximately, but this is sufficient for most applications.

Initializing the Level Set Function

If the study type Transient with Phase Initialization is used in the model, the level set variable is first initialized so that it varies smoothly between zero and one over the interface. For that study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the level set function according to the following expression:

$$\phi_0 = \frac{1}{1 + e^{-D_{wi}/\varepsilon}}$$

in domains initially outside the interface and

$$\phi_0 = \frac{1}{1 + e^{D_{wi}/\varepsilon}}$$

in domains initially inside the interface. Here, inside refers to domains where $\phi < 0.5$ and outside refers to domains where $\phi > 0.5$.

> For the initialization to work it is crucial that there are two **Initial Values** nodes and one **Initial Interface** node. One of the Initial Values nodes should use **Domain initially: Inside interface** and the other **Domain initially: Outside interface**. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the Initial interface node is empty, the initialization fails.

> - The Level Set Interface
> - Studies and Solvers and Transient with Initialization in the *COMSOL Multiphysics Reference Manual*

Variables For Geometric Properties of the Interface

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}\bigg|_{\phi = 0.5} \tag{10-4}$$

The curvature is defined as

$$\kappa = -\nabla \cdot \mathbf{n}\big|_{\phi = 0.5} \tag{10-5}$$

These variables are available in the physics interface as the interface normal and mean curvature.

> It is only possible to compute the curvature explicitly when using second-order or higher-order elements.

Reference for the Level Set Interface

1. E. Olsson and G. Kreiss, "A Conservative Level Set Method for Two Phase Flow,"
J. Comput. Phys., vol. 210, pp. 225–246, 2005.

Theory for the Phase Field Interface

The Phase Field Interface theory is described in this section:

- About the Phase Field Method
- The Equations for the Phase Field Method
- Conservative and Non-Conservative Forms
- Additional Sources of Free Energy
- Initializing the Phase Field Function
- Variables and Expressions
- Reference for the Phase Field Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the interfacial layer is governed by a phase field variable, ϕ. The surface tension force is added to the Navier-Stokes equations as a body force by multiplying the chemical potential of the system by the gradient of the phase field variable.

The evolution of the phase field variable is governed by the *Cahn-Hilliard equation*, which is a 4th-order PDE. The Phase Field interface decomposes the Cahn-Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn-Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of two immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple two-phase flows, only the mixing energy is retained, which results in a rather simple expression for the free energy.

The Equations for the Phase Field Method

The free energy is a functional of a dimensionless phase field parameter, ϕ:

$$F(\phi, \nabla\phi, T) \;=\; \int\!\Big(\tfrac{1}{2}\varepsilon^2|\nabla\phi|^2 + f(\phi, T)\Big)dV \;=\; \int f_{\text{tot}}dV$$

where ε is a measure of the interface thickness. Equation 10-6 describes the evolution of the phase field parameter:

$$\frac{\partial\phi}{\partial t} + (\mathbf{u}\cdot\nabla)\phi \;=\; \nabla\cdot\gamma\nabla\Big(\frac{\partial f_{\text{tot}}}{\partial\phi} - \nabla\cdot\frac{\partial f_{\text{tot}}}{\partial\nabla\phi}\Big) \tag{10-6}$$

where f_{tot} (SI unit: J/m^3) is the total free energy density of the system, and $\mathbf{u}$ (SI unit: m/s) is the velocity field for the advection. The right-hand side of Equation 10-6 aims to minimize the total free energy with a relaxation time controlled by the mobility γ (SI unit: m^3·s/kg).

The free energy density of an isothermal mixture of two immiscible fluids is the sum of the mixing energy and elastic energy. The mixing energy assumes the Ginzburg-Landau form:

$$f_{\text{mix}}(\phi, \nabla\phi) \;=\; \frac{1}{2}\lambda|\nabla\phi|^2 + \frac{\lambda}{4\varepsilon^2}(\phi^2 - 1)^2$$

where ϕ is the dimensionless phase field variable, defined such that the volume fraction of the components of the fluid are $(1+\phi)/2$ and $(1-\phi)/2$. The quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma \;=\; \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon} \tag{10-7}$$

The PDE governing the phase field variable is the Cahn-Hilliard equation:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi \;=\; \nabla\cdot\gamma\nabla G \tag{10-8}$$

where G (SI unit: Pa) is the chemical potential and γ (SI unit: m^3·s/kg) is the mobility. The mobility determines the time scale of the Cahn-Hilliard diffusion and must be large enough to retain a constant interfacial thickness but small enough so that the convective terms are not overly damped. In COMSOL Multiphysics the mobility is determined by a mobility tuning parameter that is a function of the interface thickness $\gamma = \chi\varepsilon^2$. The chemical potential is:

$$G = \lambda\left[-\nabla^2\phi + \frac{\phi(\phi^2 - 1)}{\varepsilon^2}\right] \tag{10-9}$$

The Cahn-Hilliard equation forces ϕ to take a value of 1 or -1 except in a very thin region on the fluid-fluid interface. The Phase Field interface breaks Equation 10-8 up into two second-order PDEs:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi \tag{10-10}$$

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2 - 1)\phi \tag{10-11}$$

Conservative and Non-Conservative Forms

If the velocity field is divergence free, use the conservative formulation:

$$\frac{\partial\phi}{\partial t} + \nabla\cdot\mathbf{u}\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi$$

Using the conservative phase field form, exact numerical conservation of the integral of ϕ is obtained. However, the non-conservative form is better suited for numerical calculations and usually converges more easily. The non-conservative form, which is the default form, only conserves the integral of the phase field function approximately, but this is sufficient for most applications.

Additional Sources of Free Energy

In some cases, the expression for the free energy can include other sources. It is possible to incorporate these by modifying Equation 10-11:

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial\phi} \tag{10-12}$$

where f is a user-defined free energy (SI unit: J/m^3).

	The expression for the external free energy must be manually differentiated with respect to ϕ and then entered into the $\partial f/\partial\phi$ field. In most cases, the external free energy is zero.

Initializing the Phase Field Function

If the study type Transient with Phase Initialization is used in the model, the phase field variable is first initialized so that it varies smoothly between zero and one over the interface. For this study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the phase field function according to the following expression:

$$\phi_0 = -\tanh\left(\frac{D_{wi}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{wi}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 2. These expressions are based on a steady, analytic solution to Equation 10-10 and Equation 10-11 for a straight, non-moving interface.

!	If the **Transient with Phase Initialization** ( ) study is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes and one **Initial Interface** node. One of the Initial Values nodes is set to *phipf* = 1 and the other to *phipf* = -1. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the Initial Interface node is empty, the initialization fails.

🔍	Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Variables and Expressions

Unlike the level set method, the phase field method does not require expressions for the unit normal to the interface or smoothed delta functions, so they are not available for analysis. Variables that are defined are the chemical potential, which can be rewritten in terms of the dependent variable ψ,

$$G = \frac{\lambda \psi}{\epsilon^2}$$

and the surface tension force $\mathbf{F} = G\nabla\phi$.

The mean curvature (SI unit: $1/\text{m}$) of the interface can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

Reference for the Phase Field Interface

1. P. Yue, C. Zhou, J.J. Feng, C.F. Ollivier-Gooch, and H.H. Hu, "Phase-field Simulations of Interfacial Dynamics in Viscoelastic Fluids Using Finite Elements with Adaptive Meshing," *J. Comp. Phys.*, vol. 219, pp. 47–67, 2006.

Theory for the Ternary Phase Field Interface

The Ternary Phase Field Interface theory is described in this section:

- About the Phase Field Method
- The Equations for the Phase Field Method
- Reference for the Phase Field Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the separating interface is identified as the region across which the phase field variables of the two adjacent phases varies between its two limiting values. The surface tension force is added to the Navier-Stokes equations as a body force by multiplying the chemical potentials of the phases by the gradient of the corresponding phase field variable.

The evolution of each phase field variable is governed by the *Cahn-Hilliard equation*, which is a 4th-order PDE. The Ternary Phase Field interface decomposes each Cahn-Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn-Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple three-phase flows, only the mixing energy is retained.

The Equations of the Ternary Phase Field Method

The ternary phase field model implemented in COMSOL is based the work of Boyer and co-workers in Ref. 1. The model is designed in order to study the evolution of the three immiscible phases, denoted phase A, phase B and phase C respectively. Each phase is represented by a phase field variable ϕ which takes values between 0 and 1. The phase field variables satisfies the constraint

$$\sum_{i = A, B, C} \phi_i = 0 \qquad (10\text{-}13)$$

and density of each phase is assumed to be constant. This implies that the phase field variable corresponds directly to the volume fraction of the phase in question.

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$F = \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 + \\ \phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2 \qquad (10\text{-}14)$$

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase i and j, and the capillary parameters Σ_i are defined as

$$\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk} \qquad (10\text{-}15)$$

and Λ is a function or parameter specifying the additional free bulk energy. By default Λ is zero. In this case it can be seen that the free energy in Equation 10-14 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

The Cahn-Hilliard equations to be solved for each phase $p = A, B, C$ are

$$\frac{\partial \phi_i}{\partial t} + \frac{\partial u_j \phi_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{M_0}{\Sigma_i}\frac{\partial \eta_i}{\partial x_j}\right) \\ \eta_i = \frac{4\Sigma_T}{\varepsilon}\sum_{j \neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial \phi_i} - \frac{\partial F}{\partial \phi_j}\right)\right) - \frac{3}{4}\varepsilon\Sigma_j\frac{\partial}{\partial x_j}\left(\frac{\partial \eta_i}{\partial x_j}\right) \qquad (10\text{-}16)$$

It can be noted that the Cahn-Hilliard equation is originally a 4th-order PDE. In COMSOL this is split up into two second order PDEs by introducing an additional dependent variable, the generalized potential η, one for each phase. In order to satisfy Equation 10-14, two sets of the equations shown in Equation 10-16 are solved, those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 10-14.

In Equation 10-16 ε (SI unit: 1/m) is a parameter controlling the interface thickness, M_0 (SI unit: m^3/s) is a molecular mobility parameter, and the parameter Σ_T is defined as

$$\frac{3}{\Sigma_T} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \tag{10-17}$$

Reference for the Ternary Phase Field Interface

1. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar and M. Quintard, "Cahn-hilliard/Navier-Stokes model for the simulation of three-phase flows", *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

11

Glossary

This Glossary of Terms contains application-specific terms used in the CFD Module software and documentation. For finite element modeling terms, mathematical terms, and geometry and CAD terms, see the glossary in the *COMSOL Multiphysics Reference Manual*. For references to more information about a term, see the index.

Glossary of Terms

Algebraic yPlus turbulence model   Low-Reynolds number, algebraic turbulence model that solves for the wall distance, y^+ (in viscous units).

anisotropy   Directional dependence. Is often obtained from homogenization of regular structures, for example, monolithic structures in tubular reactors.

Boussinesq approximation   An approximate method to include buoyancy effects, for which the density variation is only taken into account in the buoyancy term.

Brinkman equations   A set of equations extending Darcy's law in order to include transport of momentum through shear in porous media flow.

boundary layer   Region in a fluid close to a solid surface. This region is characterized by large gradients in velocity and other properties. In turbulent flow it is often treated with approximative methods because of the difficulty to resolve the large gradients.

bubbly flow   Flow with gas bubbles dispersed in a liquid.

conjugate heat transfer   heat transfer that takes place in both a solid and a fluid.

creeping flow   Models the Navier-Stokes equations without the contribution of the inertial term. This is often referred to as *Stokes flow* and is applicable when viscous flow dominates, such as in very small channels or microfluidic devices.

crosswind diffusion   A numerical technique for stabilization of convection-dominated PDEs by artificially adding diffusion perpendicular to the direction of the streamlines. It reduces oscillations near sharp gradients.

Darcy's law   Equation that gives the velocity vector as proportional to the pressure gradient. Often used to describe flow in porous media.

Euler flow   Flow of an inviscid fluid. Often used to approximate high speed compressible flows.

Euler-Euler model   A two-phase flow model that treats both phases as inter-penetrating continua.

Fick's laws   The first law states that the diffusive flux of a solute infinitely diluted in a solvent is proportional to its concentration gradient. The second law introduces the first law into a differential material balance for the temporal evolution of the solute.

fluid-structure interaction (FSI)   When a fluid flow affects the deformation of a solid object and vice versa.

fully developed laminar flow   Laminar flow along a channel or pipe that only has velocity components in the streamwise direction. The velocity profile does not change downstream.

Hagen-Poiseuille equation   See *Poiseuille's law*.

heterogeneous reaction   Reaction that takes place at the interface between two phases.

homogeneous reaction   Reaction that takes place in the bulk of a solution.

intrinsic volume averages   The physical properties of the fluid, such as density, viscosity, and pressure.

k-ε turbulence model   A two-equation RANS model that solves for the turbulent kinetic energy, k, and the dissipation of turbulence kinetic energy, ε. Utilizes wall functions to describe the flow close to solid walls.

k-ω turbulence model   A two-equation RANS model that solves for the turbulent kinetic energy, k, and the specific dissipation rate, ω. Utilizes wall functions to describe the flow close to solid walls.

L-VEL turbulence model   Low-Reynolds number, algebraic turbulence model that solves for the tangential velocity near walls, u^+ (in viscous units).

law of the wall   See *wall function*.

low-Reynolds k-ε turbulence model   Two-equation RANS model that solves for the turbulence kinetic energy, k, and the dissipation of turbulence kinetic energy, ε. Includes damping functions to be able to describe regions with low Reynolds numbers, for example close to solid walls.

low Reynolds number   The region close to the wall where viscous effects dominate.

Mach number   Dimensionless number equal to the flow velocity over the speed of sound. Compressible effects because of the flow speed can be neglected for Mach number less than 0.3.

multiphase flow   Flow with more than one phase.

Navier-Stokes equations   The momentum balance equation for a Newtonian fluid coupled to the equation of continuity. The meaning of the term originally only referred to the momentum balance but it is here used in the more general context.

Newtonian fluid   A fluid for which the stress is proportional to the rate of strain. Many common fluids such as water and air are Newtonian.

non-Newtonian fluid   A fluid for which the stress is *not* proportional to the rate of strain. Blood and suspensions of polymers are examples of non-Newtonian fluids.

Poiseuille's law   Equation stating that the mass rate of flow in a tube is proportional to the pressure difference per unit length and to the fourth power of the tube radius. The law is valid for fully developed laminar flow.

pressure work   Describes the reversible conversion of work, performed by the pressure in a fluid, into heat.

RANS   Reynolds-averaged Navier-Stokes; implying that a time-averaging operation has been performed on the equations of motion. The Reynolds' stresses (correlations between fluctuating velocity components) obtained from this averaging operation have to be obtained from an additional set of equations — a closure. Turbulence models like the k-ε and Spalart-Allmaras models constitute closures to the RANS equations.

Reynolds number   A dimensionless number that describes the relative importance between inertia and viscous effects. Flow at high Reynolds number have a tendency to undergo transition to turbulence.

Soret effect   Mass diffusion due to temperature gradients in multicomponent mixtures.

Spalart-Allmaras turbulence model   A one-equation turbulence model that solves for the undamped turbulent kinematic viscosity, $\tilde{v}_T$.

SST turbulence model   The Shear Stress Transport model is a two-equation turbulence model combining the k-ω model in the near-wall region with the k-ε model in the free stream. The SST model is a low-Reynolds number model requiring high resolution near walls. The dependent variables are the turbulent kinetic energy, k, and the turbulent dissipation rate, ω.

Stokes flow   See *creeping flow*.

streamline diffusion   A numerical technique for stabilization of convection-dominated PDEs by artificially adding upwinding in the streamline direction.

superficial volume averages   The flow velocities, which correspond to a unit volume of the medium including both pores and matrix. They are sometimes called Darcy velocities, defined as volume flow rates per unit cross section of the medium.

thin-film flow   Flow in very thin regions where the it can be assumed to always have a fully developed profile.

viscous heating   The heat irreversibly generated from work by viscous friction in a fluid.

wall function   Semi-empirical expression for the boundary-layer flow used in turbulence models. Often based on the assumption of negligible variations in the pressure gradient tangential to the surface.

Index