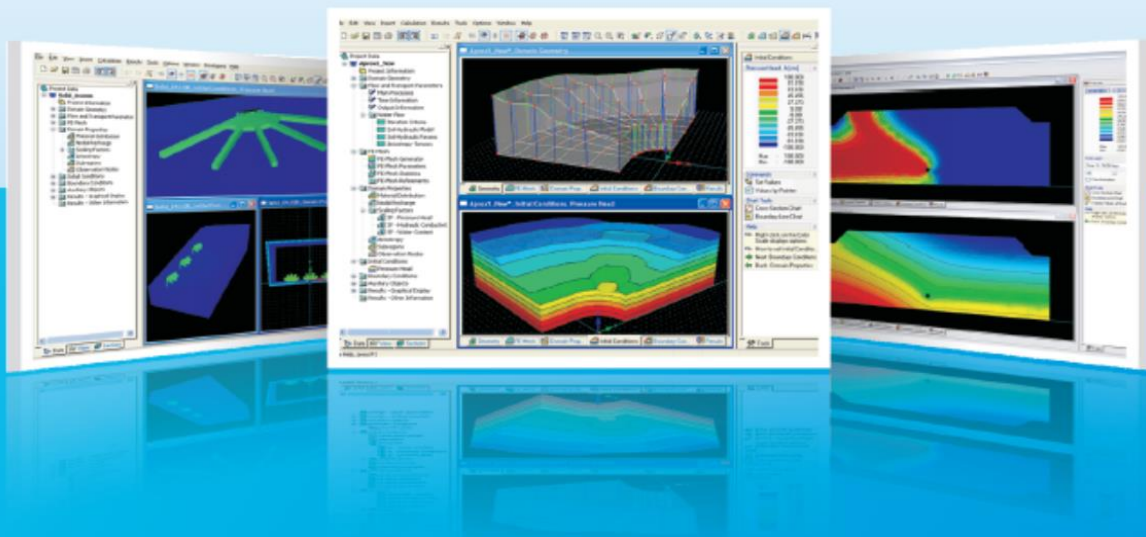




HYDRUS

User Manual

Version 5



**Software Package for Simulating
the One-, Two- and Three-Dimensional
Movement of Water, Heat and Multiple Solutes
in Variably-Saturated Media**

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***The HYDRUS Software Package for Simulating
the One-, Two-, and Three-Dimensional Movement
of Water, Heat, and Multiple Solutes
in Variably-Saturated Porous Media***

User Manual

Version 5.x

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Abstract

Šejna, M., J. Šimůnek, and M. Th. van Genuchten, The HYDRUS Software Package for Simulating One-, Two-, and Three-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Porous Media, User Manual, Version 5.x, PC Progress, Prague, Czech Republic, 352 pp., 2023.

This report documents version 5.0 of the **Graphical User Interface of HYDRUS**, a software package for simulating water, heat, and solute movement in one-, two- and three-dimensional variably saturated porous media. The software package consists of the computational computer program and the interactive graphics-based user interface. The HYDRUS program numerically solves the Richards equation for variably saturated water flow and advection-dispersion equations for both heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers transport due to conduction and convection with flowing water. The solute transport equations consider advective-dispersive transport in the liquid phase, as well as diffusion in the gaseous phase. The transport equations also include provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions. In addition, physical nonequilibrium solute transport can be accounted for by assuming a two-region, dual-porosity type formulation that partitions the liquid phase into mobile and immobile regions. Attachment/detachment theory, including filtration theory, is additionally included to enable simulations of the transport of viruses, colloids, and/or bacteria.

HYDRUS may analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media. The program can handle flow regions delineated by irregular boundaries. The flow region itself may be composed of nonuniform soils having an arbitrary degree of local anisotropy. Flow and transport can occur in the one-dimensional profile (vertical, horizontal, or in a general direction), a two-dimensional vertical or horizontal plane, a three-dimensional region exhibiting radial symmetry about the vertical axis, or a fully three-dimensional domain. The program also includes a Marquardt-Levenberg type parameter optimization algorithm for inverse estimation of soil hydraulic and/or solute transport and reaction parameters from measured transient or steady-state data for two-dimensional problems. Details of the various processes and features included in HYDRUS are provided in the **Technical Manuals** for 1D or 2D/3D [Šimůnek *et al.*, 2022ab].

The main program unit of the **HYDRUS Graphical User Interface** (GUI) defines the overall computational environment of the system. This main module controls the execution of the program and determines which other optional modules are necessary for a particular application. The module contains a project manager and both the pre-processing and post-processing units. The pre-processing unit includes specification of all necessary parameters to run the HYDRUS FORTRAN codes successfully, grid generators for relatively simple rectangular and hexahedral transport domains, a grid generator for unstructured finite element meshes for complex two-dimensional domains, a small catalog of soil hydraulic properties, and a Rosetta Lite program for generating soil hydraulic properties from soil textural data. The post-processing unit consists of simple x-y graphics for graphical presentation of soil hydraulic properties, as well as such output as distributions versus time of a particular variable at selected observation points, and actual or cumulative water and

solute fluxes across boundaries of a particular type. The post-processing unit also includes options to present results of a particular simulation by means of contour maps, isolines, spectral maps, and velocity vectors, and/or by animation using both contour and spectral maps.

This report serves as a **User Manual** and reference document of the **Graphical User Interface** of the **HYDRUS** software package. Technical aspects such as governing equations and details about the invoked numerical techniques are documented in separate **Technical Manuals**.

Other Useful Information Online:

1. Outside reviews of the HYDRUS software packages:
<https://www.pc-progress.com/en/Default.aspx?h3d-reviews>
2. HYDRUS Selected References:
<https://www.pc-progress.com/en/Default.aspx?h1d-references>
<https://www.pc-progress.com/en/Default.aspx?h3d-references>
3. HYDRUS Quick Tour and Tutorials:
<https://www.pc-progress.com/en/Default.aspx?h1d-tutorials>
<https://www.pc-progress.com/en/Default.aspx?h3d-tutorials>
4. HYDRUS Applications and Public Library of HYDRUS Projects:
<https://www.pc-progress.com/en/Default.aspx?h1d-library>
<https://www.pc-progress.com/en/Default.aspx?h3d-applications>
5. HYDRUS Book: Soil Physics with HYDRUS: Modeling and Applications:
<https://www.pc-progress.com/en/Default.aspx?h3d-book>
<https://www.pc-progress.com/en/Default.aspx?h1d-tut-TutorialBook>
6. HYDRUS FAQ:
<https://www.pc-progress.com/en/Default.aspx?hydrus-faq>
7. HYDRUS (2D/3D) Troubleshooting:
<https://www.pc-progress.com/en/Default.aspx?h3d-troubleshooting>

History of the HYDRUS Development

Version 1 of HYDRUS (2D/3D) software package [Šimůnek *et al.*, 2008] was an extension and replacement of HYDRUS-2D (version 2.0) and SWMS_3D. This software package was a complete rewrite of HYDRUS-2D and its extensions for two- and three-dimensional geometries. In addition to features and processes available in HYDRUS-2D and SWMS_3D, the new computational modules of HYDRUS (2D/3D) considered (a) water flow and solute transport in a dual-porosity system, thus allowing for preferential flow in fractures or macropores while storing water in the matrix [Šimůnek *et al.*, 2003], (b) the spatial root distribution functions of *Vrugt et al.* [2001], (c) the soil hydraulic property models of *Kosugi* [1996] and *Durner* [1994], (d) the transport of viruses, colloids, and/or bacteria using an attachment/detachment model, filtration theory, and blocking functions (e.g., *Bradford et al.*, 2002), (e) a constructed wetland module (only in 2D) [Langergraber and Šimůnek, 2005, 2006], (f) the hysteresis model of *Lenhard et al.* [1991] to eliminate pumping by keeping track of historical reversal points, (g) new print management options, (h) dynamic, system-dependent boundary conditions, (i) flowing particles in two-dimensional applications, and (j) calculations of actual and cumulative fluxes across internal meshlines.

New features of the Graphical User Interface of HYDRUS (2D/3D) included, among other things, (a) a completely new GUI based on Hi-End 3D graphics libraries, (b) the MDI architecture with multiple projects and multiple views, (c) a new organization of geometric objects, (d) a navigator window with an object explorer, (e) many new functions improving the user-friendliness, such as drag-and-drop and context-sensitive pop-up menus, (f) improved interactive tools for graphical input, (g) options to save cross-sections and mesh-lines for charts within a given project, (h) a new display options dialog where all colors, line styles, fonts and other parameters of graphical objects can be customized, (i) extended print options, and (j) extended information in the Project Manager (including project previews).

Version 2.0, which included the 3D-Professional Level of HYDRUS, included many new features as compared to version 1.0. New features and changes in the HYDRUS GUI:

- 1) Supports complex general three-dimensional geometries (Professional Level).
- 2) Domain Properties, Initial Conditions, and Boundary Conditions can be specified on Geometric Objects (defining the transport domain) rather than on the finite element mesh.
- 3) Import of initial conditions from existing HYDRUS projects even with (slightly) different geometry or FE mesh.
- 4) Import of various quantities (e.g., domain properties, initial and boundary conditions) from another HYDRUS project even with (slightly) different geometry or FE mesh.
- 5) Support of ParSWMS (a parallelized version of SWMS_3D) [Hardelauf *et al.*, 2007].
- 6) Support of UNSATCHEM (a module simulating the transport of and reactions between major ions) [Šimůnek *et al.*, 2012c].
- 7) The Mass Balance (Inverse) Information dialog window enables to display texts larger than the capacity of the Edit window.
- 8) Root distribution can be specified using GUI parallel with the slope for hillslopes.
- 9) Display of results using Isosurfaces.
- 10) Support of a new CWM1 constructed wetland module [Langergraber *et al.*, 2009].

New features and changes in the HYDRUS in the computational modules:

- 1) New initializations conditions for solute transport (initial conditions can be specified in the total solute mass, and nonequilibrium phases can be initially equilibrated).
- 2) Various new boundary conditions (e.g., gradient, surface drip, subsurface drip, and seepage face with a specified pressure head boundary condition).
- 3) Triggered Irrigation - irrigation is triggered by the program when the pressure head at a particular observation node drops below a specified value (only in 2D).
- 4) HYDRUS calculates and reports surface runoff, evaporation, and infiltration fluxes for the atmospheric boundary.
- 5) Water content dependence of solute reaction parameters using *Walker's* [1974] formula was implemented.
- 6) A new option to consider root solute uptake, including both passive and active uptake (only in 2D) [*Šimůnek and Hopmans*, 2009].
- 7) The Per Moldrup's tortuosity models [*Moldrup et al.*, 1997, 2000] were implemented as an alternative to the *Millington and Quirk* [1961] model.
- 8) An option to use a set of Boundary Condition records multiple times.
- 9) Executable programs are about 1.5 - 3 times faster than in the standard version due to the loop vectorization.
- 10) Options related to the fumigant transport (e.g., removal of tarp, temperature dependent tarp properties, additional injection of fumigant) [*Spurlock et al.*, 2013].
- 11) A new CWM1 constructed wetland module [*Langergraber et al.*, 2009].

Version 2.02 additionally supported several add-on modules that have their own user manuals:

- 1) The **DualPerm** module [*Šimůnek et al.*, 2012e],
- 2) The **UNSATCHEM** module [*Šimůnek et al.*, 2012c],
- 3) The **Wetland** module [*Langergraber and Šimůnek*, 2011],
- 4) The **C-Ride** module [*Šimůnek et al.*, 2012b], and
- 5) The **HP2** module [*Šimůnek et al.*, 2012a].

Version 2.03:

- 1) Offers some new functionality with respect to the import of various properties from either existing HYDRUS projects or from text files (see Section 6.6),
- 2) Allows users to import the definition of isolines (only in 3D-Professional). and
- 3) Resolved problems with fonts for the Chinese, Japanese, and other similar Windows systems.

Version 2.04 additionally supported two add-on modules:

- 1) the **HyPar** module (see Section 9.1) is a parallelized version of the standard two-dimensional and three-dimensional HYDRUS computational modules (h2d_calc.exe and h3d_calc.exe), and
- 2) the **Slope Classic** module is intended to be used mainly for stability checks of embankments, dams, earth cuts, and anchored sheeting structures.

Version 2.05 additionally supported the new add-on module **Slope Cube**. While the **Slope Classic** module (added in version 2.04) is based on classical engineering soil mechanics theories and uses the effective stress approach only for saturated conditions, the new add-on module "**Slope**

Cube" (Slope Stress and Stability) was developed to provide a unified effective stress approach for both saturated and unsaturated conditions [Lu *et al.*, 2010].

New features in **Version 3.01**, among many others, include:

- 1) 64bit version, which can now use all physical memory available on modern PCs.
- 2) 3D streamlines (see Section 7.1.5).
- 3) Particle animation (see Section 7.1.5).
- 4) 3D mesh clipping (see Section 7.1.6).
- 5) 3D mesh slicing (see Section 7.1.6).
- 6) Rasters for 3D Vector Fields (see Section 7.1.7).
- 7) The new "Reservoir" boundary condition (see the Technical Manual and Section 6.3.4).
- 8) A dynamic rooting system (root growth) (see the Technical Manual and Section 3.5.4).
- 9) Export data to ParaView (see Section 7.1.8).
- 10) Numbering of isolines.

New features in **Version 3.02**, among many others, include:

1. The **Furrow** module [Brunetti *et al.*, 2018, 2019].
2. The **Slope Cube** module in 3D.

New features in **Version 3.03**, among many others, include:

1. A dynamic rooting system (root growth) was also included into the UnsatChem and Wetland modules.
2. Point Probes (see Section 4.7.6).
3. Line Probes (see Section 4.7.7).
4. Inverse Solution for 3D projects.
5. Clipping of the 3D model and the FE-mesh has been extended with a new option, the "Clipper-Box" tool (see Section 7.1.6).

Version 5 of HYDRUS has been developed by merging previously independent software packages HYDRUS-1D (version 4, for one-dimensional applications) and HYDRUS (2D/3D) (version 3, for two- and three-dimensional applications).

New features in **Version 5.01**, among many others, include:

1. An option to consider sorption to the air-water interface (required to simulate the fate of PFAS chemicals) [Silva *et al.*, 2020] (in the **PFAS** Module) (for one- and two-dimensional applications).
2. An option to consider the concentration effect on surface tension and viscosity (required to simulate the fate of surfactants) [Silva *et al.*, 2020] (in the **PFAS** Module) (for one-, two-, and three-dimensional applications).
3. Reservoir Boundary Condition in 3D.
4. The **Dynamic Plant Uptake** Module [Brunetti *et al.*, 2019] (for one- and two-dimensional applications).
5. Full implementation of HYDRUS-1D, i.e., a one-dimensional version of HYDRUS, which in addition to options available in the previous version (4.x) includes:
 - The **Particle Tracking** Module [Zhou *et al.*, 2021]
 - The **Fumigant** Module [Spurlock *et al.*, 2013]

- The **PFAS** Module [Silva et al., 2020]
- The **COSMIC** Module [Brunetti et al., 2019]
- The **Dynamic Plant Uptake** Module [Brunetti et al., 2019]

New features in **Version 5.02**, among many others, include:

1. The PFAS module in 3D.
2. The PFAS computational modules print the air-water interfacial area, A_e . A_e is printed into the Nod_inf.out file in 1D instead of the $v/KsTop$ column (not displayed in GUI). A_e is printed into the new binary output file AWIArea.out in 2D and 3D (displayed in GUI).
3. The HYDRUS GUI can display the air-water interfacial area (for the PFAS module) under Results.
4. Users can display solute concentrations on the air-water interfacial area in the HYDRUS GUI (under Results) by selecting a concentration option on the View Tab of the Navigator Bar.
5. Users can display different modes (liquid, solid, AWI) of solute concentrations in the Profile Information Graph (1D).

New features in **Version 5.03**, among many others, include:

1. PFAS, Surfactant, and Reservoir BC (3D) were implemented into HyPar to make it compatible with the standard computational modules.
2. PFAS with kinetic sorption (a two-site sorption model) to the air-water interface in 1D and 2D.
3. Fluxes across cross-sections in the Wetland module.
4. Campbell model for thermal conductivity was added to 2D and 3D models.
5. Dispersive solute fluxes were included into the solute fluxes across meshlines into HP2.
6. Display of different concentration modes in the Profile Information graph of 1D.
7. The “Reverse Colors” command allows users to reverse colors in the color scale (e.g., to have dry regions red and wet regions blue, or polluted layers red).
8. Import of initial conditions from the results of another HYDRUS project in 1D (this option has been available in 2D and 3D before).
9. Water and solute fluxes across Mesh-Surfaces in 3D applications (see Fig. 102).

A detailed description of the development of various HYDRUS versions and a review of their applications can be found in:

Šimůnek, J., M. Th. van Genuchten, and M. Šejna, Development and applications of the HYDRUS and STANMOD software packages and related codes, *Vadose Zone Journal*, Special Issue “Vadose Zone Modeling”, 7(2), 587-600, doi: 10.2136/VZJ2007.0077, 2008.

Šimůnek, J., M. Th. van Genuchten, and M. Šejna, Recent developments and applications of the HYDRUS computer software packages, *Vadose Zone Journal*, 15(7), pp. 25, doi: 10.2136/vzj2016.04.0033, 2016.

Šimůnek, J., M. Šejna, and M. Th. van Genuchten, New features of version 3 of the HYDRUS (2D/3D) computer software package, *Journal of Hydrology and Hydromechanics*, 66(2), 133-142, doi: 10.1515/johh-2017-0050, 2018.

Introduction to the HYDRUS Graphical User Interface

The past several decades have seen an explosion of increasingly sophisticated numerical models for simulating water flow and contaminant transport in the subsurface, including models dealing with one- and multi-dimensional flow and transport processes in the unsaturated or vadose zone between the soil surface and the groundwater table. Even with an abundance of well-documented models now available, one major problem often preventing their optimal use is the extensive work required for data preparation, numerical grid design, and graphical presentation of the output results. Hence, the more widespread use of multi-dimensional models requires ways that make it easier to create, manipulate and display large data files, facilitating interactive data management. Introducing such techniques will free users from cumbersome manual data processing and should enhance the efficiency in which programs are being implemented, for a particular example. To avoid or simplify the preparation and management of relatively complex input data files for two- and three-dimensional applications, and to graphically display the final simulation results, we developed an interactive graphics-based user-friendly interface HYDRUS for the MS Windows 95, 98, NT, ME, XP, Vista, 7, and 10 environments. The interface is connected directly to the computational codes. The current version 4 of the HYDRUS graphical user interface represents a major upgrade of previous versions 1, 2, and 3. Version 1 itself was a complete rewrite of version 2.0 of HYDRUS-2D that expanded the capabilities of HYDRUS-2D to three-dimensional problems. Version 2, which includes the 3D-Professional Level of HYDRUS, included many new features compared to version 1. In particular, it included support for complex general three-dimensional geometries and an option to specify various domain properties and initial and boundary conditions on geometric objects, rather than directly on the finite element mesh. Version 3 of HYDRUS (2D/3D) included a flexible reservoir boundary condition, expanded root growth features, and the GUI's new graphical capabilities. The current version 5 of HYDRUS (has been developed by merging previously independent software packages HYDRUS-1D (version 4) and HYDRUS (2D/3D) (version 3)) includes options to consider sorption to the air-water interface, the concentration effect on surface tension and viscosity, a reservoir Boundary Condition in 3D, and mainly, the full implementation of HYDRUS-1D, i.e., a one-dimensional version of HYDRUS.

In addition to information given in this user manual, extensive context-sensitive on-line help is made part of the graphical user interface (GUI). By holding the F1 button or clicking on the Help button while working in any window, the user obtains information about the window content. In addition, context-sensitive help is available in every module using the "SHIFT+F1" help button. In this mode, the mouse cursor changes to a help cursor (a combination arrow + question mark), which a user can use to select a particular object for which help is needed (e.g., a menu item, toolbar button, or other features). A help file will be displayed, giving information about the item on which the user clicked. Except for the computational modules that are written in FORTRAN, the entire GUI is written in C++.

The HYDRUS Graphical User Interface (Fig. 1) is the main program unit defining the overall computational environment of the system. This main module controls the execution of the program and determines which other optional modules are necessary for a particular application. The module contains a project manager and both the pre-processing and post-processing units. The pre-processing unit includes specification of all the parameters required to successfully run the **HYDRUS** FORTRAN codes (modules H2D_CALC, H2D_CLCI, H2D_WETL, H2D_UNSC,

H3D_CALC, and many others), grid generators for relatively simple rectangular and hexahedral transport domains, a grid generator for unstructured finite element meshes appropriate for more complex two-dimensional domains, a small catalog of soil hydraulic properties, and a Rosetta Lite program for generating soil hydraulic properties from textural information. The post-processing unit consists of simple x-y graphs for graphical presentation of the soil hydraulic properties, distributions versus time of a particular variable at selected observation points, as well as actual or cumulative water and solute fluxes across boundaries of a particular type. The post-processing unit also includes options to present results of a simulation by means of contour maps, isolines, isosurfaces, spectral maps, and velocity vectors, and/or by animation using both contour and spectral maps.

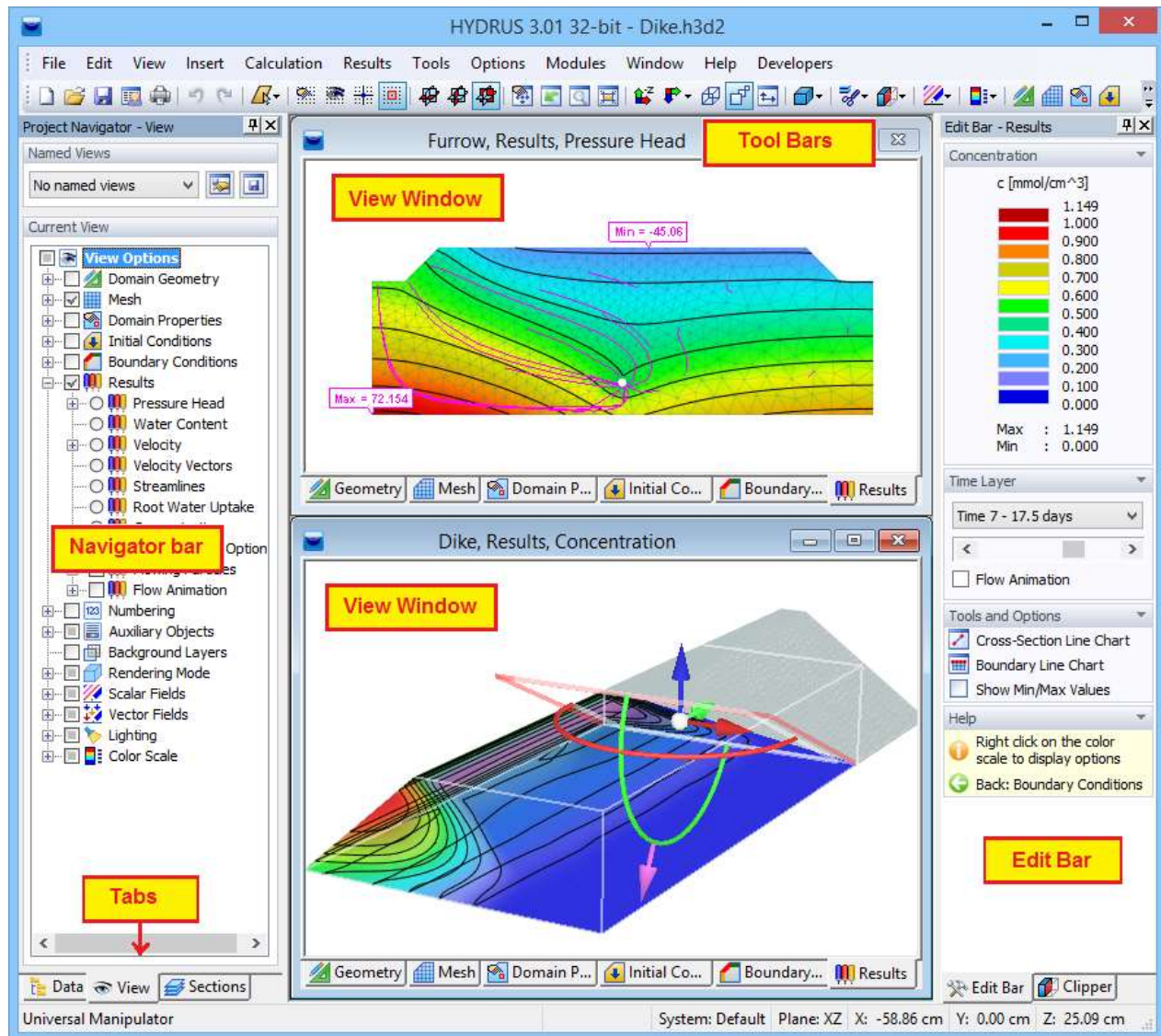


Figure 1. The HYDRUS Graphical User Interface (the main window).

Figure 1 shows the main window of the HYDRUS graphical user interface, including its main components, such as the **Menu**, **Toolbars**, the **View Window**, the **Navigator Bar**, **Tabs**, and the **Edit Bar**. These terms will be used throughout this user manual. The text below provides a

detailed description of all major components of the graphical user interface. At the end of this user manual, a list is given of all commands accessible through the menu (Table 27), as well as a brief discussion of the action taken with particular commands (Table 28). More detailed descriptions are available through the on-line help.

Work for a new project should begin by opening the Project Manager (see Chapter 1) and giving a name and a brief description of the new project. Next, the **Domain Type and Units** dialog Window (Figs. 6 and 7) appears (this window can also be selected from the Pre-processing Menu). From this point on, the program will navigate users through the entire process of entering input files. Users may either choose particular commands from a menu or allow the interface to lead them through the process of entering input data by selecting the Next button. Alternatively, clicking the Previous button will return users to the previous window. Pre- and post-processing commands and processes are also sequentially listed on the **Data Tab** of the **Navigator Bar**. Green arrows on the **Edit Bar** always direct users to subsequent or previous input processes for a particular command. Many commands and processes can be alternatively accessed using either the **Toolbars** and **Menus**, or the **Navigator** and **Edit Bars**.

1. Project Manager and Data Management

A **Project Manager** (called by the command *File->Project Manager*, Figs. 2 and 3) is used to manage the data of existing projects and helps to locate, open, copy, delete and/or rename desired projects or their input or output data. A **Project** represents any particular problem to be solved by HYDRUS. The project name, as well as a brief description of the project (Fig. 4), helps to locate a particular problem. Projects are represented by a file *project_name.hyd5* (the final digit 2 (or 3) refers to version 2 (or 3) of HYDRUS; extension h3d was used with version 1.0) that contains all input and output data when the *Temporary Working Directory* option (Fig. 4) is used. It contains only the input data when the *Permanent Working Directory* option is selected. HYDRUS input files (used by the computational modules) are extracted from the *project_name.hyd5* file into a working subdirectory; output data created by the calculation module are sent into the same folder. When saving a project, output files (created by the computational modules) are also included in the *project_name.hyd5* file (when the *Temporary Working Directory* option is used). The input and output files can be either permanently kept in the external working directory or are stored in this folder only during calculations (Fig. 4, the radio buttons *Temporary – is deleted after closing the project* and *Permanent – result files are kept in this directory*). The location of the external working directory is specified in the **Project Description** (Fig. 4) and the **Program Options** dialog window (Fig. 200).

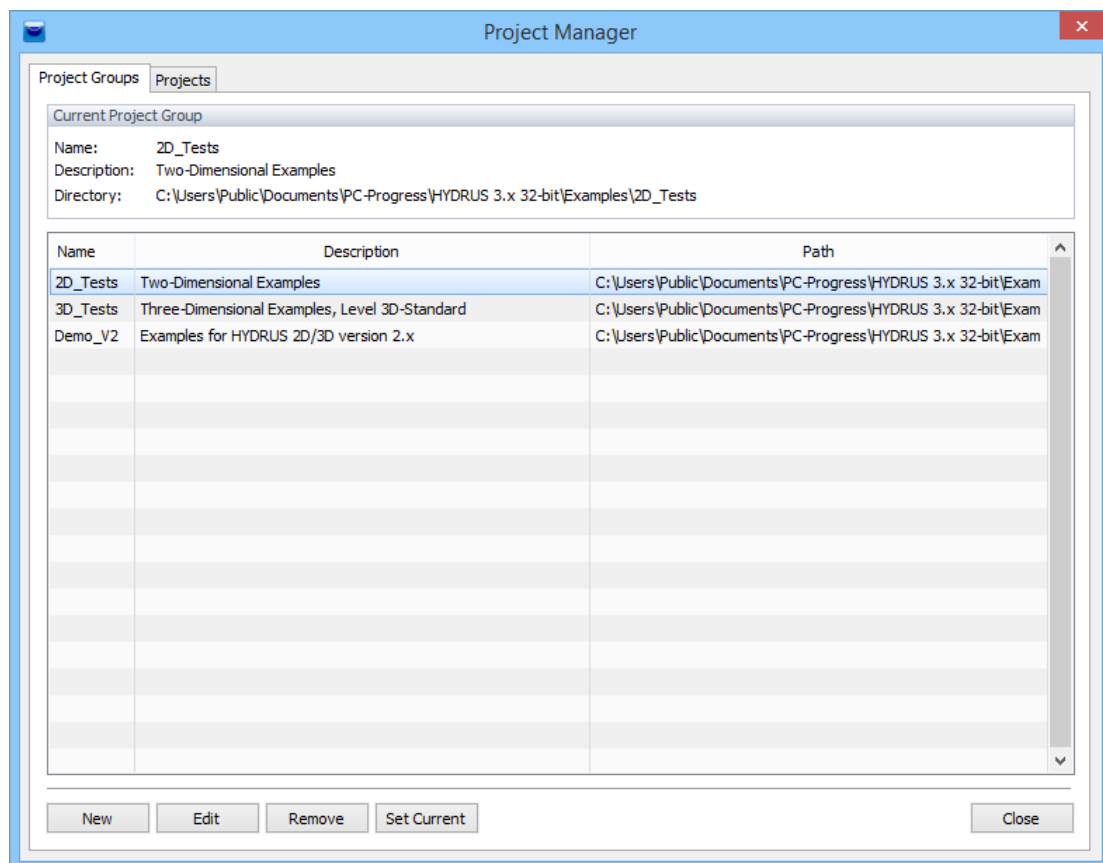


Figure 2. The project Manager with the Project Groups tab.

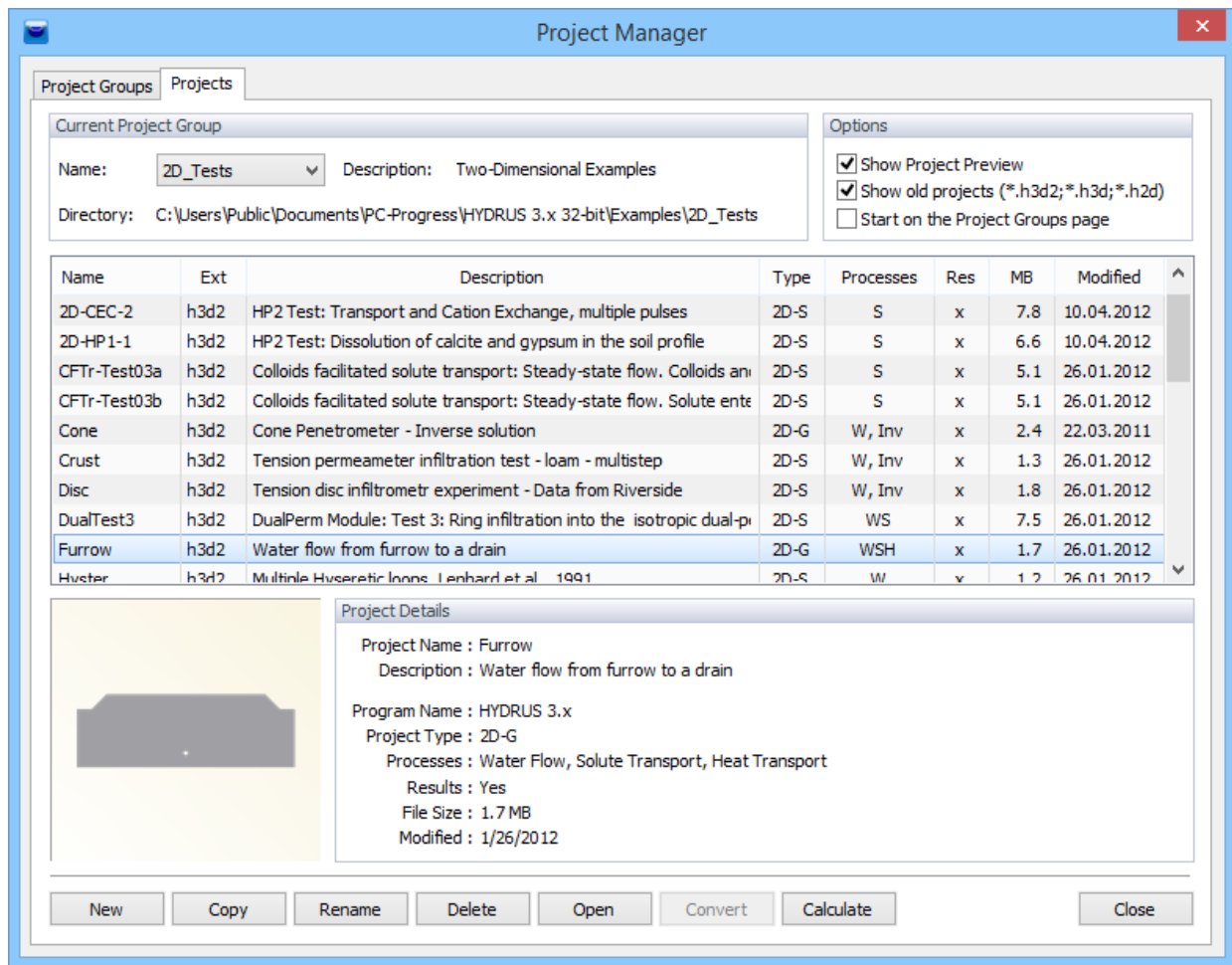


Figure 3. The Project Manager with the Projects tab.

The **Project Manager** gives users considerable freedom to organize their projects. The projects are grouped into **Project Groups** (Fig. 2), which can be placed anywhere in accessible memory (i.e., on local and/or network hard drives). **Project Groups** serve to organize projects into logical groups defined by a user. Each **Project Group** has its own *name*, *description*, and *pathway* (Figs. 2 and 5). A **Project Group** can be any existing accessible subdirectory (folder). HYDRUS is installed together with three default Project Groups *1D_Tests*, *2D_Tests*, and *3D_Tests*, located in the HYDRUS3D folder. The *1D_Tests*, *2D_Tests*, and *3D_Tests* Project Groups contain test examples for one-, two-, and three-dimensional problems, respectively. We suggest that users create their own Project Groups (e.g., the *My_1D_Direct*, *My_1D_Inverse*, *My_2D_Direct*, *My_2D_Inverse*, and *My_3D_Direct* Project Groups) and keep the provided examples intact for future reference. Projects can be copied with the **Project Manager** only within a particular Project Group. Users can copy projects between Project Groups (or share their HYDRUS projects with colleagues and clients) using standard file managing software, such as Windows Explorer. In that case, one must copy only the *project_name.hyd5* file (when the radio buttons *Temporary – is deleted after closing the project* is used, Fig. 4). When temporary data are kept permanently in the working directory (i.e., the radio button *Permanent – results files are kept in this directory* is selected, Fig. 4), the working directory must be copied together with the *project_name.hyd5* file.

In addition to a *Name* and a brief *Description* of a **Project**, the **Project Manager** also displays dimensions for a particular problem (*Type*: the dimensions are either 1D, 2D, or 3D, and the geometry is either Simple (S), Layered (L), or General (G), see Section 2), what *Processes* are involved (W – water flow, S – solute transport, T – heat transport, R – root water uptake, Inv – Inverse problem), the size of the project (MB), when the project was created (*Date*) and whether or not the *Results* exist (Fig. 3). The **Project Manager** can also display a preview of the **Project**'s geometry (see the check box *Show Project Preview* in Fig. 3). The commands of the **Project Manager** are listed in Table 1.

Table 1. Commands in the **Project Manager**.

Group	Command	Description
Project Group	New	Registers a new Project Group in the Project Manager.
	Edit	Renames the selected Project Group and changes its description and/or location.
	Remove	Removes registration of a selected Project Group from the Project Manager.
	Set As Current	Sets a selected Project Group as the active Project Group.
Project	Close	Closes the Project Manager.
	New	Creates a new project in the current Project Group.
	Copy	Copies a selected project within the current Project Group.
	Rename	Renames a selected project.
	Delete	Deletes a selected project.
	Open	Opens a selected project.
	Close	Closes the Project Manager.
	Convert	Converts projects created by earlier HYDRUS versions (i.e., either HYDRUS-1D, HYDRUS-2D, or earlier versions of HYDRUS (2D/3D)).
Options	Calculate	Calculates selected HYDRUS projects. This command allows users to calculate multiple selected projects simultaneously.
	Show Project Preview	Provides a preview of the geometry of a particular project in the bottom left corner of the Project Manager.
	Show Old Projects	Shows projects created using earlier HYDRUS versions, i.e., either HYDRUS-1D, HYDRUS-2D, or earlier versions of HYDRUS (2D/3D).
	Start on Project Groups Page	Opens the Project Manager at the Project Groups Tab.

The commands **New** and **Rename** from the **Project Tab** of the **Project Manager** dialog window (Fig. 3) call the **Project Information** dialog window (Fig. 4), which contains the *Name* and *Description* of the project, as well as information about the **Project Group** (name, description, and

pathway) to which the project belongs. It also contains information on whether or not the input and output data are kept permanently in an external directory (the radio buttons *Temporary* – is deleted after closing the project, and *Permanent* – result files are kept in this directory, Fig. 4).

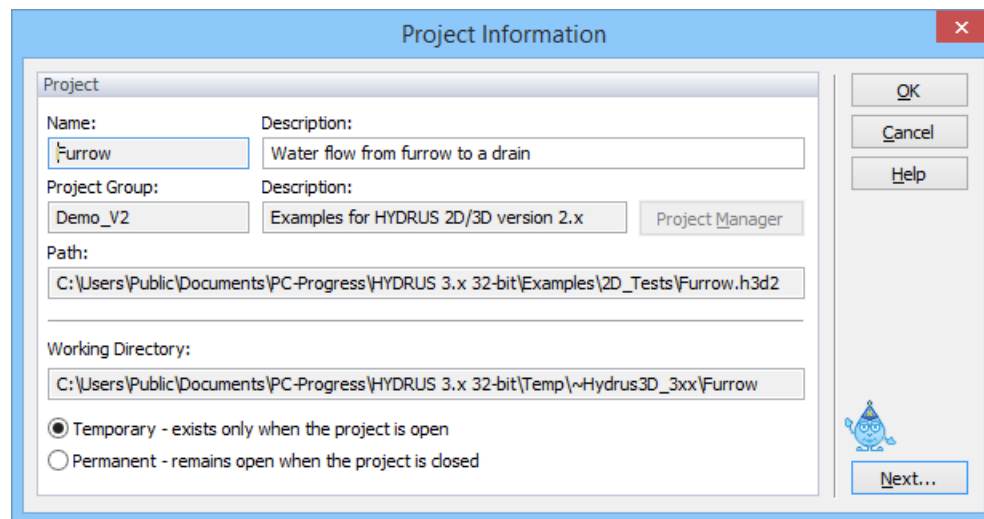


Figure 4. The Project Information dialog window.

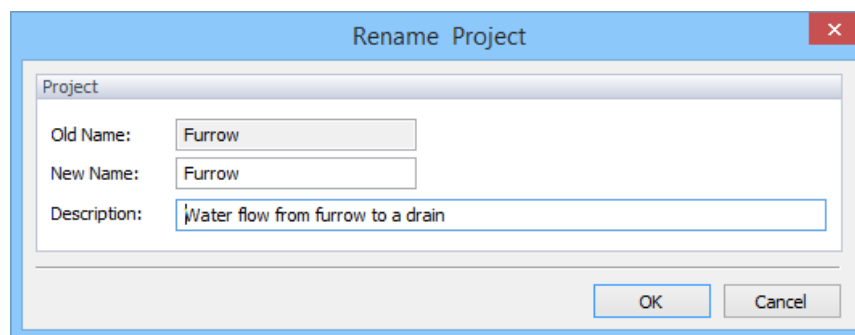


Figure 5. General description of the HYDRUS Project Group.

Projects created by the previous versions of HYDRUS (e.g., HYDRUS-1D, HYDRUS-2D) can be imported into the current version of HYDRUS using two ways:

- A. Individual projects can be converted using the command *File->Import->Import HYDRUS-2D Project*. This is done by first creating a new **Project**, and then selecting the above command and browsing for the location of a project created with a previous version of HYDRUS-2D. The input data of the older project are then converted into the new HYDRUS format. Results of the older project can then be viewed using the new version of HYDRUS, while projects can be modified or recalculated as needed.
- B. Multiple HYDRUS-1D or HYDRUS-2D projects (or HYDRUS projects created by earlier versions of HYDRUS) can be converted simultaneously using the **Convert** command of the **Project Manager**. One first creates a HYDRUS Project Group for a folder in which the

HYDRUS-1D or HYDRUS-2D projects are located and selects the **Show Old Projects** option at the **Project Tab** of the **Project Manager**. One then selects projects to be converted and clicks the **Convert** command. HYDRUS, in this way, creates HYDRUS projects and stores all input and output files in the **project_name.hyd5** files.

Input data can be edited either using the HYDRUS graphical user interface (this modifies directly the *project_name.hyd5* file) or the input data can be modified manually. In such case, HYDRUS input files need to be stored in the working external directory (sent there by the command *File->Export->Export Data for HYDRUS Solver in Text Format*), and then can be imported back into the HYDRUS *project_name.hyd5* file using the command *File->Import ->Import Input Data from *.In Files*.

The **Working Directory** is a folder into which the program stores temporary data. Each open project has its own Working Directory, where the program stores, for example, input files for computational modules, and where computational modules write the output files. When saving a project, data from the Working Directory are copied into the main project file *project_name.hyd5*. When the project is closed, the Working Directory is deleted. Only when a user selects the option “*Permanent – result files are kept in this directory*” (Fig. 4) is the Working Directory not deleted after closing the project, in which case the temporary data are not copied into the main project file. The Working Directory includes additional folders (e.g., Furrow, Genex, Genex_tmp, H_Compounds, H_Grids, H_VTK, Slope, and Textures) that contain auxiliary data that are not related to calculated results.

2. Projects Geometry Information

In the first dialog window that a user encounters after creating a new project, he/she needs to specify whether the flow and transport problem occurs in two- or three-dimensional transport domains. Geometry type is selected in the **Domain Type and Units** dialog Window (Fig. 6 and 7). In this dialog window, users specify the **Domain Type**, the **Domain Type Options**, the **Length Units**, and the size of the **Initial Project Group** (the approximate size of the transport domain).

Domain Type: This section allows a user to choose between simple geometries having a structured finite element mesh (i.e., **1D-Simple**, **2D-Simple**, and **3D-Simple**), or more general geometries having an unstructured finite element mesh (i.e., **2D-General (Boundary Rep.)**, **3D-Layered**, and **3D-General (Boundary Rep.)**). Available options depend on the level of authorization (purchased License). Only simple geometries **2D-Simple** and **3D-Simple** are available for HYDRUS Levels **2D-Lite** and **3D-Lite**, respectively. **2D-General (Boundary Rep.)** is available for the **2D-Standard** Level, **3D-Layered** for the **3D-Standard** Level, and **3D-General (Boundary Rep.)** for the **3D-Professional** Level.

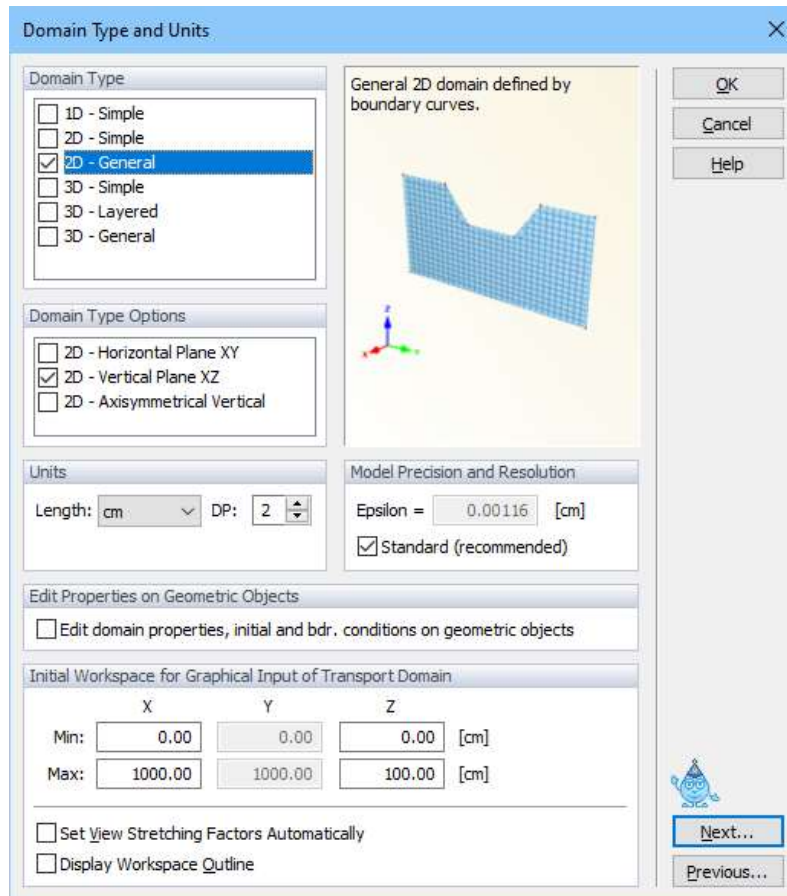


Figure 6. The Domain Type and Units dialog window (with 3D preview).

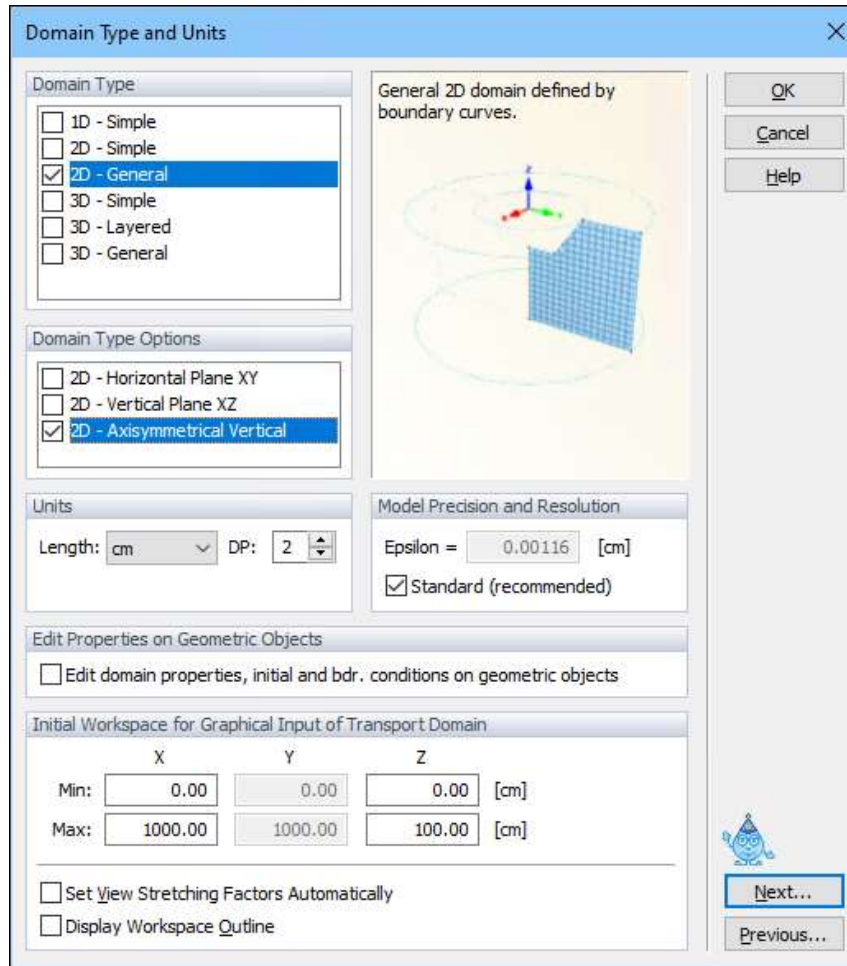


Figure 7. The Domain Type and Units dialog window (with 2D axisymmetrical preview).

There are two types of two-dimensional transport domains (Surfaces, see also Section 4.2) depending upon the selection made in the Domain Type and Units dialog window (Fig. 6 and 7):

- **2D-Simple (Parametric):** This type of solid has a **Rectangular Shape** and is defined by its basic dimensions. Rectangular domains are defined by three straight lines, one at the bottom of the domain and two at the sides, whereas the upper boundary may or may not be straight. Nodes along the upper boundary line may, in that case, have variable x- and z-coordinates. However, the lower boundary line must always be horizontal (or have a specified slope), while the left and right boundary lines must be vertical. The flow region is then discretized into a structured triangular mesh. Examples of simple rectangular geometries are shown in Figure 8 (top).
- **2D-General (Boundary Rep.):** This type of Surface is defined by a set of **Boundary Curves** see Section 4.2). Examples of general two-dimensional geometries are shown in Figure 8 (bottom) and Figure 56.

There are three types of three-dimensional transport domains (Solids, see also Section 4.4) depending upon the selection made in the Domain Type and Units dialog window (Fig. 6 and 7):

- **3D-Simple (Parametric):** This type of solid has a **Hexahedral Shape** and is defined by its basic dimensions. The base can have a certain slope in the X and Y dimensions (Fig. 9). Hexahedral domains must have similar properties as rectangular domains, i.e., vertical planes at the sides, a horizontal (or with a specified slope) plane at the bottom boundary, and with only the upper boundary not needing to be a plane. An example of a simple hexahedral three-dimensional geometry (i.e., 3D-Simple) is given in Figure 9.
- **3D-Layered:** This type of solid is defined by the **Base Surface** (see Section 4.2) and one or more **Thickness Vectors** (see Section 4.5).
- **3D-General (Boundary Rep.):** This type of solid is defined using a set of surfaces that fully form its boundaries. This type of geometries is available only in the **3D-Professional** version. **3D-General Geometries** can be formed from three-dimensional objects (**Solids**) of general shapes. Three-dimensional objects are formed by boundary surfaces, which can be either **Planar** surfaces or **Curved** surfaces (**Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**).

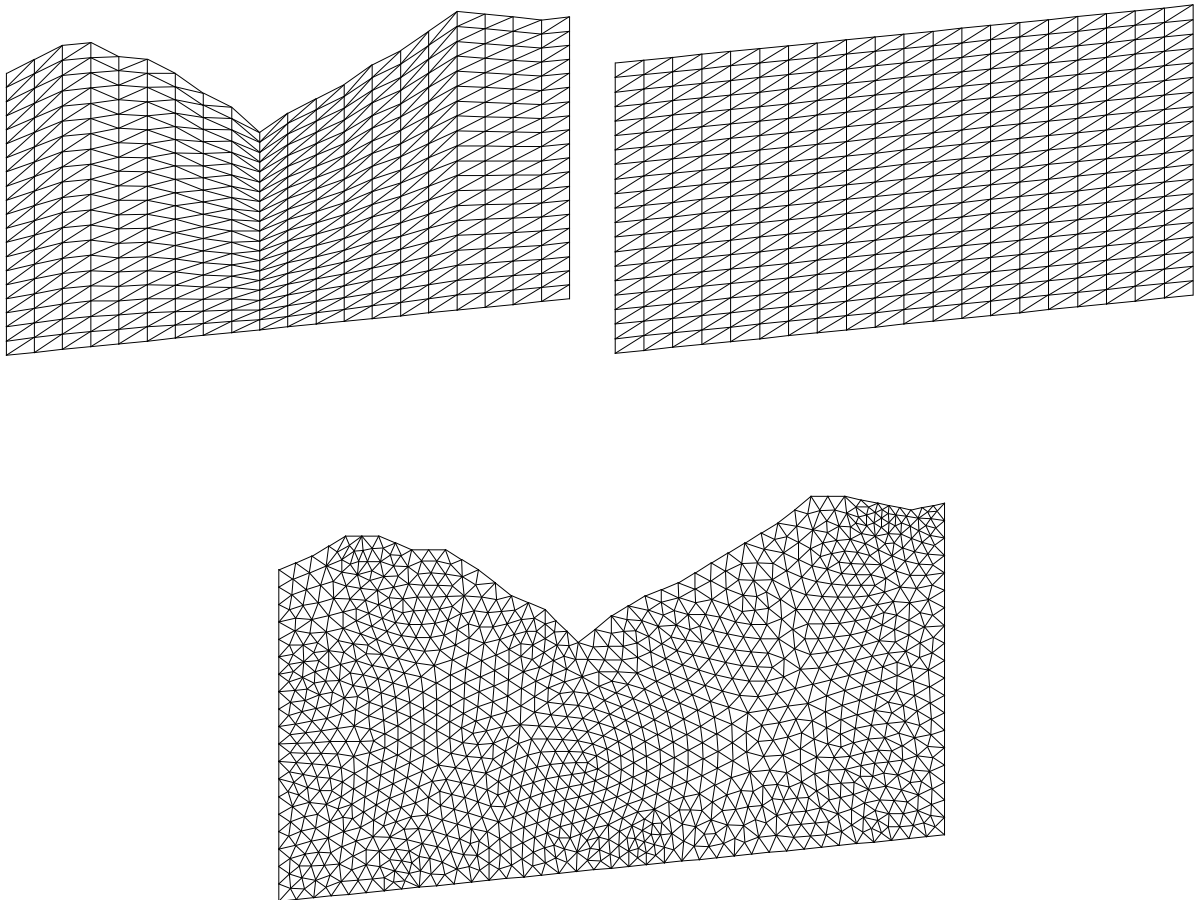


Figure 8. Examples of rectangular (top) and general (bottom) two-dimensional geometries.

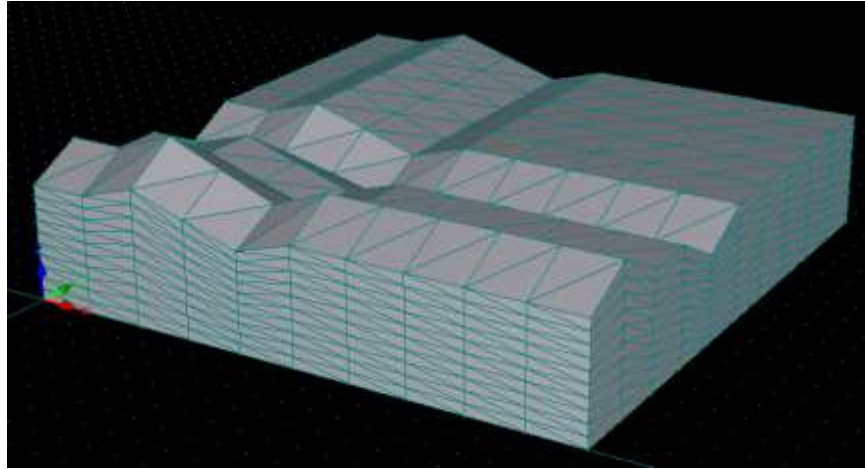


Figure 9. Example of a hexahedral three-dimensional geometry.

2D-Domain Options: Two-dimensional flow and transport can occur in a horizontal or vertical plane, or in an axisymmetrical quasi-three-dimensional transport domain. When a three-dimensional axisymmetrical system is selected, the z-coordinate must coincide with the vertical axis of symmetry. A typical example of the selected 2D or 3D geometry is shown in the preview part of the dialog window.

The simple geometries are defined in the *Rectangular* (Fig. 10) or *Hexahedral Domain Definition* (Fig. 11) dialog windows for two-dimensional and three-dimensional problems, respectively. In each of these windows, users need to specify the vertical and horizontal dimensions of the transport domain, as well as a possible slope of the base of the domain in different directions (if applicable; α is in the x-direction and β is in the y-direction). The preview in the middle of the dialog window of a simple example showing all geometry parameters should help users in specifying their desired transport domain (*Dimensions* and *Slope*).

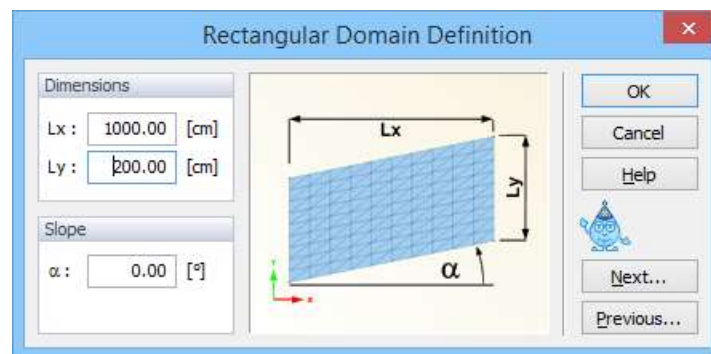


Figure 10. The Rectangular Domain Definition dialog window.

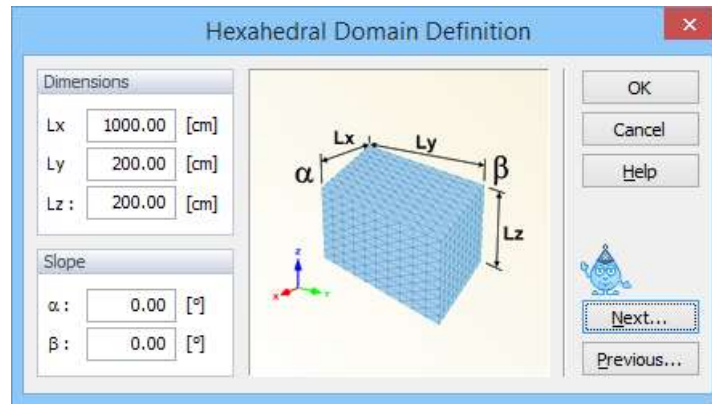


Figure 11. The Hexahedral Domain Definition dialog window.

In the **Domain Type and Units** dialog Window (Figs. 6 and 7), users also select the geometry **Units** to be used throughout the application (mm, cm, m) and the size of the **Initial Project Group**. When units are changed during specification or after reading the input data, then all input variables are automatically converted into the new units.

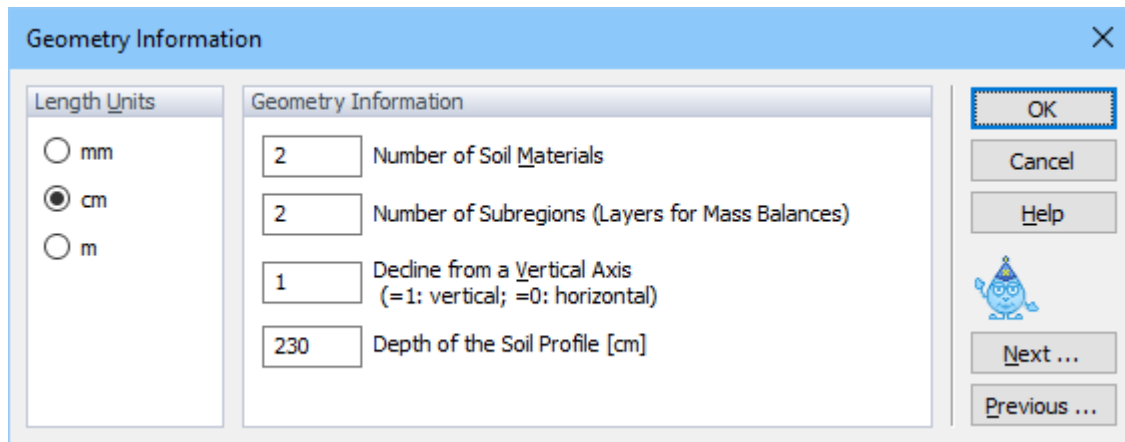
Initial Project Group: This part of the dialog allows users to define the initial dimensions of the graphical view window.

Model Precision and Resolution: *Epsilon* is a minimum resolution recognized when defining geometric objects. *Epsilon* is by default defined as $R/100,000$, where R is a domain radius, i.e., a radius of a circle/sphere circumscribing the domain. *Epsilon* is used, for example, for the evaluation of positions of two points. If their distance is less than *Epsilon*, then the two points are replaced by a single point. A user-defined epsilon may lead to unstable behavior of the program, and it is intended only for advanced users who may need it for special purposes. The correct functionality of geometrical calculations and generation of FE-meshes is not guaranteed for user-defined epsilons.

Edit Properties on Geometric Objects: When the check box "Edit domain properties, initial and boundary conditions on geometric objects" is checked, users can specify various properties and conditions on the Geometric Objects (See Section 6.5 "Defining Properties on Geometric Objects" for details), rather than only on FE-Mesh, as available in Version 1.0 of HYDRUS. This option will be by default "On" for new projects, and it is "Off" for projects converted from Version 1.0. Users can turn this option "Off" and continue defining various properties on FE-Mesh, as they have been used to. Users can turn this option "On" for projects converted from Version 1.0 of HYDRUS. However, they will lose their original definitions and have to specify them again on Geometric Objects.

In the **Geometry Information** dialog window (Fig. 12), users select for one-dimensional projects **Length Units** (used throughout the application, i.e., mm, cm, m), **Number of Soil Materials**, **Number of Subregions (Layers for Mass Balances, Decline from a Vertical Axis** (1 for vertical direction and 0 for horizontal direction), and **Depth of the Soil Profile**. Any inclined direction of the soil profile is allowed. The inclination is specified in terms of the cosine

of the angle between the vertical axis and the axis of the soil profile. Its value is equal to one for vertical soil columns and zero for horizontal soil columns.



The screenshot shows a dialog box titled "Geometry Information" with a close button (X) in the top right corner. The dialog is divided into three main sections. On the left, under the "Length Units" header, there are three radio buttons: "mm", "cm" (which is selected), and "m". The central area, also titled "Geometry Information", contains four input fields with corresponding labels: "Number of Soil Materials" (value: 2), "Number of Subregions (Layers for Mass Balances)" (value: 2), "Decline from a Vertical Axis (=1: vertical; =0: horizontal)" (value: 1), and "Depth of the Soil Profile [cm]" (value: 230). On the right side of the dialog, there is a vertical stack of buttons: "OK" (highlighted with a blue border), "Cancel", "Help", a small cartoon character icon, "Next ...", and "Previous ...".

Figure 12. The Geometry Information dialog window for one-dimensional problems.

3. Flow and Transport Parameters

Flow and transport parameters are entered in a series of dialog windows that are divided into multiple groups: a) General Information, b) Water Flow Parameters, c) Solute Transport Parameters, d) Heat Transport Parameters, and e) Root Water Uptake and Growth Parameters.

3.1. General Information

3.1.1. Main Processes

In the **Main Processes** dialog window (Fig. 13), users specify the processes to be simulated, i.e., **Water Flow**, **Solute Transport**, **Heat Transport**, and/or **Root Water Uptake**. When **Solute Transport** is selected, users can choose from multiple modules of different complexity. The **Standard Solute Transport** module is described in detail in the HYDRUS Technical Manuals [Šimůnek *et al.*, 2022ab]. This module allows consideration of individual solutes (one or several) that are either independent or subject to sequential (or consecutive) first-order decay reactions.

Other solute transport modules (briefly described below) can consider multiple solute components that can mutually interact.

Wetland Module Check this box if the Wetland module is to be used. The **Wetland Module** (for two-dimensional problems only) was developed to model biochemical transformation and degradation processes in subsurface constructed wetlands. In the wetland module, two biokinetic model formulations can be chosen: (1) the biokinetic model as described in **CW2D** [Langergraber and Šimůnek, 2005, 2006, 2011] and (2) the **CWM1** (Constructed Wetland Model #1) biokinetic model [Langergraber *et al.*, 2009]. In CW2D aerobic and anoxic transformation and degradation processes for organic matter, nitrogen and phosphorus are described, whereas in CWM1, aerobic, anoxic, and anaerobic processes for organic matter, nitrogen, and sulfur.

Unsatchem Module The **Major Ion Chemistry Module** [UNSATCHEM; Šimůnek and Suarez, 1994] can be used instead of the standard solute transport module. A detailed description of the UNSATCHEM Module is given in the UNSATCHEM user manuals [Šimůnek *et al.*, 2012c, 2021]. A more detailed description of the concepts used in the UNSATCHEM module is provided in the HYDRUS-1D manual [Šimůnek *et al.*, 2008], which provides all relevant information about the one-dimensional version of this module.

C-Ride Module The **C-Ride** module simulates one- and two-dimensional variably-saturated water flow, colloid transport, and colloid-facilitated solute transport in porous media. The module accounts for transient variably-saturated water flow and both colloid and solute movement due to advection, diffusion, and dispersion, as well as for solute movement

	facilitated by colloid transport. A detailed description of the C-Ride Module is given in the C-Ride user manual [Šimůnek <i>et al.</i>, 2012b, 2022c].
HPx Module	The HPx module is the result of coupling Hydrus (its one- and two-dimensional parts) with the PHREEQC geochemical code [Parkhurst and Appelo, 1999] [Jacques and Šimůnek, 2005, 2010; Jacques <i>et al.</i>, 2006, 2008]. HP2 has, apart from the dimensionality (2D), the same capabilities as HP1. HP2 contains modules simulating (1) transient water flow, (2) the transport of multiple components, (3) mixed equilibrium/kinetic biogeochemical reactions, and (4) heat transport in two-dimensional variably-saturated porous media (soils). A detailed description of the HP2 Module is given in the HP2 user manual [Šimůnek <i>et al.</i>, 2012a].
COSMIC Module	The COSMIC module developed by Brunetti <i>et al.</i> [2019b] calculates above-ground neutron fluxes using the physically-based COsmic-ray Soil Moisture Interaction Code (COSMIC) of Shuttleworth <i>et al.</i> [2013]. This is a one-dimensional add-on module.
DPU Module	The Dynamic Plant Uptake (DPU) module developed by Brunetti <i>et al.</i> [2019c, 2021, 2022ab] simulates the translocation and transformation of neutral compounds in the soil-plant domain. This add-on module exists for one-and two-dimensional applications.
Particle Tracking	The Particle Tracking algorithm from Šimůnek [1991] was implemented into HYDRUS [Zhou <i>et al.</i>, 2021]. The results of this module can be used to calculate soil water travel times and water age for different locations in the soil profile. This is a one-dimensional add-on module.
Slope Cube Module	While the Slope Classic module (added in version 2.04) is based on classical engineering soil mechanics theories and uses the effective stress approach only for saturated conditions, the new add-on module "Slope Cube" (Slope Stress and Stability) was developed to provide a unified effective stress approach for both saturated and unsaturated conditions [Lu <i>et al.</i>, 2010]. The module is intended to predict spatially and temporally infiltration-induced landslide initiation and to carry out slope stability analyses under variably-saturated soil conditions. Transient moisture and pressure head fields are directly obtained from the HYDRUS-2D model and subsequently used to compute the effective stress field of hillslopes [Lu and Godt, 2013]. Furthermore, instead of the methodology of one-slope for one-factor safety in the classical slope stability analysis, the SLOPE Cube module computes fields of the factor of safety in the entire domain within hillslopes [Lu <i>et al.</i>, 2012], thus allowing identification of the development of potential failure surface zones or surfaces.
Furrow Module	The Furrow module is a hybrid Finite Volume – Finite Element (FV-FE) model that describes the coupled surface-subsurface flow and transport processes occurring during furrow irrigation and fertigation [Brunetti <i>et al.</i>, 2018]. The numerical approach combines a one-dimensional description of water flow and solute transport in an open channel with a two-dimensional description of water flow and solute transport in a subsurface soil domain.

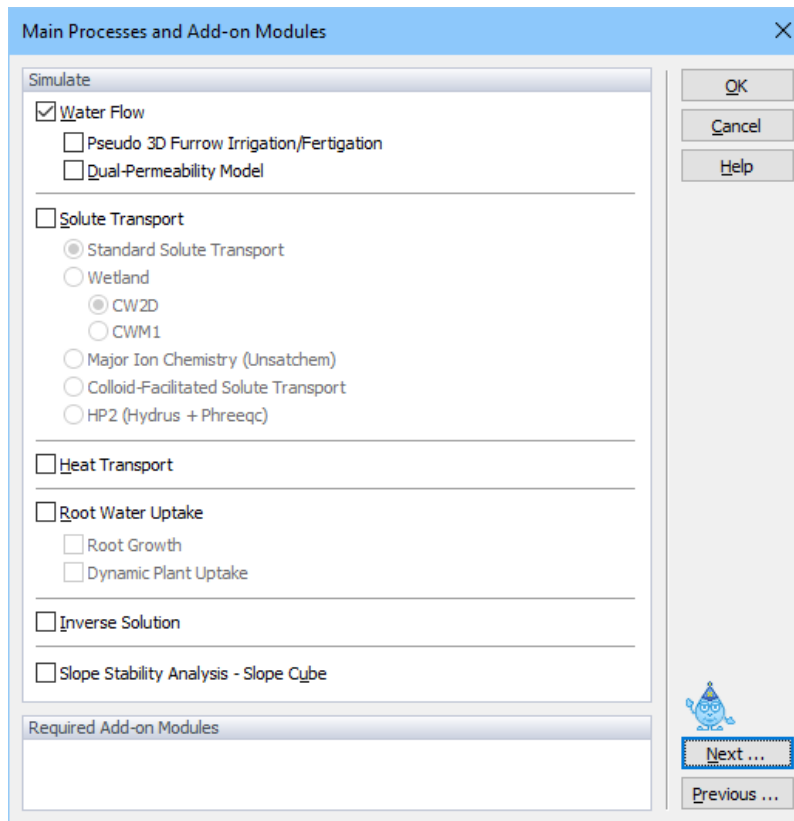
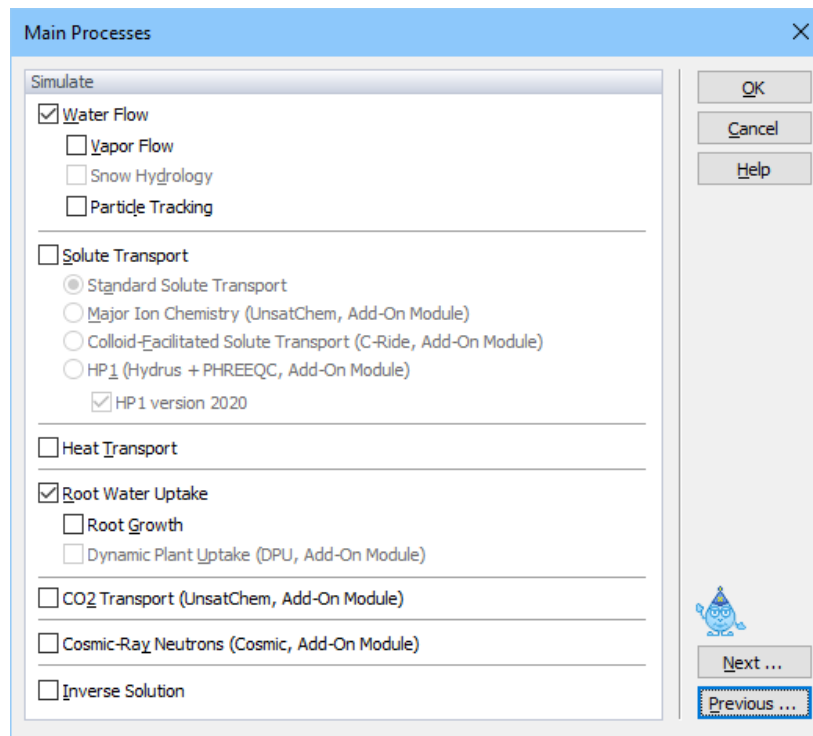


Figure 13. The Main Processes dialog window (for 1D - top, for 2D/3D - bottom).

The program automatically considers transient water flow when the “Water Flow” option is selected. Otherwise, in 2D and 3D applications, the code tries to calculate steady-state flow from the specified initial and boundary conditions. The success of such calculations depends on the complexity and/or nonlinearity of the problem. If unsuccessful, then a model run with constant boundary conditions and long simulation time may be required.

The Dual-Permeability Model can be selected as an alternative description of water flow for 2D applications.

If the solute transport, heat transport, or root water uptake options originally considered in an existing project are switched off by the user, the program issues a warning that all data related to these processes will be lost. If this loss is undesirable, we recommend that users first copy the input data of the current project to a new project before switching off the solute transport, heat transport and/or root water uptake options.

A user can also select if a **Direct** or **Inverse Problem (Inverse Solution)** is to be solved. Inverse problems involve the estimation of selected parameters from available experimental data.

A new add-on module **Slope Cube** was included in Version 2.05. Details about the **Slope Cube** module are given in its own manual.

3.1.2. Inverse Solution

HYDRUS implement a Marquardt-Levenberg type parameter estimation technique [Šimůnek and Hopmans, 2002] for inverse estimation of soil hydraulic (Hopmans et al., 2002) and/or solute transport and reaction [Šimůnek et al., 2002] parameters from measured transient or steady-state flow and/or transport data. The **Inverse Solution** dialog window (Fig. 14) appears only when the **Inverse Problem** in the **Main processes** dialog window (Fig. 13) is selected. Users select which parameters (the soil hydraulic, solute transport and reaction, and/or heat transport parameters) are to be optimized (**Estimate ...**) from the specified experimental data.

One also selects the method of **Weighting of Inversion Data** in the objective function. Users can choose between no weighting, weighting by mean ratios, or weighting by standard deviations. When no weighting is selected, one needs to supply weights for particular data points in the **Data for Inverse Solution** dialog window (Fig. 15). When weighting by mean ratio or weighting by standard deviation is selected, then the code calculates either the means or the standard deviations of the different data sets (e.g., water contents, pressure heads, concentrations, ...) and adjusts the weights proportionally. These internal weights can still be multiplied by weights from the **Data for Inverse Solution** dialog window (Fig. 15).

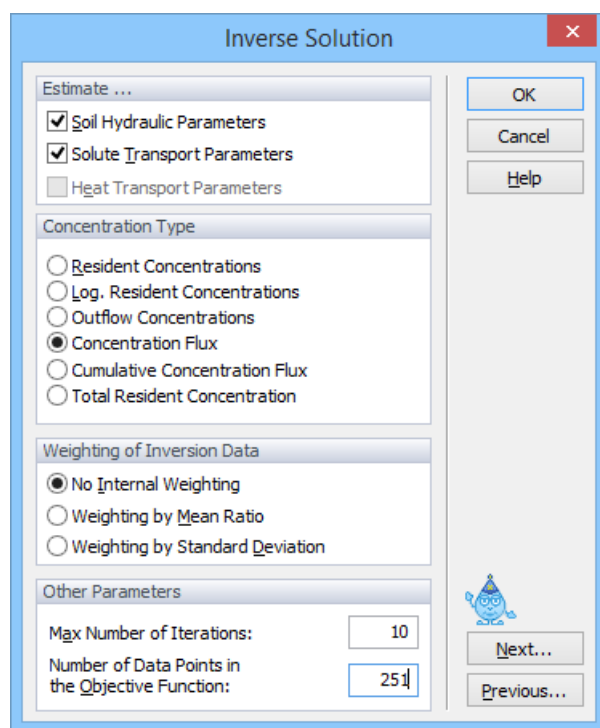


Figure 14. The Inverse Solution dialog window.

The objective function for the inverse estimation of solute transport parameters can be defined using different types of concentrations. Available **Concentration Types** are: a) the resident concentration in the liquid phase, b) a log-transformation of the resident concentration in the liquid phase, c) the outflow (flux) concentration, d) the solute flux, e) the cumulative solute flux,

and f) the total resident concentration. The total resident concentration includes concentrations in the sorbed and nonequilibrium phases.

The maximum number of iterations for the inverse solution is also specified in this dialog window. If one selects a zero number of iterations, then only the direct simulation is carried out. However, users can still enter measured data, in which case the code compares the results of the direct simulation with the measured data.

	X	Y	Type	Position	Weight
1	1	-47.61	Time - Head	2	1
2	5	-48.8	Time - Head	2	1
3	10	-48.15	Time - Head	2	1
4	15	-47.07	Time - Head	2	1
5	20	-35.77	Time - Head	2	1
6	25	-24.8	Time - Head	2	1
7	30	-19.52	Time - Head	2	1
8	35	-17.48	Time - Head	2	1
9	40	-15.33	Time - Head	2	1
10	45	-15.43	Time - Head	2	1
11	50	-14.03	Time - Head	2	1
12	55	-13.17	Time - Head	2	1
13	60	-12.42	Time - Head	2	1
14	65	-12.64	Time - Head	2	1
15	70	-13.6	Time - Head	2	1
16	75	-12.1	Time - Head	2	1

Figure 15. The Data for Inverse Solution dialog window.

In the table Data for Inverse Solution (Fig. 15), one specifies the measured data analyzed during the parameter optimization process. Many different types of data can be used to define the objective function that will be minimized for this purpose. How the values in the X and Y columns are interpreted depends on the Type and Position values. Weight is the weight associated with a particular data point. The following information can be included in the objective function:

Table 2. Data Types for the objective function (Inverse Problem).

Type	Data Point
0	Cumulative boundary fluxes across a specified boundary
1	Pressure head measurements at selected observation point(s)
2	Water content measurements at selected observation point(s)
3	Boundary flux across a specified boundary
4	Concentration or temperature measurements at observation point(s)
5	$h(\theta)$ measurements; soil water retention data
6	$K(h)$ measurements; hydraulic conductivity data point
7	Prior knowledge of parameter α
8	Prior knowledge of parameter n
9	Prior knowledge of parameter θ_r
10	Prior knowledge of parameter θ_s
11	Prior knowledge of parameter K_s

Depending upon the value of parameter **Type**, the first column (X) contains the following information:

Table 3. Definition of column X in Fig. 15 based on Data Type (Inverse Problem).

X	Type
Time	0, 1, 2, 3, 4
Pressure head	5, 6
Dummy variable	7, 8, 9, 10, 11

Depending upon the value of parameter **Type**, the second (Y) and fourth (Position) columns contain the following information:

Table 4. Definition of column Y in Fig. 15 based on Data Type (Inverse Problem).

Y	Type	Position
Cumulative boundary flux across a specified boundary	0	Code for the specified boundary*
Pressure head	1	Observation node number
Water content	2	Observation node number
Averaged water content of the entire flow domain	2	0
Averaged water content of the subregion	2	Negative subregion number
Concentrations/temperatures	4	Observation node number
Concentrations for the second solute	4	Negative observation node number
The total amount of solute in the entire flow domain	4	0
Boundary flux across a specified boundary	3	Code for the specified boundary*
Water content	5	Material number
Hydraulic conductivity	6	Material number
Particular parameter	7-11	Material number

*1 – constant pressure head or flux boundary; 2 – seepage face; 3 – variable pressure head or flux boundary 1; 4 – atmospheric boundary; 5 – drains; 6 – free or deep drainage boundary; 7, 8, and 9 – variable pressure head or flux boundaries 2, 3, or 4, respectively.

3.1.3. Time Information

The **Time Information** dialog window (Fig. 16) contains information associated with the **Time Discretization**, the **Time Units**, and the implementation of **Boundary Conditions**.

The figure displays two versions of the 'Time Information' dialog window. The top version is for 1D simulation, and the bottom version is for 2D/3D simulation.

Top Screenshot (1D):

- Time Units:** Days (selected).
- Time Discretization:**
 - Initial Time [day]: 90
 - Final Time [day]: 273
 - Initial Time Step [day]: 0.05
 - Minimum Time Step [day]: 0.0001
 - Maximum Time Step [day]: 0.5
- Time-Variable Boundary Conditions:**
 - ☒ Time-Variable Boundary Conditions
 - Number of Time-Variable Boundary Records (e.g., Precipitation): 183
 - ☐ Repeat the same set of BC records n times: 1
 - ☐ Daily Variations of Transpiration During Day Generated by HYDRUS
 - ☐ Sinusoidal Variations of Precipitation Generated by HYDRUS
- Meteorological Data:**
 - ☒ Meteorological Data
 - Number of Meteorological Records (e.g., Radiation): 183
 - ☒ Penman-Monteith Equation
 - ☐ Hargreaves Formula
 - ☐ Energy Balance Boundary Condition
 - ☐ Daily Variations of Meteo Data During Day Generated by HYDRUS

Bottom Screenshot (2D/3D):

- Time Units:** Days (selected).
- Time Discretization:**
 - Initial Time [day]: 90
 - Final Time [day]: 270
 - Initial Time Step [day]: 0.05
 - Minimum Time Step [day]: 0.001
 - Maximum Time Step [day]: 0.5
- Boundary Conditions:**
 - ☒ Time-Variable Boundary Conditions
 - Number of Time-Variable Boundary Records: 30
 - Number of times to repeat the same set of BC: 6

Figure 16. The Time Information dialog window (for 1D - top, for 2D/3D - bottom).

Table 5. Time Information variables.

Time Units	Time units [T] to be used throughout the application (years, days, hours, min, sec). When units are changed during or after data entry, then all input variables are converted automatically into the new units.
Initial Time	Starting time [T] of the calculation.
Final Time	Final time [T] of the calculation.
Initial Time Step	Initial time increment, Δt [T]. The recommended value for the initial time step depends on the type of simulation and boundary conditions used. When simulating a process that starts with a large initial pressure head or concentration gradient at the boundary (e.g., ponded infiltration or a sudden change of the boundary concentration), use a small value of the initial time step (e.g., 1 s). When simulating a long-term process with variable boundary conditions (e.g., seasonal or multiyear simulations), start with a larger time step (e.g., 15 min). This is because this initial time step is used whenever time-variable boundary conditions significantly change (e.g., the water flux changes by 25% or more). If needed (if there is no convergence for Δt_{init}), the program will still use a smaller time step than Δt_{init} , but starting with a larger Δt_{init} leads to more efficient calculations. In general, smaller initial time steps must be used for soils with more nonlinear soil hydraulic properties (e.g., coarse-textured soils), and larger initial time steps can be used for soils with less nonlinear soil hydraulic properties (e.g., loam).
Minimum Time Step	Minimum permitted value of the time increment, Δt_{min} [T]. The minimum time step must be smaller than a) the initial time step, b) interval between print times, and c) interval between time-variable boundary condition records. Always specify a small minimum allowed time step, on the order of 1 s. This value may never be used, but it provides the code with flexibility when needed, e.g., when there is a sudden change in boundary fluxes, and HYDRUS may not converge with larger time steps.
Maximum Time Step	The maximum permitted value of the time increment, Δt_{max} [T]. This is a relatively unimportant parameter, and a large value may be specified. Since HYDRUS automatically selects its optimal time step, there is usually no need to constraint that. The only time when there is a need to constrain the time step is likely for cases when HYDRUS is asked to generate intra-daily variations in temperature internally, or in evaporation and transpiration fluxes. Then there is a need to have time steps smaller (e.g., 1 h) so that these daily variations can be properly modeled.

Boundary Conditions

Time-Variable Boundary Condition - The **Number of Time-Variable Boundary Records** and time-dependent boundary conditions must be specified when this box is checked. The boundary conditions otherwise are assumed to be constant in time.

The same set of boundary records can be repeated a number of times (**Number of times to repeat the same set of BC records**) (periodically) with a time period $tPeriod = tAtmLast - tInit$, where $tInit$ is the **Initial Time** and $tAtmLast$ is the time of the last specified time boundary record. Note that $tMax < tInit + n * tPeriod$.

The **one-dimensional model** offers additional options for how to specify boundary conditions:

1. **Daily Variation of Transpiration During Day Generated by HYDRUS:** Variations in the potential transpiration rate during the day can be generated with HYDRUS using the assumption that hourly values of the potential transpiration rate between 0-6 a.m. and 18-24 p.m. represent 1% of the total daily value and that it has a sinusoidal shape during the rest of the day (see the Technical manual for details).
2. **Sinusoidal Variations of Precipitation Generated by HYDRUS:** Similarly, variations of the precipitation rate can be approximated using a cosine function.
3. **Meteorological Data:** Potential evapotranspiration can be alternatively calculated using the FAO recommended Penman-Montheith combination equation [Monteith, 1981; Monteith and Unsworth, 1990; FAO, 1990], the Hargreaves equation [Jensen et al., 1997], or by solving the surface energy balance (see the manual).
4. **Daily Variation of Meteo Data During Day Generated by HYDRUS:** HYDRUS can generate daily variations of meteo data using various meteorological models described in the Technical Manual.

3.1.4. Output Information

The **Output Information** dialog window (Fig. 17) contains information governing output from the computational module of HYDRUS.

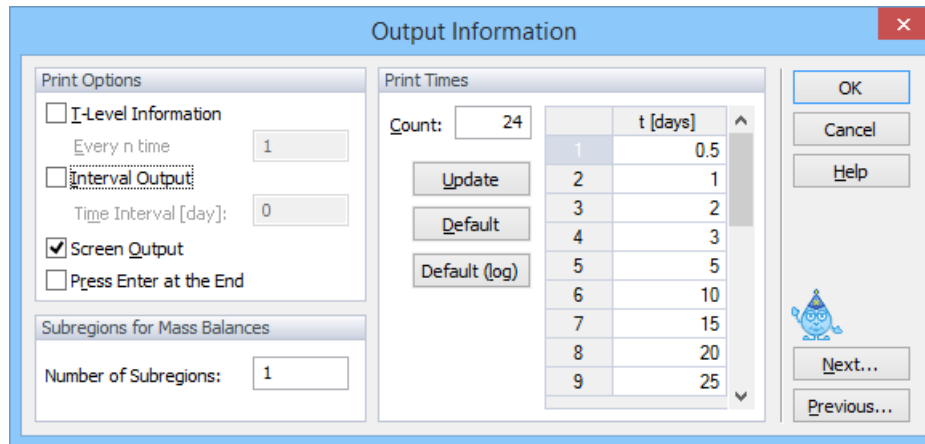


Figure 17. The Output Information dialog window.

In the **Print Options** part of the dialog window, one decides whether certain information concerning mean pressure heads and concentrations, mean water and solute fluxes, cumulative water and solute fluxes, and time and iteration information is printed at each time step (*T-Level Information*), after n time steps (*Every n time steps*), at a certain defined time interval (*Interval Output*), or if the information is sent to the screen during the calculations (*Screen Output*). When the simulation ends, users are, by default, asked to hit the Enter key of the keyboard to return to the GUI from the computational window. This action can be disabled by unchecking the Hit Enter at the End check box.

T-Level Information This check box decides whether certain information concerning mean pressure heads and concentrations, mean water and solute fluxes, cumulative water and solute fluxes, and time and iteration information, are to be printed at each time step, after n time steps, or only at preselected times (**Print Times**) or **Time Intervals**.

Interval Output Users can specify whether or not information concerning mean pressure heads and concentrations, mean water and solute fluxes, cumulative water and solute fluxes, and time and iteration information is to be printed at a regular **Time Interval**.

Screen Output Check box to decide whether or not information about the simulation run is to be printed to the screen during the execution of the HYDRUS computational code. We recommend checking this box for direct problems, but not for inverse problems.

In the **Print Times** part of the dialog window, one specifies the number of Print Times (**Count**) at which detailed information about the pressure heads, water contents, concentrations, temperatures, fluxes, and the soil water and solute balances will be printed. Clicking on the **Default** command button will cause the print times to be distributed evenly between the initial and final times. Clicking on the **Default (log)** command button will cause the print times to be distributed evenly between the initial and final times on the log scale. This option is enabled only for larger times.

Finally, in the **Subregions** part, one selects the number of regions for which a mass balance will be evaluated and printed to the Balance.out output file.

3.2. Water Flow

3.2.1. Iteration Criteria

The **Iteration Criteria** dialog window (Fig. 18) contains information related to the iterative process that is used to solve the Richards equation. Because of the nonlinear nature of the Richards equation, an iterative process must be used to obtain solutions of the global matrix equation at each new time step. For each iteration, a system of linearized algebraic equations is first derived and then solved using either Gaussian elimination or the conjugate gradient method. After solving the matrix equation, the coefficients are re-evaluated using this solution, and the new equations are again solved. The iterative process continues until a satisfactory degree of convergence is obtained, i.e., until for all nodes in the saturated (unsaturated) region, the absolute change in pressure head (water content) between two successive iterations becomes less than some small value determined by the imposed absolute **Pressure Head** (or **Water Content**) **Tolerance**. The first estimate (at zero iteration) of the unknown pressure heads at each time step is obtained by extrapolation from the pressure head values at the previous two-time levels.

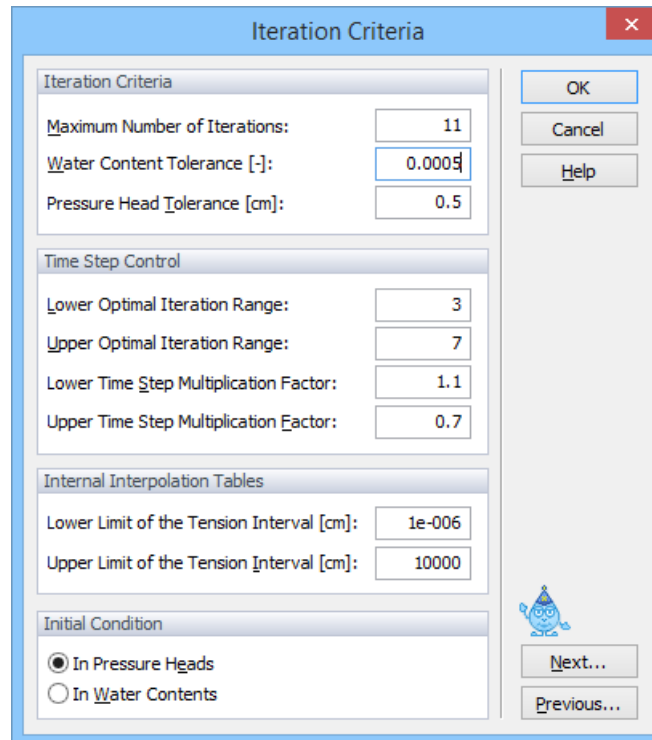


Figure 18. The Iteration Criteria dialog window.

In the **Iteration Criteria** part of the dialog window, one specifies the maximum number of iterations during one-time step, and the water content and pressure head precision tolerances.

Max. Number of Iterations Maximum number of iterations allowed during any time step while solving the nonlinear Richards equation using a modified Picard method. The

recommended and default value is 10. It is usually not helpful to use a larger value than 10. If HYDRUS does not converge in 10 iterations, then there is a relatively small probability that it will do so during more iteration. Even if it does, it is much more efficient to reduce the time step and attempt to find the solution with a smaller time step, which is done automatically by the program when It_{crit} is reached.

Water Content Tolerance Absolute water content tolerance for nodes in the unsaturated part of the flow region [-]. When the water contents between two successive iterations during a particular time step change less than this parameter, the iterative process stops, and the numerical solution proceeds to the new time step. Its recommended and default value is 0.001.

Pressure Head Tolerance Absolute pressure head tolerance for nodes in the saturated part of the flow region [L]. When the pressure heads between two successive iterations during a particular time step change less than this parameter, the iterative process stops, and the numerical solution proceeds to the new time step. Its recommended and default value is 1 cm.

Information specified in the **Time Step Control** part of the dialog window is related to the automatic adjustment of the time step during calculations. Four different time discretizations are introduced in HYDRUS: (1) time discretizations associated with the numerical solution, (2) time discretizations associated with the implementation of boundary conditions, (3) time discretizations associated with data points used in the inverse problem, and (4) time discretizations which provide printed output of the simulation results (e.g., nodal values of dependent variables, water and solute mass balance components, and other information about the flow regime).

Discretizations 2, 3, and 4 are mutually independent; they generally involve variable time steps as described in the input data file (**Time-Variable Boundary Conditions**, Fig. 48 and **Output Information**, Fig. 17). Discretization 1 starts with a prescribed initial time increment, Δt . This time increment is automatically adjusted at each time level according to the following rules:

- a. Discretization 1 must coincide with time values resulting from time discretizations 2, 3, and 4.
- b. Time increments cannot become less than a preselected minimum time step, Δt_{min} , nor exceed a maximum time step, Δt_{max} (i.e., $\Delta t_{min} \leq \Delta t \leq \Delta t_{max}$).
- c. If, during a particular time step, the number of iterations necessary to reach convergence is ≤ 3 , the time increment for the next time step is increased by multiplying Δt with a predetermined constant > 1 (usually between 1.1 and 1.5). If the number of iterations is ≥ 7 , Δt for the next time level is multiplied by a constant < 1 (usually between 0.3 and 0.9).
- d. If, during a particular time step, the number of iterations at any time level becomes greater than a prescribed maximum (usually between 10 and 50), the iterative process for that time level is terminated. The time step is subsequently reset to $\Delta t/3$, and the iterative process restarted.

We note that the selection of optimal time steps, Δt , during execution is also influenced by the adopted solution scheme for solute transport.

Table 6. Time Step Control variables.

Lower Optimal Iteration Range	When the number of iterations necessary to reach convergence for water flow is less than this number, the time step is multiplied by the lower time step multiplication factor (the time step is increased). The recommended and default value is 3.
Upper Optimal Iteration Range	When the number of iterations necessary to reach convergence for water flow is higher than this number, the time step is multiplied by the upper time step multiplication factor (the time step is decreased). The recommended and default value is 7.
Lower Time Step Multiplication Factor	If the number of iterations necessary to reach convergence for water flow is less than the lower optimal iteration range, the time step is multiplied by this number (time step is increased). The recommended and default value is 1.3.
Upper Time Step Multiplication Factor	If the number of iterations necessary to reach convergence for water flow is higher than the upper optimal iteration range, the time step is multiplied by this number (time step is decreased). The recommended and default value is 0.7.

Internal Interpolation Tables. At the beginning of a numerical simulation, HYDRUS generates for each soil type in the flow domain a table of water contents, hydraulic conductivities, and specific water capacities from the specified set of hydraulic parameters. The values of the hydraulic properties are then computed during the iterative solution process using linear interpolation between entries in the table. If the pressure head h at some node falls outside the prescribed interval (h_a, h_b) , the hydraulic characteristics at that node are evaluated directly from the hydraulic functions (i.e., without interpolation). The above interpolation technique was found to be much faster computationally than direct evaluation of the hydraulic functions over the entire range of pressure heads. Interpolation using tables can be avoided by setting h_a and h_b both to zero. Then the soil hydraulic properties are always evaluated directly from the hydraulic functions (i.e., without interpolation). Output graphs of the soil hydraulic properties will also be given for the interval (h_a, h_b) .

The lower limit of the tension interval	The absolute value of the lower limit [L] of the pressure head interval for which a table of hydraulic properties will be generated internally for each material.
The upper limit of the tension interval	The absolute value of the upper limit [L] of the pressure head interval for which a table of hydraulic properties will be generated internally for each material.

Finally, in the **Initial Conditions** part of the dialog window, a user specifies whether the initial conditions for the water flow calculations are to be specified in terms of pressure heads or water contents.

3.2.2. Soil Hydraulic Model

In the **Soil Hydraulic Model** dialog window (Fig. 19), users select the **Hydraulic Model** to describe the soil hydraulic properties and specify whether or not **Hysteresis** is to be considered during the calculations.

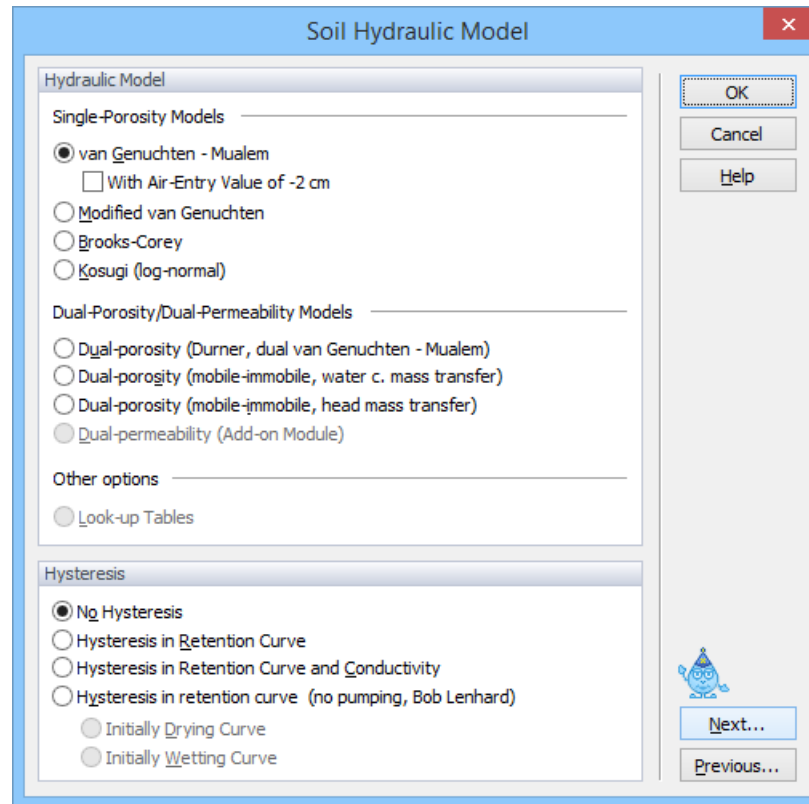


Figure 19. The Soil Hydraulic Model dialog window.

Hydraulic Model: The code allows users to select six types of models for the soil hydraulic properties: a) the van Genuchten-Mualem model [van Genuchten, 1980], b) the van Genuchten-Mualem model with an air-entry value of -2 cm, c) the modified van Genuchten type equations [Vogel and Cislérova, 1988], d) the equations of Brooks and Corey [1964], e) the lognormal distribution model of Kosugi [1996], and f) a dual-porosity model [Durner, 1994]. Additionally, users can select two dual-porosity nonequilibrium flow models with mass transfer between the mobile and immobile zones assumed to be proportional to either g) the water content or h) the pressure head [Šimůnek et al., 2003]. For a detailed description of these models, see the technical manual of HYDRUS. Two other approaches (a dual-permeability model and look-up tables) are not available in the current version of HYDRUS.

Hysteresis: When the van Genuchten model is used, either a) a non-hysteretic description (*No Hysteresis*), b) a hysteretic description only in the retention curve (*Hysteresis in Retention*

Curve), or c) hysteretic descriptions in both the retention curve and the hydraulic conductivity curve (*Hysteresis in Retention Curve and Conductivity*) can be used. When hysteresis in the soil hydraulic properties is assumed, users must specify whether the initial condition is associated with the main wetting (**Initially Wetting Curve**) or main drying (**Initially Drying Curve**) retention curve. The HYDRUS code incorporates hysteresis by using the empirical model introduced by *Scott et al.* [1983]. This model was also employed by *Kool and Parker* [1987], who modified the formulation to account for air entrapment. While relatively simple to implement, the above model has sometimes suffered from a so-called pumping effect, when the hysteresis loops can move to physically unrealistic parts of the retention function. As an alternative, we also incorporated in HYDRUS the hysteresis model of *Lenhard et al.* [1991] and *Lenhard and Parker* [1992] that eliminates pumping by keeping track of historical reversal points (*Hysteresis in Retention Curve, no pumping, Bob Lenhard*).

3.2.3. Water Flow Parameters

Parameters for the soil hydraulic models are specified in the **Water Flow Parameters** dialog window (Fig. 20).

In all models (i.e., *Brooks and Corey*, 1964; *van Genuchten*, 1980; *Vogel and Cislerova*, 1988; *Kosugi*, 1996, and *Durner*, 1994), θ_r (Q_r) and θ_s (Q_s) denote the residual and saturated water contents, respectively; K_s (K_s) [L^{-1}] is the saturated hydraulic conductivity, and l is a pore-connectivity parameter. The parameters α (Alpha) [L^{-1}] and n [-] are empirical coefficients affecting the shape of the hydraulic functions.

The modified van Genuchten model has four additional parameters: θ_a (Q_a) – a water content smaller or equal to θ_r , θ_m (Q_m) – a water content larger or equal to θ_s , K_k (K_k) [L^{-1}] – the unsaturated hydraulic conductivity at water content θ_k , and θ_k (Q_k) – the water content associated with K_k .

Water Flow Parameters

Material Properties for Water Flow

Number of Materials: Model: van Genuchten [1980] - Mualem [1976]

Mat	Name	Q_r [-]	Q_s [-]	Alpha [L^{-1}]	n [-]	K_s [m/day]	l [-]
1	Loam	0.078	0.43	3.6	1.56	0.2496	0.5
2	Sand	0.045	0.43	14.5	2.68	7.128	0.5
3	Silt modifeid	0.034	0.46	1.37	1.41	6.2	0.5

Soil Catalog: ☐ ☐ Temperature Dependence

Water Flow Parameters - Inverse Solution - Material

Material Properties for Water Flow

Number of Materials: Model: van Genuchten [1980] - Mualem [1976]

	Qr [-]	Qs [-]	Alpha[1/cm]	n [-]	Ks [cm/sec]
Initial Estimate	0.034	0.46	0.016	1.37	6.94444e-00
Minimum Value	0	0.1	0	2	0.000
Maximum Value	0	0.6	0	7	
Fitted ?	☐	☐	☒	☒	☒

Soil Catalog: Neural Network Prediction ☒ Temperature Dependence

OK Cancel Help Next ... Previous ...

Figure 20. The Water Flow Parameters dialog window for direct (top) and inverse (bottom) problems.

Durner's [1994] model has three additional parameters: w_2 (w_2), α_2 (Alpha2) [L^{-1}], and n_2 (n_2), where w_2 is the weighting factor for the second overlapping region, and α_2 and n_2 are empirical parameters for the second region.

The hysteretic model also has three additional parameters: θ_{sw} (Q_{sw}) – the saturated water content of the main wetting branch, α_w (AlphaW) [L^{-1}] – the shape parameter of the main wetting branch, and K_{sw} (K_{sw}) [LT^{-1}] – the saturated hydraulic conductivity associated with the main wetting branch (in case hysteresis also occurs in the conductivity function).

Temperature Dependence: Check this box if the hydraulic properties are considered to be temperature dependent. Using capillary theory, the influence of temperature on the soil water pressure head is then quantitatively predicted from the influence of temperature on the surface tension. The influence of temperature on hydraulic conductivity is predicted from the influence of temperature on viscosity and the density of water.

Soil Catalog: The hydraulic parameters of selected soils were included in a catalog from which users can select. The van Genuchten parameters were taken from *Carsel and Parrish* [1988] (Table 7), the Brooks and Corey parameters are from *Rawls et al.* [1982]. *Rawls et al.* (1982) used multiple linear regression to estimate the Brooks and Corey parameters from a large database of some 2540 soil horizons. Their regression equations were subsequently used by *Carsel and Parrish* [1988], but the results were further manipulated statistically to get van Genuchten parameters probability density functions (superficially, the van Genuchten parameters are the same or closely related to the BC parameters, such as $n=\lambda+1$). Hence the *Carsel and Parrish* ([1988] parameters were statistically derived from the *Rawls et al.* [1982] estimates; they were not fitted independently to the Rawls database. Some caution is needed when using these parameter values since they only represent very approximate averages for different textural classes. The soil hydraulic parameters in the catalog for Kosugi's model were obtained by fitting retention curves generated using the *Carsel and Parrish* [1988] parameters for van Genuchten's [1980] model using RETC.

The following soil textural classes are represented in the soil hydraulic catalog:

- Sand
- Loamy Sand
- Sandy Loam
- Loam
- Silt Loam
- Sandy Clay Loam
- Clay Loam
- Silty Clay Loam
- Sandy Clay
- Silty Clay
- Clay

Neural Network Prediction: The program uses pedotransfer functions (PTFs) based on neural networks [Schaap *et al.*, 2001] to predict *van Genuchten's* [1980] water retention parameters and the saturated hydraulic conductivity (K_s) based on textural information (see Section 3.8 below).

When the parameter estimation option is selected, then users have to provide initial estimates of the optimized soil hydraulic parameters, specify which parameters are to be optimized (check appropriate checkboxes), and provide parameter constraints for the optimization. Entering zeros (the default values) for the minimum and maximum values signify that the parameters are unconstrained.

Table 7. Soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA soil textural triangle, according to *Carsel and Parrish* [1988].

Textural class	θ_r [L ³ L ⁻³]	θ_s [L ³ L ⁻³]	α [cm ⁻¹]	n [-]	K_s [cm d ⁻¹]
Sand	0.045	0.430	0.145	2.68	712.8
Loamy Sand	0.057	0.410	0.124	2.28	350.2
Sandy Loam	0.065	0.410	0.075	1.89	106.1
Loam	0.078	0.430	0.036	1.56	24.96
Silt	0.034	0.460	0.016	1.37	6.00
Silty Loam	0.067	0.450	0.020	1.41	10.80
Sandy Clay Loam	0.100	0.390	0.059	1.48	31.44
Clay Loam	0.095	0.410	0.019	1.31	6.24
Silty Clay Loam	0.089	0.430	0.010	1.23	1.68
Sandy Clay	0.100	0.380	0.027	1.23	2.88
Silty Clay	0.070	0.360	0.005	1.09	0.48
Clay	0.068	0.380	0.008	1.09	4.80

Table 8. Soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA textural triangle as obtained with the Rosetta Lite program [*Schaap et al.*, 2001].

Textural class	θ_r [L ³ L ⁻³]	θ_s [L ³ L ⁻³]	α [cm ⁻¹]	n [-]	K_s [cm d ⁻¹]
Sand	0.053	0.375	0.035	3.18	643.
Loamy Sand	0.049	0.390	0.035	1.75	105.
Sandy Loam	0.039	0.387	0.027	1.45	38.2
Loam	0.061	0.399	0.011	1.47	12.0
Silt	0.050	0.489	0.007	1.68	43.7
Silty Loam	0.065	0.439	0.005	1.66	18.3
Sandy Clay Loam	0.063	0.384	0.021	1.33	13.2
Clay Loam	0.079	0.442	0.016	1.41	8.18
Silty Clay Loam	0.090	0.482	0.008	1.52	11.1
Sandy Clay	0.117	0.385	0.033	1.21	11.4
Silty Clay	0.111	0.481	0.016	1.32	9.61
Clay	0.098	0.459	0.015	1.25	14.8

Table 9. Soil hydraulic parameters for the analytical functions of *Brooks and Corey* [1964] for twelve textural classes of the USDA soil textural triangle, according to *Rawls et al.* [1982].

Textural class	θ_r [L ³ L ⁻³]	θ_s [L ³ L ⁻³]	α [cm ⁻¹]	n [-]	K_s [cm d ⁻¹]
Sand	0.020	0.417	0.1380	0.592	504.0
Loamy Sand	0.035	0.401	0.1150	0.474	146.6
Sandy Loam	0.041	0.412	0.0682	0.322	62.2
Loam	0.027	0.434	0.0897	0.220	31.7
Silt	0.015	0.486	0.0482	0.211	16.3
Silty Loam	0.015	0.486	0.0482	0.211	16.3
Sandy Clay Loam	0.068	0.330	0.0356	0.250	10.3
Clay Loam	0.075	0.390	0.0386	0.194	5.52
Silty Clay Loam	0.040	0.432	0.0307	0.151	3.60
Sandy Clay	0.109	0.321	0.0343	0.168	2.88
Silty Clay	0.056	0.423	0.0292	0.127	2.16
Clay	0.090	0.385	0.0268	0.131	1.44

Table 10. Soil hydraulic parameters for the analytical functions of *Kosugi* [1996] for twelve textural classes of the USDA soil textural triangle.

Textural class	θ_r [L ³ L ⁻³]	θ_s [L ³ L ⁻³]	α [cm ⁻¹]	n [-]	K_s [cm d ⁻¹]
Sand	0.045	0.430	303.7	0.383	712.8
Loamy Sand	0.057	0.410	12.47	0.950	350.2
Sandy Loam	0.065	0.410	27.42	1.26	106.1
Loam	0.078	0.430	101.8	1.80	24.96
Silt	0.034	0.460	510.6	2.48	6.00
Silty Loam	0.067	0.450	325.9	2.30	10.80
Sandy Clay Loam	0.100	0.390	80.89	2.04	31.44
Clay Loam	0.095	0.410	666.3	2.81	6.24
Silty Clay Loam	0.089	0.430	2853.	3.26	1.68
Sandy Clay	0.100	0.380	1129.	3.41	2.88
Silty Clay	0.070	0.360	140538.	4.49	0.48
Clay	0.068	0.380	103815.	4.67	4.80

Note that in Version 2, each material can have a name (e.g., Material 1, Sand, Clay). When soil hydraulic parameters are assigned using the **Soil Catalog**, the names of textural classes will appear in the **Name** column. These names will then appear throughout the HYDRUS GUI, e.g., at the **Edit Bar** or in the **Sort Property Object** window.

3.2.4. Neural Network Predictions

The HYDRUS code was coupled with the Rosetta Lite DLL (Dynamically Linked Library) (Fig. 21), which was independently developed by Marcel Schaap at the U.S. Salinity Laboratory [Schaap *et al.*, 2001]. Rosetta implements pedotransfer functions (PTFs), which predict *van Genuchten*'s [1980] water retention parameters and the saturated hydraulic conductivity (K_s) in a hierarchical manner from soil textural class, the soil textural distribution, bulk density, and one or two water retention points as input. Rosetta has its own help features containing all relevant information and references. Rosetta provides soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA textural triangle (Table 8).

The dialog window 'Pedotransfer Functions' is shown. It has a blue title bar with a close button. The 'Pedotransfer Model' section has two radio buttons: 'Rosetta Lite (Neural Networks) [Schaap et al., 2001]' (selected) and 'Support Vector Machines [Twarakavi et al., 2009]'. The 'Selected Model (Data Availability)' section has four radio buttons: 'Textural Classes', '% Sand, Silt, and Clay (SSC)' (selected), '% Sand, Silt, Clay, and Bulk Density (SSCBD)', and 'SSCBD + water content at 33 kPa (Theta_33)'. The 'Output' section has a radio button for 'Same + water content at 1500 kPa (Theta_1500)'. The 'Input' section has a 'Textural Class' dropdown set to 'Clay'. Below it are input fields for 'Sand' (30 [%]), 'Silt' (40 [%]), 'Clay' (30 [%]), 'Bulk Density' (1.35 [gr/cm3]), 'Theta_33' (0.33 [cm3/cm3]), and 'Theta_1500' (0.05 [cm3/cm3]). The 'Output' section has a 'Calculate output' button set to 'Predict'. Below it are output fields for 'Theta_r' (0.0795142 [cm3/cm3]), 'Theta_s' (0.437296 [cm3/cm3]), 'Alpha' (0.0101835 [1/cm]), 'n' (1.45686 [-]), and 'Ks' (10.7314 [cm/day]). At the bottom are 'OK', 'Cancel', and 'Help' buttons.

Parameter	Value	Unit
Textural Class	Clay	
Sand	30	[%]
Silt	40	[%]
Clay	30	[%]
Bulk Density	1.35	[gr/cm ³]
Theta ₃₃	0.33	[cm ³ /cm ³]
Theta ₁₅₀₀	0.05	[cm ³ /cm ³]
Theta _r	0.0795142	[cm ³ /cm ³]
Theta _s	0.437296	[cm ³ /cm ³]
Alpha	0.0101835	[1/cm]
n	1.45686	[-]
K _s	10.7314	[cm/day]

Figure 21. The Rosetta Lite (Neural Network Predictions) dialog window.

3.2.5. Anisotropy in the Hydraulic Conductivity

For two-dimensional problems, users may need to specify the principal components of the anisotropy tensor, K_1^A and K_2^A , together with the angle ω_a between the principal direction of K_1^A and the x-axis of the global coordinate system for each element (Fig. 22).

The dialog window titled "Edit Local Anisotropy" contains a sub-section "Local Anisotropy - Angle and Components". It features a "Number of Selected Elements" field set to 1. Below this, there are fields for "Angle" (set to 3) and its range "Min:" (3) to "Max:" (3). A checkbox labeled "Specify All Components Simultaneously" is checked. Underneath, there are two rows for "Component" values, each set to 1, with corresponding "Min:" and "Max:" range fields also set to 1. At the bottom are "OK", "Cancel", and "Help" buttons.

Figure 22. The Edit Local Anisotropy dialog window for two-dimensional applications.

This has been simplified for three-dimensional problems where users can specify one or more **Tensors of Anisotropy** (Fig. 23), which may be assigned to different parts of the transport domain. The anisotropy tensor is defined by three principal components, K_1^A (ConAX), K_2^A (ConAY), and K_3^A (ConAZ), and six coefficients a_{ij} that represent the cosine of angles between the i th principal direction of the tensor $\mathbf{K}^A$ and the j -axis of the global coordinate system (i.e., $\text{Cos}(X-x)$, $\text{Cos}(Y-y)$, $\text{Cos}(Z-z)$, $\text{Cos}(X-y)$, $\text{Cos}(X-z)$, $\text{Cos}(Y-z)$).

The dialog window titled "Tensors of Anisotropy" has a sub-section "Tensors of Anisotropy for Hydraulic Conductivity". It includes a "Number of Tensors of Anisotropy" field set to 1 and an "Update" button. Below is a table with 10 columns: Aniz, ConAX, ConAY, ConAZ, Cos(X-x), Cos(Y-y), Cos(Z-z), Cos(X-y), Cos(X-z), and Cos(Y-z). The first row shows values: 1, 1, 1, 1, 1, 1, 1, 0, 0, 0. To the right of the table are "OK", "Cancel", and "Help" buttons. At the bottom right, there is a cartoon character icon and "Next..." and "Previous..." buttons.

Aniz	ConAX	ConAY	ConAZ	Cos(X-x)	Cos(Y-y)	Cos(Z-z)	Cos(X-y)	Cos(X-z)	Cos(Y-z)
1	1	1	1	1	1	1	0	0	0

Figure 23. The Tensors of the Anisotropy dialog window.

3.2.6. Constraints on Hysteretic Model

In this dialog window, users can constrain optimized parameters (in the inverse mode) for problems involving hysteresis in the soil hydraulic properties. This dialog window is available only when an Inverse Problem is solved and when hysteresis is considered.

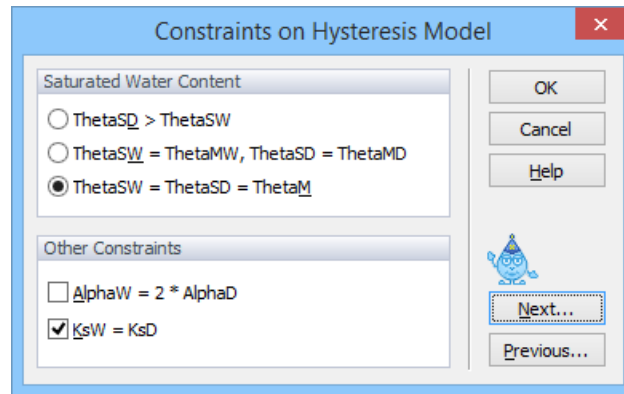


Figure 24. The Constraints on Hysteresis Model dialog window.

3.2.7. Water Flow Boundary Conditions in 1D

Users can select the upper and lower boundary conditions for water flow in one-dimensional applications in the **Water Flow Boundary Conditions** dialog window (Fig. 25).

Figure 25. The Water Flow Boundary Conditions dialog window for one-dimensional applications.

The following types of boundary conditions can be used for the soil surface boundary:

1. Constant Pressure Head (constant in time)
2. Constant Flux (constant in time)
3. Atmospheric BC with Surface Layer
4. Atmospheric BC with Surface Run-Off
5. Variable Pressure Head (variable in time)
6. Variable Pressure Head/Flux (variable in time)
7. Triggered Irrigation

The following types of boundary conditions can be used for the bottom boundary:

1. Constant Pressure Head (constant in time)
2. Constant Flux (constant in time)
3. Variable Pressure Head (variable in time)
4. Variable Pressure Flux (variable in time)
5. Free Drainage (unit gradient)
6. Deep Drainage
7. Seepage Face (with a specified pressure head value)
8. Horizontal Drains

For the **Atmospheric Boundary Conditions with a Surface Layer**, one needs to also specify the maximum thickness of the surface water layer (**Max h at Soil Surface**) before surface runoff is initiated.

Input PET and LAI: Instead of entering atmospheric fluxes (i.e., potential evaporation (E_p) and transpiration (T_p) fluxes), separately, it is also possible to enter a combined value of potential evapotranspiration (ET_p) and separate potential evaporation and transpiration fluxes from ET_p based on LAI and the extinction coefficient.

Interception: Interception can be considered in version 4.16 (and later) of HYDRUS-1D when the Leaf Area Index (LAI) is entered (see the Input PET and LAI option discussed above). One needs to specify an **Interception Constant** a (for ordinary agricultural crops $a \approx 0.25$ mm/d. For increasing amounts of precipitation, the amount of intercepted precipitation asymptotically reaches the saturation amount (the maximum interception) $a * LAI$. In principle, a must be determined experimentally and should be specified in the input file.

A detailed description of these boundary conditions and their mathematical and numerical implementation is given in the Technical Manuals.

Initial Conditions

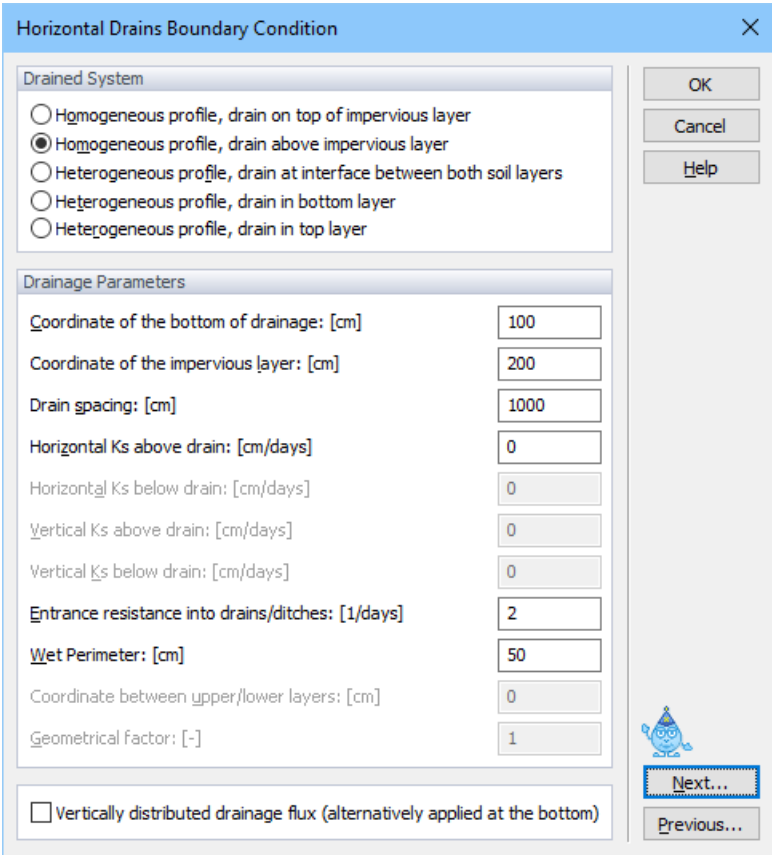
The initial condition can be specified either in terms of the pressure head or the water content. Note that when initial conditions are given in terms of water content, then for the dual-porosity model, the specified initial water content will be redistributed between the mobile and immobile domains proportionally to the saturated water contents of each domain. For the dual-permeability model, the specified initial water content will be interpreted as the initial water content in the matrix domain and the initial pressure head of the matrix domain will be calculated from this value. The fracture domain will then be assigned the same pressure head as the matrix domain.

Particle Tracking

The particle tracking module requires two input parameters: $wStand$ and $wPrec$. The $wStand$ parameter represents the water storage, which separates neighboring particles in the soil profile at the beginning of the simulation. Therefore, the particles are not geometrically evenly distributed when the soil profile's initial water content is not uniform. The $wPrec$ parameter is the amount of water that passes through the soil surface before a new particle is released. This means that particles are released at the soil surface only under wet conditions. When $wPrec$ is set to be negative, a new particle is released with each precipitation event (i.e., when $vTop$ becomes negative). Under dry conditions, the surface flux is directed out of the soil profile, and thus, new particles will not be released.

3.2.8. Water Flow to Tile Drains

When a **Horizontal** Drains boundary condition is selected as a bottom boundary condition, the description of the horizontal tile drain system is given in the **Horizontal Drains Boundary Conditions** dialog window (Fig. 26).



The dialog window titled "Horizontal Drains Boundary Condition" contains two main sections: "Drained System" and "Drainage Parameters".

Drained System: This section contains five radio button options for selecting a drainage model:

- ☐ Homogeneous profile, drain on top of impervious layer
- ☒ Homogeneous profile, drain above impervious layer
- ☐ Heterogeneous profile, drain at interface between both soil layers
- ☐ Heterogeneous profile, drain in bottom layer
- ☐ Heterogeneous profile, drain in top layer

Drainage Parameters: This section contains ten input fields with their respective units:

- Coordinate of the bottom of drainage: [cm] (value: 100)
- Coordinate of the impervious layer: [cm] (value: 200)
- Drain spacing: [cm] (value: 1000)
- Horizontal Ks above drain: [cm/days] (value: 0)
- Horizontal Ks below drain: [cm/days] (value: 0)
- Vertical Ks above drain: [cm/days] (value: 0)
- Vertical Ks below drain: [cm/days] (value: 0)
- Entrance resistance into drains/ditches: [1/days] (value: 2)
- Wet Perimeter: [cm] (value: 50)
- Coordinate between upper/lower layers: [cm] (value: 0)
- Geometrical factor: [-] (value: 1)

At the bottom, there is a checkbox labeled "Vertically distributed drainage flux (alternatively applied at the bottom)".

On the right side of the dialog, there are four buttons: "OK", "Cancel", "Help", and "Next...". The "Next..." button is highlighted with a blue border. Below the "Next..." button is a "Previous..." button.

Figure 26. The Horizontal Drains Boundary Conditions dialog window (for one-dimensional applications).

When this lower boundary condition is selected, it approximates water flow to horizontal tile drains, and the analytical solutions derived by *Houghoudt* [1940] and *Ernst* [1962] are used for this purpose. A particular analytical solution is selected depending on the description of the horizontal tile drain system.

Users must first specify the model (homogeneity of the profile and location of drains) as it applies to a specific problem involving tile drainage. The drains can be located:

- in a homogeneous soil profile on top of an impervious layer
- in a homogeneous soil profile above an impervious layer
- in a layered soil profile at the interface between two soil layers
- in a layered soil profile in the bottom layer
- in a layered soil profile in the top layer

Depending on the drainage model being used, the user has to specify the following parameters characterizing the particular model:

- Coordinate of the bottom of the drain system [L]
- Drain spacing [L]
- Entrance resistance of the drain to water flow [T]
- Horizontal saturated hydraulic conductivity of the soil layer above the drain [L/T]
- Horizontal saturated hydraulic conductivity of the soil layer below the drain [L/T]
- Vertical saturated hydraulic conductivity of the soil layer above the drain [L/T]
- Vertical saturated hydraulic conductivity of the soil layer below the drain [L/T]
- Wet perimeter of the drain [L]
- Coordinate of the impervious layer [L]
- Coordinate of the transition between the upper and lower soil layers [L]
- Geometric factor (from the table in the manual) [-]

A user can also choose if the drainage flux (to horizontal drains) should be applied at the bottom of the soil profile or vertically distributed along the saturated part of the soil profile. This selection impacts mainly the results for solute transport (concentrations may be very different at the water table than at the bottom of the soil profile), rather than for water flow.

3.3. Solute Transport

3.3.1. Solute Transport - General

The basic information needed for defining the solute transport problem is entered in the **Solute Transport** dialog window (Fig. 27 for 1D applications, Fig. 28 for 2D/3D applications). In this window, users specify the **Space** and **Time Weighting Schemes**, the **Iteration Criteria** (for nonlinear problems), and additional **Solute Information** such as mass units, pulse duration (if applicable), and a number of solutes.

The dialog window is titled "Solute Transport - General Information" and contains several sections for configuring the solute transport problem.

- Time Weighting Scheme:** Includes radio buttons for "Explicit Scheme", "Crank-Nicholson Scheme" (selected), and "Implicit Scheme".
- Space Weighting Scheme:** Includes radio buttons for "Galerkin Finite Elements" (selected), "Upstream Weighting FE", and "GFE with Artificial Dispersion".
- Solute Information:** Contains input fields for "Number of Solutes" (1), "Mass Units" (-), "Pulse Duration [day]" (273), and "Stability Criterion" (2). It also includes checkboxes for "Temperature Dependence of Parameters", "Water Content Dependence of Parameters", "Use Tortuosity" (checked), and "Millington & Quirk" (selected). Other options include "Fumigant Module", "Additional Fumigant Application at a Given Time", "Surfactant Module", and "PFAS Module (Sorption to Air-Water Interface)".
- Solute Transport Models:** Lists various models with radio buttons, including "Equilibrium Model (Standard Solute Transport Model)" (selected), "One-Site Sorption Model (Chemical Nonequilibrium)", "Two-Site Sorption Model (Chemical Nonequilibrium)", "Two Kinetic Sites Model (Particle Transport Using Attachment/Detachment, Chemical Nonequilibrium)", "Two Kinetic Sites Model (Based on Filtration Theory, Chemical Nonequilibrium)", "Dual-Porosity (Mobile-Immobile Water) Model (Physical Nonequilibrium)", "Dual-Porosity Model with Two-Site Sorption in the Mobile Zone (Physical and Chemical Nonequilibrium)", "Dual-Permeability Model (Physical Nonequilibrium)", and "Dual-Permeability Model with either Immobile Water in the Matrix or Kinetic Sorption (Physical and Chemical Nonequilibrium)".
- Iteration Criteria (Needed only for Nonlinear Adsorption or Blocking Functions):** Includes input fields for "Absolute Concentration Tolerance [M/L³]" (0), "Relative Concentration Tolerance [-]" (0), and "Maximum Number of Iterations" (1).

Navigation buttons on the right include "OK", "Cancel", "Help", "Next ..." (highlighted with a blue border), and "Previous ...". A small cartoon character is also visible near the "Next ..." button.

Figure 27. The Solute Transport dialog window for 1D applications.

Solute Transport

Time Weighting Scheme

- ☐ Explicit Scheme
- ☒ Crank-Nicholson Scheme
- ☐ Implicit Scheme

Space Weighting Scheme

- ☒ Galerkin Finite Elements
- ☐ Upstream Weighting FE
- ☐ GFE with Artificial Dispersion

Solute Information

Number of Solutes: Mass Units:

Pulse Duration [sec]: Stability Criterion:

☐ Temperature Dependence of Parameters

☐ Water Content Dependence of Parameters

☒ Use Tortuosity ☒ Millington & Quirk ☐ Moldrup

☐ Attachment/Detachment Concept (virus, bacteria transport) ☐ Filtration Theory

☐ Fumigant Module ☐ Additional Fumigant Application at a GivenTime

☐ Surfactant Module ☐ PFAS Module (Sorption to Air-Water Interface)

Iteration Criteria (for Nonlinear Adsorption only)

Absolute Concentration Tolerance [M/L³]:

Relative Concentration Tolerance [-]:

Maximum Number of Iterations:

Initial Conditions

- ☒ In Liquid Phase Concentrations [Mass_solute/Volume_water]
- ☐ In Total Concentrations [Mass_solute/Volume_soil]
- ☐ Nonequilibrium phase is initially at equilibrium with equilibrium phase

OK Cancel Help

Next ... Previous ...

Figure 28. The Solute Transport dialog window for 2D/3D applications.

a) Time Weighting Scheme

The **Time Weighting Scheme** defines the temporal weighting coefficient, ε , used in the numerical solution of the transport equation. The temporal weighting coefficient is equal to 0.0 for an *explicit scheme*, 0.5 for a *Crank-Nicholson time-centered implicit scheme*, and 1.0 for a *fully implicit scheme*. The structure of the final set of linear equations $[G] \{c\} = \{g\}$, obtained after the spatial and temporal discretization of the governing advection-dispersion equation, depends upon the value of the temporal weighing factor, ε . The explicit ($\varepsilon=0$) and fully implicit ($\varepsilon=1$) schemes require that the global matrix $[G]$ and the vector $\{g\}$ be evaluated at only one-time level (the previous or current time level). The other two schemes require evaluation at both time levels. Also, the Crank-Nicholson and implicit schemes lead to an asymmetric banded matrix $[G]$. By contrast, the explicit scheme ($\varepsilon=0$) leads to a diagonal matrix $[G]$, which is much easier to solve (but generally requires much smaller time steps).

The Crank-Nicholson-centered scheme is recommended in view of solution precision. The fully implicit scheme also leads to numerical dispersion, but is better in avoiding numerical instabilities. The explicit scheme is most prone to numerical instabilities with undesired oscillations (and is currently disabled).

b) Space Weighting Scheme

HYDRUS provides three options for the **Space Weighting Scheme**, i.e., the regular *Galerkin Finite Elements* formulation, the *Upstream Weighting Finite Elements* formulation, and the *Galerkin Finite Elements* formulation with *Artificial Dispersion*.

While the **Galerkin Finite Elements** formulation is recommended in view of solution precision, **Upstream Weighting** is provided as an option in HYDRUS to minimize some of the problems with numerical oscillations when relatively steep concentration fronts are being simulated. For this purpose, the second (flux) term of advective-dispersive equation is not weighted by regular linear basis functions, but instead using nonlinear functions [Yeh and Tripathi, 1990]. The weighing functions ensure that relatively more weight is placed on flow velocities of nodes located at the upstream side of an element.

Additional **Artificial Dispersion** may also be added to stabilize the numerical solution and to limit or avoid undesired oscillations in the Galerkin finite element results. Artificial dispersion is added so that a **Stability Criterion** involving $Pe.Cr$ (the product of the Peclet number and the Courant number) [Perrochet and Berod, 1993] is satisfied. The recommended value for $Pe.Cr$ is 2.0.

c) Solute Information

Number of Solutes	Number of solutes to be simulated simultaneously or involved in a decay chain reaction.
Pulse Duration	Time duration of the concentration pulse. Concentrations (flux or resident) along all boundaries, for which no time-variable boundary conditions are specified, are then set equal to zero for times larger the " Pulse Duration ". When the Fumigant option is active, this variable is used instead to define Time of Tarp Removal .
Mass Units	Units to be printed to the output files or displayed in various graphs. Mass units have no effect on the calculations. Concentration units, in general, should be given in $[ML^{-3}]$, where M is Mass Units specified in the Solute Transport dialog window (Fig. 22), and L is Length Units specified in the Domain Type and Units dialog window (Fig. 6). However, since the concentration variable appears in each term of the governing solute transport equations (Eq. 3.1 and 3.2 of the Technical Manual), it is possible to use different length units than those used to define geometry and fluxes (e.g., geometry may be specified in meters while concentrations are given in mg/cm^3). In such cases, the solute fluxes (cq) will then be in units of $ML_c^{-3}L_gT^{-1}$ where L_c is the length unit (e.g., cm) used to define concentrations and L_g the length unit defining geometry and fluxes (e.g., m). Similarly, the solute mass ($c\theta V$) obtained by integrating solute over the transport domain will be in units of $ML_c^{-3}L_g^2$. Similar adjustments of units

	need to be done for other variables that involve both concentration and length units.
Stability Criterion	Product of the dimensionless Peclet and Courant numbers (Pe.Cr). This criterion is used either to add artificial dispersion in the <i>Galerkin Finite Elements with Artificial Dispersion</i> scheme or to limit the time step (leading to lower Courant numbers for a given Peclet number) for the <i>Galerkin Finite Elements</i> scheme.
Use Tortuosity Factor	Check this box when molecular diffusion coefficients in the water and gas phases are to be multiplied by a tortuosity factor according to the formulation of either <i>Millington and Quirk</i> [1961] or <i>Moldrup et al.</i> [1997, 2000].
Temperature Dependence	Check this box if the solute transport and reaction parameters are assumed to be temperature dependent.
Water Content Dependence	Check this box if the solute reaction parameters are assumed to be water content dependent [Walker, 1974].
Attachment/Detachment	Check this box if the solute is assumed to be subject to attachment/detachment to/from the solid phase. This process is often used in simulations of the transport of viruses, colloids, or bacteria.
Filtration Theory	Check this box if the attachment coefficient is to be calculated from filtration theory.
Fumigant Module	Additional options related to fumigant transport (e.g., tarp removal, temperature-dependent tarp properties, an additional injection of fumigants) can be used with this module [Spurlock et al., 2013].
PFAS Module	The PFAS module includes options to consider sorption to the air-water interface and the concentration effects on surface tension and viscosity [Silva et al., 2020]. This add-on module exists for one-, two-, and three-dimensional applications.

d) Iteration Criteria

The advection-dispersion solute transport equation becomes nonlinear when nonlinear adsorption is considered. Similarly, as for the Richards equation, an iterative process must then be used to obtain solutions of the global matrix equation at each new time step. During each iteration, a system of linearized algebraic equations is derived and solved using either Gaussian elimination or the conjugate gradient method. After inversion, the coefficients are re-evaluated using the initial solution, and the new equations are again solved. This iterative process continues until a satisfactory degree of convergence is obtained, i.e., until at all nodes the absolute change in concentration between two successive iterations becomes less than some concentration tolerance (defined in HYDRUS as the sum of an **Absolute Concentration Tolerance** and the product of the concentration and a **Relative Concentration Tolerance** (the recommended and default value is 0.001)). The **Maximum Number of Iterations** allowed during a certain time step needs to be specified (recommended value is 10). When the **Maximum Number of Iterations** is reached

then the numerical solution is either (a) terminated for problems involving transient water flow or (b) restarted with a reduced time step for steady-state flow problems.

e) Initial Conditions

Initial Conditions can be specified either using liquid-phase concentrations in units of mass of solute $[M_c]$ per volume of water $[M_c L_w^{-3}]$ or using total concentrations in units of mass of solute per volume of soil $[M_c L_s^{-3}]$. In the latter case, the liquid phase concentration is calculated from the total concentration depending on the distribution coefficients (e.g., K_d , or Henry's constant) between different phases.

Rather than specifying directly the initial values of the nonequilibrium phase concentrations (e.g., concentrations in the immobile water for the dual-porosity models or concentrations kinetically sorbed to the solid phase for the two-site sorption models, or for concentrations associated with the solid phase for the attachment/detachment models), users can specify that the nonequilibrium phase concentrations are initially at equilibrium with the equilibrium phase concentrations. Initial conditions need to be then specified only for the liquid phase concentrations, and the nonequilibrium phase concentrations are calculated by HYDRUS.

In the **Solute Transport** dialog window for 1D applications (Fig. 27), users can select various equilibrium and nonequilibrium solute transport models [Šimůnek and van Genuchten, 2006]. These models include:

- Equilibrium Model

- One-Site Sorption Model (Chemical Nonequilibrium)

- Two-Site Sorption Model (Chemical Nonequilibrium)

- Two Kinetic Sites Model (Particle Transport Using Attachment/Detachment, Chemical Nonequilibrium). This model is often used for the transport of viruses, colloids, or bacteria.

- Two Kinetic Sites Model (Based on Filtration Theory, Chemical Nonequilibrium)

- Dual-Porosity (Mobile-Immobile Water) Model (Physical Nonequilibrium)

- Dual-Porosity Model with Two-Site Sorption in the Mobile Zone (Physical and Chemical Nonequilibrium)

- Dual-Permeability Model (Physical Nonequilibrium)

- Dual-Permeability Model with either Immobile Water in the Matrix or Kinetic Sorption (Physical and Chemical Nonequilibrium)

While these equilibrium and nonequilibrium solute transport models are available in 2D/3D applications (with the exception of the dual-permeability model in 3D), the model selection is recognized directly based on the values of selected parameters, such as **Frac** and **ThImob** (see Chapter 3.3.2).

The UNSATCHEM Module

When the UNSATCHEM module is used, basic information needed for defining solute transport problem is entered in the **Solute Transport** dialog window displayed in Figure 29 (instead of Figures 27 or 28, which is used for the standard solute transport module). In this window, users specify again the **Space** and **Time Weighting Schemes** and additional **Solute Information** such

as mass units. Note that all concentrations in the UNSATCHEM module are either in meq/L (in the liquid phase) or meq/kg (in the solid phase) (meq=mmol_c). The pulse duration is not used in UNSATCHEM, and the number of solutes is fixed to 8 (i.e., the number of considered major ions: Ca²⁺, Mg²⁺, Na⁺, K⁺, Alkalinity, SO₄²⁻, Cl⁻, and an independent tracer). The number of solution, adsorbed, and precipitated concentration combinations is specified when simulating the transport of major ions in the UNSATCHEM module. This value represents the maximum number of (solution, adsorbed, and precipitated) concentration combinations, which can be used to specify the initial and boundary conditions.

Users are referred to the UNSATCHEM manuals [Šimůnek *et al.*, 2012c; 2021], which provides all relevant information about this module.

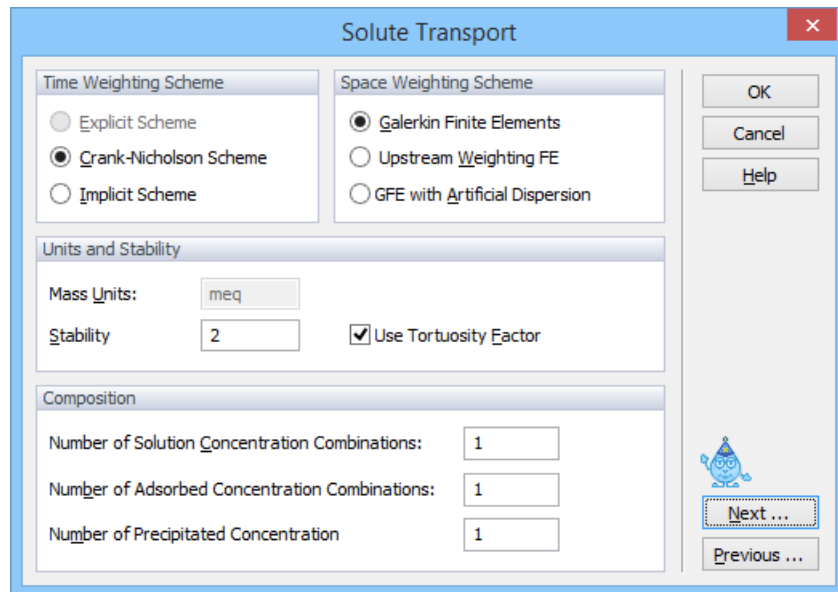


Figure 29. The Solute Transport dialog window for the UNSATCHEM module.

3.3.2. Solute Transport Parameters

Soil and Solute Specific Transport Parameters are specified in the **Solute Transport Parameters** dialog window (Fig. 30).

Mat	Bulk.D. [M/cm ³]	Disp.L. [cm]	Disp.T. [cm]	Fract. [-]	ThImob. [-]
1	1.5	0.1	0.01	1	0
2	1.5	0.1	0.01	1	0

Sol	Diffus. W. [cm ² /min]	D_soil [cm]
1	0	0
2	0	0
3	0	0

Figure 30. The Solute Transport Parameters dialog window.

The following **Soil Specific Parameters** (left part of the dialog window) are specified for each soil material:

- Bulk.d.** Bulk density, ρ [ML⁻³]
- Disp.L.** Longitudinal dispersivity, D_L [L]
- Disp.T.** Transverse dispersivity, D_T [L] (this variable is available only for 2D/3D applications)
- Frac** Dimensionless fraction of adsorption sites classified as type-1 sites, i.e., sites with instantaneous sorption when the **chemical nonequilibrium** option is considered [-]. Set this parameter equal to 1 when equilibrium transport is considered. *Frac* becomes the dimensionless fraction of adsorption sites in contact with mobile water when the **physical nonequilibrium** option is considered [-]. In that case, *Frac* should be set equal to 1 when all sorption sites are in contact with mobile water.
- ThImob** The immobile water content. Set equal to 0 when the **physical nonequilibrium** option is not considered.

The following **Solute Specific Parameters** (right part of the dialog window) are specified for each solute:

- Diffus.W** Molecular diffusion coefficient in free water, D_w [L²T⁻¹]
- Diffus.G** Molecular diffusion coefficient in soil air, D_a [L²T⁻¹]

3.3.3. Solute Reaction Parameters

The *Solute Reaction Parameters* and concentrations for *Boundary Conditions* are specified in the **Solute Reaction Parameters** dialog window (Fig. 31). Each solute has its own Solute Reaction Parameters dialog window. The **Solute Reaction Parameters** dialog window for one-dimensional applications is the same except that it does not contain the *Boundary Conditions* section.

Reaction Parameters for Solute - 1

Boundary Conditions									
	cBnd1	cBnd2	cBnd3	cBnd4	cRoot	cWell	cBnd7	cAtm	d
1	1	0	0	0	0	0	0	0	0

Reaction Parameters									
Mat	Kd=0	Nu=0	Beta=1	Henry=0	SinkL1=0	SinkS1=0	iPsi2	iPsi1	SMi
1	0	0	1	0	0	0	0	0	
2	0	0	1	0	0	0	0	0	

Figure 31. The Solute Reaction Parameters dialog window.

The following **Solute Reaction Parameters** are specified for each soil material:

Kd	Adsorption isotherm coefficient, k_s [$M^{-1}L^3$]
Nu	Adsorption isotherm coefficient, η [$M^{-1}L^3$]
Beta	Adsorption isotherm exponent, β [-]
Henry	Equilibrium distribution constant between liquid and gaseous phases, k_g [-]
SinkL1	First-order rate constant for dissolved phase, μ_w [T^{-1}]
SinkS1	First-order rate constant for the solid phase, μ_s [T^{-1}]
SinkG1	First-order rate constant for the gas phase, μ_g [T^{-1}]
SinkL1'	First-order rate constant for the dissolved phase, μ_w' [T^{-1}], as part of a solute decay chain
SinkS1'	First-order rate constant for the solid phase, μ_s' [T^{-1}], as part of a solute decay chain
SinkG1'	First-order rate constant for the gas phase, μ_g' [T^{-1}], as part of a solute decay chain
SinkW0	Zero-order rate constant for the dissolved phase, γ_w [$ML^{-3}T^{-1}$]
SinkS0	Zero-order rate constant for the solid phase, γ_w [T^{-1}]
SinkG0	Zero-order rate constant for the gas phase, γ_s [$ML^{-3}T^{-1}$]

Alpha First-order rate coefficient for one-site or two-site nonequilibrium adsorption, mass transfer coefficient for solute exchange between mobile and immobile liquid regions, ω [T⁻¹]

When the **Attachment/Detachment Model** (Fig. 28) is used, then some parameters listed above are replaced with different parameters needed for the attachment/detachment model:

D_Soil Diameter of the sand grains, d_c [L]. Note that HYDRUS allows only one value (for all materials) and that this value is used only in the Depth-dependent blocking function (iPsi=4) developed by *Bradford et al.* [2002], which was developed for homogeneous laboratory column. It is less clear what value should be used in multi-layered systems (for other than the first layer). Also, note that this blocking function depends on a vertical spatial coordinate. This means that one needs to specify the origin of the function, i.e., the inflow and inter-material interfaces. HYDRUS allows doing this for up to 2 materials using the cBnd vector, as described in the help.

iPsi2 Type of blocking on the second sorption sites:
= 0: No blocking.
= 1: Langmuirian dynamics.
= 2: Ripening.
= 3: random sequential adsorption model.
= 4: depth-dependent blocking coefficient.

iPsi1 Same for the first sorption sites.

SMax2 Parameter in the blocking function for the second sorption sites (s_{max} for blocking options (1), (2) and (3), and b for (4)).

AttachSolid2 First-order deposition (attachment) coefficient, k_a [T⁻¹], for the second sorption sites.

DetachSolid2 First-order entrainment (detachment) coefficient, k_d [T⁻¹], for the second sorption sites.

SMax1 Parameter in the blocking function for the first sorption sites.

AttachSolid1 First-order deposition (attachment) coefficient, k_a [T⁻¹], for the first sorption sites.

DetachSolid1 First-order entrainment (detachment) coefficient, k_d [T⁻¹], for the first sorption sites.

When **Filtration Theory** (Fig. 28) is used to calculate the attachment coefficient, then the following parameters must be entered instead:

D_Soil Diameter of the sand grains, d_c [L].

D_Virus Diameter of the particle, d_p (e.g., virus, bacteria) (e.g., = 0.95 μ m or 0.95e-6 m) [L].

SMax2 Parameter in the blocking function for the second sorption sites (s_{max} for model (1)).

Stick. Eff2 Sticking efficiency, a [-], for the second sorption sites.

DetachSolid2 First-order entrainment (detachment) coefficient, k_d [T⁻¹], for the second sorption sites.

SMax1	Parameter in the blocking function for the first sorption sites.
Stick. Eff1	Sticking efficiency, a [-], for the first sorption sites.
DetachSolid1	First-order entrainment (detachment) coefficient, k_d [T^{-1}], for the first sorption sites.

When the **PFAS Module** (Fig. 28) is used, then the following parameters must be entered instead of Henry, SinkL1', SinkS1', and SinkG1', respectively:

KH_AWI	Equilibrium distribution constant between the liquid phase and air-water interface, K_H , [$L^{3\beta}M^{-\beta}$].
Scal_AWI	A scaling constant k_m to linearly scale the interfacial area A_{aw} .
Nu_AWI	Parameter, K_L [$L^{3\beta}M^{-\beta}$]. Set equal to zero if Langmuir sorption to the air-water interface is not to be considered.
Beta_AWI	Coefficient, β [-]. Set equal to one if Freundlich sorption to the air-water interface is not to be considered.

Boundary Conditions:

Concentrations for time-independent Boundary Conditions are also specified in this dialog window (only for the 2D/3D applications).

cBnd1	Value of the concentration for the first time-independent boundary condition [ML^{-3}]. Set equal to zero if no time-independent boundary condition is specified. The same for cBnd2 through cBnd4
cRoot	Value of the concentration for the fifth time-independent boundary condition [ML^{-3}]. If water uptake is considered, then <i>cRoot</i> is automatically used for the maximum concentration of water removed from the flow region by root water uptake. When zero is specified, then all solute is left behind in the soil, and only a solute-free solution is being taken up. When the concentration is lower than <i>cRoot</i> , all solute is taken up. When the concentration is higher than <i>cRoot</i> , the excess solute stays behind. Set equal to zero if no fifth time-independent boundary condition and no solute uptake by roots is considered.
cWell	Value of the concentration for the sixth time-independent boundary condition [ML^{-3}]. If internal sources are specified, then <i>cWell</i> is automatically used for the concentration of water injected into the flow region through internal sources. Set equal to zero if no sixth time-independent boundary condition and no internal sources are specified.
cBnd7	Concentration of the incoming fluid for a volatile type boundary condition at the soil surface [ML^{-3}]. Set equal to zero if no volatile boundary condition is specified.
cAtm	Concentration above the stagnant boundary layer, g_{atm} [ML^{-3}], for a volatile type boundary condition. Set equal to zero if no volatile boundary condition is specified.
d	Thickness of the stagnant boundary layer, d [L], for a volatile type boundary condition. Set equal to zero if no volatile boundary condition is specified.

When the parameter estimation option is selected, users have to provide initial estimates of the optimized solute transport parameters, specify which parameters are to be optimized (select

appropriate checkboxes), and provide parameter constraints for the optimization. Zero values for minimum and maximum values signify that the parameters are unconstrained. The **Solute Transport and Reaction Parameters** dialog window for the inverse problem is not further shown here.

Mat	Bulk.d. [g/cm ³]	Dw [cm ² /day]	Disper.L. [cm]	Disper.T. [cm]	CEC [meq/kg]	Calc.SA [m ² /L]	olom.SA [m ² /L]	DOC	K[Ca.
1	1.4	2	2	0.2	10	0	0	0	
2	1.3	1	0	0	0	0	0	0	

Figure 32. The Solute Reaction Parameters dialog window for the UNSATCHEM module.

The UNSATCHEM Module

When the UNSATCHEM module is used, the *Solute Reaction* (and *transport*) *Parameters* are specified in the **Solute Reaction Parameters** dialog window displayed in Figure 32 (instead of Figure 31, used for the standard solute transport module). The following **Soil Specific Parameters** are specified for each soil material:

Bulk.d.	Bulk density, ρ [ML ⁻³]
Dw	Molecular diffusion coefficient in free water, D_w [L ² T ⁻¹]
Disper.L.	Longitudinal dispersivity, D_L [L]
Disper.T.	Transverse dispersivity, D_T [L]
CEC	Cation exchange capacity, CEC [meq/kg]
Calc.SA	Calcite surface area [m ² /dm ³]
Dol.SA	Dolomite surface area [m ² /dm ³]
DOC	Dissolved organic carbon [mmol/dm ³]
K[Ca/Mg]	Gapon constant for exchange of calcium and magnesium
K[Ca/Na]	Gapon constant for exchange of calcium and sodium
K[Ca/K]	Gapon constant for exchange of calcium and potassium

3.3.4. Temperature Dependence of Solute Reaction Parameters

Several of the diffusion (D_w , D_g), zero-order production (γ_w , γ_s , γ_g), first-order degradation (μ_w , μ_s , μ_g), and adsorption (k_s , k_g , β , η , ω) coefficients may be strongly dependent upon temperature. HYDRUS assumes that this dependency can be expressed by the Arrhenius equation [Stumm and Morgan, 1981]. This equation can be expressed in the general form

$$a_T = a_r \exp \left[\frac{E_a(T^A - T_r^A)}{R_u T^A T_r^A} \right]$$

where a_r and a_T are values of the coefficient being considered at a reference absolute temperature T_r^A and absolute temperature T^A , respectively; R_u is the universal gas constant, and E_a [$\text{ML}^2\text{T}^{-2}\text{M}^{-1}$] is the activation energy of the particular reaction or process being modeled.

The activation energy, characterizing the temperature dependence of the solute transport and reaction parameters, is entered in the dialog window shown in Figure 33.

When the Fumigant option is active, the fifth variable (normally reserved for the Freundlich exponent) is used to enter the activation energy for the resistance of the surface tarp.

	SinkWater1	SinkSolid1	SinkGas1	SinkWater1'	SinkSolid1'	S
1	51213	0	0	81171	0	
2	51213	0	0	81171	0	
3	51213	0	0	81171	0	

Figure 33. The Temperature-Dependent Solute Transport and Reaction Parameters dialog window.

3.3.5. Water Content Dependence of Solute Reaction Parameters

The water content dependence of degradation coefficients is implemented using a modified equation of Walker [1974]:

$$\mu(\theta) = \mu_r(\theta_r) \min \left[1, \left(\frac{\theta}{\theta_r} \right)^B \right]$$

where μ_r is the values of a particular coefficient (rate constant) at the reference water content θ_r , μ is the value of this coefficient at the actual water content θ , and B is a solute-dependent parameter (usually 0.7). The reference water content, θ_r , which may be different for different soil layers, is calculated from the reference pressure head, h_r , which is considered to be constant for a particular compound. The solute dependent exponent, B , and the reference pressure head, h_r , are entered in the **Water Content Dependent Solute Reaction Parameters** dialog window shown in Figure 34.

Water Content Dependent Solute Reaction Parameters

Parameter 1 (B)

Sol	SinkWater1	SinkSolid1	SinkGas1	SinkWater1'	SinkSolid1'	SinkGas1'	SinkWater0	SinkSolid0	SinkGas0
1	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0

Parameter 2 (h_ref [cm])

Sol	SinkWater1	SinkSolid1	SinkGas1	SinkWater1'	SinkSolid1'	SinkGas1'	SinkWater0	SinkSolid0	SinkGas0
1	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0

OK
Cancel
Help
Next ...
Previous ...

Figure 34. The Water Content Dependent Solute Reaction Parameters dialog window.

3.3.6. Solution Compositions for the UNSATCHEM Module

The set of solution, adsorbed, and precipitated concentration combinations for the UNSATCHEM module is specified in the **Solution Compositions** dialog window (Fig. 35). These (solution, adsorbed, and precipitated) concentration combinations can be used to specify the initial and boundary conditions. The number of solution, adsorbed, and precipitated concentration combinations is specified in the **General Solute Transport Information** window (Fig. 29). **Solution Concentrations** need to be specified for all major ions: Ca^{2+} , Mg^{2+} , Na^+ , K^+ , Alkalinity, SO_4^{2-} , Cl^- , and an independent tracer; **Adsorbed Concentrations** for all cations: Ca^{2+} , Mg^{2+} , Na^+ , and K^+ ; and **Precipitated Concentrations** for all solids that UNSATCHEM can consider: calcite, dolomite, gypsum, nesquehonite, hydromagnesite, and sepiolite. **Solution Concentrations** need to be specified in meq/L (L = liter), and **Adsorbed Concentrations** and **Precipitated Concentrations** in meq/kg (meq=mmol_c).

Solution Compositions

Solution Concentrations [meq/L]

Sol	Ca	Mg	Na	K	Alk	SO4	Cl	
1	32.6	1.05	4.8	0	0.4	32	5	1
2	32.6	9.66	4.8	0	0.4	32	4.6	

Adsorption Concentrations [meq/kg]

Ads	Ca	Mg	Na	K
1	50	20	9.5	1

Precipitated Concentrations [meq/kg]

Prec	Calcite	Gypsum	Dolomite	HydroMg	Nesqoh	Sepic
1	500	200	0	0	0	

OK
Cancel
Help
Next ...
Previous ...

Figure 35. The Solution Compositions dialog window for the UNSATCHEM module.

3.3.7. Chemical Parameters for the UNSATCHEM module.

The following chemical parameters and selections for the UNSATCHEM module are specified in the **Chemical Parameters** dialog window (Fig. 36):

- Whether the kinetic or equilibrium model for the precipitation and dissolution of calcite and dissolution of dolomite is to be used (the **Kinetic Precipitation/Dissolution** check box).
- Whether the silica content in the solution is to be calculated based on the solution pH, or whether the effect of pH is to be neglected (the **Silica in Solution (pH Dependency)** check box).
- The **Critical Ionic Strength**, i.e., the ionic strength, below which the extended Debye-Hückel equation is used to calculate ion activity coefficients. Pitzer virial-type equations are used above this value.
- The **Maximum Number of Iterations** allowed during any time step between the solute transport and chemical modules. When the maximum number of iterations is reached, then the code proceeds to the new time level. The recommended value (if the iterative approach is to be used; from our experience) is 5. Set equal to one if no iteration (we recommend this non-iterative approach) is required (this, in general, leads to significantly lower computational time without significantly altering the results in most cases).
- Whether the hydraulic conductivity is to be modified depending on the solution chemistry using the *McNeal* [1968] semi-empirical approach (the **Conductivity Reduction due to Chemistry** check box).

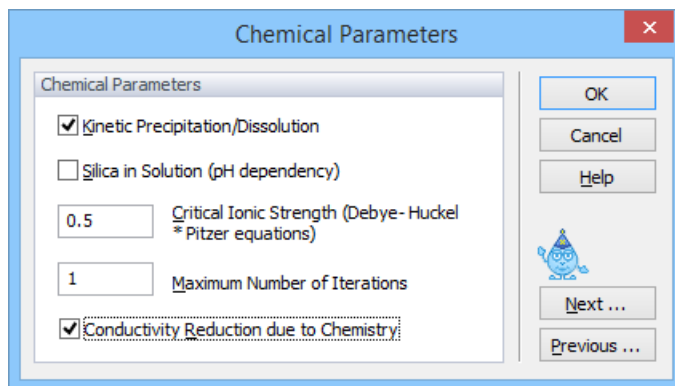


Figure 36. The Chemical Parameters dialog window for the UNSATCHEM module.

3.3.8. Additional Fumigant Application

When the **Fumigant Module** is used and an option **Additional Fumigant Application at a Given Time** is selected (Fig. 28), users can specify an additional application of a specified mass (Mass of Applied Fumigant) of a chemical into a specified location of the transport domain (defined by x, y, and z coordinates; the y-coordinate is disabled for 2D applications) at a specified time (Time of Additional Fumigant Application).

The 'Add Fumigant' dialog window is shown. It features a title bar with the text 'Add Fumigant' and a close button. The main content area is divided into two sections. The first section, 'Additional Fumigant Application', contains two input fields: 'Time of Additional Fumigant Application' with a value of 10, and 'Mass of Applied Fumigant' with a value of 25. The second section, 'Location of Fumigant Application', contains six input fields for coordinates: 'Min x-coordinate of application [cm]' (10), 'Max x-coordinate of application [cm]' (20), 'Min y-coordinate of' (100), 'Max y-coordinate of' (110), 'Min z-coordinate of application' (30), and 'Max z-coordinate of' (40). On the right side of the dialog, there are five buttons: 'OK', 'Cancel', 'Help', 'Next...', and 'Previous...'. A small cartoon character is positioned next to the 'Next...' button.

Figure 37. The Add Fumigant dialog window for the Fumigant module.

3.3.9. Surfactant Parameters

When the **PFAS Module** is used, and the Surfactant (concentration effects on surface tension and viscosity) option is selected (Fig. 28), users need to define parameters characterizing the concentration effects on surface tension and viscosity.

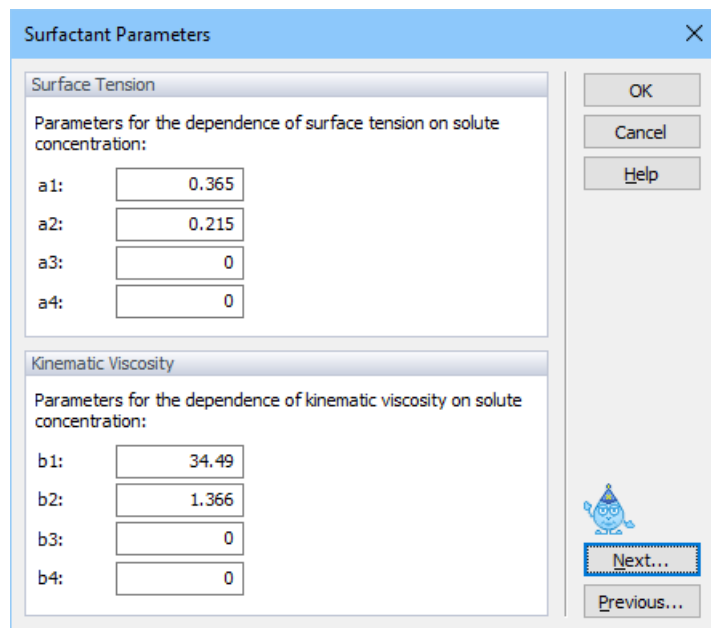


Figure 38. The Surfactant Parameters dialog window for the PFAS module.

In this dialog window, one defines parameters characterizing the concentration effects on surface tension and viscosity (used in the PFAS Module):

- a_1 Parameter a [L^3M^{-1}], describing the dependence of the surface tension on the solution concentration.
- a_2 Parameter b [-], describing the dependence of the surface tension on the solution concentration.
- a_3 Parameter currently not used
- a_4 Parameter currently not used
- b_1 Parameter d [L^3M^{-1}] describing the dependence of the kinematic viscosity on the solution concentration.
- b_2 Parameter e [-] describing the dependence of the kinematic viscosity on the solution concentration.
- b_3 Parameter currently not used
- b_4 Parameter currently not used

3.3.10. Solute Transport Boundary Conditions in 1D

Users can select the upper and lower boundary conditions for solute transport in one-dimensional applications in the **Solute Transport Boundary Conditions** dialog window (Fig. 39).

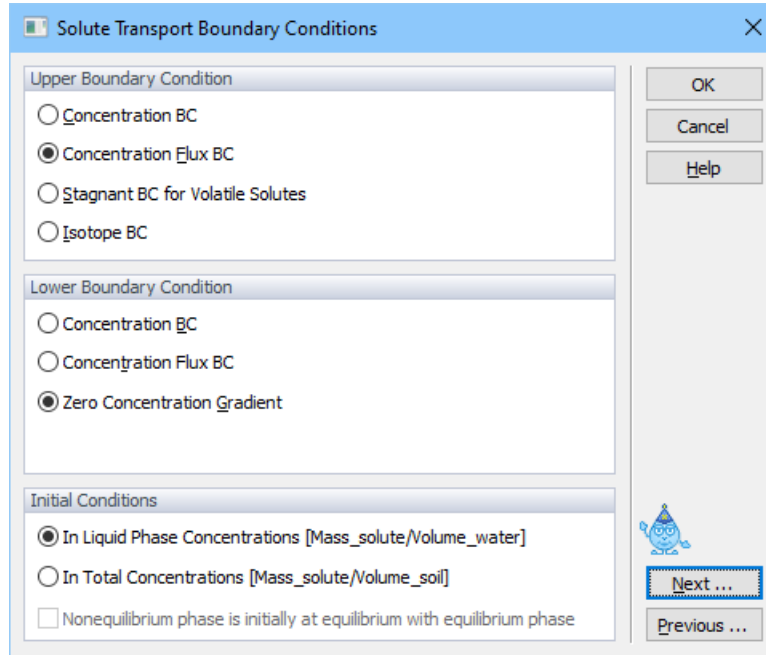


Figure 39. The Solute Transport Boundary Conditions dialog window for one-dimensional applications.

The following types of **upper boundary** conditions for solute transport are available:

- Concentration BC (user specifies a liquid phase concentration at the boundary)
- Concentration Flux BC (user specifies a liquid phase concentration of the infiltrating water)
- Stagnant BC for Volatile Solutes
- Isotope BC

Stagnant BC for Volatile Solutes: This boundary condition is used for solutes that can escape into the atmosphere by gaseous diffusion, i.e., for volatile solutes, such as fumigants, ammonium, and various organic compounds. The Thickness of the *Stagnant Boundary Layer* and the *Concentration in the Atmosphere* need to be specified for this BC.

Isotope BC: There is no solute leaving with evaporation at the atmospheric boundary for standard solutes. On the other hand, natural water isotopes are treated differently, since they do escape into the atmosphere during evaporation. When no fractionation during evaporation is considered for the isotope transport, then the concentration associated with evaporation is equal to the soil surface concentration $c(L,t)$. When constant fractionation during evaporation is considered for the isotope transport, then the concentration associated with evaporation is equal

to the soil surface concentration multiplied by a **Fractionation Ratio** r_{Fract} (input), i.e., $r_{Fract} * c(L,t)$.

The fractionation ratio r_{Fract} is defined as the fraction of isotopes that leave with evaporation. r_{Fract} is equal to zero for standard solute (no solute flux with evaporation), is equal to one when no fractionation is considered, and is smaller than one when constant fractionation is considered.

The following types of **lower boundary** conditions for solute transport are available:

Concentration BC (user specifies liquid phase concentration at the boundary)

Concentration Flux BC (user specifies liquid phase concentration of the infiltrating water)

Zero Concentration Gradient (free drainage)

Solute flux versus solute concentration boundary conditions:

A **third-type (Cauchy, solute flux) boundary condition** prescribes a solute flux (not concentration) at the boundary. Due to mixing with water (and solute) initially present in the profile, the boundary concentration does not immediately reach the value of the prescribed boundary concentration c_0 . Since this boundary condition prescribes the solute flux directly, there is complete control over the mass balance and how much solute enters into the transport domain.

If a **first-type (Dirichlet, concentration) BC** is used instead, the concentration at the boundary (not the solute flux into the domain) is prescribed. Since the solute flux consists of both advective and dispersive fluxes, both are active on the boundary as well. Initially, there is a large concentration gradient, and thus the dispersive flux is large. In this case, one has a much larger solute flux into the domain than if one uses the third-type solute flux boundary condition.

We always recommend using a third-type BC than a first-type BC since this is a more physically realistic BC. A Dirichlet BC is not physical and, for the above reasons, does not conserve mass (e.g., *van Genuchten and Parker, 1984; Leij et al., 1991*). One could use it only if there is, for example, a large reservoir of a contaminant in contact with the transport domain, and thus one can assume that the boundary concentration is fixed.

Initial Conditions:

Solute transport initial conditions can be specified either in terms of the **liquid phase concentration** c [ML⁻³; mass of solute/volume of water], or alternatively in terms of the **total concentration** S [ML⁻³; mass of solute/volume of soil]. In the latter case, the liquid phase concentration is then calculated from the total concentration by distributing the solute mass among different phases. This is straightforward for a linear case (with linear sorption), and a little more complicated for a nonlinear case (nonlinear sorption), since a root-finding problem has to be solved for this nonlinear problem.

The initial concentration of **the nonequilibrium phase** can be specified either directly or it can be assumed to be **initially at equilibrium with the equilibrium phase** concentration.

3.4. Heat Transport Parameters

3.4.1. Heat Transport Parameters

The information needed for defining the heat transport problem is entered in the **Heat Transport Parameters** dialog window (Fig. 40). In this window, users specify *Heat Transport Parameters* and temperatures for the *Boundary Conditions* (for 2D/3D applications).

Heat Transport Parameters (1D)

Heat Transport Parameters 1

Thermal Conductivity Model: ☒ Chung & Horton (1987) ☐ Campbell (1985) Loam Set Default Volumetric Heat Capacities

Temperature Amplitude [C]:

Time interval for one temperature cycle [day]:

Heat Transport Parameters 2

Mat	Solid [-]	Org.M. [-]	Disp. [cm]	b1 [kgcm/days ³ /K]	b2 [kgcm/days ³ /K]	b3 [kgcm/days ³ /K]	b4 [kg/cm/
1	0.601	0	5	1.56728e+16	2.53474e+16	9.89388e+16	1.4
2	0.661	0	5	1.56728e+16	2.53474e+16	9.89388e+16	1.4

Heat Transport Parameters (2D/3D)

Boundary Conditions

	TBound1	TBound2	TBound3	TBound4	TBound5	TWell
1	30	0	0	0	0	0

Heat Transport Parameters 1

Temperature Amplitude [C]:

Time interval for one temp. cycle [day]:

Thermal Conductivity: Loam Set Default Volumetric Heat Capacities

Heat Transport Parameters 2

Mat	Solid	Org.M.	Disp.L.	Disp.T.	b1	b2
1	0.539	0.001	0.5	0.1	1.5673e+016	2.534
2	0.539	0.001	0.5	0.1	1.5673e+016	2.534
3	0.539	0.001	0.5	0.1	1.5673e+016	2.534

Figure 40. The Heat Transport Parameters dialog window (for 1D – top; for 2D/3D- bottom).

The following **Heat Transport Parameters** (bottom part of the dialog window) are specified for each soil material:

Solid	Volume fraction of solid phase, θ_h [-]
Org.M.	Volume fraction of organic matter, θ_o [-]
Disp.L.	Longitudinal thermal dispersivity, λ_L [L]
Disp.T.	Longitudinal thermal dispersivity, λ_T [L] (only for 2D/3D applications)
b1	Coefficient b_1 in the expression for the thermal conductivity function, [W/L/K] or [ML/T ³ /K]
b2	Coefficient b_2 in the expression for the thermal conductivity function [W/L/K]
b3	Coefficient b_3 in the expression for the thermal conductivity function [W/L/K]
Cn	Volumetric heat capacity of the solid phase, C_n [J/L ³ /K] or [M/L/T ² /K]
Co	Volumetric heat capacity of organic matter, C_o [J/L ³ /K]
Cw	Volumetric heat capacity of the liquid phase, C_w [J/L ³ /K]

Boundary Conditions:

Temperatures for 2D/3D *Boundary Conditions* with time-independent boundary conditions are also specified in this dialog window.

TBound1	Value of the temperature for the first time-independent boundary condition [K]. Set equal to zero if no time-independent boundary condition is specified. The same for TBound2 through TBound4
TWell	Value of the temperature for the sixth time-independent boundary condition [K]. If internal sources are specified, then <i>TWell</i> is automatically used for the temperature of water injected into the flow region from sources in the transport domain. Set equal to zero if no sixth time-independent boundary condition and no internal sources are specified.

The boundary condition at the soil surface may be approximated using a sinus wave with the maximum one hour after noon and the minimum one hour after midnight as follows:

$$T = T_0 + A \cos \left[2\pi \left(\frac{t-13}{24} \right) \right]$$

where T_0 is the average temperature at the soil surface [K], A is the **Temperature Amplitude** at the soil surface [K], and p is the **Time Interval** for completion of one sine wave temperature (usually 1 day, the default value). The second part of the sine term is included to set the maximum temperature at 1 p.m.

Default values for the parameters in the **Thermal Conductivities** of three textural classes (sand, loam, and clay) are provided by HYDRUS for the *Chung and Horton* [1987] model. Alternatively, one can use a function suggested by *Campbell* [1985]. Default volumetric heat capacities for the solid phase (1.92 MJ m⁻³K⁻¹), organic matter (2.51 MJ m⁻³K⁻¹), and liquid phase (4.18 MJ m⁻³K⁻¹) are also given (*Set Default Volumetric Heat Capacities*).

When the parameter estimation option is selected, then users must provide initial estimates of the optimized heat transport parameters, specify which parameters are to be optimized (check appropriate checkboxes), and provide parameter constraints for the optimization. Zero values for the minimum and maximum values signify that parameters are unconstrained. The **Heat Transport Parameters** dialog window for the inverse problem is not further shown here.

Notice that thermal conductivity and volumetric heat capacity parameters have units of $[\text{Wm}^{-1}\text{K}^{-1}]$ and $[\text{Jm}^{-3}\text{K}^{-1}]$, respectively. When converted to basic SI units, these units are $[\text{ML}^{-1}\text{T}^{-2}\text{K}^{-1}]$ and $[\text{MLT}^{-3}\text{K}^{-1}]$, respectively, and thus contain the time to the negative second or third power, which needs to be taken into account during any time conversion.

3.4.2. Heat Transport Boundary Conditions for 1D

Users can select the upper and lower boundary conditions for heat transport in one-dimensional applications in the **Heat Transport Boundary Conditions** dialog window (Fig. 41).

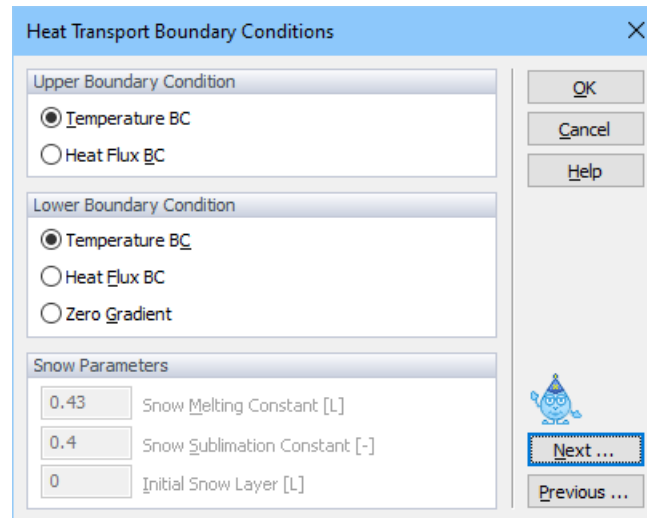


Figure 41. The Heat Transport Boundary Conditions dialog window for one-dimensional applications.

The following types of **upper boundary** conditions for heat transport are available:

- Temperature boundary condition
- Temperature flux boundary condition

The following types of lower boundary conditions for heat transport are available:

- Temperature boundary condition
- Temperature flux boundary condition
- Free drainage (zero gradient)

Snow Parameters

Snow Melting Constant: This is the amount of snow (given in length units, such as cm, of water) that will melt during one day for each °C (e.g., 0.43 cm). For example, when the temperature is equal to 5 °C, 2.15 ($=5 \times 0.43$) cm of snow (as water layer) will melt.

Sublimation Constant: A constant ($=0.4$) used to reduce the potential evaporation from an existing snow layer.

3.5. Root Uptake and Growth

3.5.1. Root Water and Solute Uptake Model

Users may select a particular **Water Uptake Reduction Model** and a **Solute Stress Model** in the **Root Water Uptake Model** dialog window (Fig. 42).

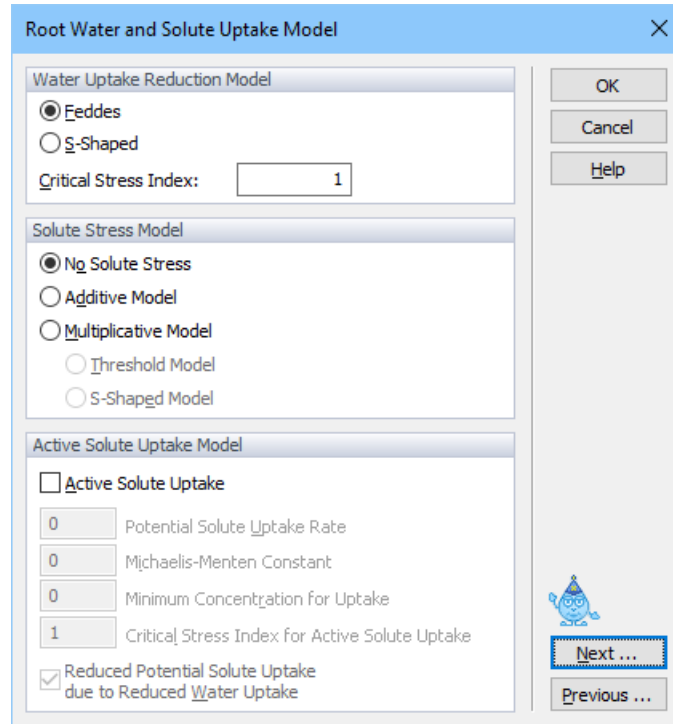


Figure 42. The Root Water Uptake Model dialog window.

a) Water Uptake Reduction Model

Either a water stress response function suggested by *Feddes et al.* [1978] or an S-shaped function suggested by *van Genuchten* [1985] can be used to reduce the potential root water uptake to the actual water uptake rate (Fig. 43). Root water uptake with compensation can be simulated when the *Critical Stress Index* is smaller than one (see the Technical Manual; *Šimůnek et al.* [2010]).

b) Solute Stress Model

The effect of salinity stress on the root water uptake can be neglected (*No Solute Stress*) or considered using the *Additive* or *Multiplicative* models, i.e., salinity stress is either added to water stress, or uptake reduction due to water stress and salinity stress are multiplied. When the multiplicative model is used for salinity stress, one can use either the *Threshold Model* [Maas, 1990] or an *S-Shaped Model* [van Genuchten, 1985] (Fig. 44).

c) Active Solute Uptake Model

Total root nutrient uptake is determined from the total of **active** (only in 2D) and **passive nutrient uptake**. The partitioning between passive and active uptake is controlled by the a priori defined concentration value **cRoot** (Fig. 31). Passive nutrient uptake is simulated by multiplying root water uptake with the dissolved nutrient concentration, for soil solution concentration values below **cRoot**. Passive nutrient uptake is thus zero when **cRoot** is equal to zero. One must therefore specify the maximum allowed concentration, **cRoot**, in the passive root solute uptake term. When zero is specified, all solute is left behind in the soil (there is no passive root solute uptake), and only the solute-free solution is taken up. When the concentration is lower than **cRoot**, all solute is taken up (unlimited passive root solute uptake). When the concentration is higher than **cRoot**, the additional solute stays behind.

As the **Active Nutrient Uptake** is obtained from the difference between plant nutrient demand (the **Potential Solute Uptake Rate** [$\text{ML}^{-2}\text{T}^{-1}$] needs to be specified) and **Passive Nutrient Uptake**, the presented model thus implies that reduced passive nutrient uptake is compensated for by active nutrient uptake. Active nutrient uptake is simulated using Michaelis-Menten kinetics (the **Michaelis-Menten constant** and a **Minimum Concentration for Uptake** need to be specified). In addition, the proposed root uptake model includes compensation for active nutrient uptake, in a similar way as used for root water uptake (using the **Critical Stress Index**).

Reduction in root water uptake will decrease passive nutrient uptake, thereby increasing active nutrient uptake proportionally. In other words, total nutrient uptake is not affected by soil water stress, as computed by the proportion of actual to potential root water uptake. This is not realistic since one would expect that plant nutrient requirements will be reduced for water-stressed plants. For that reason, the uptake model includes additional flexibility, by reducing the potential nutrient demand (**Potential Solute Uptake Rate**), in proportion to the reduction of root water uptake (see the last check box **Reduce Potential Solute Uptake due to Reduced Water Uptake**).

Active solute uptake is implemented only for a single solute (not for multiple solutes). Details about the root water and solute uptake can be found in the **Technical Manual** or Šimůnek and Hopmans [2009].

3.5.2. Root Water Uptake Parameters

Parameters for the water and salinity stress response functions are specified in the **Root Water Uptake Parameters** dialog window (Fig. 43 and Fig. 44, respectively).

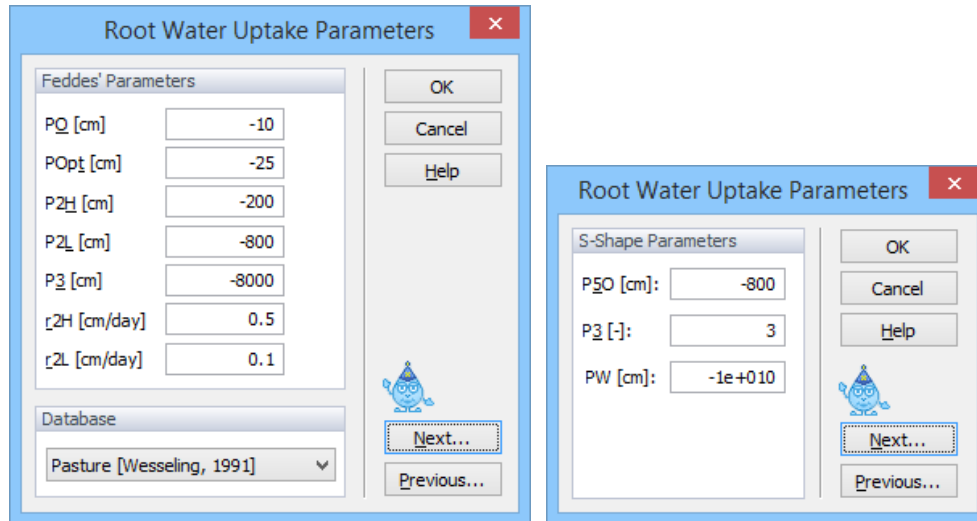


Figure 43. The Root Water Uptake Parameters dialog window for the water stress response function of *Feddes et al.* [1978] (left) and *van Genuchten* [1985] (right).

The **Root Water Uptake Parameters** for the water stress response function suggested by *Feddes et al.* [1978] (Fig. 43, left) are described in detail in the HYDRUS technical manual. Water uptake in this model is assumed to be zero close to saturation (i.e., wetter than some arbitrary “anaerobiosis point” **P0**). Root water uptake is also zero for pressure heads less (more negative) than the wilting point (**P3**). Water uptake is considered optimal between pressure heads **Popt** and **P2**, whereas for pressure heads between **P2** and **P3** (or **P0** and **Popt**), water uptake decreases (or increases) linearly with the pressure head. When root water uptake can occur at its optimal value even at full saturation, set both **P0** and **POpt** equal to zero.

- P0** Value of the pressure head [L] below which roots start to extract water from the soil.
- POpt** Value of the pressure head [L] below which roots extract water at the maximum possible rate.
- P2H** Value of the limiting pressure head [L] below which roots can no longer extract water at the maximum rate (assuming a potential transpiration rate of $r2H$).
- P2L** As **P2H**, but for a potential transpiration rate of $r2L$.
- P3** Value of the pressure head [L] below which root water uptake ceases (usually taken at the wilting point). **P3** (to avoid numerical instabilities, similarly as for h_{CritA} below) should be selected so that the corresponding water content is at least 0.005 higher than the residual water content.
- r2H** Potential transpiration rate [$L T^{-1}$] (currently set at 0.5 cm/day).

r2L Potential transpiration rate [LT^{-1}] (currently set at 0.1 cm/day).

The above input parameters permit one to make the variable P2 a function of the potential transpiration rate, T_p (P2 presumably decreases at higher transpiration rates). HYDRUS currently implements the same linear interpolation scheme as used in several versions of the SWATRE code (e.g., *Wesseling and Brandyk*, 1985). The interpolation scheme is defined in the manual.

A database of suggested values for different plants for the *Feddes et al.* [1978] model is provided in HYDRUS based on studies by *Wesseling* [1991] and *Taylor and Ashcroft* [1972].

The **Root Water Uptake Parameters** for the S-shaped water stress response function, as suggested by *van Genuchten* [1985] (Fig. 43, right) are as follows:

P50 The coefficient, h_{50} , in the root water uptake response function associated with water stress [L]. Root water uptake at this pressure head is reduced by 50%.

P3 The exponent, p_3 , in the root water uptake response function associated with water stress [-]; its recommended and default value is 3.

We have additionally included a parameter **PW**, i.e., pressure head at the wilting point [L], below which transpiration stops.

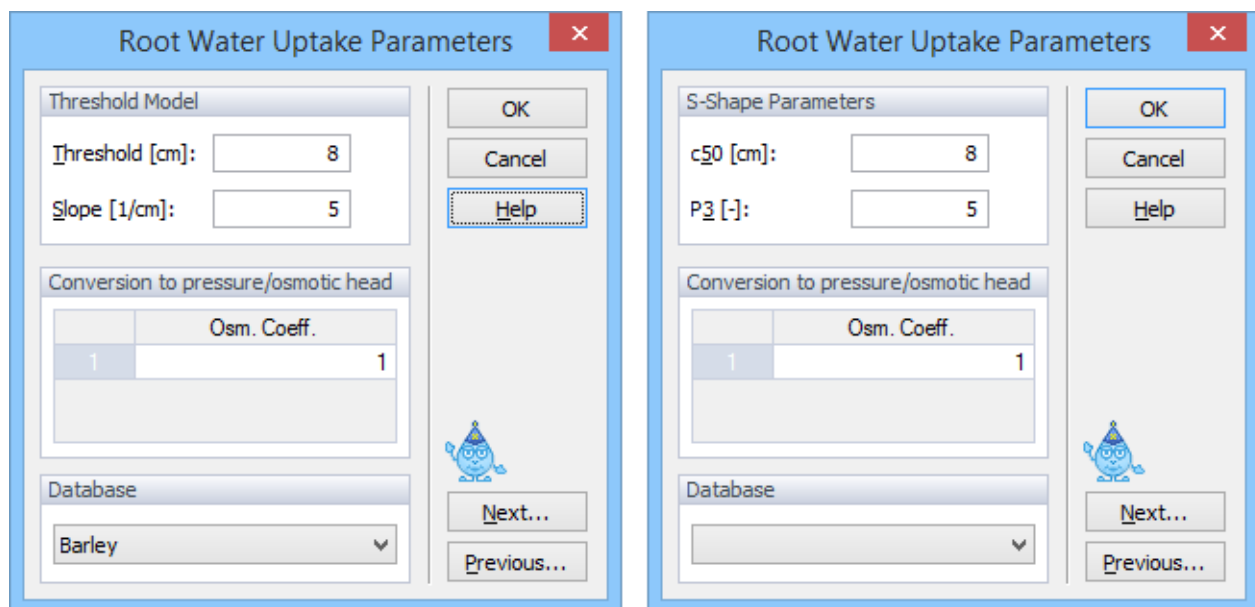


Figure 44. The Root Water Uptake Parameters dialog window for the solute stress response function based on the threshold model (left) and S-shaped model of *van Genuchten* [1985] (right).

The **Root Water Uptake Parameters** for the *Threshold Model* [Maas, 1990] of the salinity stress response function (multiplicative) (Fig. 44, left) are as follows:

Threshold Value of the minimum osmotic head [L] (the salinity threshold) above which root water uptake occurs without a reduction.

Slope Slope of the curve determining the fractional root water uptake decline per unit increase in salinity below the threshold.

The **Root Water Uptake Parameters** for the *S-Shaped Model* [van Genuchten, 1985] of the salinity stress response function (multiplicative) (Fig. 44, right) are as follows:

P3 The exponent, p , in the root water uptake response function associated with salinity stress [-]. The recommended value is 3.

c50 The coefficient, h_{50} , in the root water uptake response function associated with salinity stress [L]. Root water uptake at this osmotic head is reduced by 50%.

Both salinity stress response functions require a coefficient (*Osmotic Coefficient*) that transforms concentrations into equivalent osmotic pressure heads (Fig. 44). The osmotic coefficients should be negative for the additive model (to be added to negative pressure heads) and positive for the multiplicative model. Note that this conversion needs to be made mainly when one uses the **Additive Model**. That is because then one needs to **add** pressure heads (i.e., units of m or cm) and osmotic heads (calculated from concentrations, which likely have units of dS/m). If one uses the **Multiplicative Model**, then one does not need to use this conversion and can keep **Osm. Coeff** equal to one, since a) both water stress and salinity stress response functions can have their own units, and b) both the **Threshold Model** parameters (specified above) and selected concentrations units are likely already the same (e.g., units of EC (dS/m)).

A database of suggested values for different plants for the threshold-slope salinity stress model is provided based on the work by Maas [1990]. The database for the threshold model provides suggested values based on the electric conductivity of the saturation extract EC_e in dS/m. These values are converted internally in the GUI into the electric conductivity of soil water (at the field capacity) as follows: $EC_w \approx k_e * EC_e$, where k_e is approximately 2 [Skaggs *et al.*, 2006]. Consequently, the threshold value of Maas [1990] is multiplied by 2 (k_e), and the slope is divided by 2. A user is responsible for converting these values in the regular HYDRUS further to the osmotic pressure in the head units [L] or concentration units used in your project. For guidance, see Eqs. 13.3 and 13.4 in Maas [1990].

The threshold-slope salinity stress model is implemented in the standard HYDRUS solute transport model as $R=1-0.01(c-c_T)s$, while in the UNSATCHEM module as $R=1-0.01(h_\phi-h_{\phi T})s^*$, where c_T is the concentration threshold, $h_{\phi T}$ is the osmotic head threshold, s is the slope in HYDRUS and s^* is the slope in UNSATCHEM.

3.5.3. Root Distribution Parameters

The spatial distribution of the roots can be specified using the **Root Distribution Parameters** dialog window (Fig. 45). The following two- and three-dimensional root distribution functions are implemented in HYDRUS [Vrugt *et al.*, 2001, 2002]:

$$b(x, z) = \left(1 - \frac{z}{Z_m}\right) \left(1 - \frac{x}{X_m}\right) e^{-\left(\frac{p_z}{Z_m}|z^* - z| + \frac{p_x}{X_m}|x^* - x|\right)}$$

$$b(x, y, z) = \left(1 - \frac{x}{X_m}\right) \left(1 - \frac{y}{Y_m}\right) \left(1 - \frac{z}{Z_m}\right) e^{-\left(\frac{p_x}{X_m}|x^* - x| + \frac{p_y}{Y_m}|y^* - y| + \frac{p_z}{Z_m}|z^* - z|\right)}$$

Figure 45. The Root Distribution Parameters dialog window.

where X_m , Y_m , and Z_m are the maximum rooting lengths in the x -, y -, and z - directions [L], respectively; x , y , and z are distances from the origin of the plant (tree) in the x -, y -, and z - directions [L], respectively; p_x [-], p_y [-], p_z [-], x^* [L], y^* [L], and z^* [L] are empirical parameters (x^* , y^* , and z^* are in Fig. 45 indicated as *Depth of Maximum Intensity* or *Radius of Maximum Intensity*; parameters p_x , p_y , and p_z are assumed to be equal to one for $x > x^*$, $y > y^*$, $z > z^*$, respectively [Vrugt *et al.*, 2002]), and $b(x, z)$ and $b(x, y, z)$ denote two- and three-dimensional spatial distribution of the potential root water uptake [-]. See Vrugt *et al.* [2001, 2002] for different configurations of the normalized spatial distribution of potential root water uptake rate.

The equations above are given and used in absolute coordinates, i.e., they are independent of any actual selection in GUI. The x and y coordinates are identical to x and y coordinates for the geometry of the transport domain. The only exception is that the beginning of the z coordinate for the root distribution starts at the highest located node of the entire transport domain (again independent of any actual selection).

3.5.4. Root Growth Parameters

A simple root growth model with similar capabilities as in HYDRUS-1D (Fig 46) was implemented into Version 3 of HYDRUS (2D/3D) (its 2D version). The rooting depth, L_R , can now be either constant (the standard approach) or variable in time. Time-variable rooting depth values can be either calculated using the classical Verhulst-Pearl logistic *Growth Function* (Fig 47, top) or provided using a *Table* (Fig. 47, bottom). The user can select between three different root distribution functions, which can be either described using the Vrugt et al. (2001, 2002) or Hoffman and van Genuchten (1983) functions or can be constant with depth (*Shape of the Root Zone*). The roots can be distributed uniformly in the horizontal direction or can vary horizontally as well (*Horizontal Distribution*). When *Horizontal Distribution* of roots is considered, users have an option to specify multiple plants (*Number of Plants*), their location (*Plant Position*), and also specify the lateral extent of roots (*Half Width*), which can again be either constant or variable in time. When the Vrugt et al. (2001, 2002) function is used to describe vertical roots distribution, it can be used to describe the horizontal distribution of roots as well. When Hoffman and van Genuchten (1983) or constant functions are used, then the horizontal distribution is constant as well.

Figure 46. The Root Growth Parameters specified using the logistic growth function for 1D applications.

Root Growth Parameters

Shape of the Root Zone

☐ Vrugt et al. (2000)
☐ van Genuchten & Hoffman
☒ Constant

Horizontal Distribution of Plants

☒ Horizontal Distribution
 Root Depth: [cm]
 Half Width: [cm]
 Number of Plants:

	Plant Position [cm]
1	30
2	60

Root Depth Specified

☐ No Growth
☐ Using a Table
☒ Using a Growth Function

Root Growth Data

Root Growth Factor:

☒ From Given Data
☐ 50% after 50% Growing Season

Initial Root Growth Time: [sec]
 Harvest Time: [sec]
 Initial Rooting Depth: [cm]
 Maximum Rooting Depth: [cm]
 Initial Rooting Radius: [cm]
 Maximum Rooting Radius: [cm]
 Time - Root Data: [sec]
 Depth - Root Data: [cm]
 Time-Period: [sec]



Root Growth Parameters

Shape of the Root Zone

☐ Vrugt et al. (2000)
☐ van Genuchten & Hoffman
☒ Constant

Horizontal Distribution of Plants

☒ Horizontal Distribution
 Root Depth: [cm]
 Half Width: [cm]
 Number of Plants:

	Plant Position [cm]
1	30
2	60

Root Depth Specified

☐ No Growth
☒ Using a Table
☐ Using a Growth Function

Root Growth Data

Number of Rows:

	Time [sec]	Depth [cm]
1	10	5
2	20	15
3	30	25
4	40	35
5	50	45



Figure 47. The Root Growth Parameters specified either using the logistic growth function (top) or a table (bottom) for 2D/3D applications.

The Verhulst-Pearl logistic growth function, which may be used to describe the time-variable rooting depth, requires a parameter that characterizes the growth rate. The growth rate can be calculated either from the assumption that 50% of the rooting depth will be reached after 50% of the growing season has elapsed (*50% after 50% Growing Season*) or from a given data point of the rooting depth at a specified time (*From Given Data*). In the latter case, one data point on the root growth curve (*Time Root Data - Depth Root Data*) must be provided. The same growth pattern can be repeated at a certain time period (*Time Period*) and for multiple plants.

When the *Root Depth* is *Specified Using a Table*, users must provide a table with entries of *Time*, the *Depth* of the rooting zone, and the *Width* of the rooting zone. The same pattern is used for all plants (if multiple plant locations are specified). Rooting depths and widths are linearly interpolated between individual time entries.

3.6. Time Variable Boundary Conditions

The **Time Variable Boundary Conditions** dialog window is shown in Figure 48.

	Time [days]	Precip. [m/day]	Evap. [m/day]	Transp. [m/day]	hCritA [m]	Var.F1 [m/day]	Var.H-1 [m]	Var.F2 [m/day]	Var.H-2 [m]	V [m]
39	39	0.1	0	0.16	100	0	0	0	0	
40	40	0	0	0.18	100	0	0	0	0	
41	41	0.42	0	0.16	100	0	0	0	0	
42	42	0	0	0.18	100	0	0	0	0	
43	43	0.11	0	0.2	100	0	0	0	0	
44	44	0	0	0.21	100	0	0	0	0	
45	45	0.07	0	0.16	100	0	0	0	0	
46	46	0	0	0.2	100	0	0	0	0	
47	47	0	0	0.15	100	0	0	0	0	
48	48	0	0	0.16	100	0	0	0	0	
49	49	0	0	0.3	100	0	0	0	0	
50	50	0	0	0.22	100	0	0	0	0	
51	51	0	0	0.2	100	0	0	0	0	
52	52	0	0	0.2	100	0	0	0	0	
53	53	0	0	0.2	100	0	0	0	0	
54	54	0	0	0.18	100	0	0	0	0	

Linear interpolation of time between the initial and final time

Surface area associated with transpiration: [m]

Figure 48. The Time Variable Boundary Conditions dialog window.

The following variables are specified in the **Time Variable Boundary Conditions** dialog window:

- Time** Time for which a data record is provided [T]. Boundary condition values are specified for the time interval preceding the time given at the same line. Thus, the BC values specified in the first row are for the time interval between the initial time and time specified on the same line.
- Precip** Precipitation rate [LT^{-1}] (in absolute value) (applied to the atmospheric boundary).
- Evap** Potential evaporation rate [LT^{-1}] (in absolute value) (applied to the atmospheric boundary).
- Trans** Potential transpiration rate [LT^{-1}] (in absolute value).
- hCritA** Absolute value of the minimum allowed pressure head at the soil surface [L] (applied to the atmospheric boundary). hCritA (should be selected so that the corresponding water content is at least 0.005 higher than the residual water content (to avoid numerical instabilities, especially for coarse-textured soils).

Var.Fl1	Drainage flux [LT^{-1}] across the bottom boundary, or another time-dependent prescribed flux boundary condition (positive when the water leaves the flow region); set to zero when no time-dependent flux boundary condition is specified. Same for Var.Fl2, Var.Fl3, or Var.Fl4. The Var.Fl4 value is used for internal time-variable nodal flux sinks or sources (if they exist) (in such case, the units are [L^2T^{-1}] or [L^3T^{-1}] for 2D or 3D applications, respectively).
Var.H-1	Groundwater level [L] (usually negative), or other time-dependent prescribed head boundary condition; set equal to zero when no time-dependent head boundary condition is specified. Same for Var.H-2, Var.H-3, or Var.H-4. The Var. H-4 value is used for internal time-variable nodal pressure head sinks or sources (if they exist).
TVal1	The first time-dependent temperature [K] that can be used for nodes with time-variable boundary conditions (atmospheric BC, variable head/flux BC) (is not specified when heat transport or time-variable boundary conditions are not considered).
TVal2	The second time-dependent temperature [K] that can be used for nodes with time-variable boundary conditions (is not specified when heat transport or time-variable boundary conditions are not considered).
CVal1	The first time-dependent solute concentration [ML^{-3}] that can be used for nodes with prescribed time-variable boundary conditions (atmospheric BC, variable head/flux BC) (not specified when solute transport is not considered). This column should preferably be used only for the atmospheric boundary because the concentration value is adjusted based on values of precipitation and evaporation as follows: $\text{cVal1} = \text{Precip}/(\text{Precip} - \text{Evap}) * \text{cVal1}$. The cVal1 is adjusted to be zero when $\text{Evap} > \text{Precip}$. Similar adjustments are not made for cVal2, and other concentration values.
CVal2	The second time-dependent solute concentration [ML^{-3}] that can be used for nodes with prescribed time-variable boundary conditions (atmospheric BC, variable head/flux BC) (not specified when solute transport is not considered).
CVal3	The third time-dependent solute concentration [ML^{-3}] that can be used for nodes with prescribed time-variable boundary conditions (atmospheric BC, variable head/flux BC) (not specified when solute transport is not considered).

The last three entries are entered for each solute.

The table in Figure 48 can be edited by manually adding or deleting lines. The table has a capacity for about 32,000 records (depending on the number of columns). When a long-time record is to be simulated, then one needs to directly edit the Atmosph.in input file in the working directory using any standard software, such as MS Excel. The manually modified Atmosph.in file then needs to be imported back into the HYDRUS *project_name.h32d* file using the command *File->Import and Export->Import Input Data from *.In Files*. Data for the **Time Variable Boundary Conditions** can be prepared in any spreadsheet software and then copied into the table using Windows paste hotkeys (i.e., Ctrl+V).

The total number of atmospheric data records is given in the Main Time Information dialog window (Fig. 16).

Surface Area Associated with Transpiration: The total transpiration flux from a simulated transport domain is equal to the potential transpiration T_p (L/T) multiplied by the **Surface boundary Area** (length in 2D) **Associated with Transpiration** (see Figure 2.2. of the Technical Manual). It is usually the entire soil surface (usually the boundary area/length with an atmospheric boundary condition). By dissociating this value (i.e., the surface area associated with transpiration) from the surface boundary area/length of the transport domain, we provide HYDRUS users with more flexibility in how to specify transpiration (e.g., for sparsely vegetated soil surface, or for row crops or trees). In any case, the definition of the **Surface Area Associated with Transpiration** depends on how the potential transpiration, T_p , is calculated, which is usually done for the entire soil surface.

Linear Interpolation of Time Between the Initial and Final Time: When this option is selected, the values in the first column will be linearly interpolated between the initial and final times. For example, when the initial and final times are zero and 75 days, respectively, and there are 75 records, the first column values will be increasing by 1 d (i.e., 1, 2, 3, ..., 74, 75).

3.7. Constructed Wetlands

Two biokinetic model formulations can be chosen: (1) the biokinetic model as described in CW2D [Langergraber and Šimunek, 2005, 2006] and (2) the CWM1 (Constructed Wetland Model #1) biokinetic model [Langergraber et al., 2009]. In CW2D aerobic and anoxic transformation and degradation processes for organic matter, nitrogen and phosphorus are described, whereas in CWM1 aerobic, anoxic, and anaerobic processes for organic matter, nitrogen, and sulfur. Comparisons between CW2D and CWM1 components and processes are given in Tables 11 and 12, respectively. Details about both modules can be found in the above-referenced literature.

Parameters for constructed wetlands are entered in the **Constructed Wetland Model Parameters I and II** dialog windows for the CW2D (Fig. 49 and 51, respectively) and CWM1 (Fig. 50 and 52, respectively) modules.

Table 11. Comparison of CW2D and CWM1 components.

CW2D	CWM1
[Langergraber and Šimunek, 2005]	[Langergraber et al., 2009]
Components 1. SO: Dissolved oxygen, O ₂ . 2. CR: Readily biodegradable soluble COD. 3. CS: Slowly biodegradable soluble COD. 4. CI: Inert soluble COD. 5. XH: Heterotrophic bacteria 6. XANs: Autotrophic ammonia-oxidizing bacteria (<i>Nitrosomonas spp.</i>) 7. XANb: Autotrophic nitrite-oxidizing bacteria (<i>Nitrobacter spp.</i>) 8. NH₄N: Ammonium and ammonia nitrogen. 9. NO₂N: Nitrite nitrogen. 10. NO₃N: Nitrate nitrogen. 11. N₂: Elemental nitrogen. 12. PO₄P: Phosphate phosphorus Organic nitrogen and organic phosphorus are modeled as part of the COD. Nitrification is modeled as two-step process. Bacteria are assumed to be immobile.	Soluble components, S? 1. SO: Dissolved oxygen, O ₂ . 2. SF: Fermentable, readily biodegradable soluble COD. 3. SA: Fermentation products as acetate. 4. SI: Inert soluble COD. 5. SNH: Ammonium and ammonia nitrogen. 6. SNO: Nitrate and nitrite nitrogen. 7. SSO₄: Sulphate sulfur. 8. SH₂S: Dihydrogensulphide sulfur. Particulate components, X? 9. XS: Slowly biodegradable particulate COD. 10. XI: Inert particulate COD. 11. XH: Heterotrophic bacteria. 12. XA: Autotrophic nitrifying bacteria. 13. XFB: Fermenting bacteria. 14. XAMB: Acetotrophic methanogenic bacteria. 15. XASRB: Acetotrophic sulfate-reducing bacteria. 16. XSOB: Sulphide oxidizing bacteria. Organic nitrogen and organic phosphorus are modeled as part of the COD.

Table 12. Comparison of CW2D and CWM1 processes.

CW2D	CWM1
[Langergraber and Šimunek, 2005]	[Langergraber et al., 2009]
Heterotrophic bacteria: 3. Hydrolysis: conversion of CS into CR. 4. Aerobic growth of XH on CR (mineralization of organic matter). 5. Anoxic growth of XH on CR (denitrification on NO₂N). 6. Anoxic growth of XH on CR (denitrification on NO₃N). 7. Lysis of XH. Autotrophic bacteria: 8. Aerobic growth of XANs on SNH (ammonium oxidation). 9. Lysis of XANs. 10. Aerobic growth of XANb on SNH (nitrite oxidation). 11. Lysis of XANb.	Heterotrophic bacteria: 1. Hydrolysis: conversion of XS into SF. 2. Aerobic growth of XH on SF (mineralization of organic matter). 3. Aerobic growth of XH on SA (mineralization of organic matter). 4. Anoxic growth of XH on SF (denitrification). 5. Anoxic growth of XH on SA (denitrification). 6. Lysis of XH. Autotrophic bacteria: 7. Aerobic growth of XA on SNH (nitrification). 8. Lysis of XA. Fermenting bacteria: 9. Growth of XFB (fermentation). 10. Lysis of XFB. Acetotrophic methanogenic bacteria: 11. Growth of XAMB: Anaerobic growth of acetotrophic, methanogenic bacteria XAMB on acetate SA. 12. Lysis of XAMB. Acetotrophic sulphate reducing bacteria: 13. Growth of XASRB: Anaerobic growth of acetotrophic, sulphate reducing bacteria. 14. Lysis of XASRB. Sulphide oxidizing bacteria: 15. Aerobic growth of XSOB on SH₂S: The opposite process to process 13, the oxidation of SH₂S to SSO₄. 16. Anoxic growth of XSOB on SH₂S: Similar to process 15 but under anoxic conditions. 17. Lysis of XSOB.

Solute Transport - Constructed Wetland Model (CW2D) Parameters I ✕

Hydrolysis

Hydrolysis Rate: 0.05	Sat./Inh. Coeff. for: 0.1
--	--

Heterotrophic Organisms: Mineralization

Max. Aerobic Growth Rate: 0.1	Sat./Inh. Coeff. for Substr.: 2
Rate Constant for Lysis: 0.0025	Sat./Inh. Coeff. for NH4: 0.05
Sat./Inh. Coeff. for O2: 0.2	Sat./Inh. Coeff. for P: 0.01

Heterotrophic Organisms: Denitrification

Max. Denitrification Rate: 0.08	Sat./Inh. Coeff. for NO2: 0.5
Sat./Inh. Coeff. for O2: 0.2	Sat./Inh. Coeff. for Substr.: 2
Sat./Inh. Coeff. for NO3: 0.5	Sat./Inh. Coeff. for NH4: 0.05
Sat./Inh. Coeff. for P: 0.01	

Autotrophic Bacteria: Nitrosomonas

Max. Aerobic Growth Rate: 0.015	Sat./Inh. Coeff. for NH4: 0.5
Rate Constant for Lysis: 0.0015	Sat./Inh. Coeff. for P: 0.01
Sat./Inh. Coeff. for O2: 1	

Autotrophic Bacteria: Nitrobacter

Max. Aerobic Growth Rate: 0.0167	Sat./Inh. Coeff. for NO2: 0.1
Rate Constant for Lysis: 0.0015	Sat./Inh. Coeff. for NH4: 0.05
Sat./Inh. Coeff. for O2: 0.1	Sat./Inh. Coeff. for P: 0.01

OK

Cancel

Help



Next ...

Previous ...

Figure 49. The Constructed Wetland Model (CW2D) Parameter I dialog window.

Table 13. Kinetic parameters in the CW2D biokinetic model [Langergraber and Šimůnek, 2005].

Description [unit]		Value
Hydrolysis		for 20°C (10°C)
K_h	hydrolysis rate constant [1/d]	3 (2)
K_X	saturation/inhibition coefficient for hydrolysis [g COD _{CS} /g COD _{BM}]	0.1 (0.22)
Heterotrophic bacteria (aerobic growth)		
μ_H	the maximum aerobic growth rate on CR [1/d]	6 (3)
b_H	rate constant for lysis [1/d]	0.4 (0.2)
K_{het,O_2}	saturation/inhibition coefficient for S _O [mg O ₂ /L]	0.2
$K_{het,CR}$	saturation/inhibition coefficient for substrate [mg COD _{CR} /L]	2
K_{het,NH_4N}	saturation/inhibition coefficient for NH ₄ (nutrient) [mg N/L]	0.05
$K_{het,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01
Heterotrophic bacteria (denitrification)		
μ_{DN}	the maximum aerobic growth rate on CR [1/d]	4.8 (2.4)
K_{het,O_2}	saturation/inhibition coefficient for S _O [mg O ₂ /L]	0.2
K_{het,NO_3N}	saturation/inhibition coefficient for NO ₃ [mg N/L]	0.5
K_{het,NO_2N}	saturation/inhibition coefficient for NO ₂ [mg N/L]	0.5
$K_{het,CR}$	saturation/inhibition coefficient for substrate [mg COD _{CR} /L]	4
K_{het,NH_4N}	saturation/inhibition coefficient for NH ₄ (nutrient) [mg N/L]	0.05
$K_{het,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01
Ammonia oxidizing bacteria (<i>Nitrosomonas</i> spp.)		
μ_{ANs}	the maximum aerobic growth rate on S _{NH} [1/d]	0.9 (0.3)
b_{ANs}	rate constant for lysis [1/d]	0.15 (0.05)
K_{ANs,O_2}	saturation/inhibition coefficient for S _O [mg O ₂ /L]	1
K_{ANs,NH_4N}	saturation/inhibition coefficient for NH ₄ [mg N/L]	0.5
$K_{ANs,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01
Nitrite oxidizing bacteria (<i>Nitrobacter</i> spp.)		
μ_{ANb}	the maximum aerobic growth rate on S _{NH} [1/d]	1 (0.35)
b_{ANb}	rate constant for lysis [1/d]	0.15 (0.05)
K_{ANb,O_2}	saturation/inhibition coefficient for S _O [mg O ₂ /L]	0.1
K_{ANb,NO_2N}	saturation/inhibition coefficient for NO ₂ [mg N/L]	0.1
K_{ANb,NH_4N}	saturation/inhibition coefficient for NH ₄ (nutrient) [mg N/L]	0.05
$K_{ANb,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01

Table 14. Kinetic parameters in the CWM1 biokinetic model [Langergraber et al., 2009].

Parameter	Description [unit]	Value
Hydrolysis		for 20°C (10°C)
K_h	hydrolysis rate constant [1/d]	3 (2)
K_X	saturation/inhibition coefficient for hydrolysis [g COD _{SF} /g COD _{BM}]	0.1 (0.22)
η_H	correction factor for hydrolysis by fermenting bacteria [-]	0.1
Heterotrophic bacteria (aerobic growth and denitrification)		
μ_H	the maximum aerobic growth rate on S_F and S_A [1/d]	6 (3)
η_g	correction factor for denitrification by X_H [-]	0.8
b_H	rate constant for lysis [1/d]	0.4 (0.2)
K_{OH}	saturation/inhibition coefficient for S_O [mg O ₂ /L]	0.2
K_{SF}	saturation/inhibition coefficient for S_F [mg COD _{SF} /L]	2
K_{SA}	saturation/inhibition coefficient for S_A [mg COD _{SA} /L]	4
K_{NOH}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5
K_{NHH}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.05
K_{H2SH}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Autotrophic bacteria		
μ_A	the maximum aerobic growth rate on S_{NH} [1/d]	1 (0.35)
b_A	rate constant for lysis [1/d]	0.15 (0.05)
K_{OA}	saturation/inhibition coefficient for S_O [mg O ₂ /L]	1
K_{NHA}	saturation/inhibition coefficient for S_{NH} [mg N/L]	0.5 (5)
K_{H2SA}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Fermenting bacteria		
μ_{FB}	the maximum aerobic growth rate for X_{FB} [1/d]	3 (1.5)
b_{FB}	rate constant for lysis [1/d]	0.02
K_{OFB}	saturation/inhibition coefficient for S_O [mg O ₂ /L]	0.2
K_{SFB}	saturation/inhibition coefficient for S_F [mg COD _{SF} /L]	28
K_{NOFB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5
K_{NHFB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01
K_{H2SFB}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Acetotrophic methanogenic bacteria		
μ_{AMB}	the maximum aerobic growth rate on for X_{AMB} [1/d]	0.085
b_{AMB}	rate constant for lysis [1/d]	0.008
K_{OAMB}	saturation/inhibition coefficient for S_O [mg O ₂ /L]	0.0002
K_{SAMB}	saturation/inhibition coefficient for S_A [mg COD _{SA} /L]	56
K_{NOAMB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.0005
K_{NHAMB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01
K_{H2SAMB}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Acetotrophic sulfate-reducing bacteria		
μ_{ASRB}	the maximum aerobic growth rate for X_{ASRB} [1/d]	0.18
b_{ASRB}	rate constant for lysis [1/d]	0.012
K_{OASRB}	saturation/inhibition coefficient for S_O [mg O ₂ /L]	0.0002
K_{SASRB}	saturation/inhibition coefficient for S_A [mg COD _{SA} /L]	24
K_{NOASRB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.0005
K_{NHASRB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01
K_{SOASRB}	saturation/inhibition coefficient for S_{SO4} [mg S/L]	19
$K_{H2SASRB}$	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140

Sulfide oxidizing bacteria

μ_{SOB}	the maximum aerobic growth rate for X_{SOB} [1/d]	5.28
η_{SOB}	correction factor for anoxic growth of X_{SOB} [-]	0.8
b_{SOB}	rate constant for lysis [1/d]	0.15
K_{OSOB}	saturation/inhibition coefficient for S_O [mg O_2 /L]	0.2
K_{NOSOB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5
K_{NHSOB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.05
K_{SSOB}	saturation/inhibition coefficient for S_{H_2S} [mg S/L]	0.24

Solute Transport - Constructed Wetland Model No1 (CWM1) Parameters I

Hydrolysis

Hydrolysis Rate Constant: 0.125 Sat./Inh. Coef. Hydrolysis: 0.1 XFB Correction Factor: 0.1

Heterotrophic Bacteria (aerobic growth and denitrification)

Max. Aerobic Growth Rate: 0.25 Sat./Inh. Coef. for SO : 0.2 Sat./Inh. Coef. for SNO : 0.5
 Anoxic Correction Factor: 0.0333333 Sat./Inh. Coef. for SF : 2 Sat./Inh. Coef. for SNH : 0.05
 Rate Constant for Lysis: 0.4 Sat./Inh. Coef. for SA : 4 Sat./Inh. C. for SH_2S : 140

Autotrophic Bacteria

Max. Growth Rate XA : 0.0416667 Sat./Inh. Coef. for SO : 1 Sat./Inh. Coef. for SH_2S : 140
 Rate Constant for Lysis: 0.00625 Sat./Inh. Coef. for SNH : 0.5

Fermenting Bacteria

Max. Growth Rate XFB : 0.125 Sat./Inh. Coef. for SF : 28 Sat./Inh. Coef. for SNH : 0.01
 Rate Constant for Lysis: 0.000833333 Sat./Inh. Coef. for SNO : 0.5 Sat./Inh. Coef. for SH_2S : 140
 Sat./Inh. Coef. for SO : 0.2

Acetotrophic Methanogenic Bacteria

Max. Growth Rate $XAMB$: 0.00354167 Sat./Inh. Coef. for SA : 56 Sat./Inh. Coef. for SNH : 0.01
 Rate Constant for Lysis: 0.000333333 Sat./Inh. Coef. for SNO : 0.0005 Sat./Inh. Coef. for SH_2S : 140
 Sat./Inh. Coef. for SO : 0.0002

Acetotrophic Sulfate Reducing Bacteria

Max. Growth Rate $XASRB$: 0.0075 Sat./Inh. Coef. for SA : 24 Sat./Inh. Coef. for SSO_4 : 19
 Rate Constant for Lysis: 0.0005 Sat./Inh. Coef. for SNO : 0.0005 Sat./Inh. Coef. for SH_2S : 140
 Sat./Inh. Coef. for SO : 0.0002 Sat./Inh. Coef. for SNH_4 : 0.01

Sulphide Oxidising Bacteria

Max. Aerobic Growth Rate: 0.22 Sat./Inh. Coef. for SO : 0.2 Sat./Inh. Coef. for SNH : 0.05
 Anoxic Correction Factor: 0.8 Sat./Inh. Coef. for SNO : 0.5 Sat./Inh. Coef. for SH_2S : 0.24
 Rate Constant for Lysis: 0.00625

OK
 Cancel
 Help

Next ...
 Previous ...

Figure 50. The Constructed Wetland Model (CWM1) Parameter I dialog window.

Solute Transport - Constructed Wetland Model (CW2D) Parameters II

Temperature Dependence	
Heterotrophic Organisms:	47800
Autotrophic Organisms:	69000
Hydrolysis:	28000
Factor KX for Hydrolysis:	-53000
Factor KNHA for Nitrification:	-160000

Stoichiometric Parameters	
Production of CI in Hydrolysis:	0
Fraction of CR in biomass Lysis:	0.1
Fraction of CI in biom.	0.02

Yield Coefficients	
Yield Coeff. for Heterotr.:	0.65
Yield Coeff. for N Somonas:	0.24
Yield Coeff. for N.Bacter.:	0.24

Composition Parameters	
N Content of CR:	0.03
N Content of CS:	0.04
P Content of CR:	0.01
P Content of CS:	0.01
N Content of CI:	0.01
N Content of biomass:	0.07
P Content of CI:	0.01
P Content of biomass:	0.02

Oxygen	
O2 Saturation:	9.18
Temp. Dep. O2 Saturation:	-15000
Rate O2:	10

OK
Cancel
Help

Next ...
Previous ...

Figure 51. The Constructed Wetland Model (CW2D) Parameter II dialog window.

Table 15. Temperature dependencies, stoichiometric parameters, composition parameters, and parameters describing oxygen transfer in the CW2D biokinetic model [Langergraber and Šimunek, 2005].

Parameter	Description [unit]	Value
Temperature dependences (activation energy [J/mol] for Arrhenius equation)		
Tdep_het	activation energy for processes caused by XH [J/mol]	47800
Tdep_aut	activation energy for processes caused by XA [J/mol]	69000
Tdep_Kh	activation energy Hydrolyses [J/mol]	28000
Tdep_KX	activation energy factor KX for hydrolyses [J/mol]	-53000
Tdep_KNHA	activation energy for factor KNHA for nitrification [J/mol]	-160000
Stoichiometric parameters		
$f_{Hyd,CI}$	production of CI in hydrolysis	0.0
$f_{BM,CR}$	a fraction of CR generated in biomass lysis	0.1
$f_{BM,CI}$	a fraction of CI generated in biomass lysis	0.02
Y_{Het}	yield coefficient for XH	0.63
Y_{ANs}	yield coefficient for XANs	0.24
Y_{ANb}	yield coefficient for XANb	0.24
Composition parameters		
$i_{N,CR}$	N content of CR [g N/g COD _{CR}]	0.03
$i_{N,CS}$	N content of CS [g N/g COD _{CS}]	0.04
$i_{N,CI}$	N content of CI [g N/g COD _{CI}]	0.01
$i_{N,BM}$	N content of biomass [g N/g COD _{BM}]	0.07
$i_{P,CR}$	P content of CR [g P/g COD _{CR}]	0.01
$i_{P,CS}$	P content of CS [g P/g COD _{CS}]	0.01
$i_{P,CI}$	P content of CI [g P/g COD _{CI}]	0.01
$i_{P,BM}$	P content of biomass [g P/g COD _{BM}]	0.02
Oxygen		
cO2_sat_20	saturation concentration of oxygen [g/m ³]	9.18
Tdep_cO2_sat	activation energy for saturation concentration of oxygen [J/mol]	-15000
rate_O2	re-aeration rate [1/d]	240

Solute Transport - Constructed Wetland Model No1 (CWM1) Parameters II ✕

Temperature Dependence

Hydrolysis:	28000	XFB Growth:	47800
KX (Hydrolysis):	-54400	XFB Lysis:	0
XH:	47800	XAMB:	0
XA:	75800	XASRB:	0
KNHA (nitrification):	-160000	XSOB:	0

Stoichiometric Parameters

Production of SI (Hydrolysis):	0	Fraction of XI generated (Lysis):	0.1
Fraction of SF Generated	0.05		

Yield Coefficients

Yield Coefficient for XH:	0.63	Yield Coefficient for XAMB:	0.032
Yield Coefficient for XA:	0.24	Yield Coefficient for XASRB:	0.05
Yield Coefficient for XFB:	0.053	Yield Coefficient for XSOB:	0.12

Composition Parameters

N Content of SF:	0.03	N Content of XI:	0.03
N Content of SI:	0.01	N Content of Biomass:	0.07
N Content of XS:	0.04		

Oxygen

O2 Saturation:	0.3825	Rate O2:	240
Temp. Dep. O2 Saturation:	-15000		



Figure 52. The Constructed Wetland Model (CWM1) Parameter II dialog window.

Table 16. Temperature dependencies, stoichiometric parameters, composition parameters, and parameters describing oxygen transfer in the CWM1 biokinetic model [Langergraber *et al.*, 2009].

Parameter	Description [unit]	Value
Temperature dependences (activation energy [J/mol] for Arrhenius equation)		
Tdep_HyKh	activation energy Hydrolyses [J/mol]	28000
Tdep_HyKX	activation energy factor KX for hydrolyses [J/mol]	-54400
Tdep_H	activation energy for processes caused by XH [J/mol]	47800
Tdep_A	activation energy for processes caused by XA [J/mol]	75800
Tdep_KNHA	activation energy for factor KNHA for nitrification [J/mol]	-160000
Tdep_mueFB	activation energy for XFB growth [J/mol]	47800
Tdep_bFB	activation energy for XFB lysis [J/mol]	0
Tdep_AMB	activation energy for processes caused by XAMB [J/mol]	0
Tdep_ASRB	activation energy for processes caused by XASRB [J/mol]	0
Tdep_SOB	activation energy for processes caused by XSOB [J/mol]	0
Stoichiometric parameters		
$f_{Hyd,SI}$	production of S_I in the hydrolysis	0.0
$f_{BM,SF}$	a fraction of S_F generated in biomass lysis	0.05
$f_{BM,XI}$	a fraction of X_I generated in biomass lysis	0.1
Y_H	yield coefficient for XH	0.63
Y_A	yield coefficient for XA	0.24
Y_{FB}	yield coefficient for XFB	0.053
Y_{AMB}	yield coefficient for XAMB	0.032
Y_{ASRB}	yield coefficient for XASRB	0.05
Y_{SOB}	yield coefficient for XSOB	0.12
Composition parameters		
$i_{N,SF}$	N content of S_F [g N/g COD _{SF}]	0.03
$i_{N,SI}$	N content of S_I [g N/g COD _{SI}]	0.01
$i_{N,XS}$	N content of X_S [g N/g COD _{XS}]	0.04
$i_{N,XI}$	N content of X_I [g N/g COD _{XI}]	0.03
$i_{N,BM}$	N content of biomass [g N/g COD _{BM}]	0.07
Oxygen		
cO2_sat_20	saturation concentration of oxygen [g/m ³]	9.18
Tdep_cO2_sat	activation energy for saturation concentration of oxygen [J/mol]	-15000
rate_O2	re-aeration rate [1/d]	240

3.8. The Slope Cube Module

The **Slope Cube** (Slope Stress and Stability) module (added in version 2.04) was developed by the Soil Water Retention, LLC as a supplemental module of the HYDRUS (2D/3D) software package to simulate two-dimensional transient fields of soil moisture, soil suction, suction stress, total and effective stresses, and local factor of safety. While the SLOPE Stability module is based on classical and engineering soil mechanics theories and uses the effective stress approach only for saturated conditions, a new add-on module "**SLOPE Cube**" (Slope Stress and Stability), recently developed in cooperation with Dr. Ning Lu from the Colorado School of Mines, uses a unified, effective stress approach for both saturated and unsaturated conditions [Lu *et al.*, 2010]. The module is intended to predict spatially and temporally infiltration-induced landslide initiation and to carry out the slope stability analysis under variably-saturated soil conditions. Transient moisture and suction fields are directly obtained using the HYDRUS model and are used to compute the effective stress field in hillslopes [Lu and Godt, 2013]. Furthermore, instead of the methodology of one-factor safety for the entire slope in the classical slope stability analysis, the **SLOPE Cube** module computes the field of the factor of safety in the entire domain within hillslopes [Lu *et al.*, 2012], allowing identification of the development of potential failure surface zone or surface.

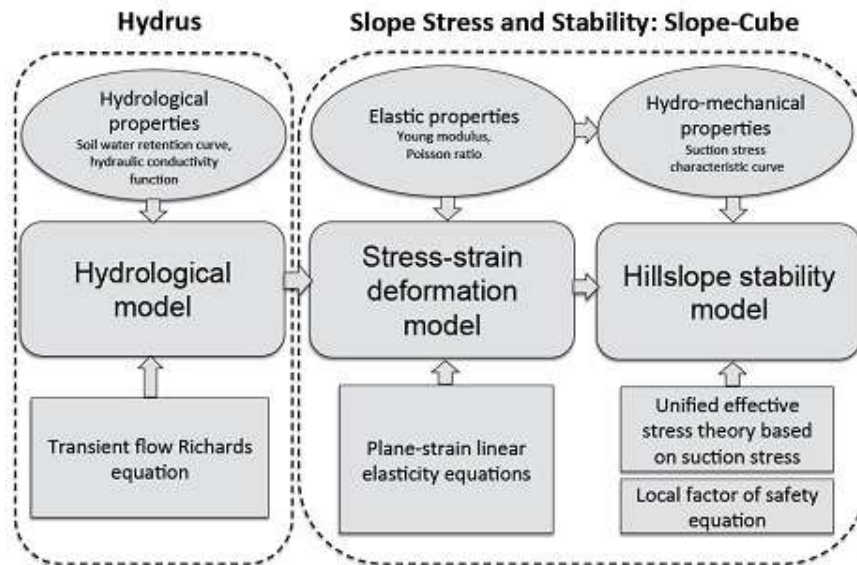


Figure 53. Illustration of the physical processes in the SLOPE Cube module.

Slope Cube is a physically-based hydro-mechanical framework focusing on assessment and prediction of the initiation and locations of landslide occurrences under rainfall conditions. **Slope Cube** couples variably-saturated flow and stress fields to simulate transient hillslope hydrologic and mechanical responses to rainfall events (Fig. 53). Two recent advancements are implemented in **Slope Cube** that are beyond the traditional, physically based landslide models. The first is the utilization of the suction stress-based effective stress to unify the description of effective stress distribution in hillslopes under variably-saturated conditions. The second is to employ a recently established concept of the local factor of safety to capture the evolution of stress paths toward the failure state in hillslopes.

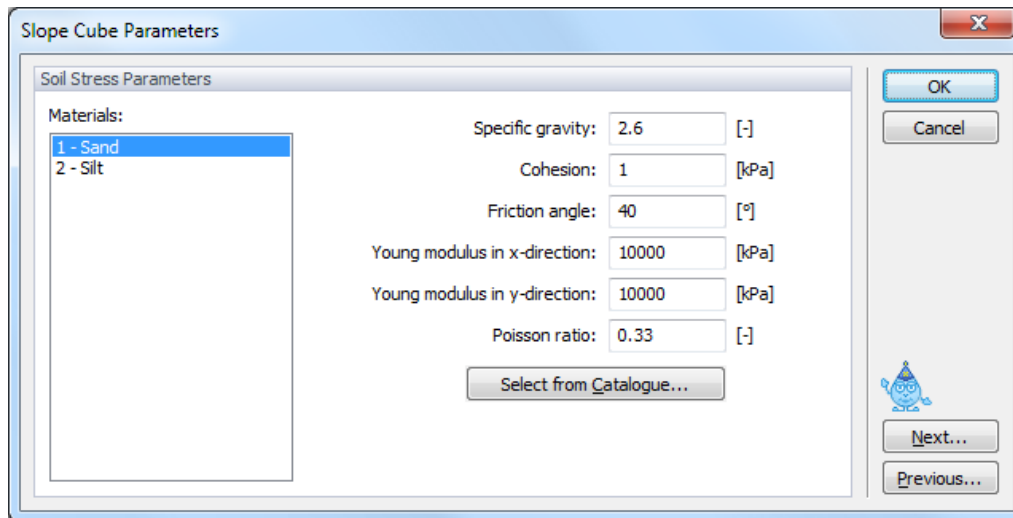


Figure 54. The Slope Cube Parameters dialog window.

The inputs for the Slope Cube module are entered in the Slope Cube Parameter dialog window (Fig. 54). Here is the link to the [Slope Cube Manual](#) [Lu et al., 2016]. Examples of selected outputs (maximum and minimum effective stresses, suction stress, and local factor of safety; other parameters not shown here are maximum and minimum total stresses) from the Slope Cube module are given in Figure 55.

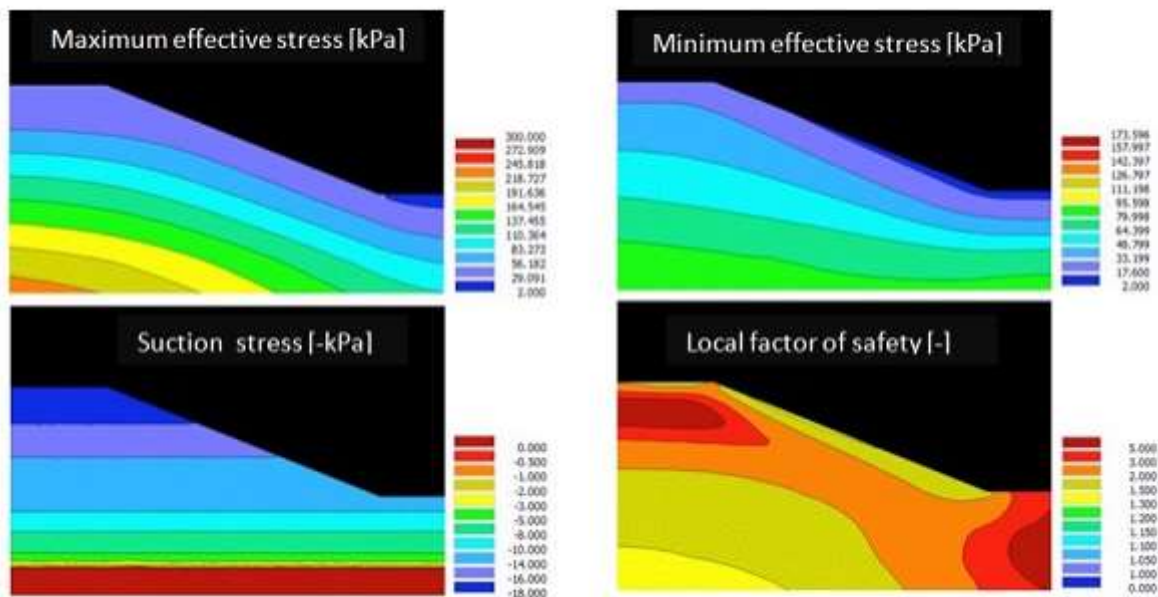


Figure 55. Examples of selected outputs (maximum and minimum effective stresses, suction stress, and local factor of safety) from the Slope Cube module.

4. Geometry of the Transport Domain

The transport domain may be defined using relatively simple one-dimensional (Fig. 12), two-dimensional rectangular (Fig. 10), or three-dimensional hexahedral (Fig. 11) objects. In that case, the dimensions and other parameters of the transport domain are specified numerically using either the *Rectangular* (Fig. 10) or *Hexahedral Domain Definition* (Fig. 11) dialog windows. In both of these cases, the transport domain is discretized into a structured finite element mesh. Alternatively, a more general two-dimensional geometry can be defined from basic boundary objects, such as points, lines, splines, polylines, arcs and/or circles. Boundary curves can consist of any combination of polylines, arcs, circles, or cubical splines. The program permits one to specify internal boundaries (e.g., drains, wells, impermeable objects), as well as internal curves. A user can define from these boundary objects either a two-dimensional transport domain, the base plane (**base surface**) of the **three-dimensional layered domain**, or multiple surfaces that can then define the **three-dimensional general domain**. In the former two cases, the two-dimensional transport domain or the base plane of the three-dimensional domain is discretized into an unstructured finite element mesh.

4.1. Boundary Objects

The **computational domain** (the two-dimensional transport domain or the **base surface** of the three-dimensional domain) is formed by an arbitrary number of mutually nonintersecting **curves**. Each curve can be formed by connecting an arbitrary number of **objects**. Objects are defined by nodes, the positions of which can be specified either graphically with the mouse with possibilities to use **grid** alignment (Fig. 185) or by numerically defining their coordinates *X*, *Y*, and *Z*. It is also possible to read in the objects with a large number of nodes (**spline**, **polyline**) from a file containing the *x*-(, *y*-,) and *z*-coordinates for each node using the command *Insert->Domain Geometry->Points->Read from File* The order of inputting particular objects is arbitrary; the code automatically forms the desired curves. In order to have a physically realistic domain, only one closed outer curve can exist (for multicomponent domains, such a curve must exist for each component of the domain). The domain can have an arbitrary number of **holes** or **internal curves**. The consistency of the geometry can be verified at any time using the command **Check Data Consistency (Tools Menu)**. Any change in geometry can be undone using the **undo** command (up to ten levels backward in time) or redone using the **redo** command (again up to 10 levels).

An object type (e.g., polyline, spline, arc, or circle) must be selected first when designing a new object from the **Edit Bar** on the right side of the view window or from the menu (e.g., *Insert->Domain Geometry->Nodes*). Then points defining a particular object should be entered. The manner in which nodes are entered depends on the selected input style. When entering data graphically, an appropriate **Work Plane** (*x-y*, *y-z*, *x-z*) and a grid with appropriately set parameters (Fig. 185 and Section 8.1.2) can be used to facilitate the input, while the coordinates *X*, *Y*, and *Z* of the cursor are continuously displayed in the bottom right corner of the window.

It is possible to edit existing objects by double-clicking on a particular object. The current selection, displayed in yellow, may be modified (edited) using the following operations: **delete**,

copy (Fig. 66), **move** (Fig. 66), **rotate** (Fig. 67, left), and **mirror** (Fig. 67, right). Note that, in addition to objects, particular nodes of an object can belong to a selected set as well, in which case the edit operations are carried out also for these points. Editing of selected objects (e.g., moving objects) also depends on the currently selected input style. The objects are moved with the cursor when the graphical mode is selected, while in numerical mode, a vector of translation (X , Y , and Z) must be specified. It is possible to directly edit nodes of objects with the commands **insert point** (Fig. 58), **delete point**, and/or **move point**.

Before saving the data, an option is always displayed whether or not to verify the consistency of the geometry. We strongly recommend to regularly perform this test in order to prevent errors in subsequent calculations, e.g., during mesh generation.

Table 17. Definition of terms related to geometry design.

Objects Objects are basic elements for building a geometric model of the computational domain and for defining other properties of the computational problem. Objects are divided into several categories (e.g., Geometry, FE-mesh, or Auxiliary), with each category containing several fields of objects of the same type. The shape (boundary) of the computational domain is defined using Geometric objects. Basic types of geometric objects are: - points - curves (polylines, arcs, circles, splines) - surfaces - openings - thickness vectors - solids Points A point is a basic geometric object which is used to define Curves and other objects. A point location is defined using two or three coordinates depending on the dimensions of a particular problem. Curves A curve is a set consisting of a finite number of objects connected by boundary nodes. Except at point nodes, objects cannot intersect with each other or themselves. A curve can be open or closed. Outer Boundary Curves An outer boundary curve is a boundary curve with the following properties: the curve is closed, positively oriented (i.e., in a counter-clockwise direction), does not intersect any other curve or itself, and has the computational domain (surface) located on its left side (in the sense of positive orientation), while the right side is not part of a computational domain. Internal Curves

An internal curve must be located entirely within the computational domain. It can touch (but not intersect) the outside boundary of the computational domain at its definition points. An internal curve can be open or closed, and can intersect itself, provided the intersect occurs at a definition point of the internal curve.

Openings

An opening is defined by one or more boundary **curves** that form a closed boundary.

Lines

Lines and polylines are the most commonly used objects for describing the boundaries of a domain or internal curves. Lines are defined by two points specifying their beginning and end. Several lines can be connected to form “polylines” by connecting the beginning and end of two neighboring lines. Nodes cannot coincide, while lines cannot intersect with each other.

Arcs

An arc can be defined either by a) **three points** on its circumference, b) a **center**, a **radius**, **two angles** (starting and final angle) and its orientation, and c) **two points**, a **center**, and a **radius**.

Circles

A circle can be defined either by **a center and a radius**, or by **three different points**.

Surface

A **surface** (the **computational domain** of two-dimensional applications) is defined by a finite number of continuous disjunctive bounded two-dimensional subdomains (Fig. 56). This means that the domain can be multicomponent, but that each of its components must have only one **outer boundary curve**. The domain can contain any finite number of **internal holes** or **internal curves**. **Surfaces** can be either **planar surfaces** (defined in a single plane) or **curved surfaces** (e.g., **Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**). The **base surface** is a two-dimensional **planar surface** that can be extended into a three-dimensional **solid** (the **computational domain** of three-dimensional applications) using **thickness vectors**.

Thickness Vectors

The term **thickness vector** is used for a vector perpendicular to the **base surface** that extends the Base Surface to form a **solid** (three-dimensional **computational domain**).

Solids

The term **solid** represents a three-dimensional **computational domain** that is formed either by the **base surface** and **thickness vectors** (**3D-Layered Solids**), or **boundary surfaces** (**3D-General Solids**), which can be either planar or curved (e.g., **Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**).

Computational Domain

A **Computational Domain** is a continuous part of a two- or three-dimensional space for which water flow or solute transport is simulated. The **Domain Geometry** term relates to the shape of this space. The **Domain Geometry** can be defined for simple cases using parameters (using a Generalized Rectangle in 2D projects or a Generalized Hexahedral in 3D projects) and for

general cases using boundaries (boundary curves for two-dimensional domains and boundary surfaces for three-dimensional domains).

In the **3D-Standard** version, the **Geometry** is defined using the **Base Surface**, which is a 2D domain of an arbitrary shape, and a set of **Thickness Vectors** that define the variable thickness of the 3D domain or thicknesses of an arbitrary number of **Geo-Layers** (the term **Sublayers** was used in version 1, and is used alternatively in the text below). Such a domain is then called the **3D-Layered** domain. Although such domains cannot be fully general, they allow the definition of a majority of realistic 3D problems. In the **3D-Professional** version, the **Geometry** is defined using three-dimensional objects (Solids, bodies) of general shapes, which are formed by boundary surfaces, which can be either planar or curved.

A **Computation domain** can be formed using several surfaces that can touch each other, but cannot overlap (Fig. 56). It is possible to create an opening in the base surface and then enter another surface into it. The division of the transport domain into individual surfaces enables easier work with it. The program creates for each surface its own section, and users can then specify different domain properties and initial and boundary conditions on these sections.

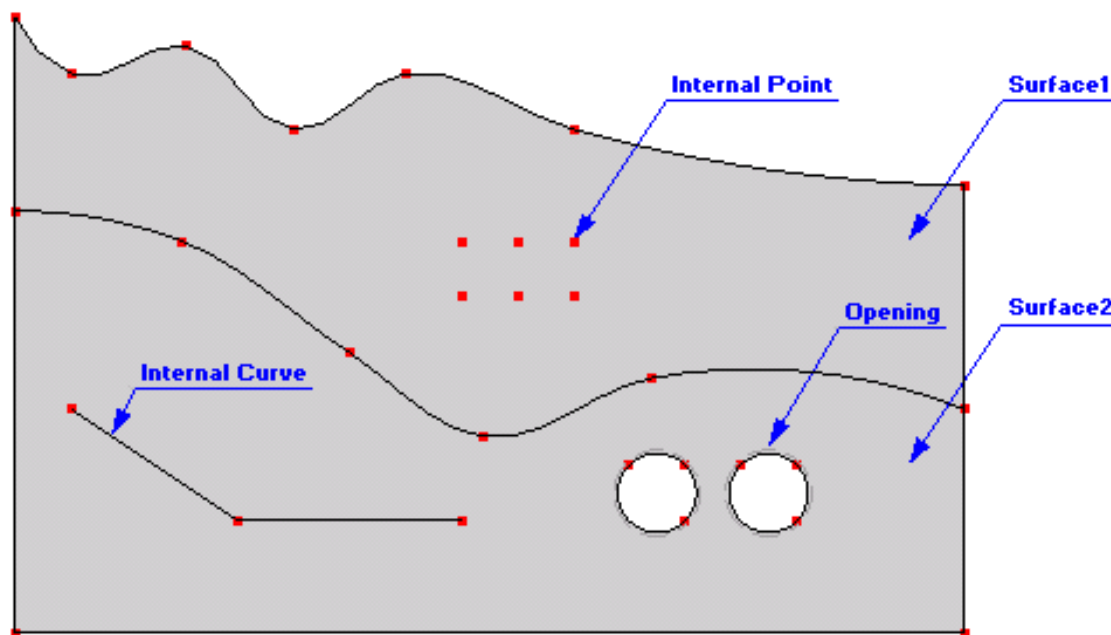


Figure 56. A base surface showing several basic geometric objects.

4.1.1. Points

Points can be either used to define **Boundary Objects** or can be located inside of the **Surface** (computational domain) and not be associated with any boundary object (**Single Points**). Points can be entered either graphically using a cursor (most common) or using the **New Point** dialog window (identical to the **General Tab** of the **New Point** dialog, Fig. 58). To enter a new point graphically, select the command *Insert->Domain Geometry->Point->Graphically* from the

menu, or **Points** from the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window**, and then enter the points using a cursor.

Once a command for defining a **new point** graphically is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 57 (left). The **Edit Bar** will also show which point (its number) is being defined and what reference coordinate system (the current coordinate system or the grid origin) is used. The process of defining new points is ended by pressing the Esc keyboard button, the right mouse button (see the **Help** part of the Edit Bar), or clicking the Stop button on the Edit Bar.

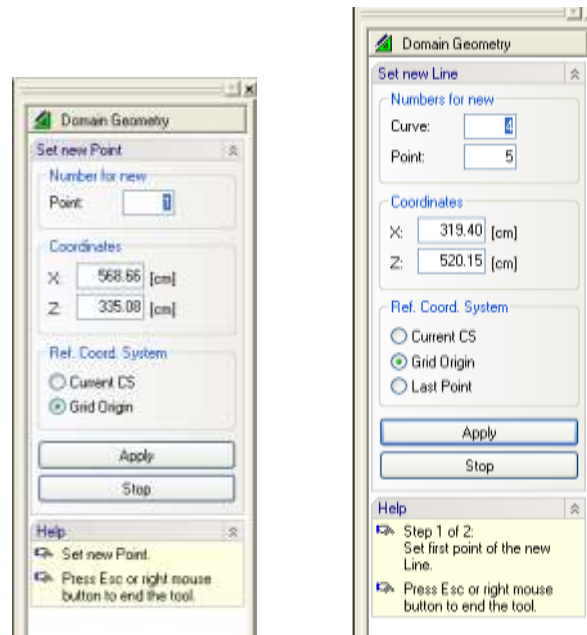


Figure 57. The Edit Bar during the process of defining a new point (left) and a new line (right) graphically.

Double-clicking on an existing point will recall the **Edit Point** dialog window (Fig. 58). In addition to the **General Tab** (Fig. 58, left) in the **New Point** dialog window, the **Edit Point** dialog window also has the **FE-Mesh Tab** (Fig. 58, right). Coordinates of a point and its number are entered in the **General Tab**, while the **FE-Mesh Refinement** at a given point can be defined in the **FE-Mesh Tab**.

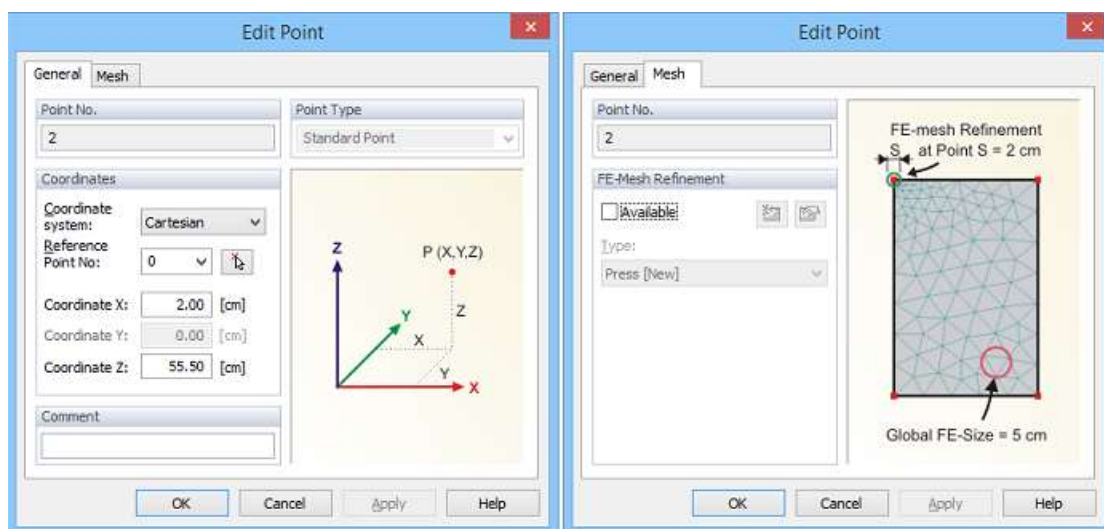


Figure 58. The Edit Point dialog window.

Although Cartesian Coordinates are usually used, it is possible to use also other coordinate systems:

Coordinate Systems in 3D Projects	Coordinate Systems in 2D Projects
• Cartesian • X-cylindrical • Y-cylindrical • Z-cylindrical • Spherical	• Cartesian • Polar

Reference Point: Point coordinates are usually related to the defined origin of the coordinate system. They can nevertheless be also related to another existing point, whose index is specified in the box **Reference Point No.** Locations of all related points are automatically adjusted when the location of the reference point is changed. The dependence of points on the Reference Point is, however, canceled during more complex operations, such as Copy, Rotate, or Drag and Drop. The coordinates of such points are then recalculated using the absolute Cartesian coordinate system.

Point Type: Current version of HYDRUS recognizes two types of points:

- **Standard** – These are regular points defined using two or three coordinates.
- **Parametric** – These points are located on a curve. Their location is calculated using a specified parameter from the interval (0.1), where 0 and 1 represent the beginning and end of the curve, respectively. For example, a point with a parametric coordinate $t=0.5$ is located exactly in the middle of the curve. A parametric point is not a defining point of a curve; i.e., it does not define its shape. On the contrary, the shape of a curve defines the location of a parametric point. A **Parametric Point** can be redefined as a

Standard Point in the **Edit Point** dialog window (Fig. 58). **Parametric Points** can be added on a curve using the command **Insert Points on Line** on the **Edit Bar**, using the menu command *Tools -> Insert Points On Line->Graphically*, or by clicking on a curve with the right mouse button and selecting the *Insert Points On Line->Graphically* from the popup menu (Fig. 59). Either the parametric coordinate of a point or its distance from boundary points (L) of a curve is displayed on the Edit Bar when specifying a **Parametric Point**.

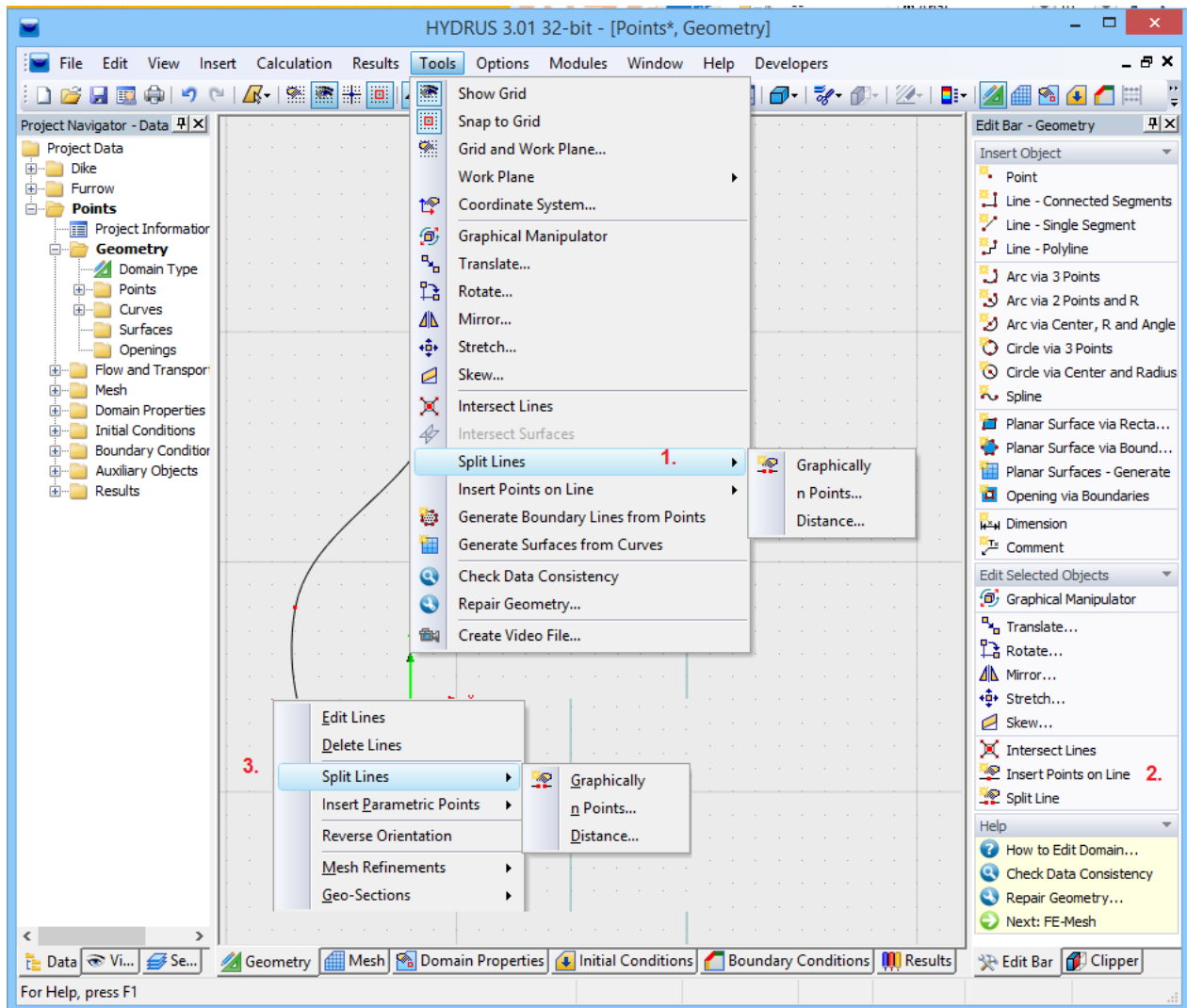


Figure 59. Different ways of adding Parametric Points on a curve.

4.1.2. Lines and Polylines

Lines and **Polylines** are the most commonly used objects for describing the boundaries of a two-dimensional domain and its internal curves. Similarly, as above for **Points**, **Lines** and **Polylines** can be entered either graphically using a cursor (most common) or using the **New Line** dialog window (identical to the **General Tab** of the **Edit Line** dialog, Fig. 60). When entering a new

line graphically, users can select the command *Insert->Domain Geometry->Line(Polyline)->Graphically* from the menu, or **Line - Abscissa** or **Line - Polyline** from the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window** and then enter the lines using a cursor.

Once a command for defining a **New Line** (a single abscissa) or a **New Polyline** is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 57 (right). The **Edit Bar** will also show which point and curve (their numbers) are being defined and what reference coordinate system (the current coordinate system, the grid origin, or the last inserted point) is used. Once a single **Line** is specified (for a new line), one can immediately continue in specifying the second one, while the last point of the first line will be the beginning point of the second line. Each abscissa is considered to be a single curve. When a **New Polyline** is being created, the entire polyline is considered to be a single curve. The process of defining new lines is ended by pressing the Esc keyboard button, the right mouse button (see the **Help** part of the Edit Bar), or clicking the Stop button on the Edit Bar.

Double-clicking on an existing line will recall the **Edit Line** dialog window (Fig. 60). Before using the **New Line** dialog window, a user needs to first define points that are then used to define the line. In addition to the **General Tab** (Fig. 60, left) in the **New Line** dialog window, the **Edit Curve** dialog window also has the **FE-Mesh Tab** (Fig. 60, right). Points defining the line are entered in the **General Tab**, while the **FE-Mesh Refinement** along a given line can be defined in the **FE-Mesh Tab**.

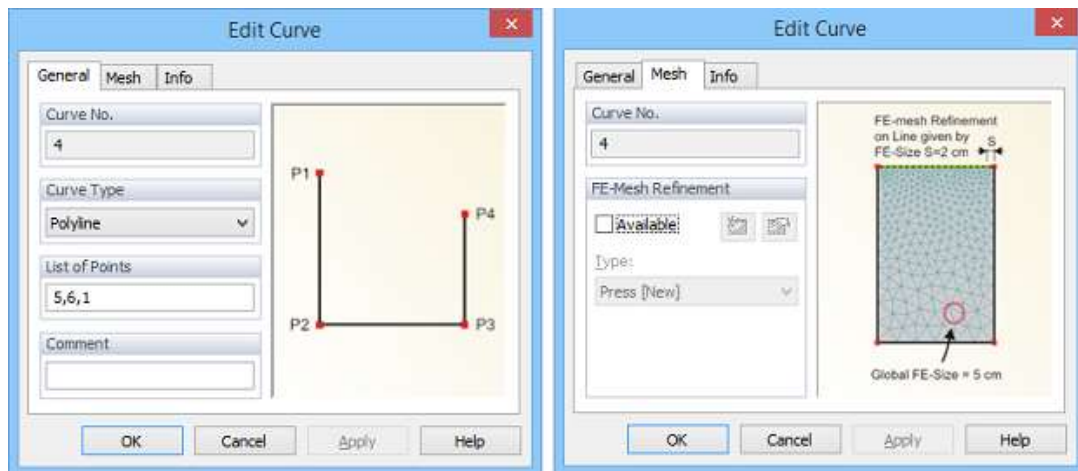


Figure 60. The Edit Curve dialog window.

4.1.3. Arcs and Circles

An **arc** is part of a **circle**. An object **arc** is always internally defined using three definition points. However, to simplify its specification, it is possible to define an **arc** graphically in multiple ways using: a) **three points** on its circumference, b) a **center**, a **radius**, **two angles** (starting and final angle) and its orientation, or c) by **two points**, a **center**, and a **radius**. Again, **arcs** can be entered

either graphically using a cursor (most common) or using the **New Line** dialog window (Fig. 62). When entering a new **arc** or circle graphically, a user must select the command *Insert->Domain Geometry->Arc->Graphically* from the menu, or one of the following commands (a) **Arc by 3 Points**, b) **Arc by 2 Points and R**, or c) **Arc by Center, R, and Angle**) from the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window** and then enters **arc** using a cursor.

The graphical definition of **Arcs** and **Circles** is rather similar to the definition of **Points** and **Lines**. Differences occur when **Radii** or **Angles** are used to define these objects. For example, when a user defines **Arc by 2 Points and Radius**, he/she first needs to define the two points, after which both the cursor and the **Edit Bar** change (Fig. 61, left) for the definition of the third type of information defining the arc. This can be a radius, an internal angle, or a height. The selection can be made on the **Edit Bar** that also displays the magnitude of this variable (R , A) and a step (dR , dA) in which it can be increased.

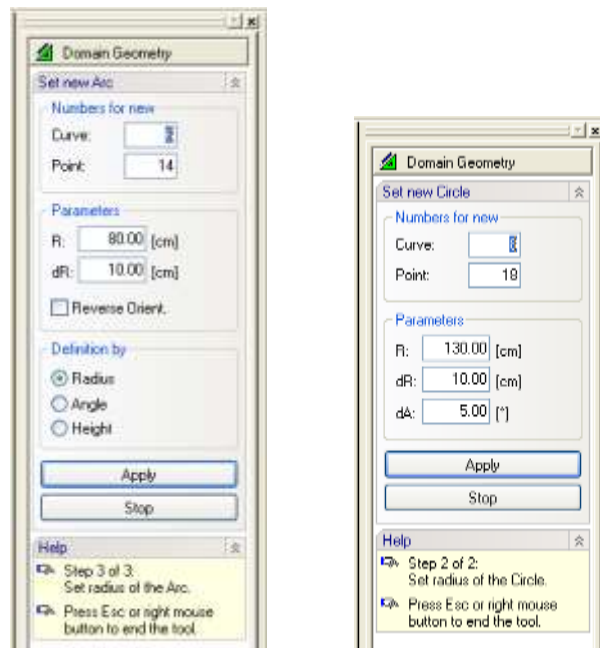


Figure 61. The Edit Bar during the process of defining a radius for a new arc (left) or a new circle (right) graphically.

In addition to the **General Tab** (Fig. 62, left) in the **New Line** dialog window, the **Edit Line** dialog window also has the **Arc Tab** (Fig. 62, right). A list of points defining the arc is given in the **General Tab**, while coordinates of points defining the arc, its center, and other parameters are entered in the **Arc Tab**. Double-clicking on an existing line will recall the **Edit Curve** dialog window (Fig. 62). The **Edit Curve** dialog window (Fig. 62) has an additional **FE-Mesh Tab** (similarly as for a line in Fig. 60; not shown here) where a user can refine the **FE-Mesh** along a given arc.

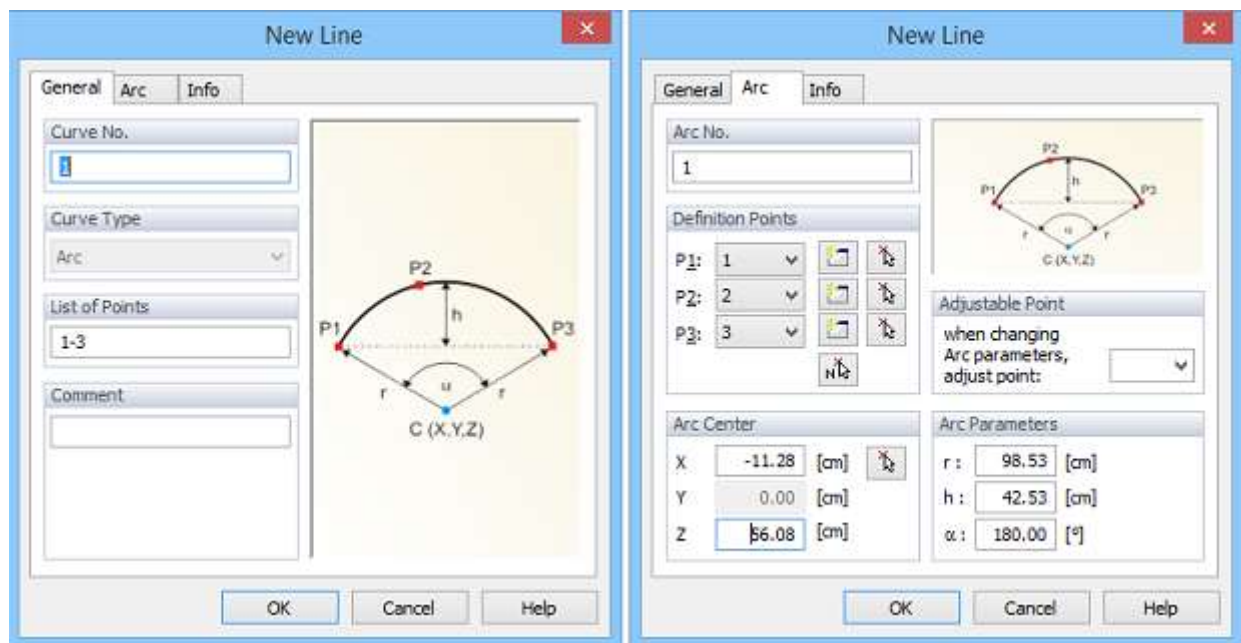


Figure 62. The New Line (Arc) dialog window.

An object **circle** is always defined internally using **three definition points**. However, to simplify its specification, it is possible to define a **circle** also using **a center and a radius**. Three definition points are then created automatically. Again, **circles** can be entered either graphically using the cursor (most common) or using the **New Line** dialog window (Fig. 62). A new **circle** can be entered graphically by selecting the command *Insert->Domain Geometry->Arc(Circle)->Graphically* from the menu, or by using one of the following commands (a) **Circle by 3 Points**, or b) **Circle by Center and Radius**) from the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window**, and then entering lines using the cursor. The list of points defining the circle must be entered in the **General Tab** (Fig. 63, left), while coordinates of points defining the circle, its center, and radius are entered in the **Circle Tab** (Fig. 63, right). When a **Circle** is defined **by Center and Radius** graphically, then the first definition point is created at the mouse click, while the other two are at the circle circumference at -90 and -180 degrees.

Adjustable Point: When a radius or the center of an arc is modified, it is usually also necessary to modify the location of one of the arc definition points. An adjustable point enables one to choose a point whose coordinates are to be changed.

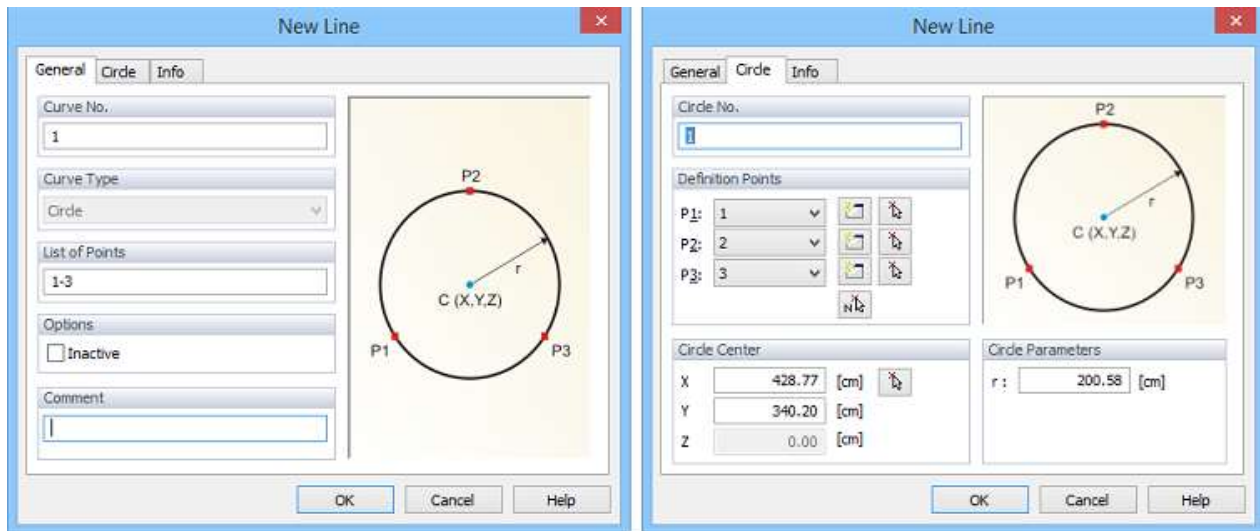


Figure 63. The New Line (Circle) dialog window.

4.1.4. Curves and Splines

The term “**Curve**” is used in the program and its documentation in two ways, while the meaning depends on where it is used.

- 1/ The term **Curve** is a general term for objects **Line**, **Polyline**, **Arc**, **Circle**, **Spline**.
- 2/ The term **Curve** can also refer to multiple objects (ad 1/) connected in their boundary points.

This meaning of the term **Curve** is mainly used in connection with “**Boundary Curve**”, “**Internal Curve**”, and so on.

There are several rules that need to be followed during the definition of a **Curve**.

- Curves cannot intersect with each other or themselves except at their definition nodes.
- No point that is not either its definition or **Parametric Point** can lie on a **Curve**.

Curves are always defined using their definition points (their indexes). The list of indexes can be checked or changed using the **Edit Curve** dialog (the first Tab “General”).

A **Spline** is a set of more than 2 points connected smoothly by cubic arcs. Splines are general smoothed curves defined using points in the 2D or 3D space. Three-dimensional splines do not generally have to lie in the same plane. However, if a spline is used to define a boundary of a surface, then all its definition points need to lie on this surface. A spline can be defined either graphically using a command on the **Edit Bar** or in the dialog where we select a particular type of spline. HYDRUS allows three types of splines:

- cubic spline, i.e., a curve defined by multiple polynomials of the third order. It passes smoothly through all points.
- Bezier's curve – a smooth curve that passes through boundary points, but does not have to pass through internal points .
- B-spline – a general Bezier's curve.

More information can be found at

<http://mathworld.wolfram.com/BezierCurve.html>

<http://mathworld.wolfram.com/B-Spline.html>

Once a command for defining a **new spline** graphically is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 64. The **Edit Bar** will also show which point and curve (their numbers) are being defined and what reference coordinate system (the current coordinate system, the grid origin, or the last inserted point) is used. One node is specified after the other. A user can also select on the **Edit Bar** the type of the spline (standard spline, B-spline, or Bezier curve). The process of defining a new spline is ended by pressing the Esc keyboard button, the right mouse button (see the **Help** part of the **Edit Bar**), or clicking the Stop button on the **Edit Bar**.

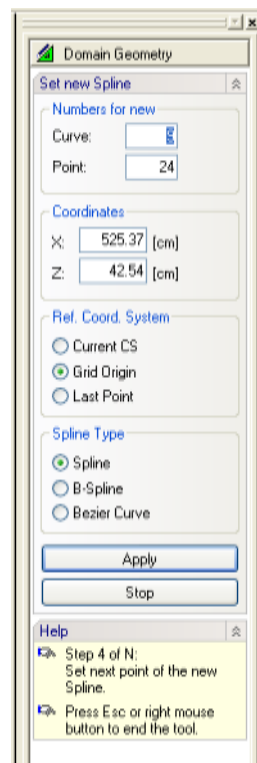


Figure 64. The Edit Bar during the process of defining a spline graphically.

4.1.5. Common Information for a Graphical Input of Objects

A/ A Numerical Input of Values. Edit controls displayed on the **Edit Bar** can be used to enter some values that are difficult to enter graphically as follows. Using a mouse, one defines the approximate shape of an object. Then using a keyboard, one enters selected values numerically. While entering values using a keyboard one cannot move a mouse, or entered values will be lost. One needs to use the „Tab“ key or „Shift + Tab“ keys at the keyboard to move forward or backward from one edit controls to another one, respectively. A control of Combo Boxes and Radio buttons is done using a standard way as in dialog windows, i.e., using keys Arrow Up or Arrow Down, etc. After all values are entered, one pushes the Enter key to finish the actual step of the running tool.

B/ Adjusting View. When graphically entering objects, one often needs to move or turn the scene, or to enlarge or reduce a selected detail. This can be done without interrupting the input of a particular object. The fastest way is to press the center mouse button (a wheel) and then a) dragging the scene with the mouse move, b) moving forward or backward an object by scrolling the wheel, or c) rotating the scene by simultaneously also pushing the right mouse button. After releasing the center mouse button, one can continue in the graphical input of an object. Similar operations can also be performed using the button on the **View Toolbar**:



A majority of buttons on the View Toolbar do not interrupt the graphical input of an object, i.e., after the adjustment of the **View Window** one can continue in the graphical input of an object.

C/ Snapping. When entering Points graphically (points created when entering curves or surfaces), a process called **Snapping** is taking place. This means that a cursor snaps to points of a **Grid** (Fig. 65, left) or to existing points. **Snapping** can be disabled using a button **Snap to Grid** on the **Tools Toolbar**. **Snapping** on existing points or curves cannot be disabled. **Snapping** occurs when a center of a cursor comes close to an existing point and when this point is redrawn with a yellow color (or any pre-select color assuming that redrawing of preselected points is not switched off). One can simultaneously observe on the **Edit Bar** that an index of a preselected point and its coordinates are displayed in edit controls. These controls are disabled since displayed values cannot be changed. **Snapping** on curves (Fig. 65, right) occurs in addition to **Snapping** on existing points. An automatic calculation of coordinates of a point on a curve and snapping to this point occurs when a center of a cursor comes close to an existing curve. A location of this point is marked using a yellow cross, which indicates that after this point is entered, it becomes a definition point of a curve. This is important since entering a point on a curve that is not its definition point leads to the wrongful definition of a domain. A **Check of a Geometry** discovers such errors, and the **Repair Geometry** function will automatically correct it.

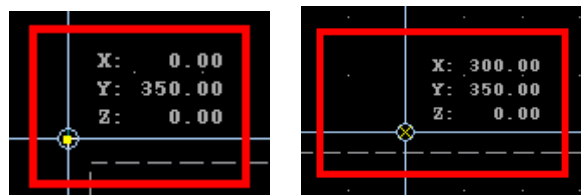


Figure 65. Snap to a point (left) and snap to a curve (right).

4.1.6. Translate, Copy, Rotate, Mirror, Stretch, and Skew Operations

All boundary objects can be manipulated using the **Translate**, **Copy**, **Rotate**, **Mirror**, **Stretch**, or **Skew** operations in the **Translate – Copy** (Fig. 66), **Rotate** (Fig. 67, left), **Mirror** (Fig. 67, right), **Stretch** (Fig. 68, left), and **Skew** (Fig. 68, right) dialog windows. These commands can be accessed either from the **Tools Menu** or from the **Transform Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window**. Users first select an object to be manipulated, then click on the command, and specify the **Vector of Translation** for the **Translate** or **Copy** operations, or the **Angle of Rotation** for a **Rotation**, or define the **Mirroring Plane/Axis** for a **Mirroring** operation.

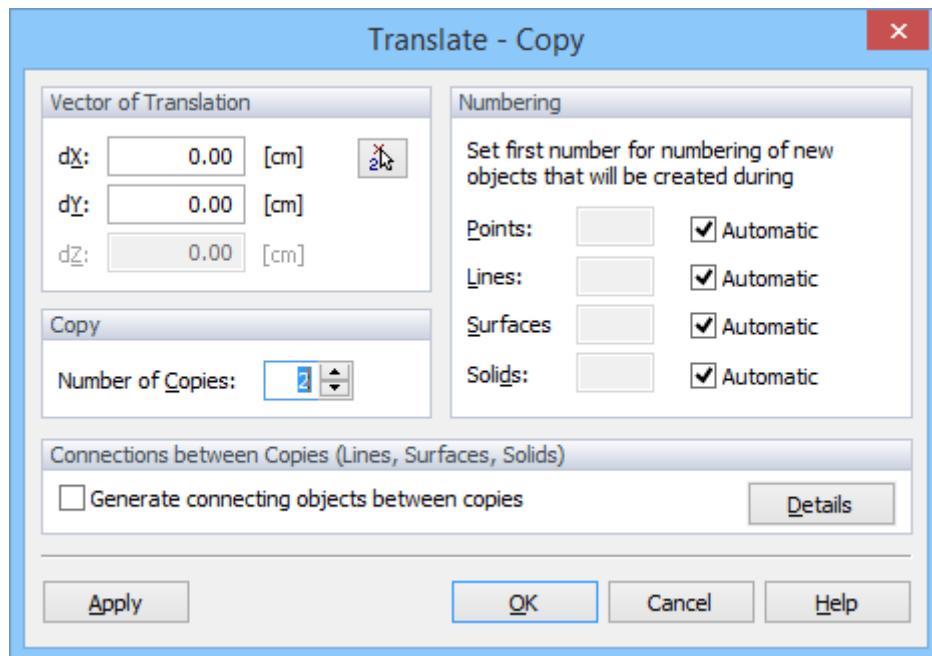


Figure 66. The Translate - Copy dialog window.

Rather than simply **Translating** or **Rotating** a given object, one can choose to use this operation (e.g., **Translate/Move** or **Rotate**) to create one or multiple copies of a given object by specifying the **Number of Copies** (see Figs. 66 and 67, left). Once one or more copies of a given object are to be created, one can also choose to **Generate Connecting Objects Between Copies** (e.g., Fig. 66). What types of connecting objects are to be created is selected in the **Manipulation Options** window (Figs. 69). HYDRUS can generate a) lines between selected nodes and their copies, b) surfaces between selected lines and their copies, and c) solids between selected surfaces and their copies). Lines can be either straight or curved when a copy is created using the Rotate operation.

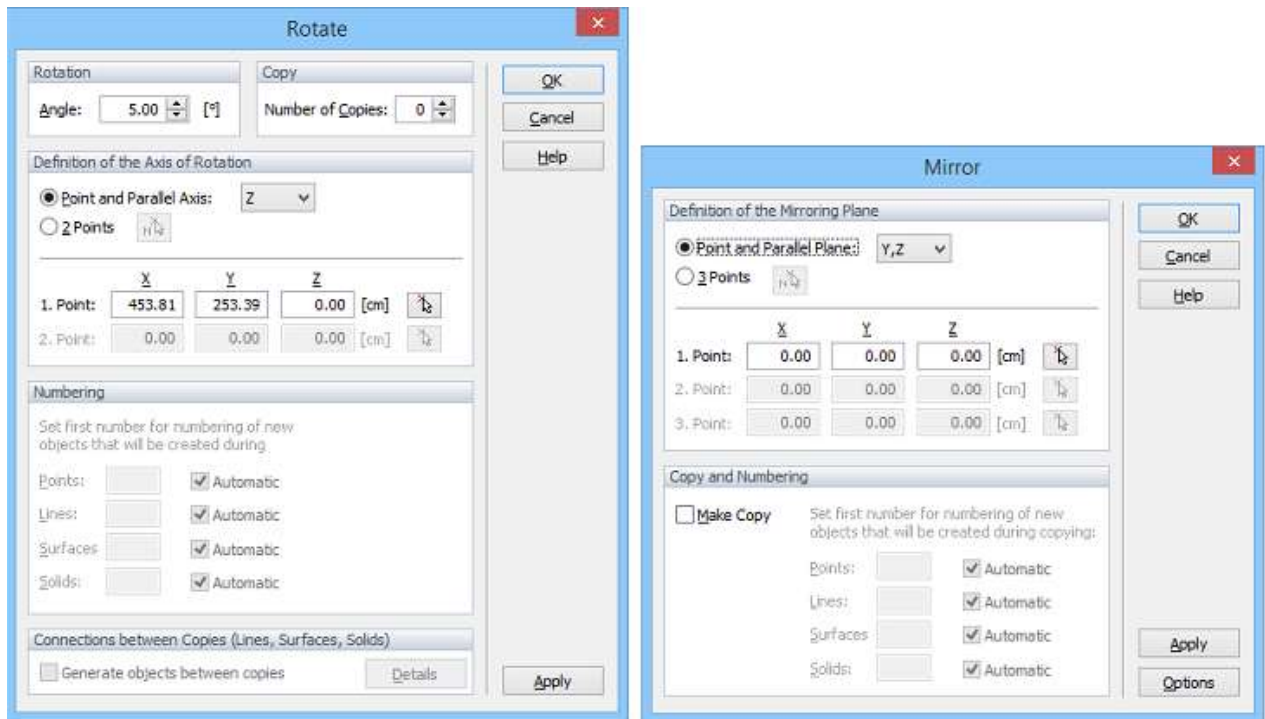


Figure 67. The Rotate (left) and Mirror (right) dialog windows.

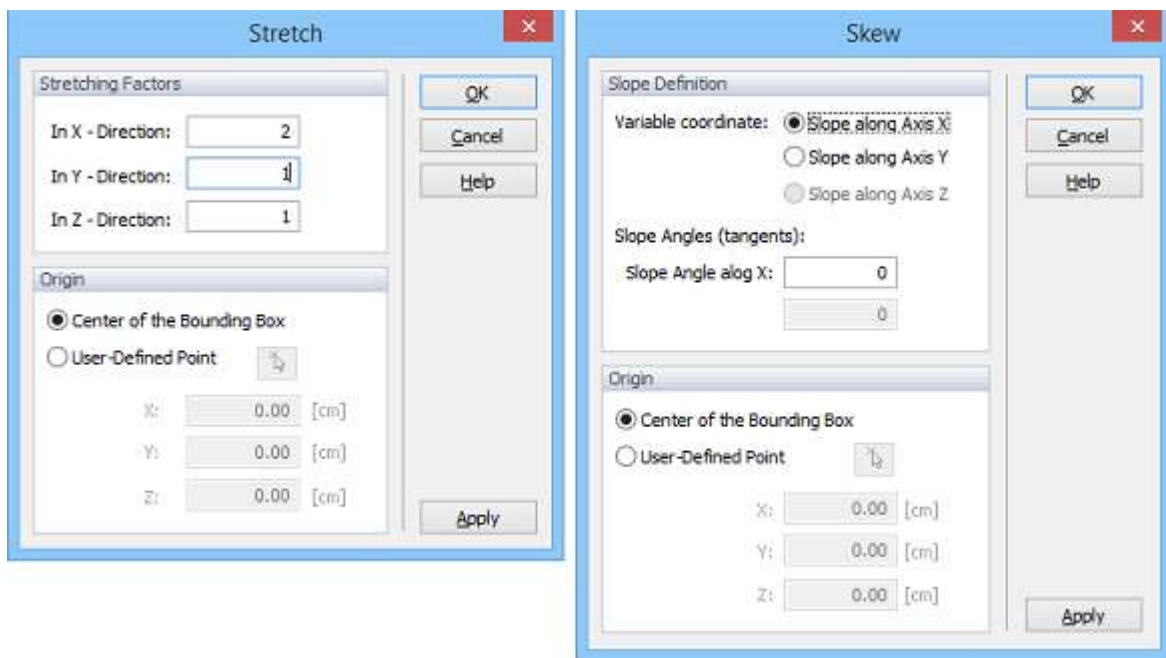


Figure 68. The Stretch (left) and Skew (right) dialog windows.

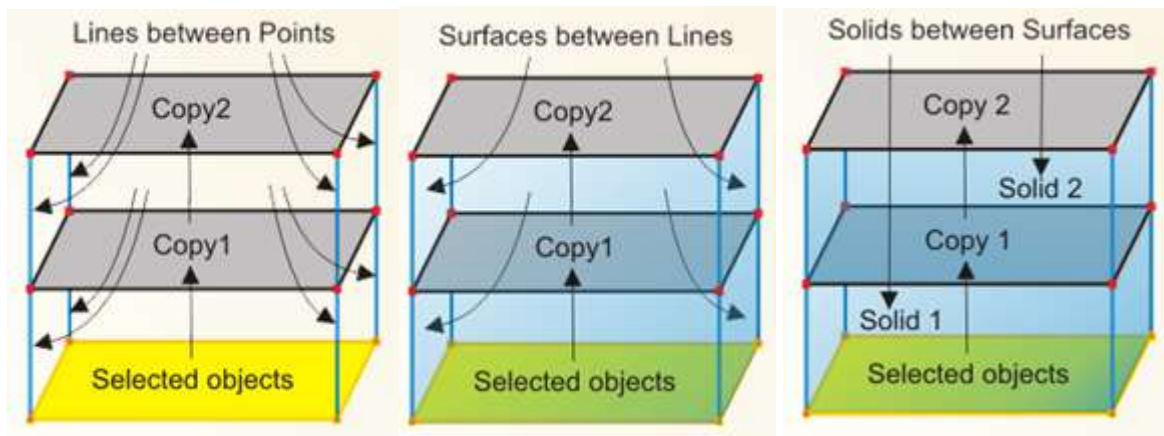
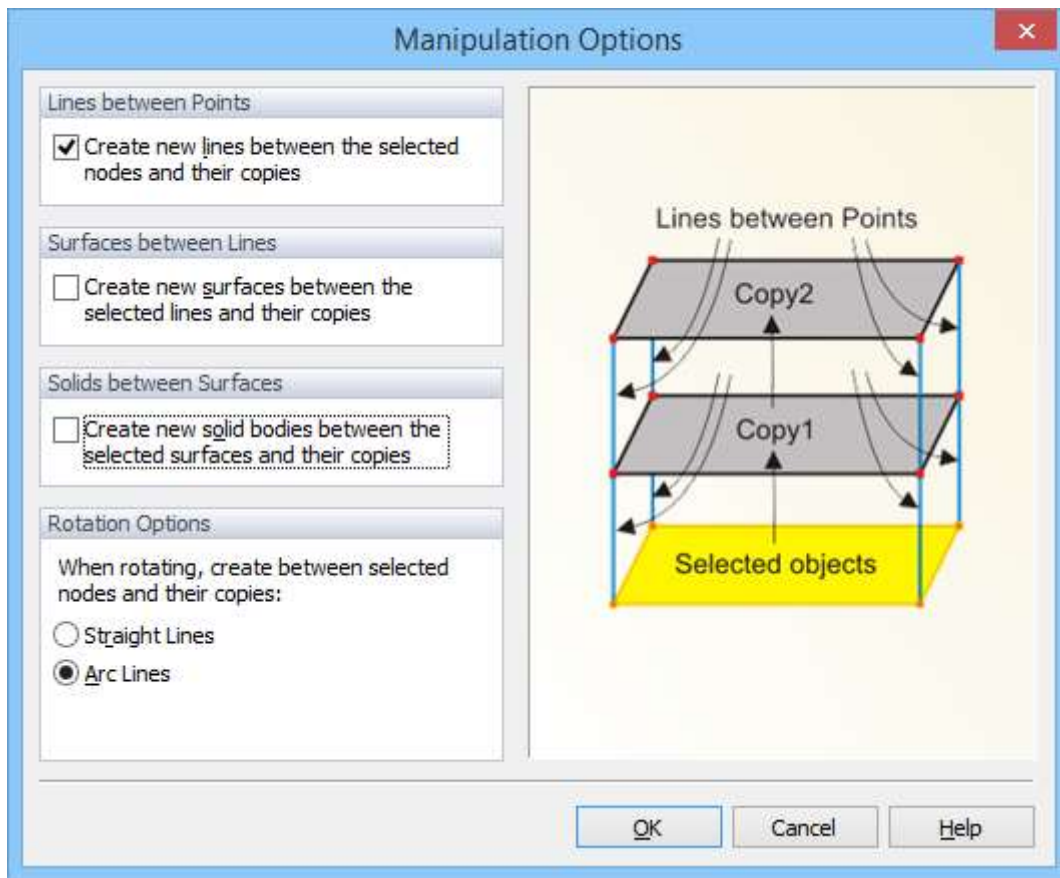


Figure 69. The Manipulation Options dialog window. The bitmaps indicate connecting lines between points, surfaces between lines, and solids between surfaces.

4.1.7. Additional Operations

Additional operations that can be used to manipulate boundary objects are **Intersect Lines**, **Insert Points on Line**, and **Split Line**. All three commands again can be accessed either from the **Tools** menu or from the **Transform Object** part of the **Domain Geometry** version of the **Tool Bar** on the right side of the **View Window**. The first command (**Intersect Lines**) finds the **Intersect** of two lines, whereas the second command **Inserts Points on a Line**. This can be done either graphically or numerically by specifying the number of nodes to be inserted on the line or distance of the point from the beginning of the line (Fig. 70). The third (**Split Line**) command can be used to split a line into two or more parts.

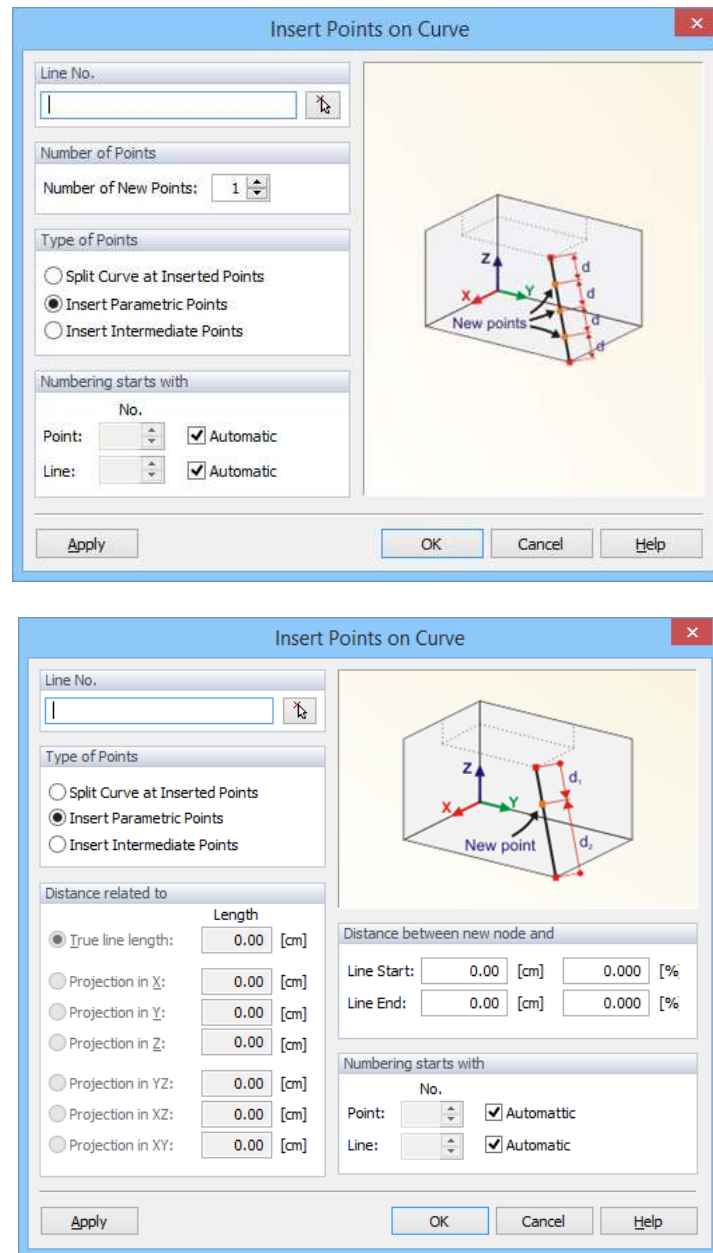


Figure 70. The Insert Point on Curve dialog window.

4.2. Surfaces

4.2.1. General Definitions

An object **Surface** refers to, depending on the problem type and the selection made in the **Domain Type and Units** dialog window:

- **2D-General:** For two-dimensional problems, a **Surface** serves to define the shape of the computational domain or its parts. See also **Geometry Information**.
- **3D-Layered:** In this case, the term **Surface** is used to define the **Base Surface** for **Solid - 3D-Layered** domains. This type of **Solids** is available in the **3D-Standard** version.
- **3D-General:** The term **Surface** serves to define boundary surfaces of a general 3D solid. This type of **Solids** is available only in the **3D-Professional** version. More detailed information can be found in the section about **Solid – General** (Section 4.4).

In the **3D-Standard** version, the only available type of a **Surface** is a **Planar Surface**. This type of **Surface** is defined by its boundary curves that must all lie in the same plane and cannot cross each other. In the **3D-Professional** version, also the **Curved Surfaces** (**Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**) are available.

A **surface** is a closed two-dimensional domain that is either the computational domain for two-dimensional applications or the **base surface** that can be extended into a **solid** for three-dimensional applications. A **surface** is defined by the **List of Boundary Curves**. It can be created using either the *Insert->Domain Geometry->Surfaces->Graphically* or *Insert->Domain Geometry->Surfaces->Graphically Rectangle* commands. Alternative commands on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** are **Planar Surface via Rectangle** and **Planar Surface via Boundaries**. In the first case, a cursor appears, and users can create a rectangular surface using the mouse. The **Edit Bar** displayed during this operation is similar to the one displayed in Figure 57 (right). The **Edit Bar** will also show which point, curve, and surface (their number) are being defined. In the second case, users can create a surface by clicking on a closed curve (one or more boundary objects forming a close curve). The **Edit Bar** displayed during the operation will list **Boundary Curves** defining the **Surface** (Fig. 72, left). A **surface** can be edited using the **Edit Surface** dialog window (Fig. 72, right), which specifies the surface type, the number of boundary curves defining the surface, its number, and had a box for possible comments or a description. A **surface** must be created before one can do finite element discretization.

A **Surface** can also be created automatically by using the menu command *Tools->Generate Domain Surfaces* or the **Edit Bar** command *Planar Surfaces - Generate*. After this command is clicked on, the program analyses existing boundary curves and attempts to generate planar surfaces automatically, i.e., without the user being required to define its boundaries. This operation is usually successful when there is a single uninterrupted boundary curve. The operation may fail when there are some ambiguities, such as when there are multiple curves or when boundary curves are not closed. If this operation fails, the following warning is displayed (Fig. 71) and the user needs to define Surfaces manually.

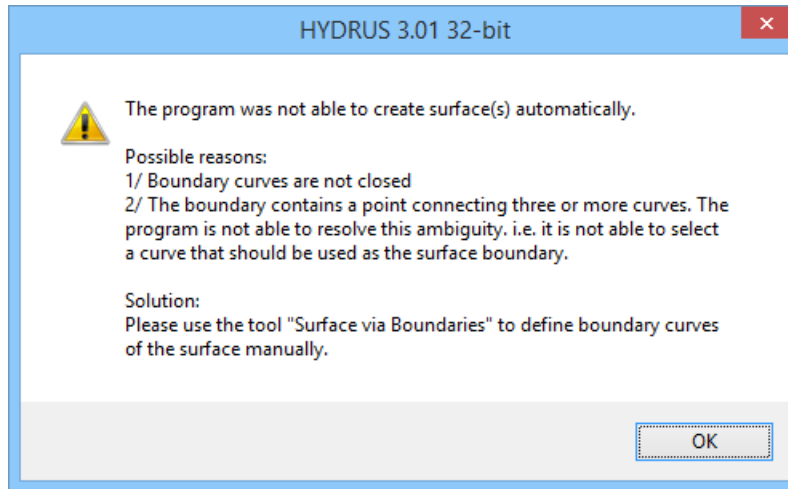


Figure 71. The warning issued when Surfaces cannot be created automatically and must be defined manually.

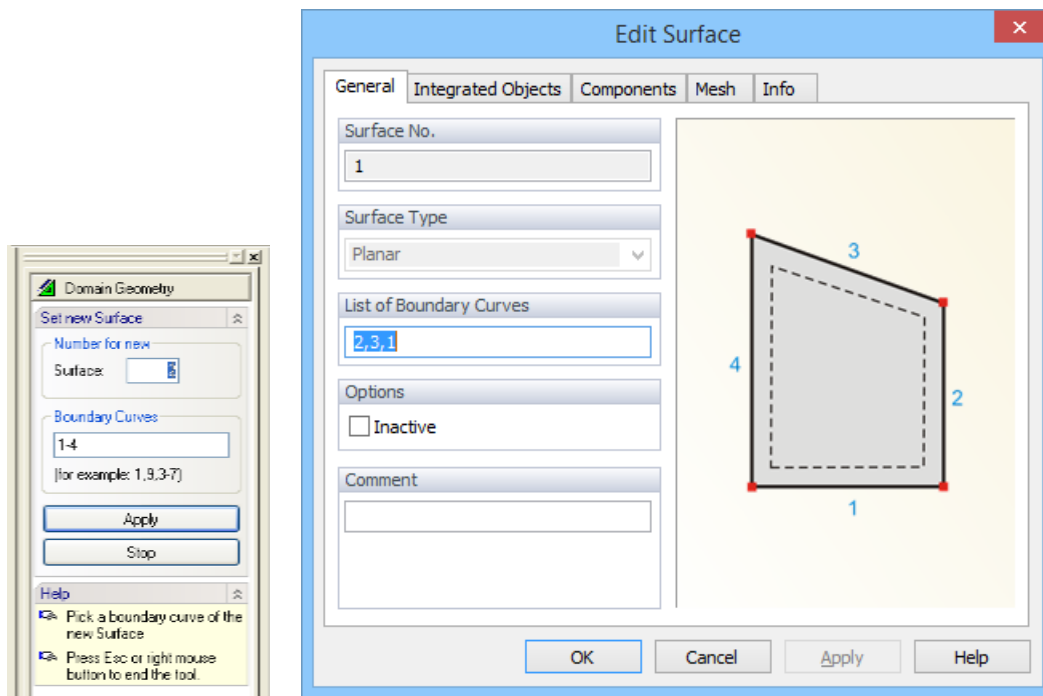


Figure 72. The Edit Bar during defining a surface graphically (left) and the General tab of the Edit Surface dialog window (right).

4.2.1.1. Planar Surfaces

A **base surface** is formed by a **planar surface** of arbitrary shape. The base surface can contain **openings**, **internal curves**, and **internal points** (Fig. 73). In the current version of HYDRUS, a base surface can be formed by a single surface. Future versions will permit multiple surfaces to form one single base surface.

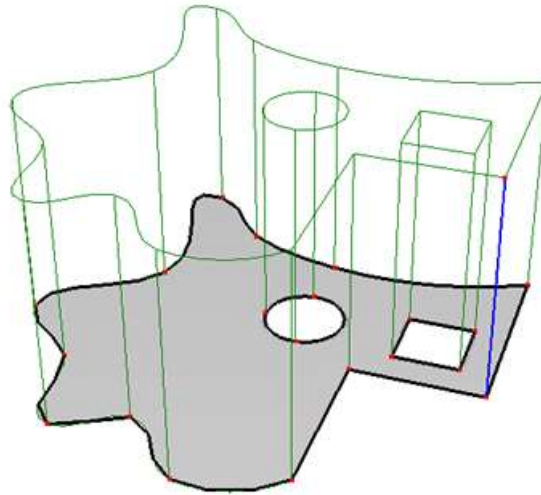


Figure 73. A solid showing the base surface.

If the solid needs to be divided into vertical columns, then these columns must be defined using internal curves in the base surface. The FE-mesh then follows exactly the specified shape of these internal curves (Fig. 74):

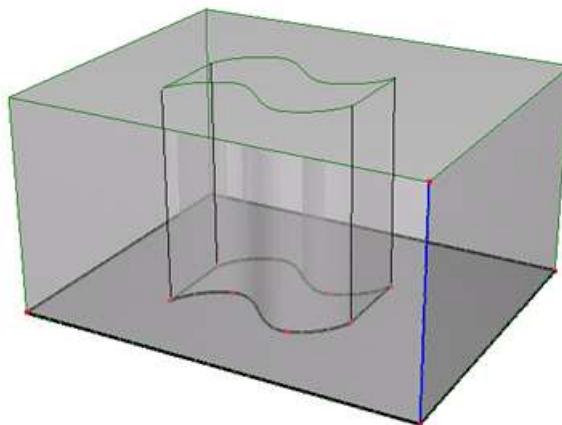


Figure 74. Solid showing separate vertical columns.

A **base surface** can be defined by a plane other than the horizontal plane, while thickness vectors can be defined in other than the vertical direction. Figures 75 and 76 show an example of a solid that has a base surface in the XZ plane and thickness vectors in the Y direction.

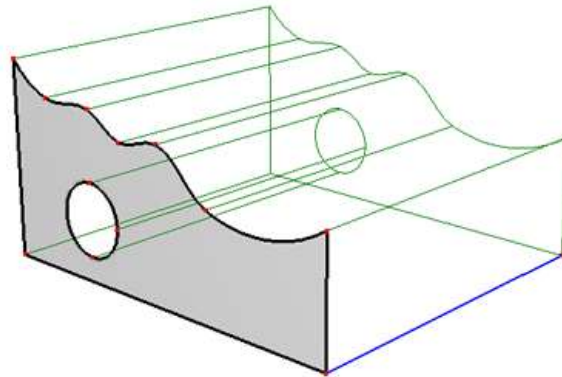


Figure 75. A solid with its base surface in the XZ plane and thickness vectors in the Y direction.

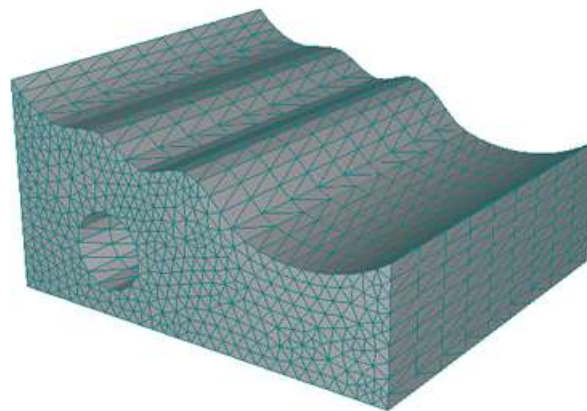


Figure 76. FE-Mesh for a solid with its base surface in the XZ plane and thickness vectors in the Y direction.

4.2.1.2. *Curved Surfaces*

There are currently four types of **Curved Surfaces** (Fig. 77) available in the **3D-Professional** version: **Quadrangle**, **Rotary**, **Pipe**, and **B-Spline**. While the boundary of a **Planar Surface** must be formed by multiple different **Curves**, the boundary of a **Curved Surface** can contain one curve two times. An example is a **Pipe Surface** (Fig. 77), in which the curve along a pipe occurs twice, each time with a different orientation. Note that the list of curves defining **Pipe** and **Rotary** Surfaces is generated automatically and cannot be edited, contrary to the list of curves defining **Quadrangle** or **B-Spline**, for which curves are selected by a user.

A **Quadrangle** is a **Surface** defined by its boundary curves of an arbitrary type (except a circle). Curves do not have to be placed in a single plane, that is, in general, a **Quadrangle** can be a curved surface. This type of surface corresponds to a general surface with four corners, i.e., it is

typically defined by four boundary curves (although this is not a necessary condition). If there is another number of boundary curves than four, it is necessary to define corner nodes of a **Quadrangle**.

A **B-Spline Surface** is a **Surface** defined using **Boundary Curves** (similarly as a **Quadrangle**). However, for this type of **Surface**, one needs to also define an additional matrix of $N*N$ internal nodes, which allows one to curve the inside of a **Surface**. One needs to define a number of internal nodes N and an order of the **Surface Spline**. Internal nodes are created automatically when a **B-Spline Surface** is defined. Their coordinates can be subsequently edited. An order of the Surface Spline is an order of the polynomial, which is used for modeling the surface (either quadratic or cubic).

A **Rotary Surface** is defined by an **Axis of Rotation** (defined using two nodes), a **Rotated Curve** (of arbitrary type, as long as the created surface makes sense), and an **Angle of Rotation** (from 0 to 360 degrees).

A **Pipe Surface** is defined by an **Axis Curve** (a smooth curve of an arbitrary type – only a polyline does not have to be smooth) and a radius.

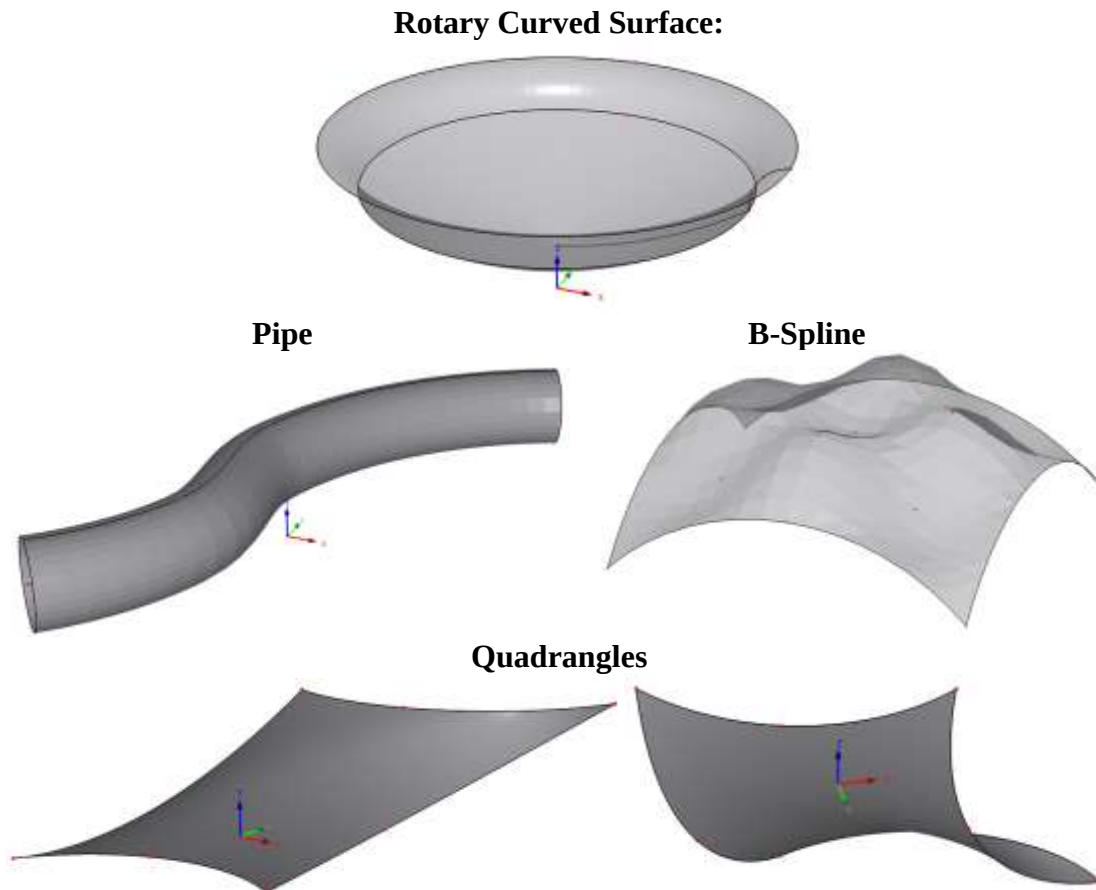


Figure 77. Examples of Curved Surfaces (Rotary, Pipe, B-Spline, and Quadrangle Surfaces).

4.2.1.3. *Partial Surfaces*

A **Partial** (or **Component**) **Surface** (Fig. 95) is created by an **Intersection of Surfaces** or **Solids** (see Section 4.6), which divides an original **Surface** into smaller **Sub-Surfaces**, or the so-called **Component Surfaces**. Although this **Surface** has its own number and can be used to define, for example, a **Solid**, its shape and boundaries are defined (generated) by the shape of its original **Surface** and a given **Intersection**. A list of **Components** resulting from the division of the original **Surface** by an **Intersection** can be found on the **Tab Components** of the **Edit Surface** dialog window. Since **Partial Surfaces** are generated objects, they cannot be deleted, or their shape cannot be edited (only the parental **Surfaces** can be edited). When a parental **Surface** is divided into **Components**, it still exists (is listed in the Navigator), but is not displayed in the **View** anymore; only its **Components** can be displayed.

One can define for each **Component** its activity (using commands **Activate Partial Surface** and **Deactivate Partial Surface**), i.e., whether it should be a part of the domain and whether an FE-Mesh should be generated on it or not. In this way, one can cut from the original **Surface** unneeded parts. When an option „**Display components as independent surfaces**“ is selected, **Components** are displayed in the **Navigator Data Tree** as independent **Surfaces**, and it is possible to select them graphically and use them for a definition of **Solids**. A selected **Component** is displayed in a view, in order to facilitate visual identification of **Components**.

4.2.2. *Steps to Define a Two-Dimensional Domain*

1/ **Definition of Boundary Curves of Particular Surfaces**

Boundary Curves are formed using basic geometric objects, such as **Points** and **Curves**. These objects can be specified in three different ways:

1. **Graphically.** One selects on the **Edit Bar** an appropriate tool and specifies new objects graphically in the **View Window**. This is usually done by specifying coordinates of points while using the **Grid Alignment** or snapping to already existing objects (points).
2. **Numerically.** Objects can be entered numerically by defining their X, Y, and Z coordinates and indexes in a dialog window. The dialog is obtained by using the **Menu** command *Insert → Domain Geometry* or the **Navigator Bar** command *Data Tab → Domain Geometry* and selecting the desired object type with a click of the right mouse button and the **New** command ...
3. **Import from a File.** Particular objects (with a large number of nodes (**spline**, **polyline**) or the entire Geometry can be read from the text file using several formats. More detailed information is at **Read points from a text file** and **Import Geometry from a Text File**.

The order of inputting particular objects is arbitrary.

2/ **Definition a Surfaces**

Boundary Curves do not yet form the **Computational Domain**. The **Computational Domain** is formed using one or more **Surfaces** that need to be defined. A **Surface** is defined using a list of **Curves** that form a closed external boundary. A **Surface** can be defined **Graphically** by sequentially clicking on particular **Boundary Curves** or **Numerically** in a dialog where one can define a list of indexes of **Boundary Curves**.

3/ Internal Objects

Any surface can have an arbitrary number of **Openings (Holes)**, **Internal Curves**, or **Internal Points**. Additional information can be found at **Internal Objects**.

4/ Openings

Each surface can have an arbitrary number of **Openings (Holes)**. An **Opening** is defined by a closed internal boundary (one or more **Internal Curves**), which entirely lies inside of a **Surface**. An **Opening** can be formed by clicking with the right mouse button in the **View Window** on the closed internal boundary and selecting from the popup menu the "**Create Opening**" command. Additional information can be found at **Openings**.

5/ Geometry Check

The consistency of the geometry can be verified at any time using the command **Check Data Consistency (Tools Menu)**.

6/ Remarks

- Any change in geometry can be undone using the **undo** command or redone using the **redo** command. The number of undo or redo steps is limited by the buffer memory, which can be set in the **Program Options** dialog window (Tab **Options and Directories**).
- When the **Computation Domain** is formed by several subdomains with different properties (e.g., different materials, and so on), one can form this domain from multiple **Surfaces** corresponding to these subdomains. An advantage is that after the **FE-Mesh** is generated, it is possible to automatically form **Mesh Sections** for particular **Surfaces** and use them to easily define materials and other properties or initial and boundary conditions. Additional information can be found at **FE-Mesh Sections** (Section 5.7).

4.2.3. Several Notes on Rules for Correct Definition of Surfaces

1. Contrary to the old HYDRUS-2D program, internal curves can touch or cross other internal curves and can touch boundary curves. A point where two curves intersect (or touch) must be a definition point of both curves (must be a part of the Geometry). This point can be found automatically using commands **Intersect Lines (Tools->Intersect Lines)** or **Intersect Lines** from the Edit Bar) or **Repair Geometry (Tools->Repair Geometry)**.
2. Curves cannot lie upon each other.
3. Multiple points cannot be defined at the same location. A frequent error is when the initial and final points of a curve are defined at the same location. The curve is then not closed, and

a surface cannot be defined using this curve. The initial and final points of a closed curve must be defined using the same point.

4. A point cannot lie on a curve without being its definition point.
5. All the above-mentioned errors in the definition of the Geometry can be automatically solved using the command **Repair Geometry** (*Tools->Repair Geometry*).
6. Contrary to the old HYDRUS-2D program, the number of **Surfaces** is virtually unlimited (up to 30,000). **Surfaces** can touch each other (in a point or on a boundary line), or one Surface can lie inside of the other Surface. In this case, one needs to first create an internal **Hole** in the first Surface and then insert the second Surface into this hole. This process can be recursive, i.e., it is possible to create a Hole in the internal Surface and insert an additional Surface there). When defining a new Surface graphically (e.g., using a rectangle), HYDRUS recognizes when the new Surface is located inside the existing Surface and automatically offers its integration.
7. Surfaces cannot partially cover each other (see also 6).
8. Points located outside of Surfaces are ignored when generating FE-Mesh.

4.2.4. Internal Objects

Internal Objects are objects of the type **Point**, **Curve**, or **Opening**, integrated in the **Surface** object. Objects are by default integrated into the Surface automatically (see Option “Autodetect” in Figure 1). It is possible to edit objects manually when the “**Autodetect**” option is turned off.

{bmct Internal_Object_Dlg.bmp}

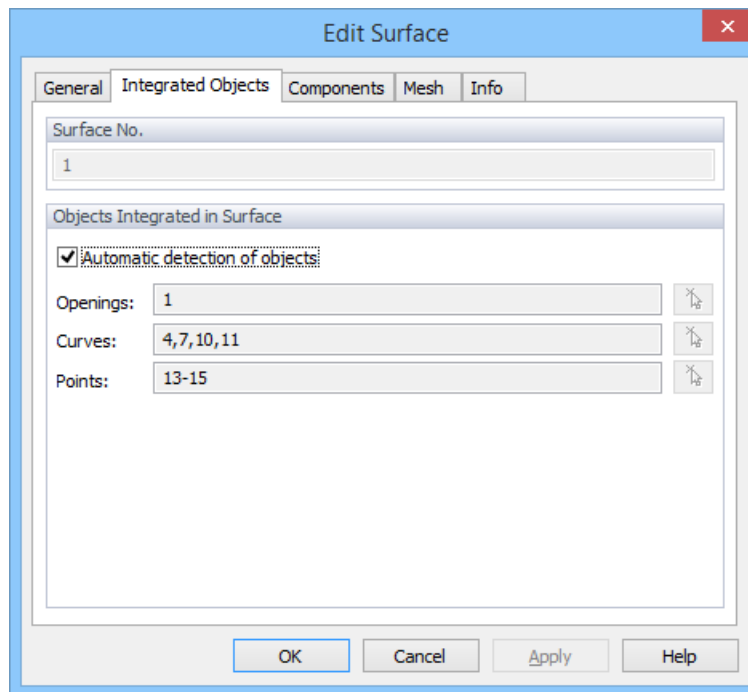


Figure 78. The Integrated Tab of the Edit Surface dialog window.

Main reasons for integrating objects into a **Surface**:

- Objects integrated into a **Surface** are respected when the FE Mesh is generated. On the other hand, objects that lie on a Surface but are not integrated into it are ignored during the FE Mesh generation.
- **Internal Points** allow users to precisely define the location of **Observation Points** and other objects.
- **Internal Curves** allow users to precisely define geometric boundaries inside of the transport domain. They can be used for many different purposes (e.g., **Mesh Lines**, **Material Boundaries**, etc.).
- Curves integrated into a **Surface** that is used as a **Base Surface** for the **3D-Layered Solid** are also projected at the Upper Surface and enable thus more precise modeling of its shape (see Figs. 79 and 80).

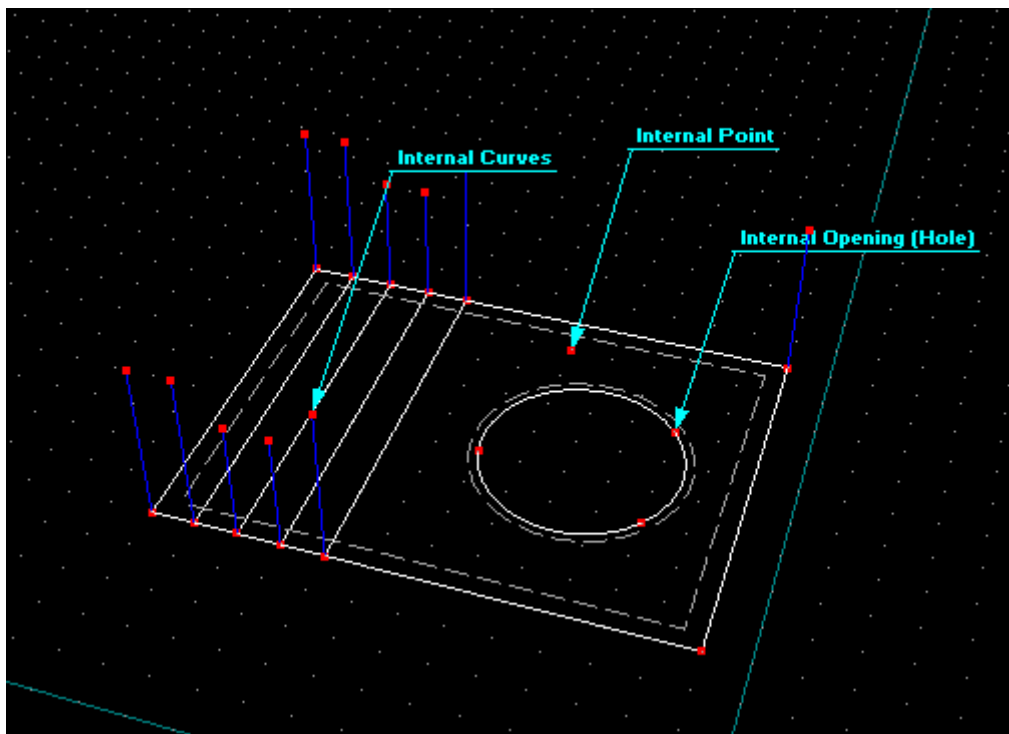


Figure 79. An example of internal objects.

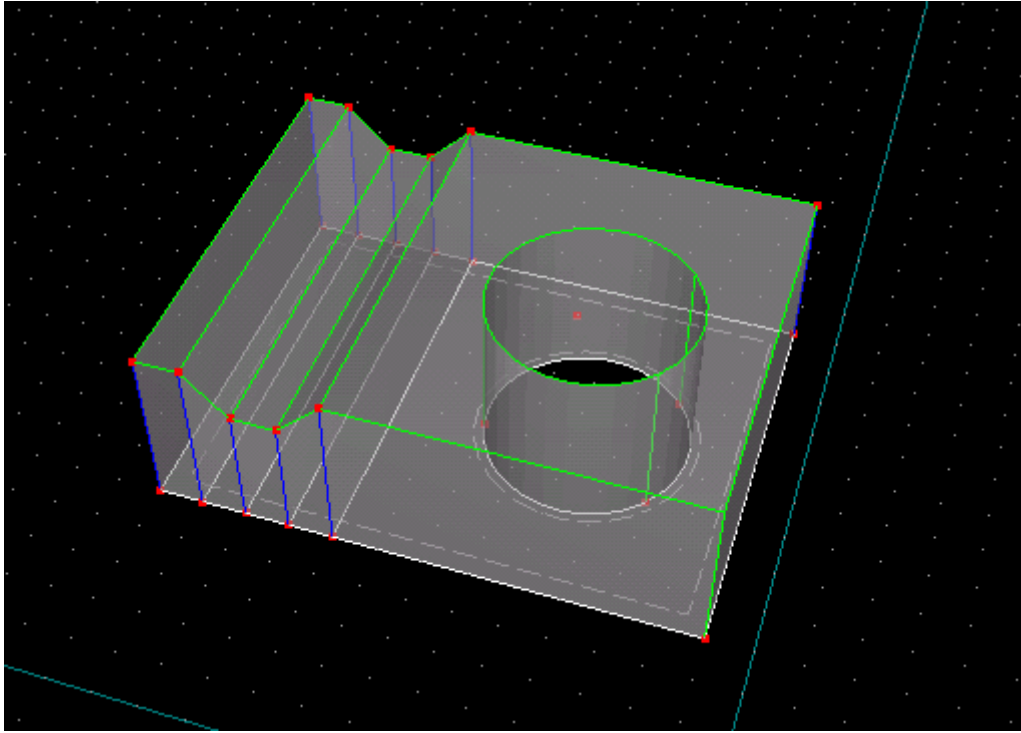


Figure 80. An example of an Upper Surface definition using Internal Curves and Thickness Vectors.

There are several rules that must be followed when defining **Internal Objects**:

- An **Internal Curve** must be entirely within a **Computational Domain**.
- An **Internal Curve** can touch (but cannot intersect) the outside boundary of a parent **Surface** at its definition points (definition points of its boundary curves).
- An **Internal Curve** can be open or closed, and can intersect itself, provided that the intersect occurs at a definition point of an Internal Curve.

An **Internal Curve** or an **Opening** must lie entirely inside of the parent **Surface**. Common reasons why a **Curve** or an **Opening** are not automatically integrated into a **Surface** is that there exist small deviations between them and a **Surface** that are not visible, but are larger than allowed tolerance (usually 0.1 mm).

4.2.5. Check and Repair Geometry

The **Check Data Consistency** command performs a consistency test of the domain boundaries. It checks especially whether each domain component is bounded by an outer boundary curve and whether or not the curves are intersecting each other. When the geometry is not correct, the code sends a warning and select those curves which do not fulfill the rules for a correct definition of boundaries. The command **Repair Geometry** may then be used to fix existing problems.

The **Repair Geometry** command attempts to fix errors in the ill-defined **Geometry** that were found using the command **Check Data Consistency**. This command calls the **Repair Domain Definition** dialog window (Fig. 81). The **List of Corrections** section of this dialog lists various operations that can be used automatically by the program when attempting to correct the ill-defined **Geometry**. Some of these corrections depend on the model precisions, which are defined in the **Model Precision and Precision of Corrections** section. Users can define these precision criteria or use those suggested by HYDRUS.

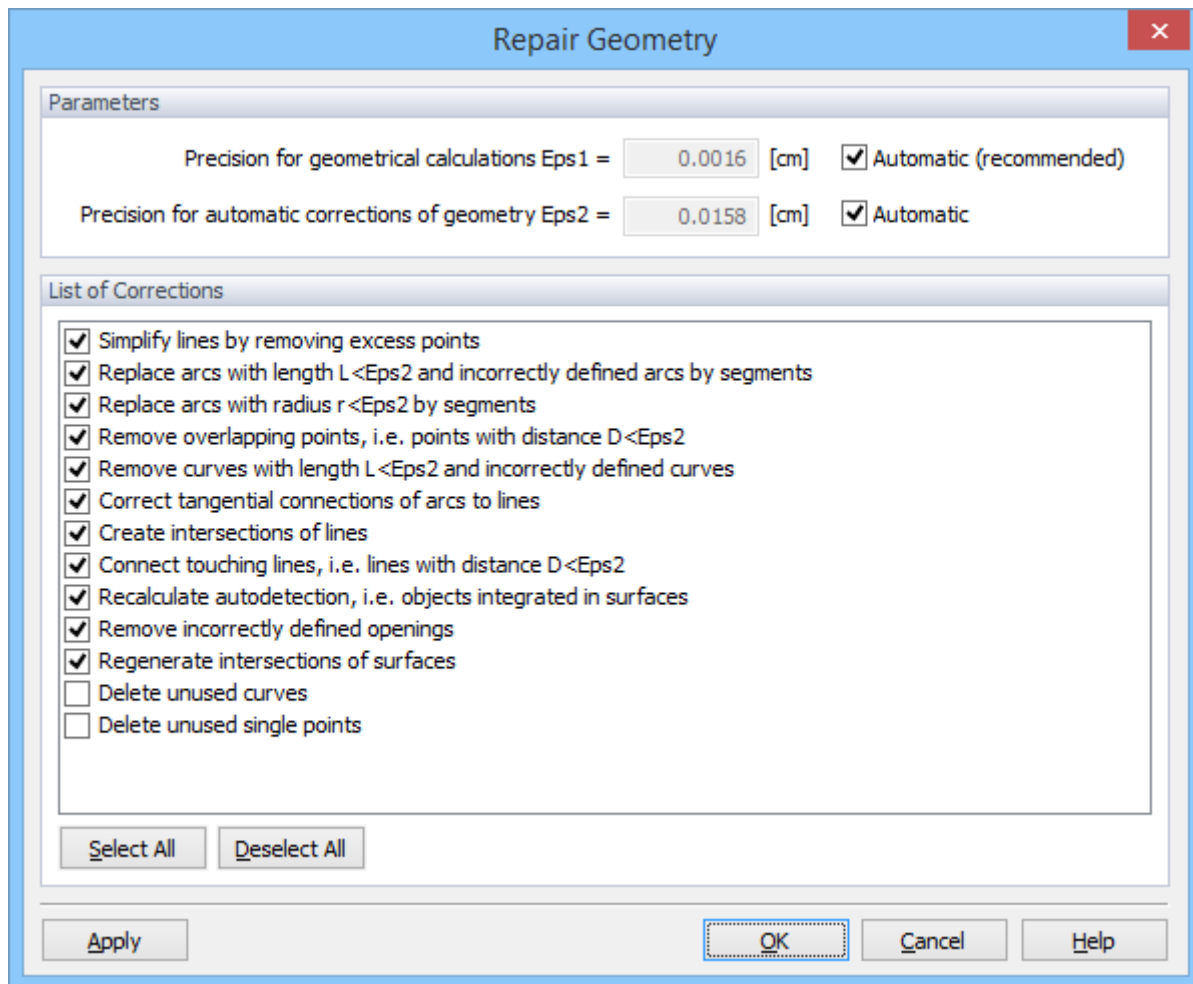


Figure 81. The Repair Domain Definition dialog window.

HYDRUS automatically analyzes defined Geometry, and if it is not consistently defined, it displays a warning at the Edit Bar in its Help section: **Errors in Domain Definition**. After double-clicking on this warning, HYDRUS displays a message informing what is wrong (incorrect), similarly as when using the **Check Data Consistency** command.

4.3. Opening

An **opening** is an internal hole defined by a **boundary curve** having the following properties: the curve is closed, positively oriented (in a counter-clockwise direction), does not intersect any other curve or itself, and has the computational domain located on its right-hand side (in the sense of positive orientation), while the left side is not part of a computational domain. An **opening** is not part of the computational domain or surface. An **opening** is created graphically as follows: One first defines boundary objects that create a closed boundary curve. One then uses the command *Insert->Domain Geometry->Opening->Graphically* from the menu, or alternatively, the command **Opening via Boundaries** on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar**. A user creates an **opening** by clicking on the closed curve (one or more boundary objects forming a closed curve). The **Edit Bar** displayed during the operation will list **Boundary Curves** defining the **Opening** (similar to Fig. 72, left). Alternatively, an **opening** can be created using the **New Opening** dialog window (Fig. 82) by clicking on the command *Insert->Domain Geometry->Opening->Dialog* from the menu. An **opening** can be edited using the **Edit Curve** dialog window (Fig. 60), which specifies the number of boundary curves defining the opening, its number, and has a box for possible comments or a description.

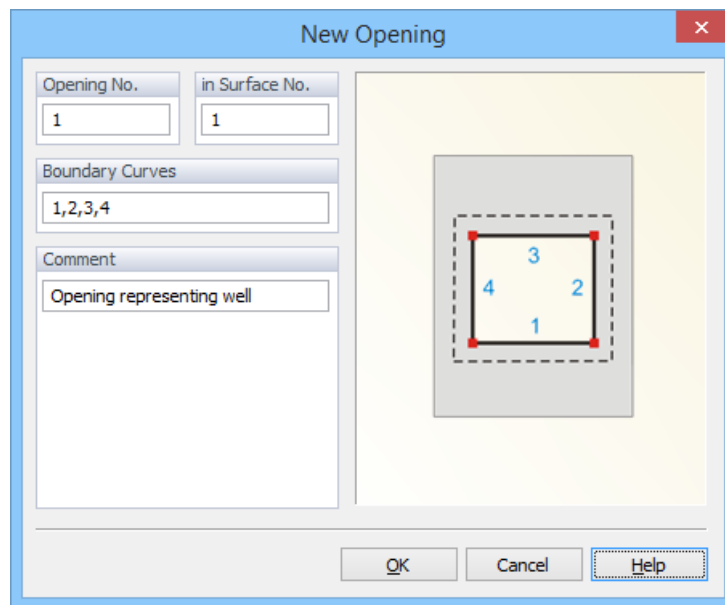


Figure 82. The New Opening dialog window.

4.4. Solids

Solids are three-dimensional objects defined by the **base surface** and one or more **thickness vectors** (See also Section 2 - **Projects Geometry Information**). There are three types of Solids depending upon the selection made in the **Domain Type and Units** dialog window (Figs. 6 and 7):

- **3D-Simple (Hexahedral):** This type of solid has a **Hexahedral Shape** and is defined by its basic dimensions (Figs. 6 and 9). The base can have a certain slope in the X and Y dimensions.
- **3D-Layered:** This type of solid is defined by the **Base Surface** and one or more **Thickness Vectors**.
- **3D-General:** This type of solid is defined using a set of surfaces (either **Planar** or **Curved Surfaces**) that form its boundaries. This selection is available only in the **3D-Professional** version of HYDRUS.

4.4.1. 3D-Simple (Hexahedral) Solids

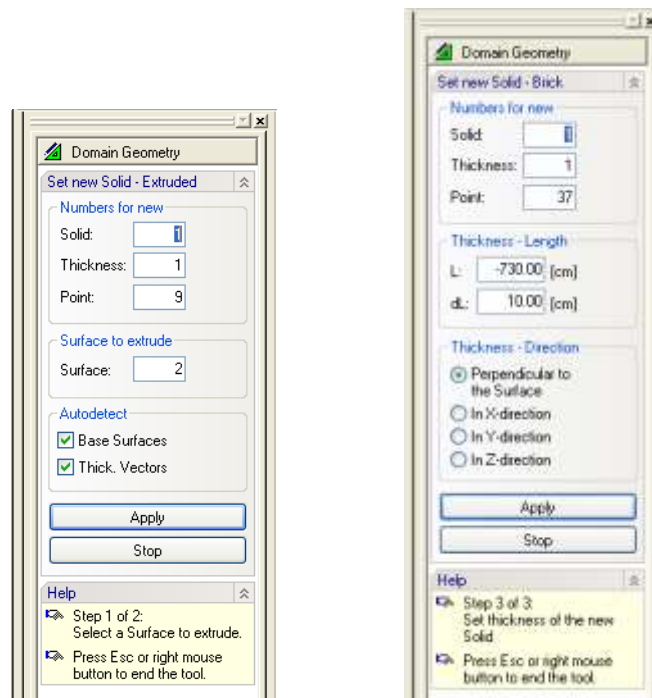


Figure 83. The Edit Bar during the process of graphically defining a Hexahedral Solid. Definition of a Base Surface on the left and a Thickness on the right.

A simple **Hexahedral Solid** can be created graphically using the menu command *Insert->Domain Geometry->Solid->Graphically* or alternatively the command **Solid - Extruded** on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar**. Once a command for

defining a new **Hexahedral Solid** is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 83 left. The **Edit Bar** will also show which point, curve, and surface (their numbers) are being defined and what reference coordinate system (the current coordinate system, the grid origin, or the last inserted point) is used. After two points defining a surface are specified, both the cursor and the **Edit Bar** change (Fig. 83 right) for the definition of the Thickness Vector. The selection can be made on the **Edit Bar** that also displays the height of the Thickness Vector (L) and a step (dL) in which it can be increased. The Thickness Vector can be created (a) Perpendicular to the Base Surface, b) in X-direction, c) in Y-direction, or d) in Z-direction). The process of defining a new Hexahedral solid is ended after the Thickness Vector is defined.

4.4.2. 3D-Layered Solids

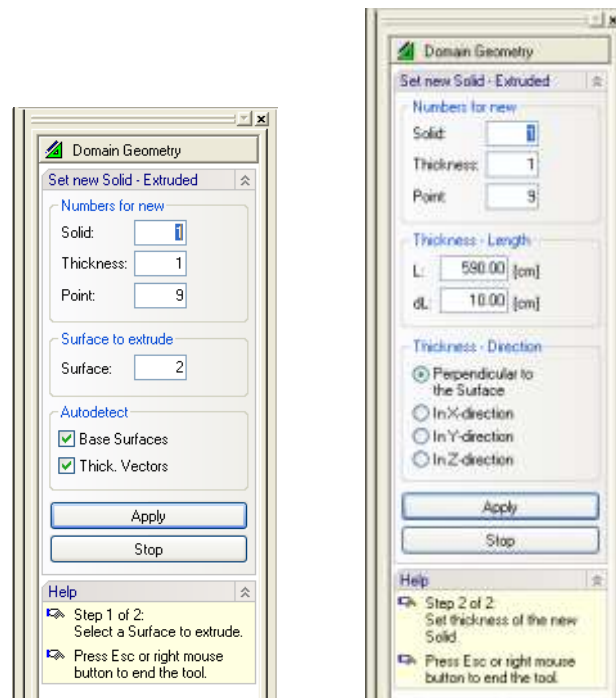


Figure 84. The Edit Bar during the process of graphically defining a Solid by extruding a Base Surface. Selection of a Surface (left) and definition of a Thickness Vector (right).

A **Solid** can be created graphically (*Insert->Domain Geometry->Solid->Graphically* from the menu or alternatively the command **Solid - Extruded** on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar**) by clicking on one point defining the **Base Surface** and extruding the base to form a three-dimensional solid. During the first part of the operation, the **Edit bar** (Fig. 84 left) displays numbers for a Solid, a Thickness Vector, a Point, and a Surface, while during the second part, it (Fig. 84, right) displays the Thickness Vector length (and increment) and in which direction it is created (a) Perpendicular to the Base Surface, b) in X-direction, c) in Y-direction, or d) in Z-direction). A user should, during the first step, select (click

on) the **Base Surface** that is to be used to define the **Solid**. It is also possible to click on any **Point** that defines the **Base Surface**. The second step depends on whether **Thickness Vectors** are already defined in **Points** of the **Base Surface**. If they are, they are used to define the **Solid**, and the second step is not done. If they are not, the thickness of the solid needs to be defined during the second step. The length and direction of the **Thickness Vector** are defined using a mouse in the **Point** on the **Base Surface** closest to the mouse click, which selected it.

How to create a **Solid** once the **Base Surface** and multiple **Thickness Vectors** are defined?

1. Graphically: Use the “**Solid Extruded**” tool and click on the **Base Surface**. A **Solid** is created using existing **Thickness Vectors**.
2. Numerically: By using a command from the **Insert** menu or by clicking with the right mouse button on **Solids** in the **Data** tree of the **Navigator Bar**. From the popup menu, select the **New Solid** command. In the **New 3D-Layered Solid** dialog, select the **Base Surface** and **Thickness Vectors**. Since the **Autodetect** function is automatically on, the **Base Surface** and **Thickness Vectors** will likely be detected automatically.

Thickness vectors do not have to be perpendicular to the **base surface**. A **Solid**, i.e., its **base surface** and **thickness vectors**, is defined and can be edited in the **Edit Solid** dialog window (Fig. 85) that has four tabs: **General**, **Sub-Layers**, **Thickness Profiles**, and **FE-Mesh**. The **General Tab** provides information on which **base surface** and which **thickness vectors** define the solid. The **Sub-Layers Tab** informs whether the solid is divided into one or more **Layers**. **Layers** are other objects that can be used to subdivide a single solid. These layers can be used, for example, to keep constant thicknesses of selected horizons or constant discretization close to the soil surface (to get good estimates of evaporation) across the entire transport domain (solid). Layers can have different **Thickness Profiles (the Thickness Profiles Tab)**. One profile is created by the code automatically. Users can then define one or more **Thickness Profiles** that are associated with different **Thickness Vectors**. These profiles can then be subdivided into multiple layers that can have either constant or variable thickness (**T**) across the transport domain. Thicknesses and the mode (constant or variable) of particular layers are specified in a table. Thickness Sum (**TS**) is then calculated by adding thicknesses of particular layers. At least one layer thickness must be variable. The finite element discretization then follows these layers. Finally, the **FE-Mesh Tab** (Fig. 86) specifies how many horizontal FE-Layers are used to discretize the solid. When only one layer exists then users can specify relative finite element spacing (spacing of vertical discretization layers) on the vertical side (*FE-Mesh Layer Spacing*) using the RS1 (relative size at the top) and RS2 (relative size at the bottom) factors below *Generate Mesh Layer Spacing*. The element sizes are then proportionally distributed. The preview part of the dialog window shows the main terms used on each Tab. When multiple layers exist, then users can specify relative sizes of elements for each layer (*FE-Mesh Density in Layers*).

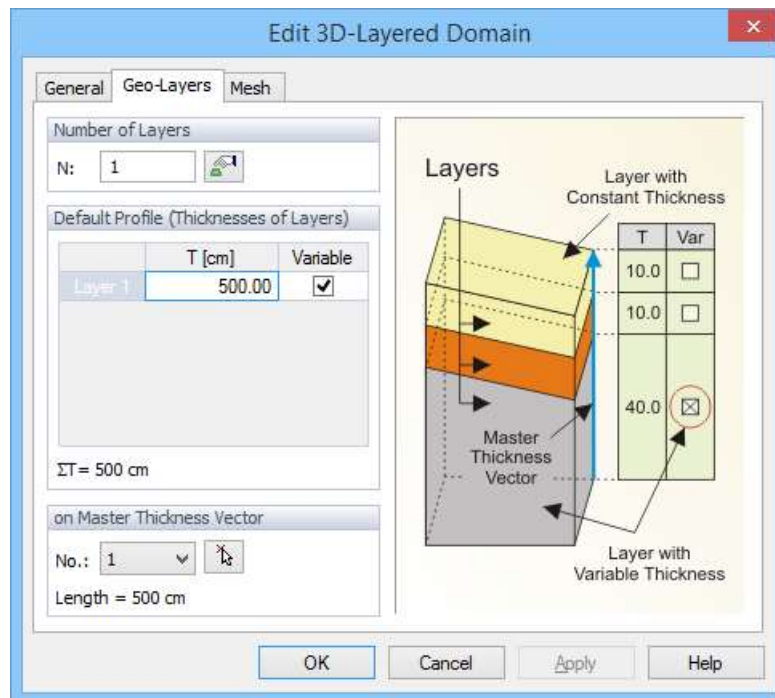
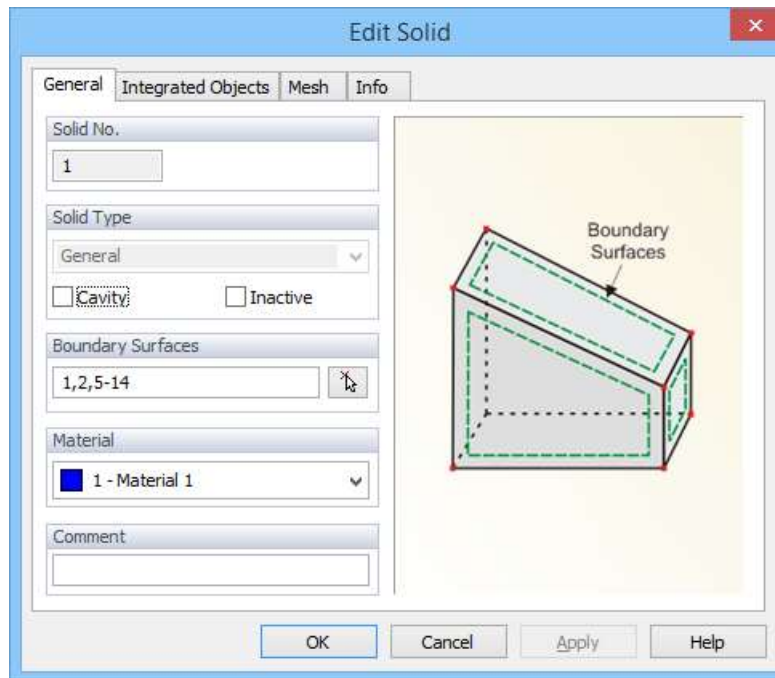


Figure 85. The Edit Solid dialog window: the General and Geo-Layers Tabs.

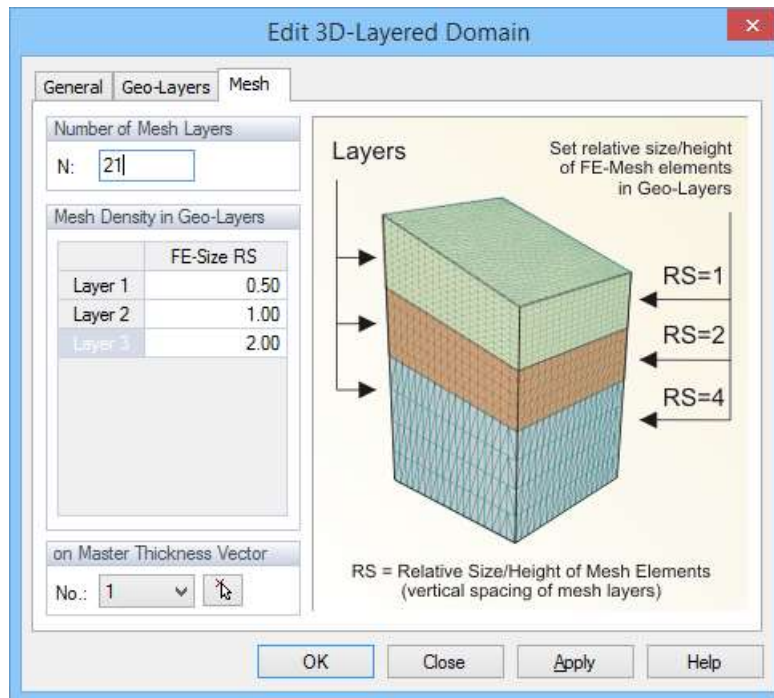
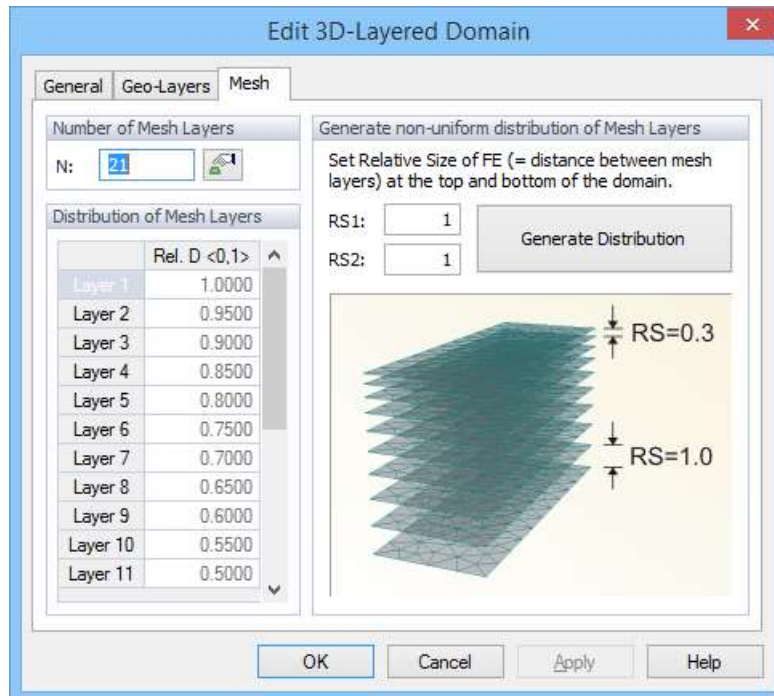


Figure 86. The Edit Solid dialog window; the FE-Mesh Tab for a single and multiple layers.

4.4.2.1. Division of a Solid into Columns

Notice that the **Base Surface** must be defined using several **Surfaces** (see Fig. 73). Parts of the **Solid** above each **Surface** are called **Columns** and serve to geometrically divide the **Solid** in the vertical direction. All **Surfaces** defining the **Base Surface** must lie in a single plane. A list of these **Surfaces** can be defined manually using indexes or can be **Autodetected** by the program (the “**Autodetect**” option). A division of a **Solid** into **Columns** leads to automatic creation of **Mesh Sections** that correspond with **Columns** after the generation of the **FE-Mesh**. These **Mesh Sections** can be used to define various properties (e.g., materials distribution) or initial and boundary conditions.

4.4.2.2. Division of a Solid into Geo-Layers

Geo-Layers (alternative term **Sublayers**, which was used in Version 1 is used alternatively below) are used to divide a **Solid** in the horizontal direction (Fig. 85).

It is possible in the **Edit Solid** dialog to define the number of **Layers** and their **Thicknesses**. A **Solid** always has one **Master Thickness Vector**, which is one of the **Thickness Vectors** of a **Solid**, that has a special meaning as described below.

A thickness of a **Layer** is calculated as follows:

- **Thicknesses of Layers** given in the Table are calculated on the **Master Thickness Vector**
- The sum of the **Thicknesses of all Layers** should be equal to the length of the **Master Thickness Vector**. If it is not so, a program will issue a warning and recalculate the **Thicknesses of Layers** automatically.

A **Solid** can have more **Thickness Vectors** of different lengths so that specified **Thicknesses of Layers** cannot be maintained. The program then does the following: For **Geo-Layers** with the **Constant Thickness Type**, the specified thickness is maintained at all **Thickness Vectors**, i.e., over the entire computational domain. For **Geo-Layers** with the **Variable Thickness Type**, their thicknesses are linearly increased or decreased so that the sum of the **Thicknesses of all Layers** corresponds with the length of a particular **Thickness Vector**.

4.4.2.3. Individual specification of different Thicknesses of Geo-Layers at different Thickness Vectors.

In the preceding paragraph, we have described how to define **Thicknesses of Layers** on the **Master Thickness Vector** using a table (Fig. 85). This table represents the so-called **Profile**, i.e., a particular distribution of thicknesses. If one wants to define precisely the division of thicknesses also on other vectors than the **Master Thickness Vector**, then it is necessary to create additional **Special Profiles** and use then on corresponding **Thickness Vectors**. There is always a **Default Profile**, which corresponds to the table described in 4.4.2 above. One can create new profiles, change their thicknesses, or delete them. One can simultaneously also see a list of **Thickness Vectors** where the selected **Profile** is used.

The desired **Profile** can be associated with a particular **Thickness Vector** after opening a dialog with its properties (e.g., by double-clicking on a vector) and selecting a **Profile** from a Combo Box “**Thickness Profile No.**” (see Fig. 89). This operation can even be carried out globally by first selecting desired **Thickness Vectors**, then opening a dialog with their properties (Alt + Enter), and finally repeating the above-described process. Note that one **Profile** can be associated with many **Thickness Vectors**, which enables one to change **Thicknesses of Layers** easily on all **Thickness Vectors** by changing a single **Profile**.

4.4.2.4. Steps to Define a 3D-Layered Domain

1/ Definition of the Base Surface

The **Base Surface** is a **2D domain of an arbitrary shape**. How to specify the **Base Surface** is described in **Building a Two-Dimensional Domain**.

2/ Definition of Thickness Vectors

One inserts one or more **Thickness Vectors** in points that lie in the **Base Surface**, so that the shape of a **Solid** is defined as needed.

3/ Definition of a Solid

On the **Edit Bar** (or the Menu command *Insert → Domain Geometry*), one clicks on the **Solid – > Extruded** command and selects (clicks on) one of the **Surfaces** defining the **Base Surface**. This operation creates the **3D-Layered Solid**. One can do this even when no **Thickness Vectors** are defined. In such a case, after clicking on the **Base Surface**, a graphical tool is started, using which one can extrude the **Solid** into space. A **Thickness Vector** is simultaneously created in the **Point** on the **Base Surface** that is closest to the location of the click.

4/ Formation of a Solid

A **Solid** can be further formed using additional **Thickness Vectors** and **Internal Lines**.

5/ Definition of Geo-Layers

A **Solid** can be vertically divided into **Layers**.

4.4.3. 3D-General Solids

Solids in the 3D-Professional version are defined using boundary **Surfaces** (either **Planar** (see Section 4.2.1.1) or **Curved** (see Section 4.2.1.2)) and identified as **3D-General Solids**. In one project, one cannot use at the same time **3D-General Solids** and **3D-Layered Solids** (created in the 3D-Standard Version) or the parametric blocks (created in the **3D-Lite Version**). It is,

however, possible to convert **3D-Layered Solids** into **3D-General Solids** by changing the project type from **3D-Layered** to **3D-General**.

Boundary Surfaces of a **Solid** must enclose a closed space and cannot intersect with each other. Interior of a **Solid** must form a three-dimensional “simply continuous space”, i.e., it must be possible to connect any two internal points using a polyline that is entirely located inside of a **Solid**. Boundaries of a **Solid** thus can be formed by any number of either **Planar** or **Curved Surfaces**. Figure 87 shows two examples of 3D-General solids. While the **Solid** at the top is formed using 8 **Planar Surfaces** and 4 **Quadrangles**, the **Solid** at the bottom is formed by multiple **Curved Surfaces**.

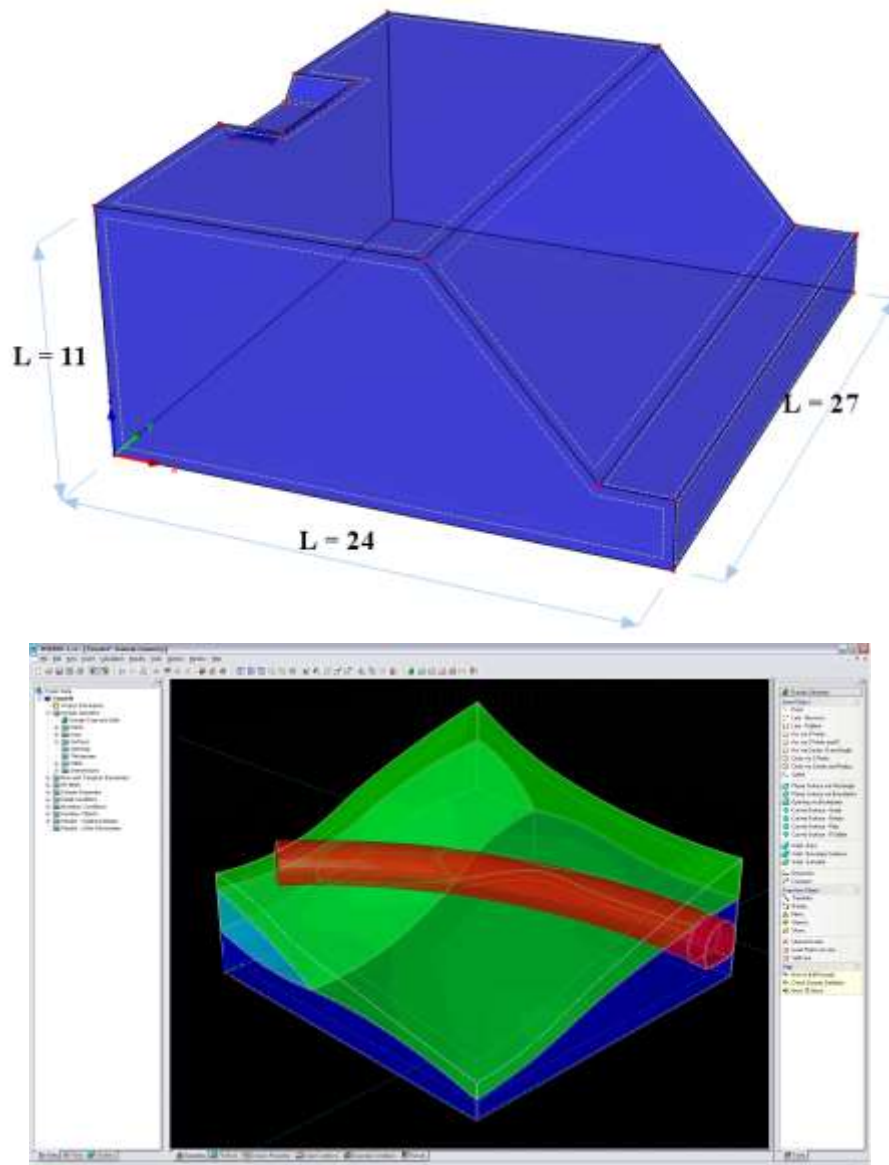


Figure 87. Examples of 3D-General Solids. Top - formed by Planar Surfaces, bottom – formed by Curved Surfaces.

General Solids can be created in the following ways:

1. Using a standard dialog, from which **Boundary Surfaces** can be picked graphically (individually, or using a **Quadrilateral** or **Rhomboid Selection Tool**).
2. Creating a **Simple Block (Brick)**.
3. **Extruding** a **Solid** from a **Surface** (one or multiple simultaneously).

Process of Extruding:

Approach 1: Start a tool and click on a given **Surface**, which is to be extruded. It is important where a click occurs. The program finds the closest **Node** on a **Surface Boundary**, and the extruding distance (height) is measured in this node. The extruding height is measured on a line passing through this node.

Approach 2: When you want to extrude multiple surfaces at the same time, you need to press the **Left Shift** keyboard button before selecting the desired **Surfaces** (you can add or remove **Surfaces**). After a selection is made, release the Left Shift button and start extruding selected surfaces.

Approach 3: First select desired **Surfaces** and then click the **Edit Bar** command “**Solid – Extruded**”. This will start the extruding process for all selected surfaces.

One can extrude **Surface** in the direction of *X*, *Y*, and *Z* axis, or in the direction perpendicular to an extruded **Surface**. When a **Surface** is not in a plane (e.g., is curved) and perpendicular extruding is selected, extruding is done in directions of local perpendicular lines to an extruded **Surface**.

During extruding, one can select on the **Edit Bar** the length step (*dL*) or enter the numerically desired length of extruding (*L*).

Note that the command **Extrude** can be used only for **Planar**, **Quad**, and **B-Spline Surfaces**, and it cannot be used for **Partial Surfaces** and for **Surfaces** containing a zero **Curve** (i.e., a curve with a zero length from point *P* to point *P*).

4.5. Thickness Vectors

The term **Thickness Vector** is used for a vector (usually but not always perpendicular to the **Base Surface**) that extends the Base Surface to form a **solid** (the three-dimensional **computational domain**). A new **Thickness Vector** can be defined either graphically or numerically (Fig. 89).

There are several ways in which a **Thickness Vector** can be specified graphically and these are displayed at the **Edit Bar** (Fig. 88), which appears once a command for defining a **Thickness Vector** is selected.

- a) **Point and Length:** A user specifies the length of the **Thickness Vector** on the **Edit Bar (Vector Length)** and with the mouse selects the point to which the Thickness vector is assigned.
- b) **Point and Coordinate:** A user specifies the End Coordinate of the **Thickness Vector** on the **Edit Bar (End Coordinate)** and with the mouse selects the point to which the Thickness vector is assigned. This method is suitable, especially in the case, when points located at the upper surface of the domain already exist (see Tutorial 2.07). In this case, we need to specify **Thickness Vectors** whose upper points were read in from a GIS file, and we need to create the lower (beginning) points that would be located in the plane of the **Base Surface**. Note (in the Tutorial) that the **Reverse Points** option was automatically checked on the **Edit Bar**. This is because the thickness Vectors have to originate from the **Base Surface** and not from the upper surface. If the **Reverse Points** option was not checked, Thickness Vectors would originate from the upper surface and end at the **Base Surface**.
- c) **Two Points:** A user selects graphically two existing Points to form the **Thickness Vector**. In this case, an **Anchoring** (beginning) **Point** of a **Thickness Vector** is the first selected point. Therefore, it is important to select points defining a **Thickness Vector** in the right order, i.e., to first select a point at the **Base Surface** and only then a point at the upper surface of the domain.
- d) **Three Points:** A Thickness Vector is, in general, defined by three points: an **Anchoring Point**, a **Beginning Point**, and an **End Point** (Fig. 89). The **Anchoring Point** must be located on the **Base Surface**. The **Anchoring Point** is usually the same as the **Beginning Point** (i.e., both Point indices are the same), and one does not have to pay attention to it. However, in general, the **Anchoring Point** can be different than the **Beginning Point**, which leads to the so-called “offset”. This option allows defining **Domains** that have both upper and lower surfaces deformed, i.e., not a plane.

Vector Direction can be specified to be a) Perpendicular to the Base Surface, b) in X-direction, c) in Y-direction, or d) in Z-direction.

Thickness Vectors can be defined by:

- clicking on individual Points
- selecting points with a rectangle (rhomboid, circle, polygon)
- clicking on a curve – Thickness Vectors will be added to all points of a curve.

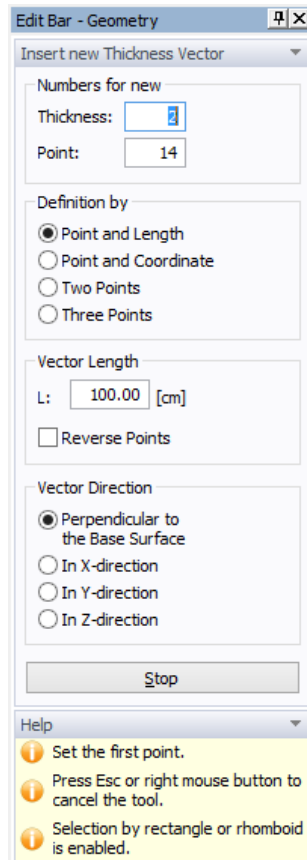


Figure 88. The Edit Bar during the process of graphically defining a Thickness Vector.

A definition of the **Thickness Vector** (i.e., its **Boundary Points**) is given and can be edited in the **Thickness** dialog window (Fig. 89).

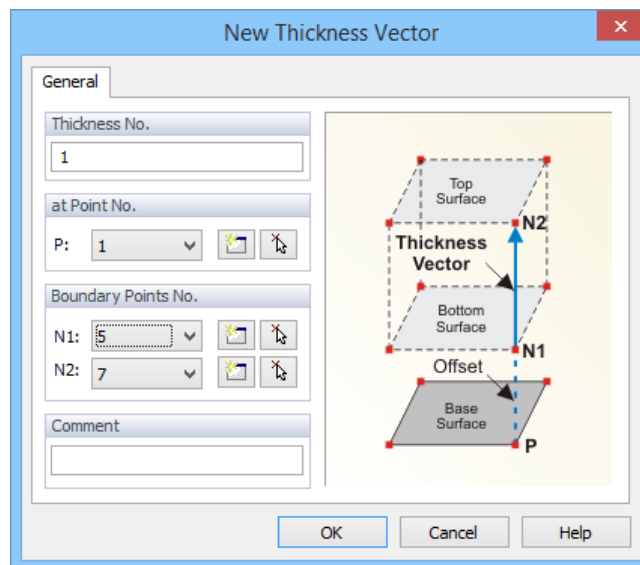


Figure 89. The New Thickness dialog window.

The height of a solid is defined using one or more **Thickness vectors**. Each thickness vector is defined by an **Anchor Point P** and two **Boundary Points N1** and **N2**. The anchor point P must be part of the base surface, i.e., it must be either a defining point of the external boundary or the internal curve, or an internal point in the base surface. Boundary points N1 and N2 are arbitrary points in 3D space. Coordinates of these points can be edited, thus allowing one to specify the thickness vector in an arbitrary direction (i.e., not necessarily perpendicular to the base surface). Usually, the anchor point P is the same as boundary point N1 so that one can use the same index for both P and N1. If, for whatever reason, we do not want to have the base surface on the bottom of the transport domain (Solid) (e.g., when the bottom of the transport domain is not in the same plane), users can make the N1 node different from P (the red part in Fig. 90).

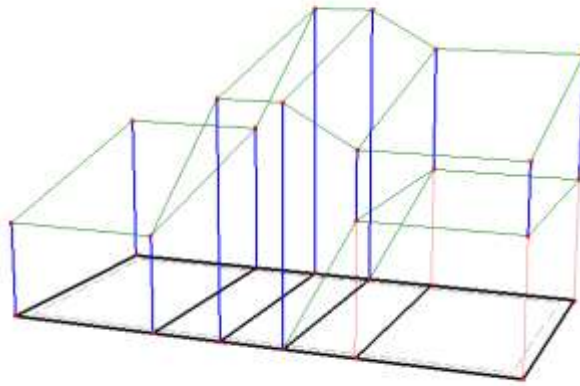


Figure 90. A solid with several thickness vectors.

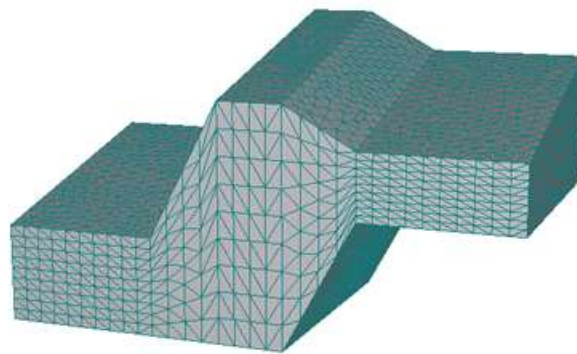


Figure 91. FE-Mesh for the solid in Figure 90.

The height of a solid is constant when less than three thickness vectors are used. Three thickness vectors define a linear plane (with generally an inclined surface). More than three thickness

vectors with different lengths then define the top surface that is formed by triangles, whose coordinates are calculated from the thickness vectors using linear interpolation or extrapolation.

When breaks in the slope of the top surface are to be defined exactly, then it is necessary to define internal curves in the base surface. Figures 92 and 93 show the importance of having internal curves (or not having them) in the Y direction for a proper definition of the solid (compare Figures 90 and 92 Figures 91 and 93).

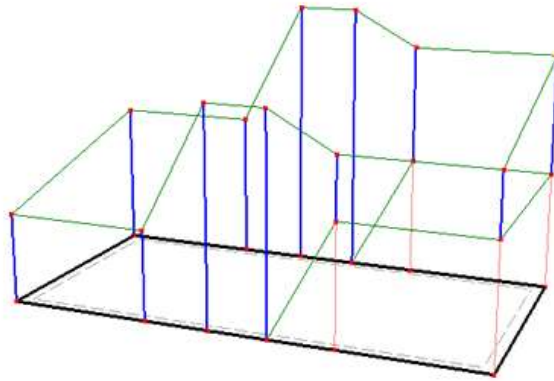


Figure 92. Missing internal curves in the base surface.

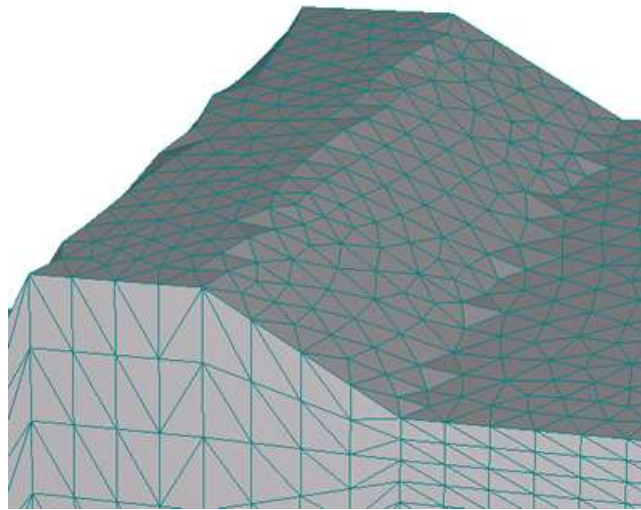


Figure 93. A consequence of missing an internal curve in the base surface on the FE-Mesh of the top surface.

Note: Three **Thickness Vectors** need to be specified to define a **Domain** with a linearly changing thickness. As long as only two **Thickness Vectors** are specified, the thickness of the **Domain** is constant and defined using the first **Thickness Vector** (with lower index) (since three points are needed to define a plane).

4.6. Intersections of Surface and Solids

Intersections of Surfaces and Solids (Fig. 94) can be created using the following approaches:

- A. **Intersection of Surfaces:** Select two or more **Surfaces**, click with the right mouse button on these selected **Surfaces**, and select the command “**Create Intersection**”. When more types of different objects are selected (e.g., nodes, lines, or surfaces), which can, for example, occur when selection is made by a **Rectangle** (or a **Rhomboid**), then the command is located in the submenu “**Surfaces**”.
- B. **Intersection of Solids** (this option not yet available): Select two or more **Solids**, click with the right mouse button on these selected **Solids**, and select the command “**Create Intersection**”. When more types of different objects are selected (e.g., nodes, lines, or surfaces), which can, for example, occur when selection is made by a **Rectangle** (or a **Rhomboid**), then the command is located in the submenu “**Solids**”. For the **Intersection „Solids A-B”** (Fig. 94), Solid A will remain in its original shape, and Solid B will be cut off. For the **Intersection „Solids B-A”**, Solid B will remain in its original shape, and Solid A will be cut off.
- C. **Intersection of Surfaces and Solids** (this option not yet available): It is possible to create this intersection using the menu command *Insert->Domain Geometry->Intersection* or by clicking with the right mouse button on the item “**Intersections**” in the data tree of the **Navigator bar** and selecting “**Insert Intersections**” from the displayed popup menu. In the dialog, select a desired type of Intersection (e.g., surfaces or solids).

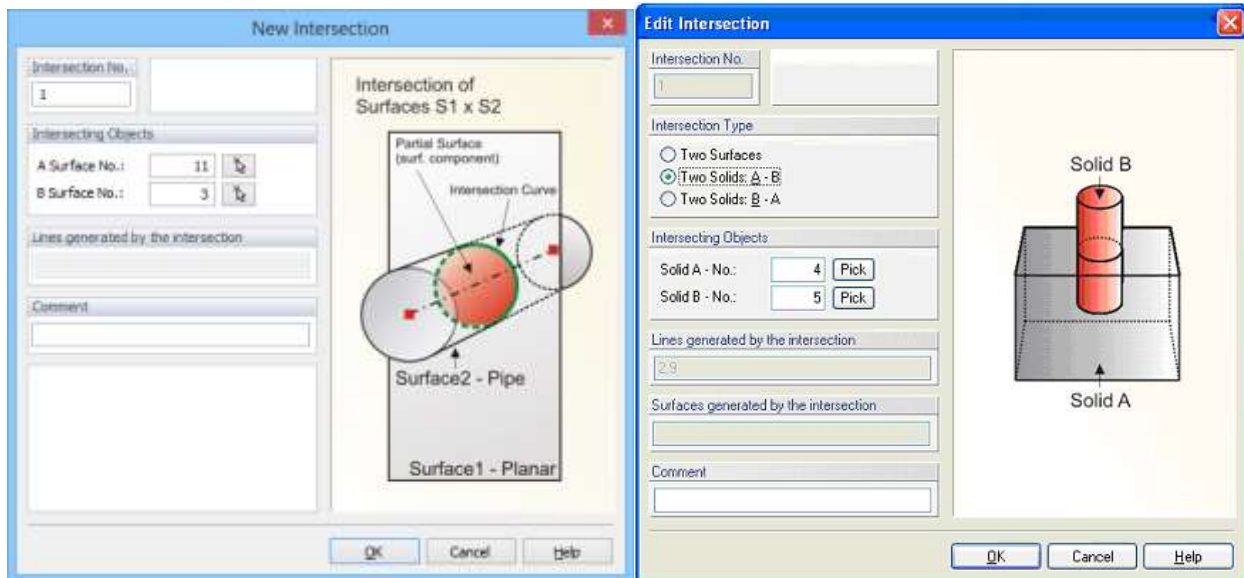


Figure 94. The Edit Intersection dialog window (for two Surfaces (left) and two Solids (right)).

A **Partial** (or **Component**) **Surface** (Fig. 95) is created by an **Intersection of Surfaces** or **Solids**, which divides an original **Surface** into smaller **Sub-Surfaces**, or the so-called **Component Surfaces**. Although this **Surface** has its own number and can be used to define, for example, a **Solid**, its shape and boundaries are defined (generated) by the shape of its original **Surface** and a given **Intersection**. A list of **Components** resulting from the division of the original **Surface** by an **Intersection** can be found on the **Tab Components**.

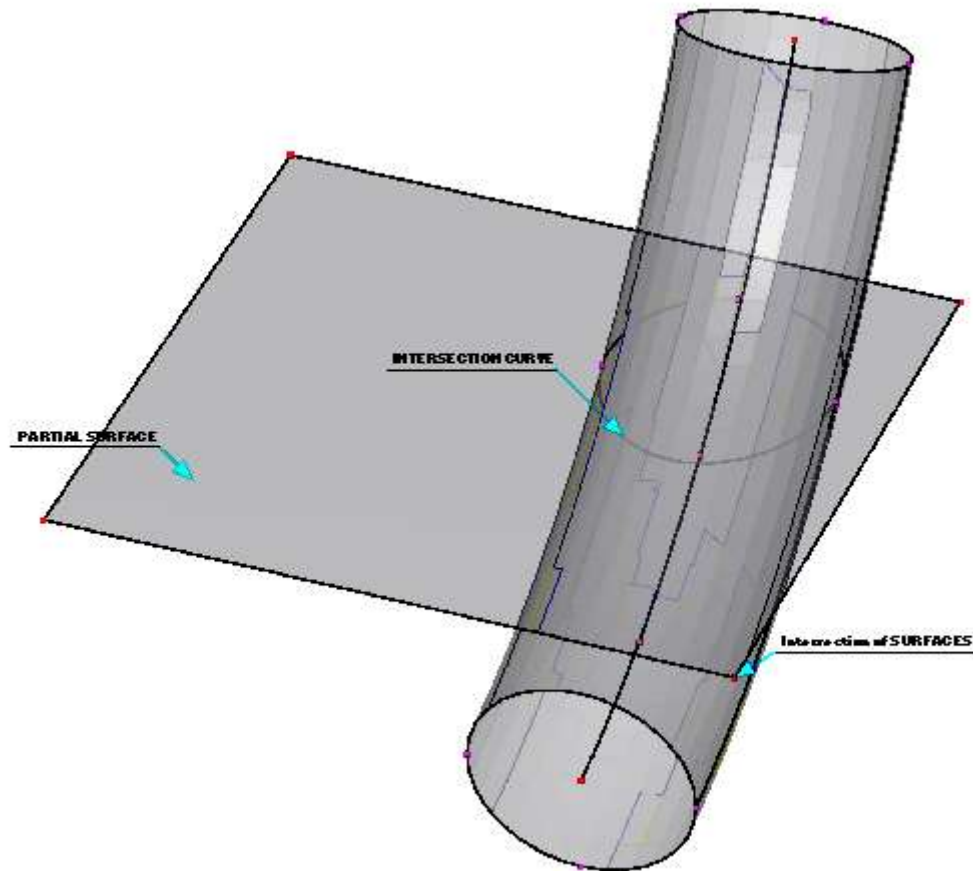


Figure 95. An example of an Intersection of two Surfaces and a resulting **Partial Surface** and **Intersection Curve**.

4.7. Auxiliary Objects

In addition to objects that define the computational domain, the HYDRUS GUI allows users to employ several **Auxiliary Objects** that can be used to, for example, add **Dimensions** to the computational domain, include various **Labels**, or define permanent **Cross Sections** or **Mesh-Lines**.

4.7.1. Dimensions

Dimensions can be added to describe spatial properties of the computational domain in the **View** window using the *Insert->Auxiliary Objects->Dimensions* command or the **Dimensions** command from the **Insert Object** part of the **Domain Geometry** version of the **Edit Bar**. Then one needs to click on two points defining the computational domain and drag **Dimensions** to the required position. Figure 126 shows an example of how **Dimensions** can be used.

After a command for defining a **Dimension** is selected, a user needs to first select by a cursor two existing points, the distance between which is to be labeled. The **Edit Bar** lists during this operation two definition points and the Dimension number (Fig. 96 left). After the second point is selected, a cursor in the **View window** and the **Edit Bar** (Fig. 96 right) change and allow a user to define where a Dimension is to be displayed. In which plane a Dimension is to be displayed can be done on the **Edit Bar** (Fig. 96 right).

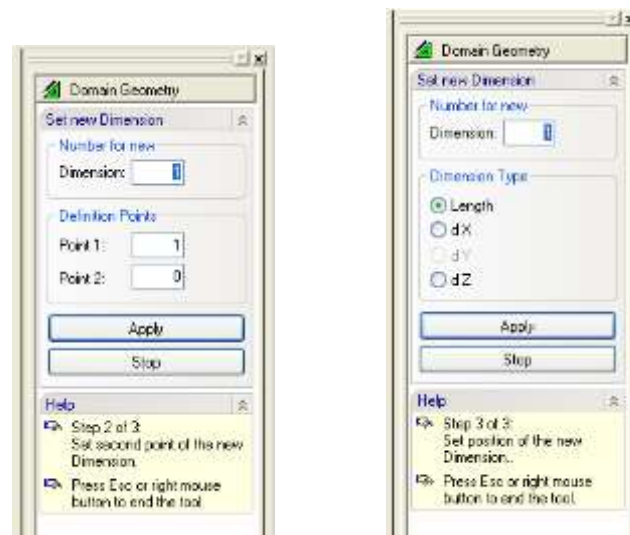


Figure 96. The Edit Bar during the process of graphically defining a Dimension. Selection of two definition points, the distance of which is to be labeled (left) and the dimension type (right).

4.7.2. Labels

Labels can add any desired text to the computational domain in the **View** window using the *Insert->Auxiliary Objects->Dimensions* command or the **Comments** command from the **Insert Object** part of the **Domain Geometry** version of the **Edit Bar**. One then clicks simply anywhere in the **View** window and write the desired text. The text itself, its color, frame, and its offset can be specified in the **Edit Comment** dialog window (Fig. 97). Figure 126 shows an example of how the “Furrow” **Label** is used.

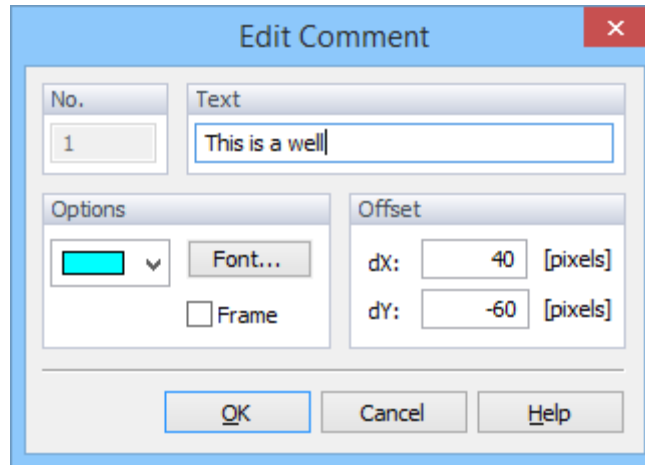


Figure 97. The Edit Comment dialog window.

After a command for defining a **Comment** is selected, a user needs first to select a location to which the comment will point using a cursor. The **Edit Bar** lists during this operation the coordinates of a cursor (**Position**), the color to be used for a comment, and the comment text (**Text**) (Fig. 98 left). A user can also select the **Font** to be used for the comment text. After the position is selected, a user defines an **Offset** of the Comment text. The comment text, the comment font and color, and offset are displayed at the **Edit Bar** (Fig. 98 right).

4.7.3. Bitmaps (Textures)

Bitmaps (Textures) serve to use scanned figures (maps) as a means to define the computational domain in the **View** window. **Bitmaps** can be added using the *Insert->Auxiliary Objects->Textures* command. Corners of the **Bitmap** must be anchored at 4 points, coordinates of which must be selected such that the scale of the Bitmap corresponds with the scale of the View window. Anchor points can be selected one at a time using either a Listbox (containing a list of all defined nodes) or using a command **Pick** and selecting nodes using a cursor. All anchor points can also be selected simultaneously using the command **Pick ABCD**. The **Edit Bitmap** dialog window then provides information about the selected Bitmap, such as its **Size** in *pixels* and *kB*. One can then simply trace the bitmap to specify the computational domain.

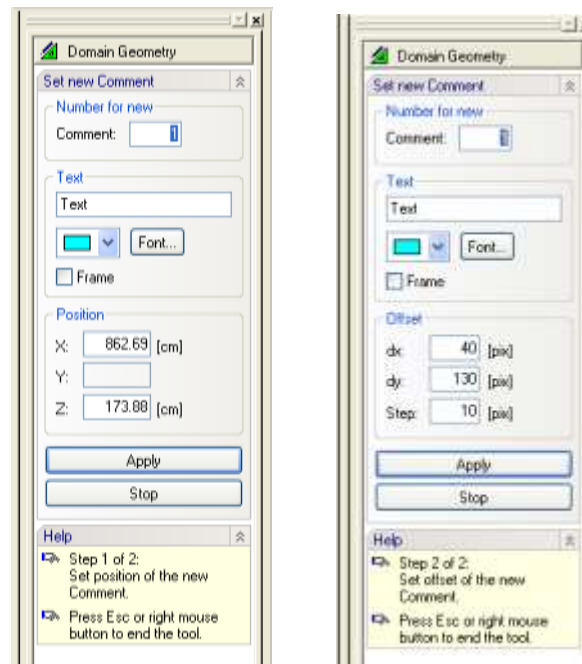


Figure 98. The Edit Bar during the process of graphically defining a Comment. Selection of the Comment Position, Comment Text, Font, and Color (left), and Offset (right).

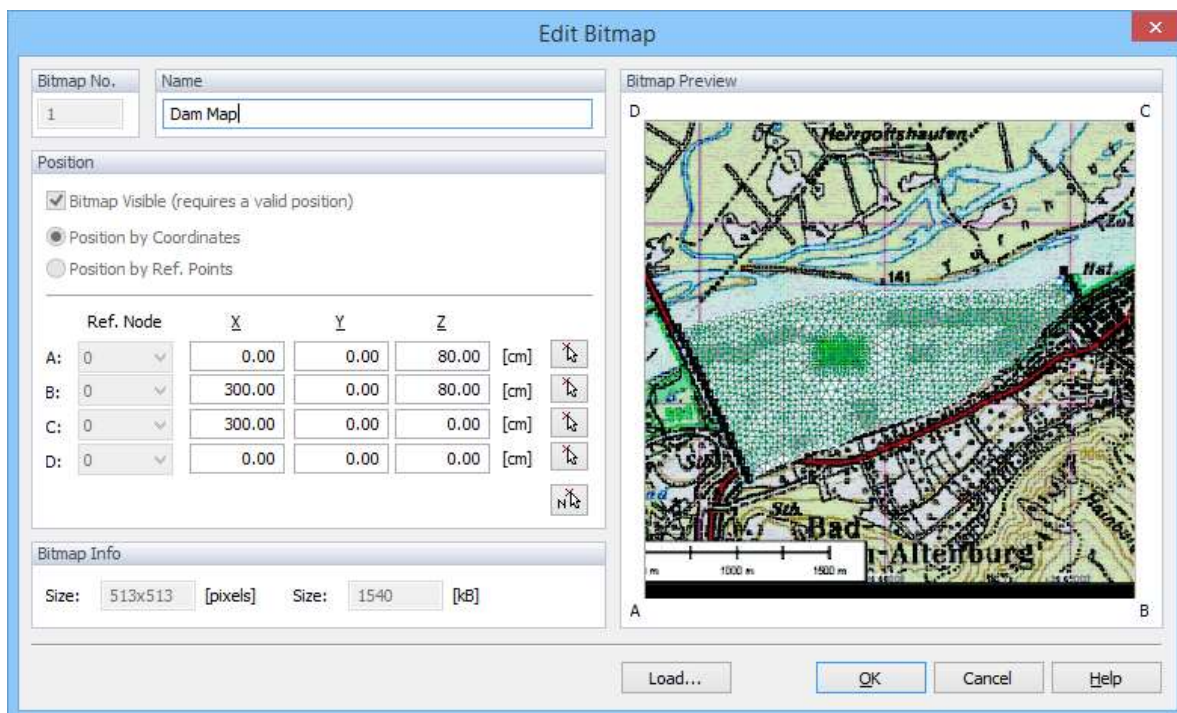


Figure 99. The Edit Bitmap dialog window.

4.7.4. Cross-Sections

In the HYDRUS-2D software package, one could click at any two points of the transport domain to display the results of selected variables between those two points, i.e., along a specified cross-section. The exact location of these cross-sections was not saved, and they had to be redefined whenever a new graph was required. In HYDRUS, one can define the cross-sections and save their locations so that graphs along the cross-sections can be recalled at any time by simply clicking at them. Graphs along pre-defined cross-sections can be displayed for both the initial conditions and the output results. For example, if a plot of the pressure head along a predefined cross-section at a particular time is needed, one needs to display the pressure head outputs, find a particular time, and then click on the predefined cross-section. The graph is displayed instantaneously. Specifying the cross-section within a two-dimensional domain is straightforward.

In 3D problems, a Cross-Section is a plane that is defined using two points, which are defined (either graphically or numerically (in the **Cross-Section** dialog window (Fig. 100))) in a currently active Workplane, and is perpendicular to this Workplane. When a 2D Mesh-Section is displayed in the View Window, the Cross-Section Chart displays a particular variable at the cross-section of this 2D Mesh-Section with the Cross-Section Plane. When a 3D Mesh-Section is displayed, the Cross-Section Chart displays a particular variable at the cross-section of this 3D Mesh-Section with the Cross-Section Plane.

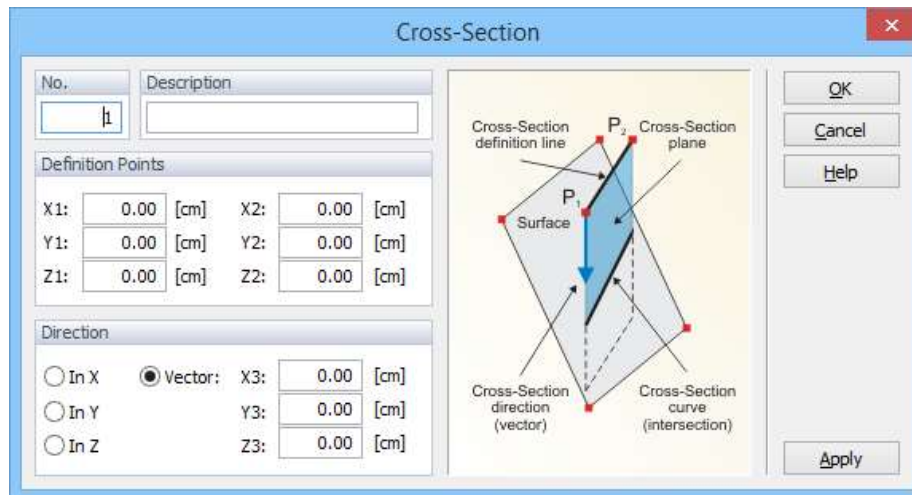


Figure 100. The Cross-Section dialog window.

The ability of charts displaying the distribution of various quantities along boundary-lines and cross-section lines has been extended in Version 3. The GUI now allows the display of results at multiple time-layers simultaneously in one chart. This feature allows one to compare the values of a given quantity very easily at different times. Note that cross-section lines and charts can also be applied to mesh slices created by the Clipper tool as described below and shown in Figure 169.

4.7.5. Mesh-Lines and Mesh-Surfaces

Mesh-Lines (in 2D) are very similar to **Cross-Sections**, except that **Mesh-Lines** follow edges of the finite elements and do not have to be straight. They are used, similarly to **Cross-Sections**, to display selected variables along defined **Mesh-Lines**. Similarly to **Cross-Sections**, the locations of **Mesh-Lines** are saved and can be recalled at any time.

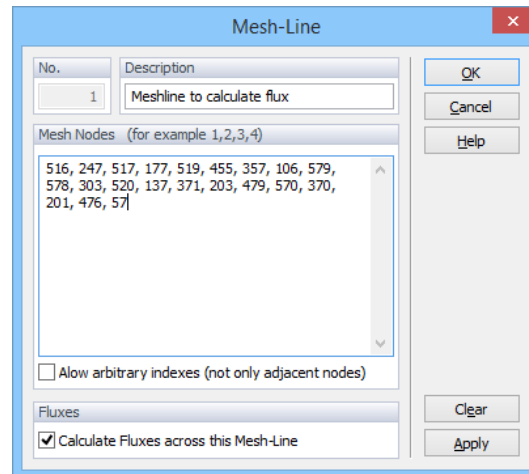


Figure 101. The Mesh-Line dialog window.

A description of the **Mesh-Line** is given in the **Mesh-Line** dialog window (Fig. 101), which contains the Mesh-Line number, its description, a list of nodes defining the Mesh-Line, and whether or not the computational module should calculate (actual and cumulative) water and solute fluxes across this Mesh-Line. The fluxes across the Mesh-Line are then displayed using the **Fluxes across Mesh-Lines** dialog window (Fig. 103) after using the *Results->Fluxes across Mesh-Lines* command. This dialog displays actual and cumulative, water and solute (includes both convective and dispersive) fluxes across individual **Mesh-Lines**.

Similarly to Mesh-Lines, in three-dimensional applications one can define Mesh-Surfaces (Fig. 102), and request HYDRUS to calculate actual and cumulative water and solute fluxes across these Mesh-Surfaces.

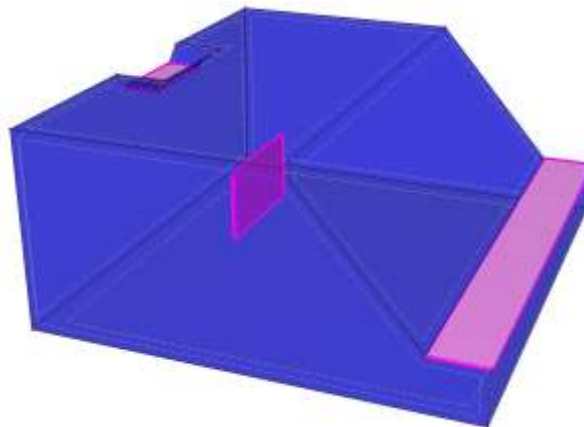


Figure 102. An example of a 3D domain with three Mesh-Surfaces.

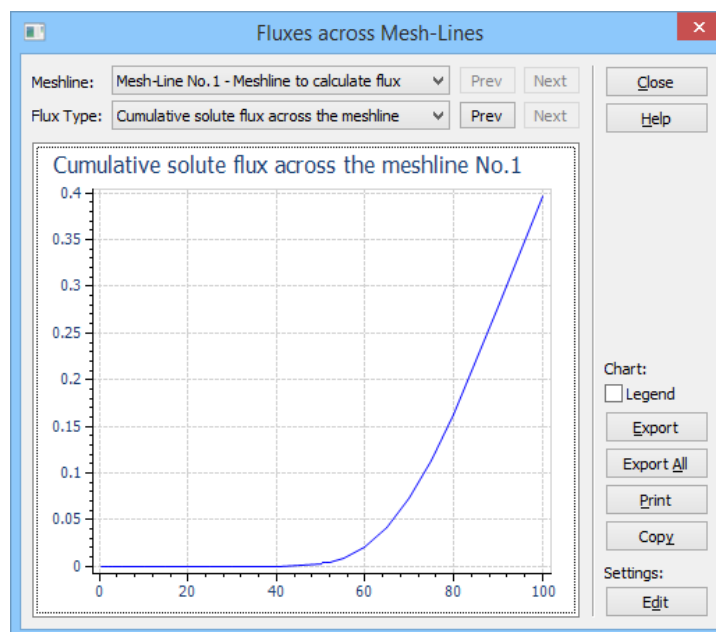


Figure 103. The Fluxes across Mesh-Line dialog window.

Information for this graph is read from the CrossSect.out file that contains data organized into the following columns:

Variable	Description	Units
Time	Time	[T]
Flux(i)	Water flux across the ith cross-section	$[L^2/T]$ or $[L^3/T]^{\dagger}$
CumFlux(i)	Cumulative water flux across the ith cross-section	$[L^2]$ or $[L^3]^{\dagger}$
SolFlux(i)	Convective solute flux across the i-th cross-section	$[M/L^3 * L^2/T = M/L/T]$ or $[M/L^3 * L^3/T = M/T]^{\dagger}$
CumSFlx(i)	Cumulative solute flux across the i-th cross-section	$[M/L^3 * L^2 = M/L]$ or $[M/L^3 * L^3 = M]^{\dagger}$

[†] for 2D and three-dimensional (or axisymmetrical) problems, respectively.

Water Fluxes across internal lines (**mesh-lines**) are calculated in HYDRUS similarly as fluxes through the boundary nodes with prescribed Dirichlet boundary conditions (see the Technical Manual). Nodal fluxes are calculated from the finite element matrix equation that is obtained by the discretization of the Richards equation and assembled for all elements on one side of the selected internal line. The finite element matrix equation for internal fluxes is calculated at the last iteration after convergence for a given time level had been achieved. Fluxes calculated directly from the Richards equation are much more accurate than fluxes calculated using Darcy's law and have the same accuracy as the overall solution. **Solute Fluxes** are then calculated simply by multiplying water flux values with nodal concentrations and adding dispersive solute fluxes (which are calculated similarly as water fluxes above). Note that the reported solute fluxes across mesh-lines in Version 5 (contrary to earlier versions) include the total (dispersive/diffusive and

convective) solute fluxes. Note that mesh-lines are oriented (from the first selected node to the last one), and reported fluxes are positive or negative depending on this orientation.

4.7.6. Points Probes

As an alternative to “**Observation Nodes**,” which need to be defined on FE nodes and before calculations are carried out, Hydrus also provides an option to specify “**Point Probes**,” which can be defined anywhere in the transport domain (independent of FE nodes) and after calculations are done.

When presenting simulation results, HYDRUS displays these “**Point Probes**” and values of a particular displayed quantity (e.g., water contents or concentrations) (Fig. 105). Since “**Point Probes**” are specified after the simulation is finished, HYDRUS cannot display continuous time series as for **Observation Nodes**, but only values at pre-specified **Print Times**. When the **Point Probe** is not located directly on a FE node, the quantity value is linearly interpolated from the corner values of a particular finite element.

A **Point Probe** can be inserted using the **Point Probe** command, available on the **Insert Menu**. One can create a set of **Point Probes** either a) numerically using a table in the **New Point Probe** dialog window (Fig. 104) or b) graphically after clicking on the button “**Set Graphically**.” When defining **Point Probes** numerically, one must predefine their number (**Number of Points**) and click on the **Update** button to update the table before entering **Point Probe** coordinates.

	X [m]	Y [m]	Z [m]
1	0.000	0.000	0.000
2		4	0.000
3	0.000	0.000	0.000

Figure 104. The New Point Probe dialog window.

When defining **Point Probes** graphically (after clicking the button **Set graphically**), one defines Points in the **View** window directly on the Transport Domain using the mouse (clicking the left mouse button at selected locations):

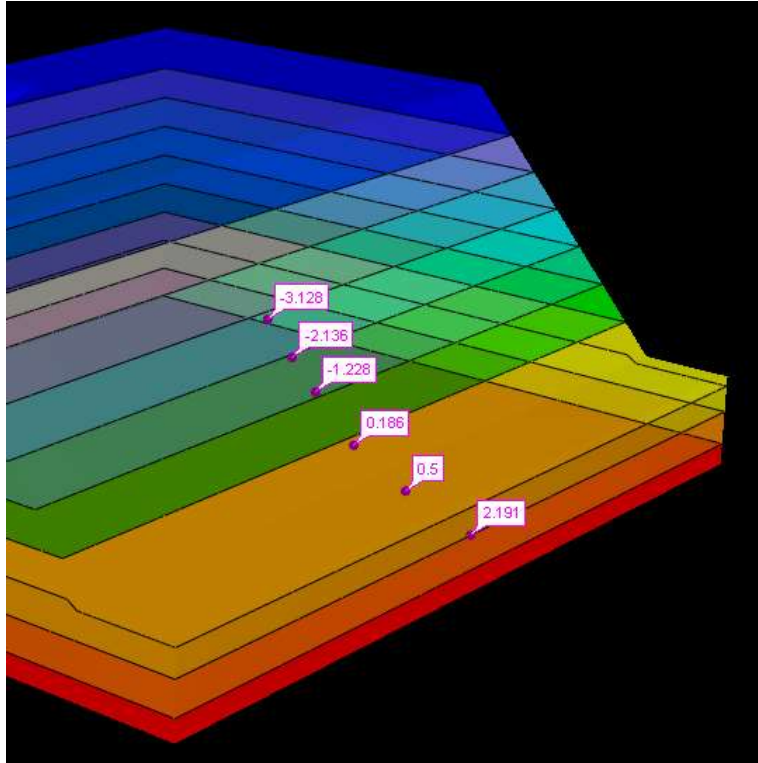


Figure 105. The display of Point Probes with their values.

Point Probes (and associated quantity values) can be displayed or hidden using the **Show Point Probes** check box on the “**Edit bar – Results**” tab (in the section “**Tools and Options**”).

The **Point Probes** can be **Deleted**, **Inserted**, **Saved**, and **Edited** using the command in the “**Current Point Probe**” section of the “**Edit bar – Results**” tab (Fig. 106).

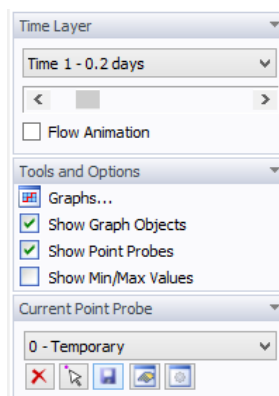


Figure 106. The Tools and Options section of the Results Edit Bar with Point Probes commands.

The **Point Probes** can be grouped into multiple named groups. The initial set of **Point Probes** is denominated **0 - Temporary**. To save it permanently, use the **Save Probe Copy** button on the

Edit Bar below the list of point probes. A new dialog box is opened where you can define the **Name** of the Group of **Probe Points** and check the coordinates of each point.

There are several **Snap** modes (**Points Probes** can be defined on different geometrical objects) that can be used when inserting **Probe Points** graphically (Fig. 107).

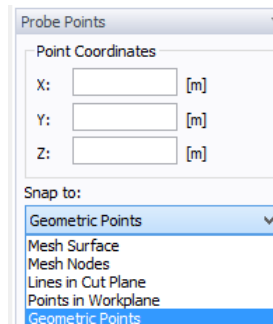


Figure 107. The Probe Points section of the Results Edit Bar when Point Probes are defined.

All saved **Point Probes** are shown on the **Navigator Bar** under the **Auxiliary Objects**, where one can select various Edit Commands using the right mouse button click, for example, **Edit** and **Delete**.

4.7.7. Lines Probes

As an alternative to “**Mesh-lines**,” which need to be defined along edges of finite elements (and thus are broken lines) before calculations are carried out, and “**Cross-Sections**,” which are straight lines through the transport domain (independent of finite elements) that can be defined after calculations are done, HYDRUS also provides an option to specify c) “**Line Probes**,” which are broken lines defined anywhere in the transport domain (also possibly independent of finite elements) and which can be specified after calculations are done.

When presenting simulation results, HYDRUS displays these “**Line Probes**” and values of a particular displayed quantity (e.g., water contents or concentrations) along these lines. HYDRUS can display graphs of a particular quantity along a **Line Probe** for a particular **Print Time** or for all **Print Times**. When **Points** defining a **Line Probe** are not located directly on FE nodes, the quantity values are linearly interpolated from the values in FE nodes.

A **Line Probe** can also be inserted using the **Line Probe** command, available on the **Insert Menu**. One can create a set of definition points for the new **Line Probe** either a) numerically using a table in the **New Line Probe** dialog window (Fig. 108), or b) graphically after clicking on the button “**Set Graphically**.” When defining a **Line Probe** numerically, one must predefine the number of definition points (**Number of Points**) and click on the **Update** button to update the table before entering definition points coordinates

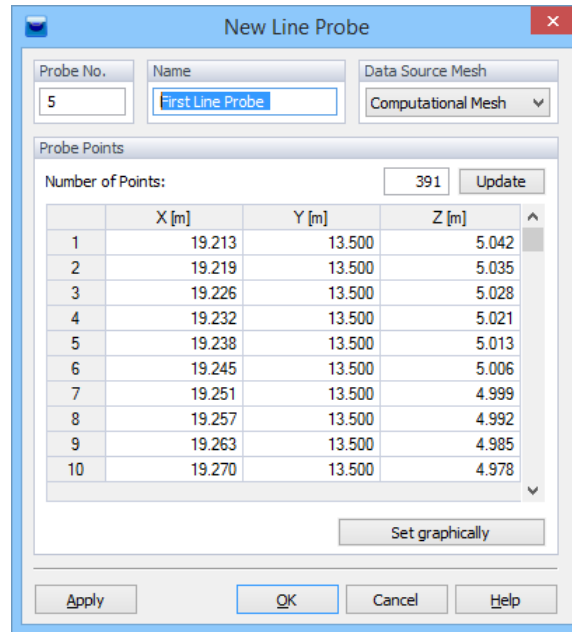


Figure 108. The New/Edit Line Probe dialog window.

The **Graph Polyline Probe** function (on the “**Edit bar – Results**” tab, in the section “**Tools and Options**”) enables you to define a line in the transport domain or in the slicer plane and, thus, create a sectional diagram of the results along the line (Fig. 109).

To display a line chart, use a) the **Graphs -> Polyline Probe** command which is available on the **Results** menu, or b) double-clicking on a **Line Probe**. When the line is activated, you can select the relevant points of the line (or polyline) by mouse-clicks. The coordinates of the points are displayed in the panel, which has a specific layout for this purpose. Here, you can also modify the Snap object, if necessary (Fig. 109).

The **Line Probes** can be grouped into multiple named groups. The initial set of **Line Probes** is denominated **0 - Temporary**. To save it permanently, use the **Save Probe Copy** button on the **Edit Bar** below the list of point probes. A new dialog box is opened where you can define the **Name** of the Group of **Probe Points** and check the coordinates of each point.

All saved **Line Probes** are shown on the **Navigator Bar** under the **Auxiliary Objects**, where can select various **Edit** commands, such as **Delete All Line Probes**.

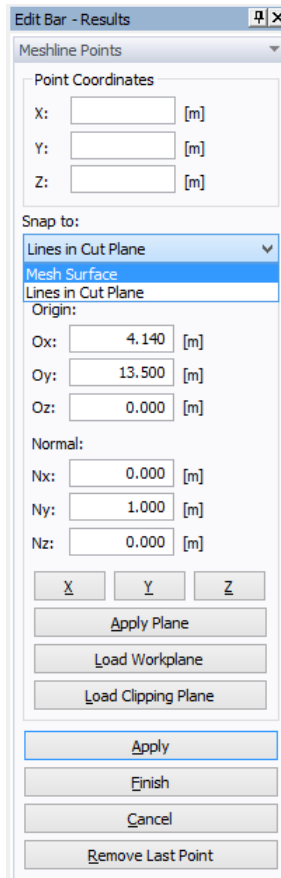


Figure 109. The Line Points section of the Results Edit Bar when Line Probes are defined.

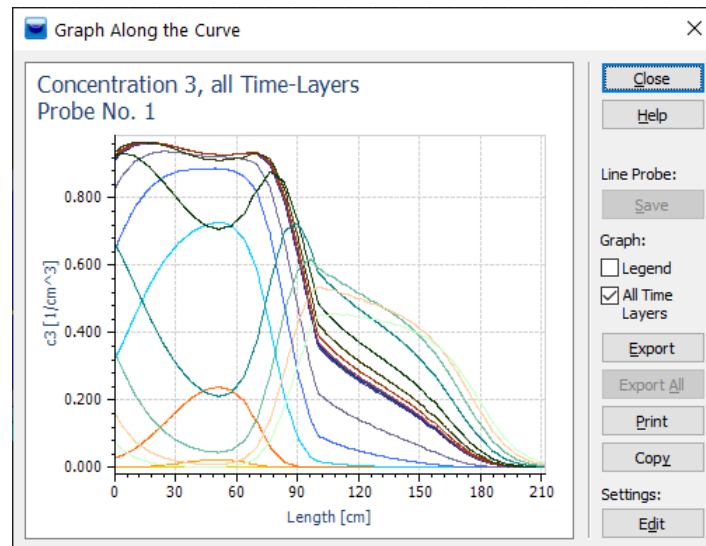


Figure 110. An example of the Line Probes graph.

4.7.8. Background Layers

Background Layers are geometric objects that can serve as a template for defining the transport domain. A **Background Layer** consists of nodes and curves that are not part of the transport domain, but its components can be used to define the transport domain. A **Background Layer** is usually read from the DXF file (AutoCAD) (Figure 113), but may also be read from another HYDRUS project (h3d, h3d2, or h3d3), or from STL (stereolithography), TIN (Triangular Irregular Network), or BMT (bitmap) formats (Figure 112). An example of a very complex Background Layer (unrelated to hydrology) read from the DXF file is given in Figure 111.

In the **New Background Layer** dialog window (Figure 112), one selects a) the format of the imported file (i.e., either HYDRUS formats h3d, h3d2, and h3d3, or DXF, STL, TIN, or BMT formats), b) units of the imported file, c) whether or not to place the Background Layer so that its bottom-left corner is located in the origin of the coordinate system, d) whether or not to make the Background Layer visible in the View window, and e) whether or not the **Grid and Workspace** settings should be adjusted according to the Background Layer dimensions.

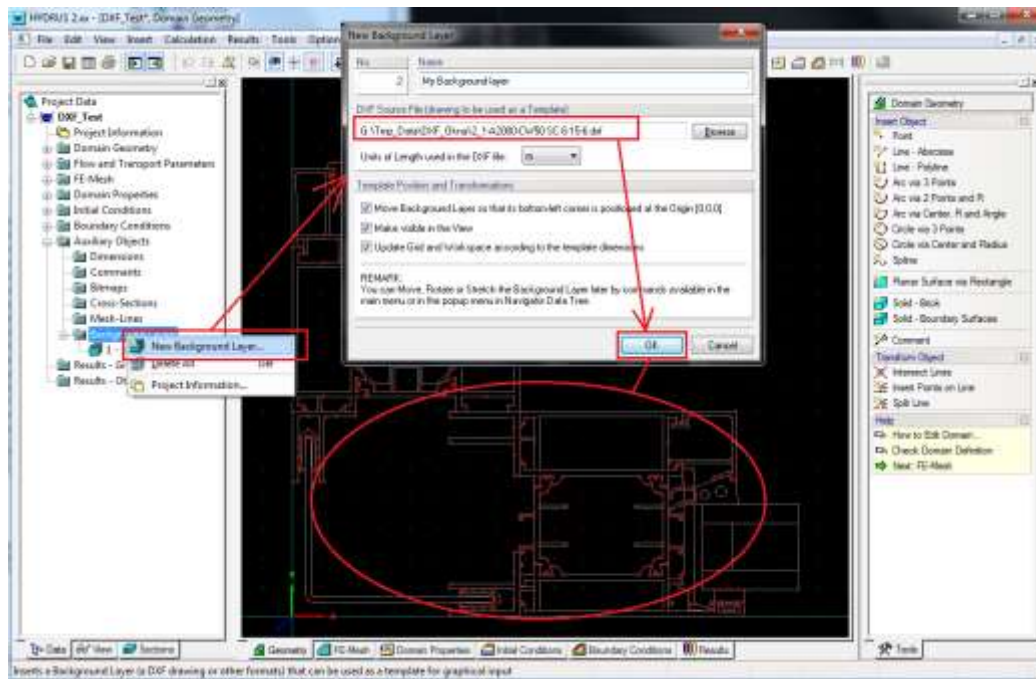


Figure 111. An example of the Background Layer.

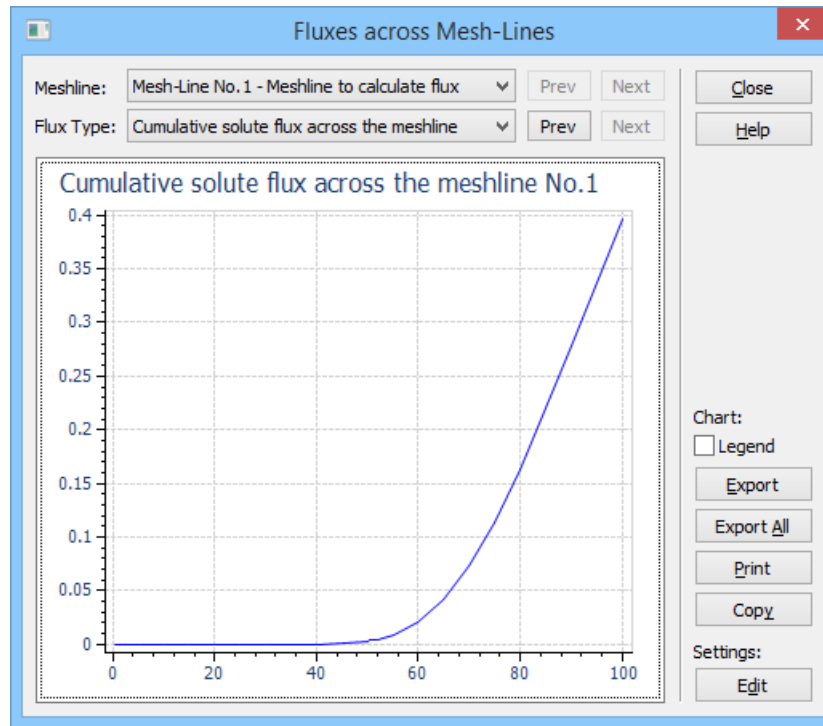


Figure 112. The New Background Layer dialog window.

STL is a file format native to the stereolithography CAD software created by 3D Systems. This file format is supported by many other software packages; it is widely used for rapid prototyping and computer-aided manufacturing. STL files describe only the surface geometry of a three-dimensional object without any representation of color, texture or other common CAD model attributes. The STL format specifies both ASCII and binary representations. Binary files are more common since they are more compact. An STL file describes a raw unstructured triangulated surface by the unit normal and vertices of the triangles using a three-dimensional Cartesian coordinate system. The STL file specifications are at: [http://en.wikipedia.org/wiki/STL_\(file_format\)](http://en.wikipedia.org/wiki/STL_(file_format)).

TIN files are used for storing triangulated irregular networks using a simple set of xyz coordinates. The TIN file specifications are at: http://www.ems-i.com/wmshelp/Files/File_Formats/TIN_Files.htm.

The project may have at the same time multiple **Background Layers** (virtually any number) and their visibility can be turned on and off using the View Tab at the Navigator Bar (*Auxiliary Objects->Background Layers*). **Background Layers** are displayed in the View window using suppressed (less intense) colors so that they do not visually disturb when objects of the geometry are being defined. The intensity of display and other parameters can be set (intensity of their display can be set between 0 and 1) in the **Display Options** dialog window (the Menu command *Options->Display Options->Edit*) (Fig. 157). If the location of the template (background layer) is not satisfactory, it can be **Moved** (Fig. 66), **Rotated** (Fig. 67, left), **Mirrored** (Fig. 67, right), **Stretched** (Fig. 68, left), and/or **Skewed** (Fig. 68, right) as needed.

4.8. Other Notes on Objects

Objects **Mesh Refinement** define a local density of the FE-Mesh in the vicinity of a particular object. Possible types of Mesh Refinement are:

- Mesh Refinement at Point
- Mesh Refinement on Curve given by a number of points
- Mesh Refinement on Curve given by FE size
- Mesh Refinement on Surface

4.8.1. Object Numbering

Each object has its own number (index) that serves for the unique identification of an object for operations such as Edit, Delete, or Find. Object numbering is fully controlled by the user (a user specifies the object index) and does not have to be continuous (indexes do not have to sequentially increase).

4.8.2. Relations among Objects

More complex objects are defined using simpler objects. For example, a surface is defined by indices of its boundary curves, and a boundary curve is defined by indices of its points. The curve, however, does not own its points since these points can also be used to define other curves. This is especially true for points at the beginning and end of a curve, since these points are usually used also by neighboring curves. A relation „Parent – Descendent“ exists among objects. In the case of a curve, points are „Parent“ objects, and a Surface is its „Descendent“.

4.8.3. References among Objects and Convention for Writing a List of Indices

Objects are referenced using a list of indices. A list of indices is written using a text format, where individual indices are separated by a comma and dash (-) between two indices indicates a range “from-to” (e.g., 1,5-10,35-30,8,11). After inserting new indices, the list is always reformatted to minimize the length of the text. Depending on circumstances, the list of indices respects/does not respect the sequence, in which objects were defined.

4.9. Import Geometry from a Text File

It is possible to **Import** the definition of objects defining the **Geometry** of the transport domain from a text file using the command “*Import Geometry from a Text File*”. It is possible to import (export) points, curves (polylines, circles, arcs, and splines), surfaces, openings, and thickness vectors.

- a) The definition of each object starts with the word **OBJECT=KEY_WORD**, followed by coordinates of points defining the given object. Two or three coordinates (for two- and three-dimensional problems; units must always be in meters) of a single point are given on a single line. Numbers can be delimited using a space, a semicolon, or a tabulator.

- b) Points associated with higher objects, i.e., lines, openings, or surfaces, are listed as part of this object. Similarly, lines associated with higher objects, i.e., openings or surfaces, are listed as part of this object. Only points that are not part of any higher object should thus be listed under the object POINTS, and only lines that are not part of any higher object (e.g., that do not form boundaries of surfaces) should thus be listed under the object LINES.
- c) Lines with a semicolon at the beginning are ignored as „Comments“. Note that comment lines can appear only between blocks, but not inside of any particular block.
- d) It is possible that exported Geometry once imported back into HYDRUS can have different numbering, i.e., the project may not be identical.
- e) Below is a list (**KEY_WORD**) of all possible objects. "**POLYLINE**" is a single line defined by multiple nodes, while "**LINES**" is a series of lines (multiple objects). **Surfaces** or **Openings** must be defined by a single closed curve, the type of which is given in the name of the object (e.g., SURFACE_CIRCLE). When this rule is not fulfilled (e.g., for a surface with complex boundary), this complex boundary will be saved as a series of lines, i.e., SURFACE_LINES.
- f) The **THICKNESS_ARR3Z_NLAYERS** command allows importing multiple **Thickness Vectors** to define the variable thickness of a **Solid**. On each Thickness Vector, one can define multiple z-coordinates that are used to divide a Solid automatically into Layers with variable thicknesses. The number of Layers is arbitrary (min=1, max=100), and their number is given by the number of columns in the file.

KEY_WORD for Import/Export:

```
POINTS
LINES
POLYLINE
SPLINE
CIRCLE
ARC
SURFACE_LINES
SURFACE_POLYLINE
SURFACE_SPLINE
SURFACE_CIRCLE
OPENING_LINES
OPENING_POLYLINE
OPENING_SPLINE
OPENING_CIRCLE
THICKNESS
THICKNESS_ARR3Z
THICKNESS_ARR3Z_NLAYERS
```

Notes on the **THICKNESS_ARR3Z_NLAYERS** command (the **THICKNESS_ARR3Z** command has only the first five columns):

Particular columns in the input file have the following meaning:

1. X coordinate (m).
2. Y coordinate (m).
3. Z coordinate (m) of the Definition Point of the Thickness Vector (Anchor Point, see Figure 89 of the User Manual with the Edit Thickness Vector dialog and the point denoted "P"). The Definition (Anchor) Point must lie in the plane of the Base surface. The Z-coordinate in the third column will thus likely be constant for all Thickness Vectors unless the Base Surface is inclined.
4. Z coordinate (m) of the lower point of the first layer of the Thickness Vector (a point denoted "N1" in Figure 89 of the User Manual). When P=N1, this coordinate is the same as the 3rd coordinate.
5. Z coordinate (m) of the upper point of the first layer of the Thickness Vector.
6. Z coordinate (m) of the upper point of the second layer of the Thickness Vector.
7. ...
8. Z coordinate (m) of the upper point of the last layer of the Thickness Vector, i.e., the coordinate of the surface of the solid.

Here is an example of the file for the import of a Solid divided into three Geo-Layers:

```
OBJECT=THICKNESS_ARR3Z_NLAYERS
4.500000e+000 4.000000e+000 0.000000e+000 0.000000e+000 1.300000e+000 2.100000e+000 3.300000e+000
5.500000e+000 2.500000e+000 0.000000e+000 0.000000e+000 1.300000e+000 2.200000e+000 3.400000e+000
7.000000e+000 4.500000e+000 0.000000e+000 0.000000e+000 1.400000e+000 2.300000e+000 3.000000e+000
7.000000e+000 2.500000e+000 0.000000e+000 0.000000e+000 1.200000e+000 2.600000e+000 3.500000e+000
6.500000e+000 9.999999e-001 0.000000e+000 0.000000e+000 1.600000e+000 2.400000e+000 3.600000e+000
5.000000e+000 2.000000e+000 0.000000e+000 0.000000e+000 1.200000e+000 2.500000e+000 3.700000e+000
4.500000e+000 2.000000e+000 0.000000e+000 0.000000e+000 1.400000e+000 2.400000e+000 3.400000e+000
5.000000e+000 9.999999e-001 0.000000e+000 0.000000e+000 1.500000e+000 2.500000e+000 3.300000e+000
5.500000e+000 9.999999e-001 0.000000e+000 0.000000e+000 1.100000e+000 2.100000e+000 3.200000e+000
;
```

Other notes:

9. The minimum number of columns is 5 (this corresponds to a single layer).
10. Z coordinates must be entered in the correct sequence, i.e., from the bottom (Base Surface) up towards the end of the Thickness Vector.
11. If layers are to be defined in a different direction than Z (e.g., when the Base Surface lie in the XZ plane), one needs to first carry out the standard import in the Z direction and then to rotate the entire domain using the Rotate function.
12. When the "THICKNESS_ARR3Z_NLAYERS" is used, i.e., the input file includes data of thickness vectors with multiple geo-layers, this keyword can be processed fully only if the domain already contains a 3D-Layered Solid. If there is no Solid defined yet, then HYDRUS is not able to create a Solid automatically from imported points because its Base Surface can have a very complex shape. There are two ways how to proceed:
 - a) Press "OK" to continue. HYDRUS will import first only thickness vectors without geo-layers. Then define a 3D-Layered Solid using imported points and import the same file again. Geo-layers will be added to the Solid during this second import.
 - b) Press "Cancel" to cancel this import. First, define a 3D-Layered Solid and then import this file again. Thickness vectors with layers will be added to the Solid.

4.10. Import Geometry from a DXF File

It is possible to **Import** the definition of objects defining the **Geometry** of the transport domain from a file in the DXF format. **AutoCAD DXF** (Drawing Interchange Format, or Drawing Exchange Format) is a CAD data file format developed by Autodesk for enabling data interoperability between AutoCAD and other programs. Autodesk now publishes the [DXF specifications](#) on its website for versions of DXF dating from AutoCAD Release 13 to AutoCAD 2010. The menu command **Import Geometry from a DXF File** calls the dialog window (Fig. 113) of the same name that allows users to select (or browse for) the DXF file with the description of the transport domain and to specify units that are used in this file.

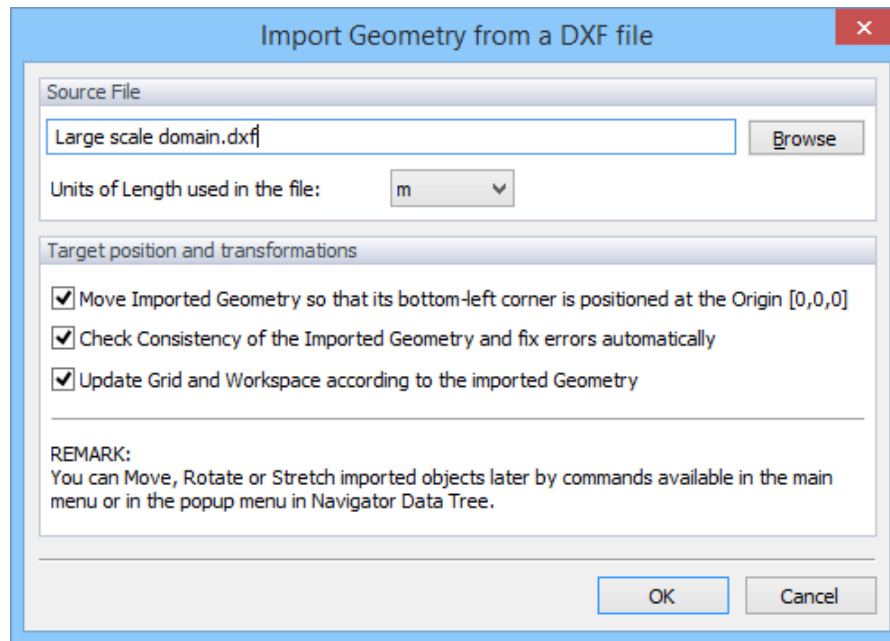


Figure 113. The Import Geometry from a DXF File dialog window.

Since local coordinates defining the transport domain in the coordinate system used in the DXF files may include very large numbers, users can ask the HYDRUS GUI to convert these coordinates so that the bottom-left corner of the transport domain is located in the origin of the computational coordinate system. This will likely lead to much smaller values of local coordinates. Finally, users can ask the HYDRUS GUI to automatically adjust the Grid and Workspace variables to accommodate the imported geometry.

4.11. Import Geometry from a TIN File

It is possible to also Import the definition of objects defining the Geometry of the transport domain from a file in the TIN format. TIN files are used for storing triangulated irregular networks using a simple set of xyz coordinates. The TIN file specifications are at: http://www.ems-i.com/wmshelp/Files/File_Formats/TIN_Files.htm.

5. Finite Element Mesh

5.1. Finite Element Mesh Generator

The **Finite Element Mesh Generator** dialog window was used in earlier versions to select a structured finite element mesh for a relatively simple rectangular or hexahedral domain, or a more general unstructured finite element mesh. The dialog provided a brief description of each mesh generator and a simple bitmap with an explanation of the main terms involved. In later versions (after 1.03), a decision on which generator to use is made in the Domain Type and Units Window (Fig. 6 and 7). While the structured finite element generator can be used only for simple rectangular (i.e., the Geometry Type "2D-Simple (Parametric)" - see the Projects Geometry Information Section 2) or hexahedral domains (3D-Simple (Parametric)), the unstructured finite element generator is used for more complicated geometries (i.e., 2D-General (Boundary Rep.), 3D-Layered, and 3D-General (Boundary Rep.)). While the unstructured mesh generator **MeshGen2D** is used to generate FE meshes for two-dimensional domains (2D-General (Boundary Rep.)) and for the **Base Surface** of three-dimensional layered domains (3D-Layered), the mesh generator **Genex/T3D** is used to generate three-dimensional FE meshes for the 3D-General (Boundary Rep.) geometry.

5.2. Structured Finite Element Mesh Generator

Soil Profile Depth

Depth: 230 [cm] Update

Fixed Points and Mesh Density

URS = Upper Relative Size of FE
LRS = Lower Relative Size of FE

No.	z [cm]	URS	LRS
1	0.00000	1.000	1.000
2	-230.00000	1.000	1.000

New Delete Delete All

FE-Mesh Nodes

Number of Mesh Nodes: 33

No.	z [cm]
1	0.00000
2	-1.00000
3	-2.00000
4	-4.00000
5	-6.00000
6	-10.00000
7	-15.00000
8	-20.00000
9	-25.00000
10	-30.00000
11	-40.00000
12	-50.00000
13	-60.00000
14	-70.00000
15	-80.00000
16	-90.00000

Update Mesh Nodes

OK Cancel Apply Help

Next... Previous...

Figure 114. The FE-Mesh dialog window for one-dimensional applications.

The finite element discretization for one-dimensional applications can be done either in a graphical mode or in the FE-Mesh dialog window (Fig. 114). The FE-Mesh for one-dimensional domains is

defined by the **Soil Profile Depth** (the upper left part of the dialog window) and z-coordinates of FE nodes (the right part of the dialog window). The **Number of Mesh Nodes** is defined in the edit box on the upper right side of the dialog window. The default **Number of Mesh Nodes** is 100. The finite element nodes are by default distributed uniformly, i.e., having the same distances between nodes.

The *relative size of finite elements* can be modified using the **URS** (upper relative size of FE) and **LRS** (lower relative size of FE) factors in the subsection **Fixed Points and Mesh Density** (Fig. 114, left). The node at the soil surface (with a z-coordinate=0 cm) has only the LRS factor and the node at the soil bottom (with a z-coordinate=-Soil Profile Depth) has only the URS factor. Users can also define coordinates of internal **Fixed Points**, and define both URS and LRS factors for these internal nodes. The element sizes are then proportionally distributed.

As discussed in Section 2, two-dimensional transport domains can be defined using modified rectangles. Simple rectangular domains are defined by three straight lines, one at the bottom of the domain and two at the sides, while the upper boundary may or may not be straight (see examples in Fig. 8). Nodes along the upper boundary may, in that case, have variable x- and z-coordinates, but the lower boundary line must be straight (horizontal or with a specified slope), whereas the left and right boundary lines must be vertical. The flow region can then be discretized into either a structured or an unstructured triangular finite element mesh.

The dialog window is titled "Rectangular Domain Discretization". It contains the following sections:

- Horizontal Discretization in X:**
 - Count: 10 (with an Update button)
 - Table with columns x [cm] and dz [cm]:

	x [cm]	dz [cm]
1	0.00	0.00
2	0.11	0.00
3	0.22	0.00
4	0.33	0.00
5	0.44	0.00
6	0.56	0.00
7	0.67	0.00
8	0.78	0.00
9	0.89	0.00
10	1.00	0.00
- Vertical Discretization in Z:**
 - Count: 41 (with an Update button)
 - Table with column z [cm]:

	z [cm]
1	8.00
2	7.80
3	7.60
4	7.40
5	7.20
6	7.00
7	6.80
8	6.60
9	6.40
10	6.20
11	6.00
12	5.80
13	5.60
- Generate Z - Coordinates:**
 - Set relative size of finite elements:
 - RS1: 1
 - RS2: 1
 - Generate button
 - Preview: A rectangular domain with a triangular mesh. Labels RS1=1.0 and RS2=5.0 are shown.
- Buttons:** OK, Cancel, Help, Next..., Previous..., Apply.

Figure 115. The Rectangular Domain Discretization dialog window.

When the structured mesh is used, one then needs to specify in the **Rectangular Domain Discretization** dialog window the number of nodes (*Count*) on the horizontal (*Horizontal Discretization in X-Direction*) and vertical (*Vertical Discretization in Z-Direction*) sides of the rectangular region, including their nodal coordinates (Fig. 115). The *relative size of finite elements* on the vertical side can be modified using the RS1 (relative size at the top) and RS2 (relative size at the bottom) factors below *General Vertical Coordinates*. The element sizes are then proportionally distributed. Smaller RS factor leads to smaller elements.

The upper boundary is by default parallel with the bottom boundary. Any possible vertical deviations from this parallel line can be defined using *dz* values (in the *Horizontal Discretization in X-Direction* part of the window). Relatively general domains can still be defined by properly adjusting the *dz* values (see Fig. 8).

A similar approach can be used to discretize simple hexahedral domains in three dimensions. Hexahedral domains must have similar properties as rectangular domains in that they are defined by vertical planes at the sides, a horizontal plane (possibly with a certain slope) at the bottom boundary, and with only the upper boundary not having to be a plane. The discretization of the hexahedral domain is then defined in the **Hexahedral Domain Discretization** dialog window. Again, one needs to specify the number of nodes (*Count*) on the horizontal (*Horizontal Discretization in X*, *Horizontal Discretization in Y*) and vertical (*Vertical Discretization in Z-Direction*) sides of the hexahedral region and their nodal coordinates (Fig. 116). The *relative size of finite elements* on the vertical side can again be modified using RS1 (relative size at the top) and RS2 (relative size at the bottom) factors (*General Vertical Coordinates*). The vertical final element sizes are then proportionally distributed.

Any possible vertical deviations from the plane parallel with the bottom of the domain can be defined using the *dz* values (in the *Horizontal Discretization in X* and *Horizontal Discretization in Y* parts of the window). This feature still allows relatively general domains to be created (see Fig. 9).

Hexahedral Domain Spatial Discretization

Horizontal Discretization in X

Count: 5

Update

	x [cm]	dz [cm]
1	0.00	0.00
2	0.25	0.00
3	0.50	0.00
4	0.75	0.00
5	1.00	0.00

Horizontal Discretization in Y

Count: 11

Update

	y [cm]	dz [cm]
1	0.00	0.00
2	0.10	0.00
3	0.20	0.00
4	0.30	0.00
5	0.40	0.00
6	0.50	0.00
7	0.60	0.00
8	0.70	0.00
9	0.80	0.00
10	0.90	0.00
11	1.00	0.00

Vertical Discretization in Z

Count: 62

Update

	z [cm]
1	61.00
2	60.00
3	59.00
4	58.00
5	57.00
6	56.00
7	55.00
8	54.00
9	53.00
10	52.00
11	51.00
12	50.00
13	49.00

Element Type

☐ Tetrahedral

☒ Triangular Prism

Generate Z - Coordinates

Set relative size of finite elements:

RS1: 1

RS2: 1

Generate

RS1=1.0

RS2=5.0

OK

Cancel

Help

Next...

Previous...

Apply

Figure 116. The Hexahedral Domain Discretization dialog window.

5.3. Unstructured Finite Element Mesh Parameters

Parameters for generating the *Unstructured Finite Element Mesh* are specified in the **FE-Mesh Parameters** dialog window (Figs. 117 through 123). This dialog window has six and four Tabs for the MeshGen2D and T3D generators, respectively, in which various parameters of the unstructured finite element mesh can be specified.

The Main Tab

The *Targeted FE size* (i.e., the average size of the triangular elements in the generated finite element mesh) is specified on the **Main** Tab (Figs. 117). The program selects by default a **Targeted FE Size**. Users can change this value by deselecting the **Automatic** check box. The finite element mesh with this *Targeted FE size* can be further modified using various tools, such as *Stretching* in different directions (on the **Stretching** Tab, Fig. 118) to make the mesh anisotropic, specifying the *Maximum Number of Nodes on Boundary Curve* (on the **MG-Options** Tab, Fig. 122) and *Minimum Number of Nodes on Boundary Curve* (on the **Options** Tab, Fig. 123), and using **Finite Element Mesh Refinement** (Fig. 125). While the **Default** command sets default values on a particular tab of the **FE-Mesh Parameters**, the **All Default** command sets default values on all four tabs. For three-dimensional applications (only for 3D-Layered geometries), a user can specify on the **Main** Tab the **No. of Horizontal Layers**, which are layers parallel with the **Base Surface** to add the third dimension to the problem and if the finite elements used to discretize the three-dimensional domain are to be **Tetrahedrals** or **Triangular Prisms** for 3D-Layered geometries, or **Tetrahedrals** or **Mixed Elements** (multiple types of elements) for 3D-General geometries. It is recommended to use Triangular Prisms or Mixed Elements rather than Tetrahedrals since then the number of finite elements is three or more times smaller, and thus, the calculations are faster.

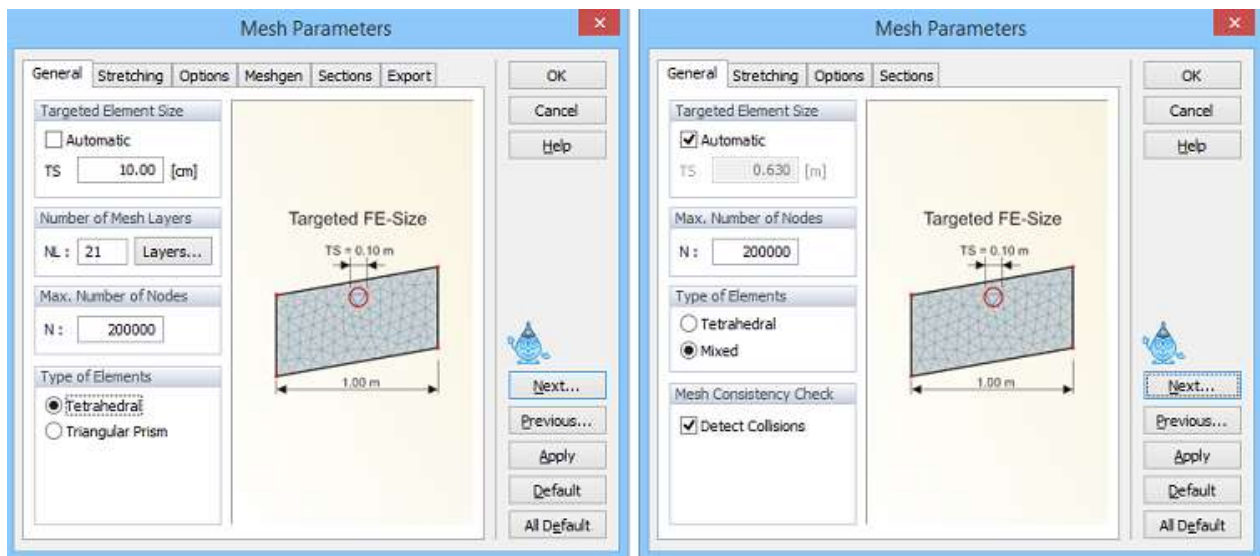


Figure 117. The FE-Mesh Parameters dialog window (the Main Tab for 3D-Layered (left) and 3D-General (right) geometries).

For 3D-General geometries, users also need to specify the **Maximum Number of Nodes** in the FE mesh. This is the maximum number of finite element nodes in the entire three-dimensional domain. Similarly, as below for MeshGen, when this is specified for a two-dimensional domain (Fig. 122) when this maximum number is reached a warning will appear ***Achieved the maximum number of nodes!*** This means that the maximum allowed number of nodes was reached during the mesh generation process and the user needs to decide whether or not so many nodes are needed for the envisioned FE mesh and either increase this number or adjust other parameters so that fewer nodes (and FE elements) are generated.

For 3D-General geometries, there is in the **Mesh Consistency Check** section an additional check box **Detect Collisions**. This check box is important only for complex 3D-General geometries consisting of multiple solids. When this check box is on, the program checks "collisions" of different objects. The solids cannot intersect each other without having the intersections properly defined using boundary curves. The program also detects if one **Solid** is entirely inside of another Solid (i.e., its boundaries do not intersect). The former Solid has to be in such a case defined as an **Opening** (Hole, **Cavity**). The check box "Detect Collisions" enables users to turn off this check in cases, when they are absolutely sure that there are no such collisions, and they still receive a warning about a collision of solids.

The Stretching Tab

Stretching of the finite element mesh (i.e., the degree of mesh anisotropy in a certain direction) is defined using the **Stretching Factor** and **Stretching Direction** (Fig. 118). The finite elements are made larger in the particular **Stretching Direction** if the **Stretching Number** is larger than one and smaller if smaller than one. The result of this transformation is a mesh deformed in the given direction, which can be desirable for problems that, for example, require different spatial steps (mesh sizes) in the *X* and *Y* directions.

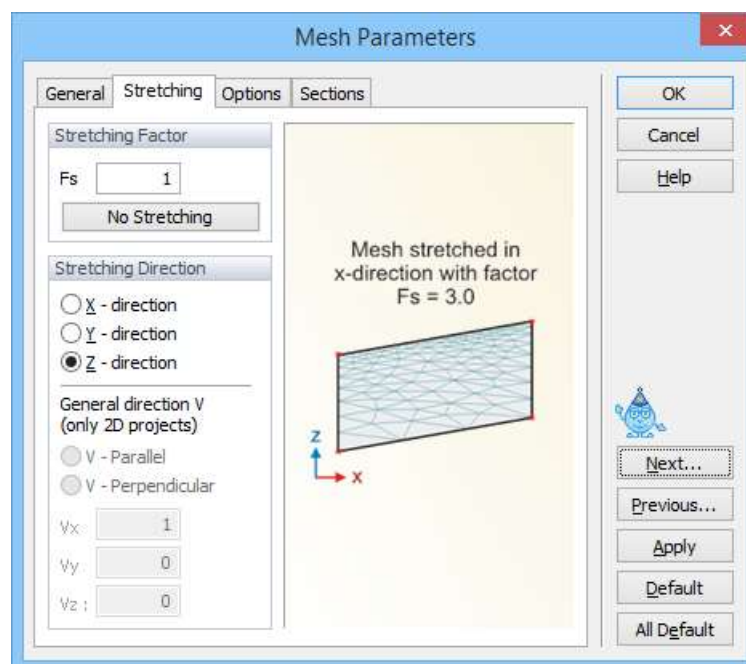


Figure 118. The FE-Mesh Parameters dialog window (Tab Stretching).

The **Stretching Direction** is defined either by the direction of main X, Y, and Z coordinates (in both 2D and 3D projects) or by a general vector V with two coordinates (V_x and V_z for vertical two-dimensional domains and V_x and V_y for horizontal two-dimensional domains). An example of a mesh stretched using a **Stretching Factor** of 3 in the x-direction is shown in Figure 131.

One can define a **Global FE-Mesh Stretching** using the Stretching Tab (Fig. 118) of the FE-Mesh Parameters window or a **Local FE-Mesh Stretching**, using the Insert->FE-Mesh->Mesh Stretching command. While a Global FE-Mesh Stretching is applied to the entire transport domain, a Local FE-Mesh Stretching can be assigned to individual **Surfaces** (*On Surface No.*). A local FE-Mesh Stretching can be defined in the direction of main coordinates or parallel (*V-Parallel*) or perpendicular (*V - Perpendicular*) to a general vector V , which is defined by two (or three) coordinates (V_x and V_z or V_x and V_y (or V_x , V_y , and V_z)) or by selecting two points in the transport domain (*Pick Two Points*). Note that Local FE-Mesh Stretchings are ignored when a Global FE-Mesh Stretching is defined (i.e., a Global FE-Mesh Stretching has to be equal to 1 if one wants to consider Local FE-Mesh Stretchings). FE-Mesh Stretching is available only for 2D-General and 3D-Layered domains.

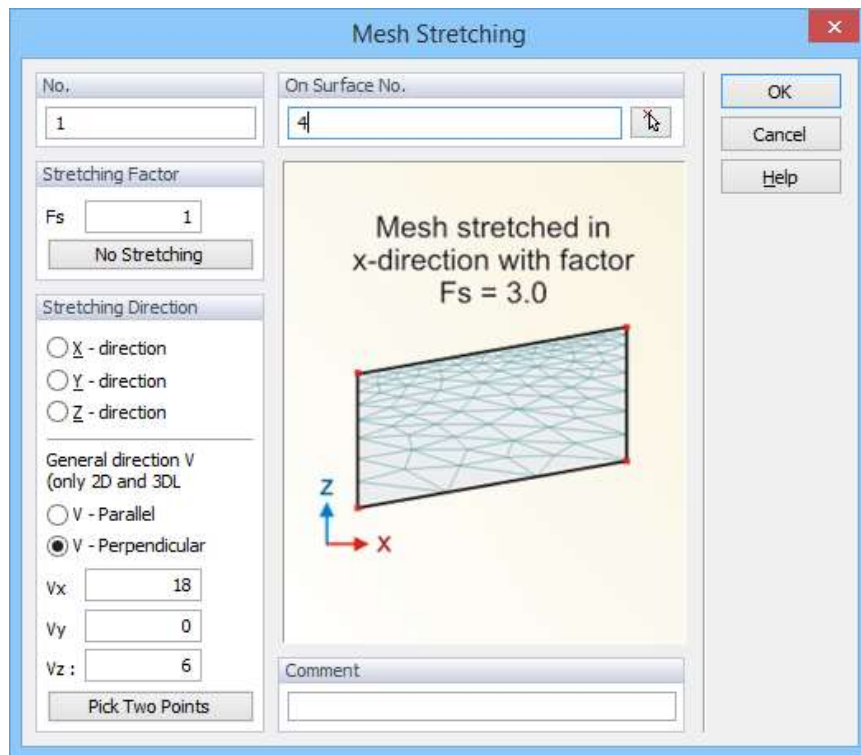


Figure 119. The Mesh Stretching dialog window for a Local FE-Mesh Stretching.

In the example below (a listing from the Navigator Bar), the first FE-Mesh Stretching has a Stretching Factor of 0.03 in the direction of the Z coordinates assigned to Surface 3, the second FE-Mesh Stretching has a Stretching Factor of 0.01 in the direction of the general V_2 vector assigned to Surface 2, etc.

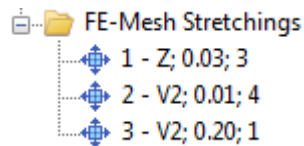


Figure 120. Listing of FE-Mesh Stretchings on the Navigator Bar.

Local FE-Mesh Stretchings can be edited by clicking at them at the Navigator Bar. Figure 121 below shows an example of the finite element mesh with three **FE-Mesh Stretchings** assigned to areas below the domain surface. These Stretchings were defined either using the Menu Command "Insert->FE-Mesh->Mesh Stretching - Dialog" or the Edit Bar Command "Insert Mesh Stretching". All Local FE-Mesh Stretchings can be deleted using the Edit Bar Command "Delete All Stretching".

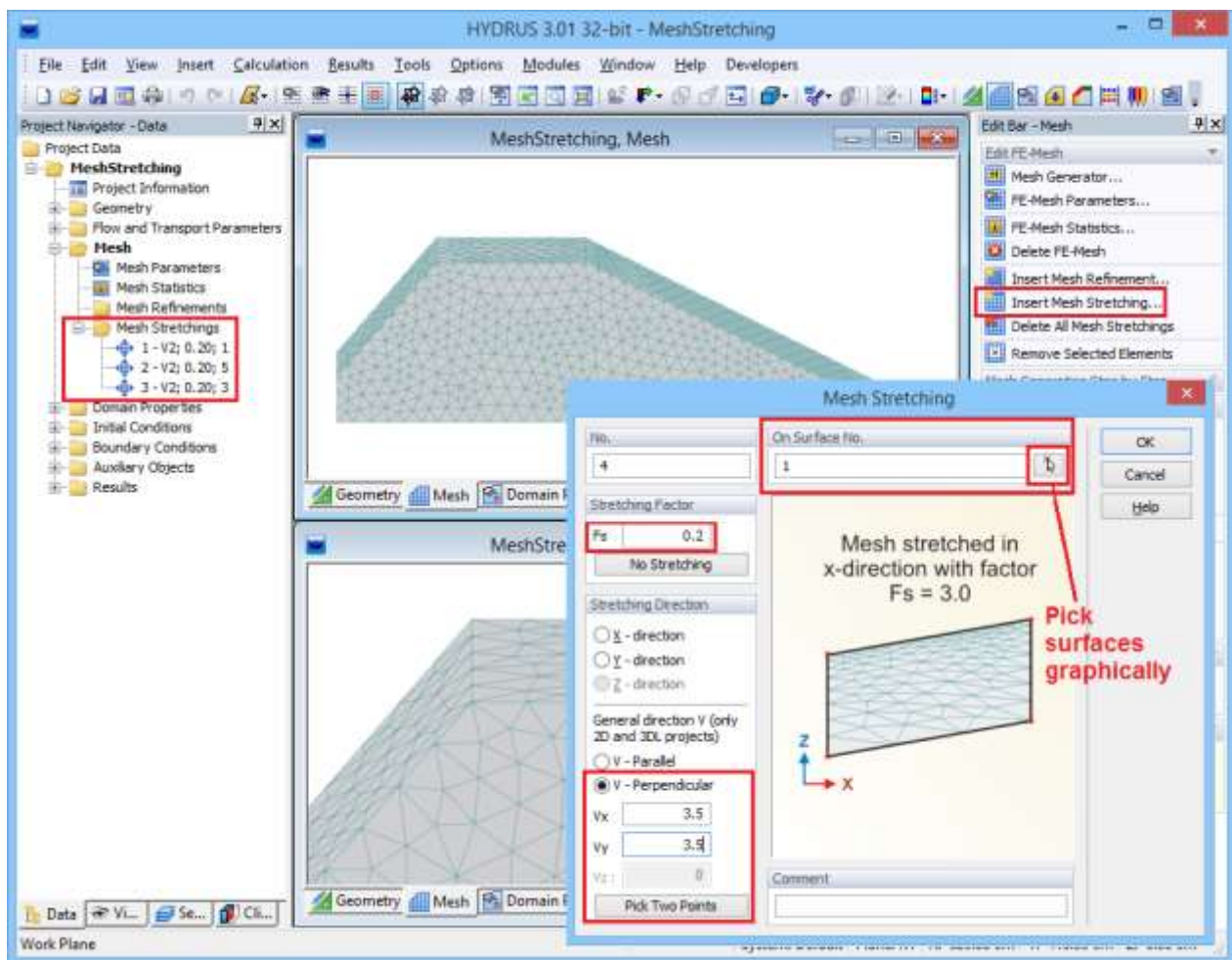


Figure 121. An example of the FE-Mesh with three FE-Mesh Stretchings assigned to areas below the domain surface.

The MG-Options Tab

Parameters for the unstructured triangular finite element generator are given in the **MG-Options** (Meshgen) Tab of the **FE-Mesh Parameters** dialog window (Fig. 122). The parameters are divided into *FE-Mesh Limits* (which limits the number of elements) and *FE-Mesh Quality* (which affects the smoothness of the FE mesh) groups.

The following parameters are specified in the **FE-Mesh Limits** group:

Maximum Number of Nodes on Boundary Curves: This is the maximum total number of nodes on all boundary curves for two-dimensional applications, or on all boundary curves defining the bottom plane (base surface) for three-dimensional applications.

Maximum Number of FE-Mesh Nodes (2D Mesh): This is the maximum total number of finite element nodes in two-dimensional domains, or on the bottom plane (base surface) of three-dimensional domains.

Both parameters are mainly informative and may lead to an interruption of the FE-mesh generation process. The mesh generation is interrupted by the message: **Achieved the maximum number of nodes!** This means that the maximum allowed number of nodes (either on the boundary curves or in the two-dimensional domain) was reached during the mesh generation process. This is usually a consequence of having too many nodes along the boundaries (the number of mesh nodes inside a domain increases approximately with the square of the number of boundary nodes). It is then necessary to decide whether or not so many nodes are needed for the envisioned triangular mesh. If the answer is ‘yes’ then the maximum number of nodes must be increased in this dialog window. If the answer is ‘no’, then it is necessary to decrease the **Targeted FE Size** (Figs. 117) or to increase the **Smoothing Factor** (in the *FE-Mesh Quality* group discussed below).

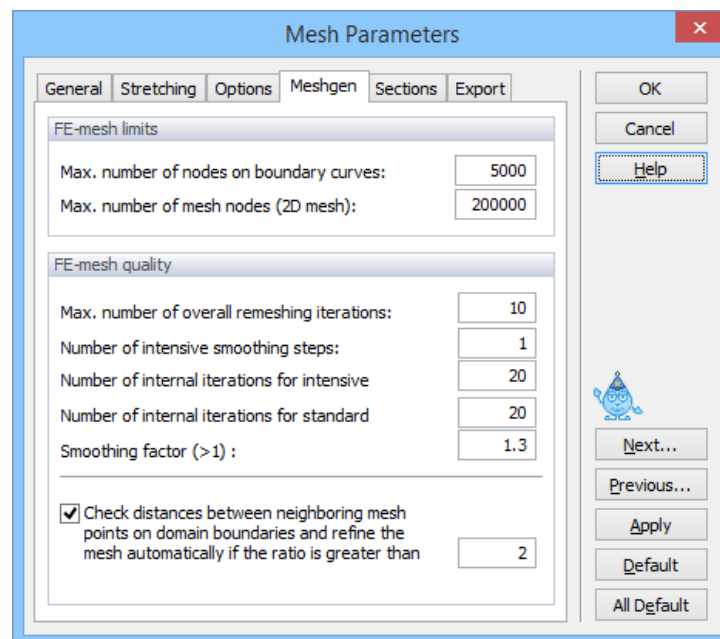


Figure 122. The FE-Mesh Parameters dialog window (Tab MG-Options).

The following parameters are specified in the **FE-Mesh Quality** group:

Maximum Number of Overall Remeshing Iterations:

This number defines the maximum number of iterations during finite element mesh remeshing. In most cases, the resulting mesh is obtained within fewer iterations than the default value of 10. In some cases, the repeated adding and removing of nodes can cause an infinite loop. In that case (or when the mesh generation process converges very slowly) the code terminates after reaching the maximum number of iterations as defined by this value.

The number of Intensive Smoothing Steps:

Intensive smoothing repeats the operations of Delaunay remeshing and smoothing until there are no more changes during the Delaunay remeshing step. This parameter specifies the number of intensive smoothing cycles at the beginning of the mesh generation process, which can significantly influence the mesh smoothness. However, too many smoothing cycles can significantly slow down the mesh generation process. The recommended value is between 1 (less smoothing) and 3 (more smoothing).

The number of Internal Iterations for Intensive Smoothing:

This number defines the maximum number of iterations during one intensive smoothing step. This number guarantees that intensive smoothing will stop after a specified number of iterations, even when the prescribed criterion is not reached (i.e., some changes would still occur during Delaunay remeshing).

The number of Internal Iterations for Standard Smoothing:

This number defines the maximum number of iterations while solving the elliptic equations, a process needed during mesh smoothing; it significantly influences the final smoothness of the mesh. A higher number of iterations improves mesh smoothness. It serves little purpose to increase the number above 20 since the mesh is then virtually constant anyway, while the whole process of mesh generation would be slowed down significantly.

Smoothing Factor:

The smoothing factor is the ratio of the maximum and minimum height of a finite element triangle. For a triangle with equal sizes, this factor is equal to 1 (which is theoretically not achievable for finite element meshes). The smoothing factor can be decreased to a value of about 1.1 when a highly smooth finite element mesh is required and, vice-versa, can be increased when a course mesh can be tolerated. The smoothing factor significantly affects the final number of elements.

In general, the default values in the FE-Mesh Parameters dialog window should be preserved; only experienced users should modify the various parameters needed for the mesh generation process.

When the option at the bottom of Figure 122 is checked, HYDRUS compares distances between the neighboring nodes on the domain boundaries. When the ratio of distances between two neighboring nodes is larger than F , the FE mesh is automatically refined.

The Options Tab

Minimum Number of Points Boundary Curves is set by default equal to 15. This number can be changed in the **FE-Mesh Parameters** dialog window of the **Options** Tab (Fig. 123). This parameter is important when such objects as openings representing wells or drains are included in the transport domain. These objects may be very small compared to the global finite element mesh (i.e., smaller than the targeted finite element size). Having a minimum number of nodes on boundary curves will then lead to local refinement of the finite element mesh around these objects, thereby ensuring that relatively small objects are accurately represented in the numerical solution.

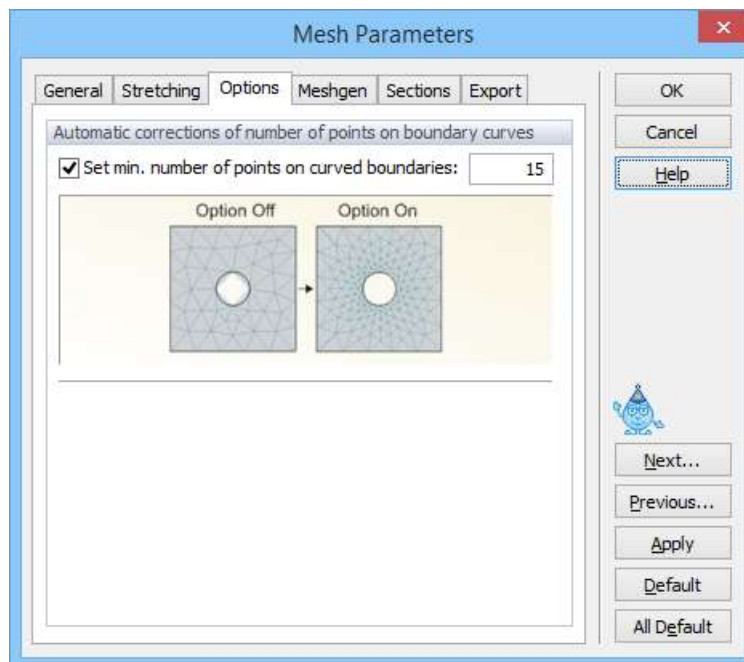


Figure 123. The FE-Mesh Parameters dialog window (Tab Options).

The Export Tab

In the **Export Tab** (not shown), users can select options for export of the FE-Mesh to a text file. One can, for example, choose, which points to export (including or excluding the intermediate points on boundary curves) and whether or not to include in the export also internal curves.

The Mesh Section Tab

The program can generate default **FE-Mesh Sections** (the **Mesh Section** Tab of the **FE-Mesh Parameters** dialog window, Fig. 124) or FE-Mesh Sections (for detailed description, see Section 5.7) can be created by a user. Default FE-Mesh Sections depend on the geometry of the transport domain. For example, the default section includes a) Entire FE Mesh, b) Vertical (horizontal) shell, and c) Each horizontal (vertical) layer. Mesh Sections can also be generated for each **Geo-Section** (see Section 8.1.8). The **Mesh Sections** are generated automatically when the FE-Mesh is generated or anytime using the menu command *Edit->Sections->Generate Sections* (note that the dialog window to **Options for Generation of Geo-Sections and FE-Mesh Sections** (Fig. 190) is similar to the **Sections** Tab of the **FE-Mesh Parameters** window (Fig. 124)).

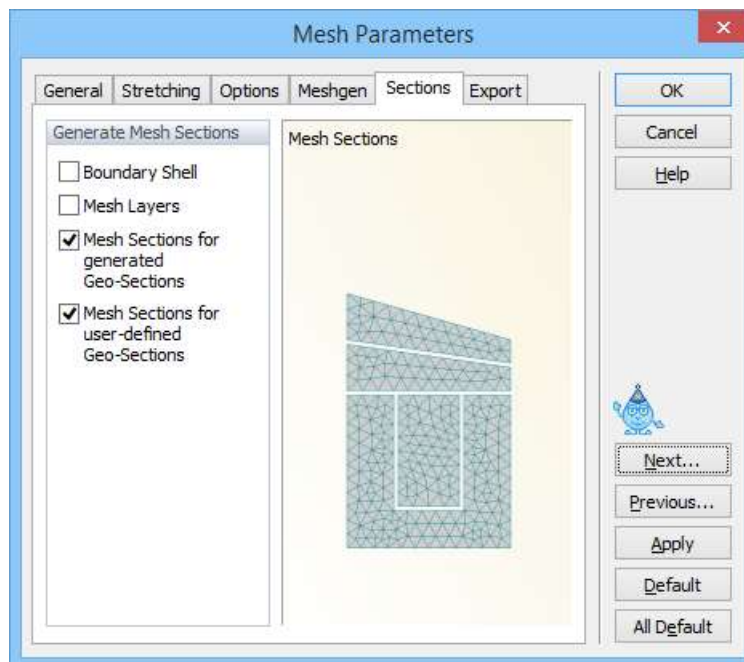


Figure 124. The FE-Mesh Parameters dialog window (Mesh Section Tab).

5.4. Finite Element Mesh Refinement.

The Finite Element Mesh Refinement is carried out in two steps:

1. One must first define the desired type of **FE Mesh Refinement** using the dialog window shown in Figure 125. Mesh refinement can be defined around **Points**, **Lines**, **Number of Points on the Line**, **Surfaces**, or **Solids**.
2. Next, users must assign the refinement to particular Points, Lines, or Surfaces, so the program knows where the refinement should take place. After double-clicking on a particular point, line, arc, circle, or spline, the corresponding dialog window will appear (the **Edit Point** dialog window, Fig. 58; or the **Edit Curve** dialog window, Fig. 60), where users should select **FE-Mesh Refinement** in the **FE-Mesh Tab**. The code will then create a list of nodes (or lines or surfaces) for a particular refinement that can be further edited by a user. **FE Mesh Refinement** is graphically displayed using red dots in green circles for nodes, green nodes for lines, and a small square in the corner of a surface. By clicking on these colored items, the **FE Refinement** can be deleted or edited. Editing of the FE mesh refinement will affect all objects to which a particular refinement was assigned.

5.4.1. Finite Element Mesh Refinement for MeshGen2D

Figure 125 below shows the **New FE-Mesh Refinement** dialog windows that are used with the **MeshGen** module for four different types of refinements. **FE-Mesh Refinements** can be applied to a **Point**, a **Line**, and a **Surface**.

When the **FE-Mesh Refinement** is assigned to a **Point** (Figure 125 top left), users only need to define the finite element size that is to be used at a given point. This FE-size will be used around a given point, while the sizes of neighboring FE will be gradually increased until the **Targeted FE Size** is reached further away in the computational domain. Notice that the dialog window also displays the **Global Targeted FE Size**. The same **FE-Mesh Refinement**, i.e., the same refined FE size, can be assigned to multiple **Points** in the transport domain.

There are two ways how the **FE-Mesh Refinement** can be assigned to a **Line** (Figure 125 top right and bottom left). Users can either specify the **FE-Size (Line – FE-Size;** Figure 125 top right) or the **Number of Points (Line – Number of Points;** Figure 125 bottom left) to be used on the entire line. Similarly, as for points, the **FE-Size** (either given directly or calculated from the number of points) will be used on the **Line**, while the sizes of FE away from the **Line** will gradually increase until the **Targeted FE Size** is reached further away in the computational domain. Again, the same **FE-Mesh Line Refinement**, i.e., the same refined FE size, can be assigned to multiple **Lines** in the computational domain. The size of FEs specified by the Number of Points (on the Line) does not affect the sizes of FEs on neighboring lines.

The **FE-Mesh Refinement** can also be assigned to a selected **Surface** (Figure 125 bottom right). In this case, users need to define FE-Size for a selected **Surface**. Note that this option is useful only when multiple **Surfaces** are used in the computational domain. The refined FE-Size is then used on the entire surface, including boundaries with other **Surfaces**, and the **Targeted FE Size** is reached only further away in the other **Surfaces** of the computational domain.

The **Point** or **Surface** with an assigned **FE-Mesh Refinement** are indicated using the following marks:  and , respectively. **FE-Mesh Refinement** is marked on curves using green points, visible in the edit mode. Contrary to other green points on the curves, they can be selected.

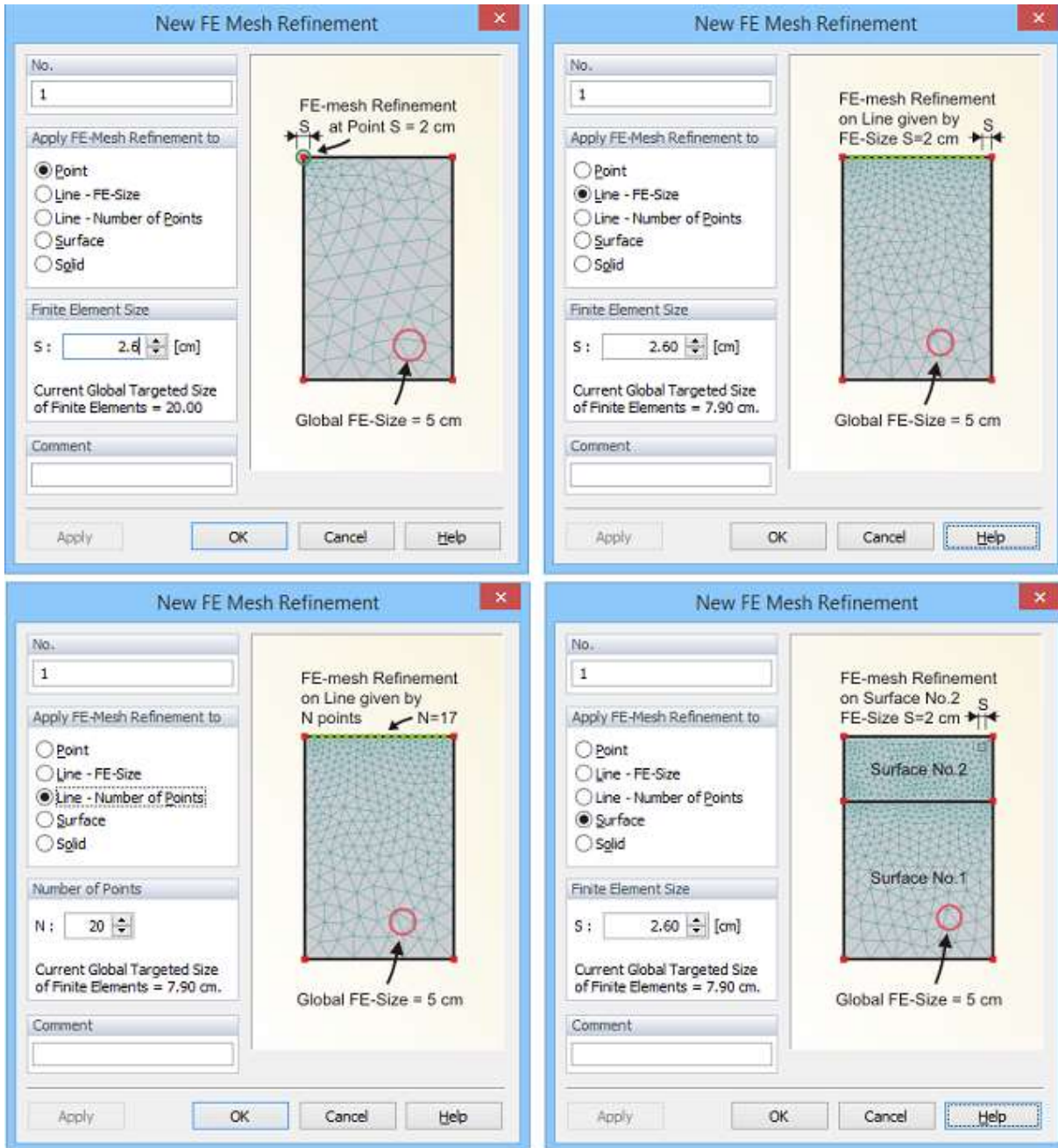


Figure 125. The FE-Mesh Refinement dialog window for the **MeshGen2D** module with four different types of refinements (applied to a Point, a Line with a given FE-size or the number of Points, and to a Surface).

As an example, Figure 126 shows the transport domain (700 * 650 cm) and the finite element mesh of a problem with a furrow and a drain. The mesh was generated with a **Targeted FE Size** of 50 cm and three **FE-Mesh Refinements** (Fig. 126, top). Refinement 1 (with a finite element size of 10 cm) was assigned to nodes 1, 2, 4, and 5, refinement 2 (5 cm) to node 3, and refinement 3 (15 cm) to nodes 8 and 9. There were 15 nodes on the drain boundary (due to the command **Minimum Number of Points on Each Closed Boundary Curve**). The resulting finite element mesh is shown in Figure 126 (bottom).

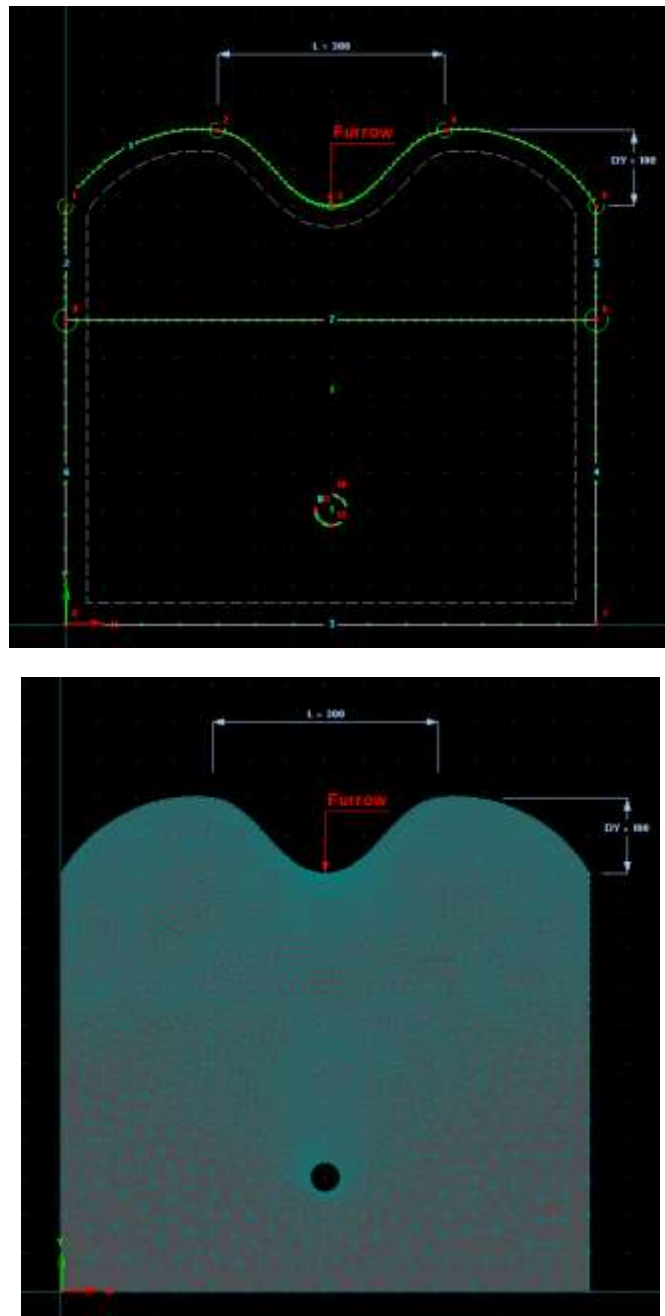


Figure 126. Example of FE-Mesh Refinements (top) and FE-Mesh (bottom).

5.4.2. Finite Element Mesh Refinement for Genex/T3D

While the **MeshGen2D** module discretizes the computational domain into unstructured FE-mesh using triangles (in 2D) and tetrahedrals (in 3D), the **Genex/T3D** module uses primarily quadrilateral (in 2D) and hexahedral (in 3D) finite elements. **Genex/T3D** uses triangles only in parts of the domain where needed, e.g., when it refines the grid. Although quadrilateral or hexahedral elements may be generated by **Genex/T3D**, the computational module subdivides these elements into triangles or tetrahedrals, respectively. While the transition between domains with refined FE-mesh and domains with global mesh size in **MeshGen2D** is relatively smooth and gradual (see Figure 126), in **Genex/T3D** the extent of this transition zone is defined exactly by users (see Figures below). Similarly, as **MeshGen2D**, the same **FE-Mesh Line Refinements** can be assigned to multiple **Points**, **Lines**, **Surfaces**, and **Solids** in the computational domain.

There are two ways how the **FE-Mesh Refinement** can be assigned to a **Point** (Figure 127). Users can use either **Circular** or **Rectangular** refinement. For a **Circular Refinement** around a point, a radial refinement area is defined around a node in all directions. Users need to specify the **Radius** of the refinement area, the **Inner Targeted FE-Size** (i.e., an FE-size immediately around a point), and the **Outer Targeted FE-Size** (i.e., an FE-size at the outer end of the radial refinement area) (Fig. 130). The **Outer Targeted FE-Size** should be equal or slightly smaller than the **Global Targeted FE-Size**. When generating the FE mesh, the mesh refinement is carried out gradually towards the center because the FE length at the periphery of the refinement area is usually identical to the global mesh width. For larger differences between the inner and outer FE length, it is recommended to set the radius not too small to avoid acute-angled triangular finite elements in the refinement area. For a **Rectangular Refinement**, a rectangular refinement area is defined around a node in all directions. Users need to specify the **Side Length** of the refinement area and the **Inner Targeted FE-Size** (i.e., an FE-size immediately around a point) (Fig. 130).

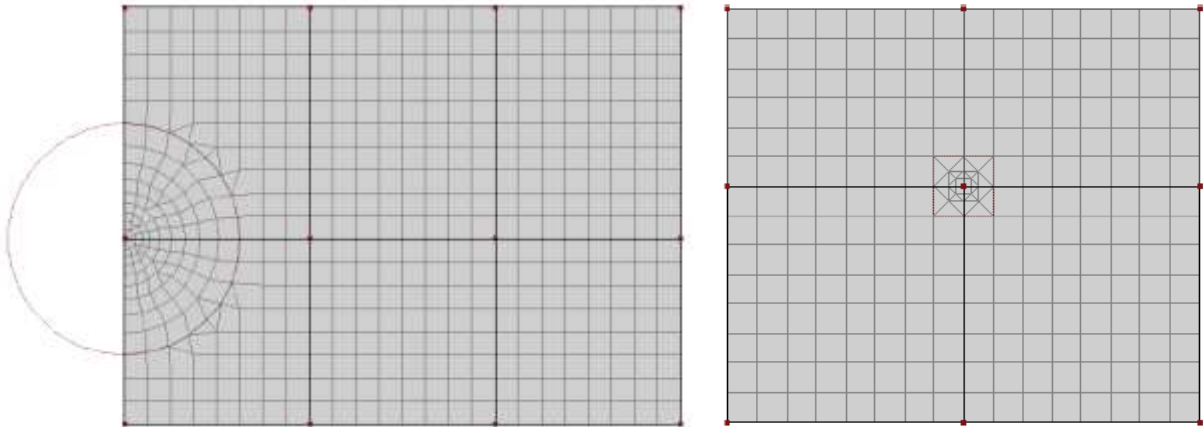


Figure 127. Circular (left) and rectangular (right) refinements around a node.

FE-Mesh Refinements assigned to a **Line** are handled in **Genex/T3D** similarly as in **MeshGen2D**. One can again define either the size (spacing; **Line through FE-Length**) or the number (a specific number of equidistant sub-divisions; **Line through Division**) of finite

elements along a line. In the former case, one needs to define the **Target FE Length**, in the latter case, the **Number of Division FE Nodes**. However, while in **MeshGen2D** there was a gradual increase in sizes of finite elements away from the **Line**, in **Genex/T3D** the refinement affects only one row of finite elements (Figure 128).

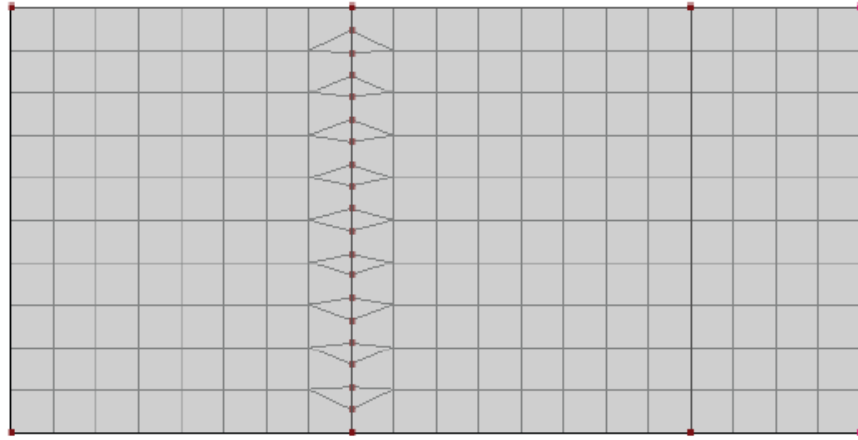


Figure 128. Refinement on a line (by defining either the size or the number of finite elements along a line).

It is also possible to define **Fe-Mesh Refinements** for **Surfaces** or **Solids** (Figure 129). In both cases, users need to specify the **Targeted FE-Size**, which will be set as the target size of the finite elements for the entire surface or solid.

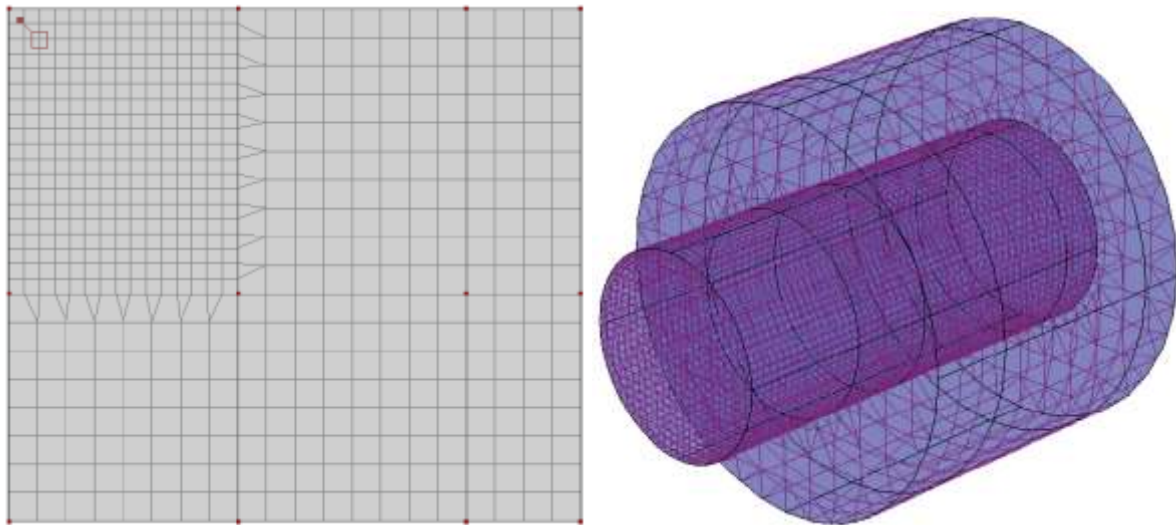


Figure 129. Refinements on a surface (left) or solid (right).

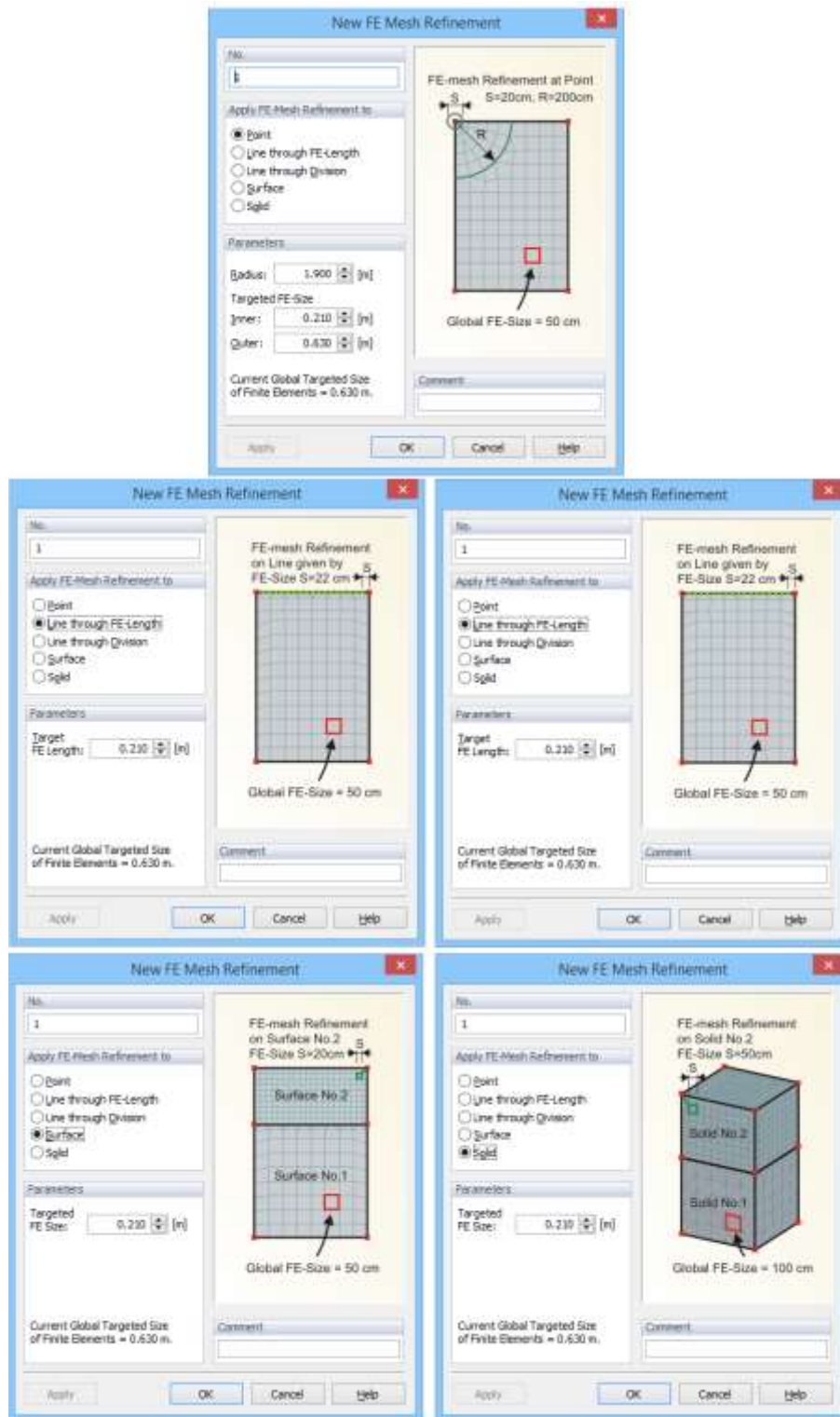


Figure 130. The **FE-Mesh Refinement** dialog window for the **Genex/T3D** module with six different types of refinements (applied to a **Point**, a **Line** with a given FE-size or a number of points, to a **Surface**, and to a **Solid**).

5.5. Unstructured Finite Element Mesh Generator MeshGen2D

The **MeshGen2D** module may be used to discretize a two-dimensional flow region (or a base plane of the three-dimensional domain) into an unstructured triangular mesh. The algorithm used for this purpose is general and can be applied to virtually any two-dimensional computational domain. The first step of the mesh generation process discretizes the boundary curves, while the second step generates the unstructured triangular mesh.

Generation of Boundary Points

The first step of the mesh generation process involves discretization of the boundary curves. During this step, boundary nodes are generated on all boundaries and internal curves by dividing them in abscissas (i.e., short boundary edges). If no previous boundary nodes existed, the program automatically generates a default equidistant point distribution. Boundary nodes can be edited by users to optimize the lengths of the boundary edges using the **FE-Mesh Parameters** dialog window (Figs. 117 through 123). The local density of the mesh can thereby be determined in any part of the domain (also taking into account the use of internal curves). There are two ways to obtain appropriate distributions of the boundary nodes, i.e., by (1) specifying the *Targeted FE size* (Figs. 117, the Main Tab), and (2) refining the FE-Mesh (the **FE Mesh refinement** dialog window, Fig. 125).

- 1) A global **Targeted FE Size** (Fig. 117) is the main variable of the FE-Mesh process. Although a default Targeted FE-Size is specified by the program, this value should be adjusted by users in most applications. The default value is used to generate at least a reasonable initial mesh, even for inexperienced users.
- 2) The finite element mesh can be adjusted locally in the domain by using **FE-Mesh Stretching** (Fig. 118 and 131) or **FE-Mesh Refinement** (Figs. 58, 35, and 125). **FE-Mesh Refinement** can be implemented for various geometric objects, including **Points**, **Lines**, or **Surfaces** (Fig. 125). When several **FE-Mesh Refinements** overlap in one location (such as when the **FE-Mesh Refinement** is defined for both a point and a line), then the FE-Mesh Refinement specified for the lower-level objects (i.e., a point rather than a line) is used.

The boundary nodal distribution determines in a very substantial manner the ultimate quality and size of the unstructured finite element mesh. Optimally distributing nodes along the boundaries of relatively complicated domains (e.g., a very irregular anisotropic domain) can be a very difficult problem and may require some experience.

Table 18. Definition of terms related to the boundary discretization.

Boundary Nodes	Boundary nodes are points marked by green squares, which discretize boundary curves. These nodes are generated along every boundary curve and are ordered in a counter-clockwise direction (on closed curves). Boundary nodes determine the local densities of the triangular mesh generated for a given boundary nodal distribution and are part of the triangular mesh.
----------------	---

Boundary Edges	Boundary edges are abscissas discretizing boundary curves. They connect generated boundary nodes, are oriented in a counter-clockwise direction, and are located on the edge of the mesh.
Fixed Points	Fixed points are points on boundary curves marked by red squares. These points may be used to adjust the local density of boundary nodes (using FE Mesh refinement). By default, fixed points are placed on all nodes of polylines and on all object boundary points describing the boundary, but they can also be inserted or deleted at any other point on boundary curves.

Generation of the Unstructured Triangular Mesh

The unstructured triangular mesh is generated by means of five operations:

- (1) discretization of the flow domain into triangles with vertices at given boundary nodes (**Fundamental Triangulation**),
- (2) inserting new points in all triangles which do not fulfill a certain smoothness criterion (**Mesh Refinement**),
- (3) implementation of Delaunay's retriangulation for the purpose of eliminating all nodes surrounded by more than six triangles, as well as to avoid extreme angles (**Remeshing**),
- (4) smoothing of the mesh by solving a set of coupled elliptic equations in a recursive manner (**Smoothing**), and
- (5) correction of possible errors that may appear during the smoothing of the finite element mesh (**Convexity Check**).

Operations 2 through 5 are repeated until a prescribed smoothness of the mesh has been achieved.

An unstructured triangular mesh for a given boundary nodal distribution can be generated in two different ways: a step-by-step approach (*Calculation->Advanced FE-Mesh Generation->Fundamental Triangulation* and subsequent commands, or by clicking on the **Fundamental Triangulation** command of the **FE-Mesh Advanced** part of the **FE-Mesh** version of the **Tool Sidebar**), or by using automatic mesh generation (*Calculation->Generate FE-Mesh* or the **Generate FE-Mesh** command on the **Edit FE-Mesh** part of the **FE-Mesh** version of the **Tool Sidebar**). The step-by-step approach should be used only for special cases and then only by experienced users. Automatic generation (recommended) is a much faster and easier approach. The mesh generation parameters must be specified before the mesh generation process is started. By modifying the mesh generation parameters, users can influence the smoothness of the mesh (**Smoothing Factor**, Fig. 122), its anisotropy (Figs. 118 and 131), computational time, and the possible display of intermediate results, among other features. The most important mesh generation parameter is the "smoothing factor", which can significantly affect the final number of elements. The smoothing factor is defined as the ratio of the minimum and maximum dimensions of a triangle. When a very smooth finite element mesh is required, the smoothing factor should be decreased to about 1.1; when a coarser mesh is possible, the smoothing factor can be increased.

The code saves mesh data, by default, in a binary format (the file MESHTRIA.000). However, users have the option to also save mesh data into a file (MESHTRIA.TXT) in ASCII format (the Program Options dialog window, Fig. 200), and then use possibly the data later for other calculations.

When users do not have the authorization to use the MeshGen2D module, they can employ the internal mesh generator for relatively simple rectangular or hexahedral transport domains.

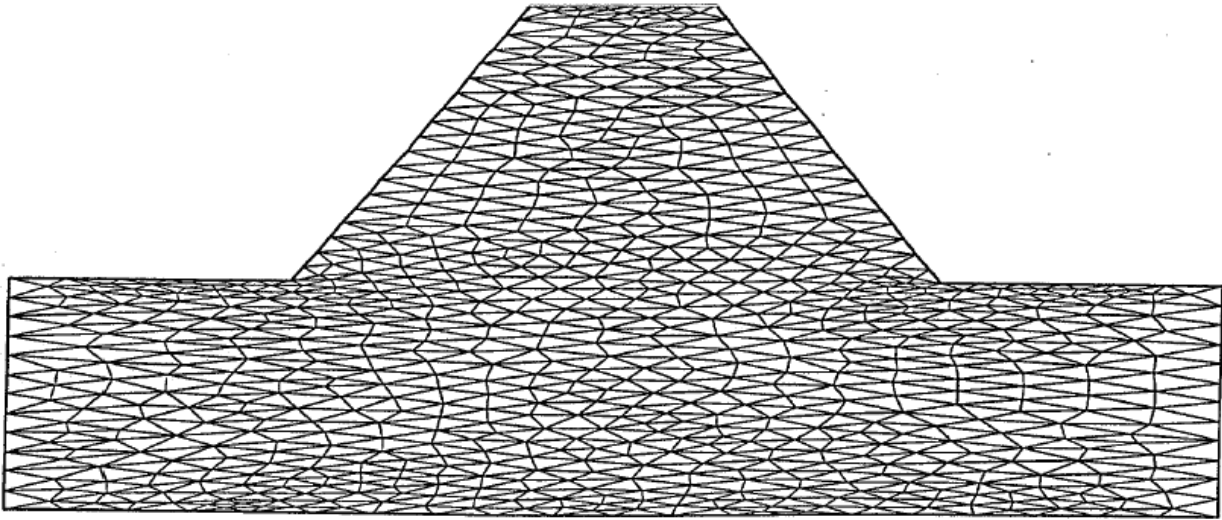


Figure 131. Example of mesh stretching using a stretching factor of 3 in the x -direction.

5.6. Finite Element Mesh Statistics

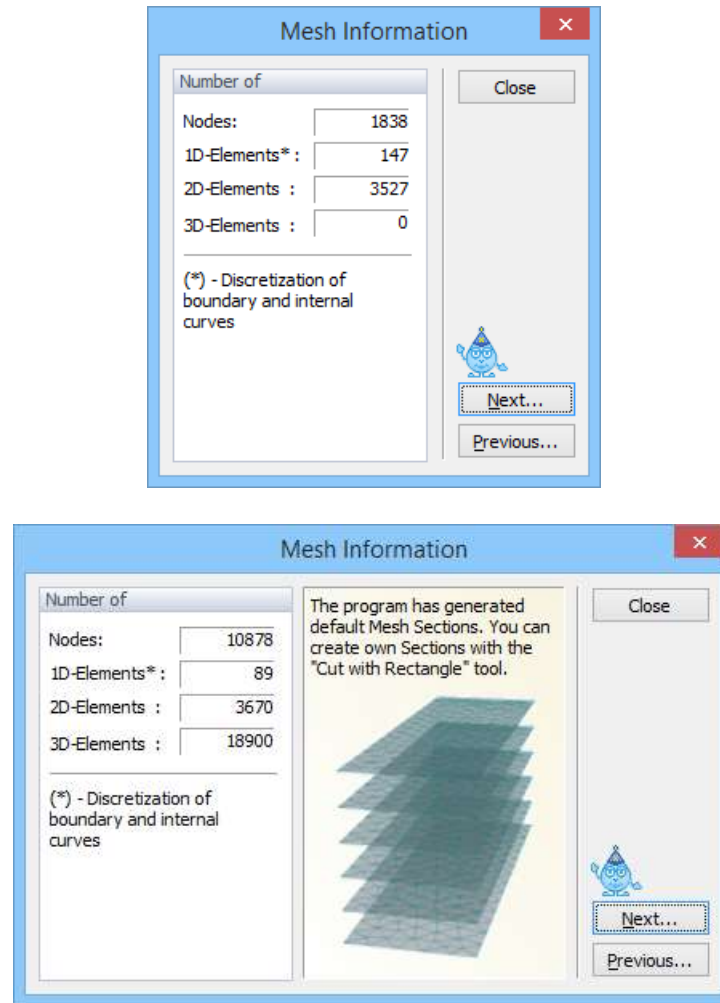


Figure 132. The FE-Mesh Information dialog window for a two-dimensional problem (top) and a three-dimensional problem (bottom).

Figure 132 shows dialog windows that provide information about the finite element mesh for two- and three-dimensional applications. For two-dimensional grids, the window shows the number of finite element *Nodes*, the number of boundary *1D-Elements* (boundary edges between boundary nodes), and the number of *2D-Elements* (triangles). For three-dimensional grids, the window shows again the number of finite element *Nodes* (in the entire 3D domain), the number of boundary *1D-Elements* (boundary edges between boundary nodes on the bottom plane, i.e., the 2D base surface of the transport domain), the number of *2D-Elements* (the number of triangles on the bottom plane of the domain), and the number of *3D-Elements* (tetrahedrons) in the entire transport domain.

5.7. Finite Element Mesh Sections

FE-Mesh Sections allow users to split the computational (transport) area into arbitrarily complicated shapes that are defined by external 3D points. These **FE-Mesh Sections** can then be used, for example, to define the material distribution or other properties. **FE-Mesh Sections** are parts of the FE-Mesh used to specify input variables and to display results of calculations. By default, two-dimensional problems have only one section consisting of the entire transport domain. For three-dimensional problems, one section by default is formed by the *Whole FE-Mesh* (Section D0_000 in Fig. 133), whereas each horizontal (vertical for some applications) layer forms one additional section (Sections ML_001 through ML_010 – *Mesh Layer* in Fig. 133), while the last section is made up by the vertical surface (Section ML_000 *Shell* Fig. 133). For example, the bottom Mesh Layer can be displayed when the bottom boundary conditions are specified, while the top Mesh Layer (Section) can be displayed when the surface boundary conditions are provided. One can similarly display results at different depths using different horizontal sections (Mesh Layers). The **Mesh Sections** are generated automatically when the FE-Mesh is generated or anytime using the menu command *Edit->Sections->Generate FE-Mesh Sections*. Automatically generated FE-Mesh Sections in different HYDRUS versions are listed in Table 19. Mesh Sections can also be generated for each Geo-Section (see Section 8.1.8).

Additional sections can be created using commands from the **FE-Mesh Sections** part of the **FE-Mesh** version of the **Edit Bar**. One can display any existing section (or set of sections) and modify them using the *Cut with Rectangle* command, and then create a new section using the *New Section from View* command. This new section will then appear in the list of sections in the **Section** Tab of the **Navigator Bar** and can be recalled at any time. Existing sections can be manipulated (*Display, Hide, Select, Unselect, Rename, Delete, Move Up, and Move Down*) using the *Edit Section* command from the **Edit Bar**, or using *Edit->Sections->Edit Sections*.

Table 19. Finite element mesh sections generated in different HYDRUS versions.

HYDRUS Version	Generated FE-Mesh Sections
2D-Lite	Nothing
2D-Standard	For each Surface (of more than one) and each Geo-Section (see Section 8.1.8) defined by user.
3D-Lite	For each layer of the FE-Mesh
3D-Standard	For each FE layer, each geometric layer, and for each Column
3D-Professional	For each Geo-Section as defined in Section 8.1.8.

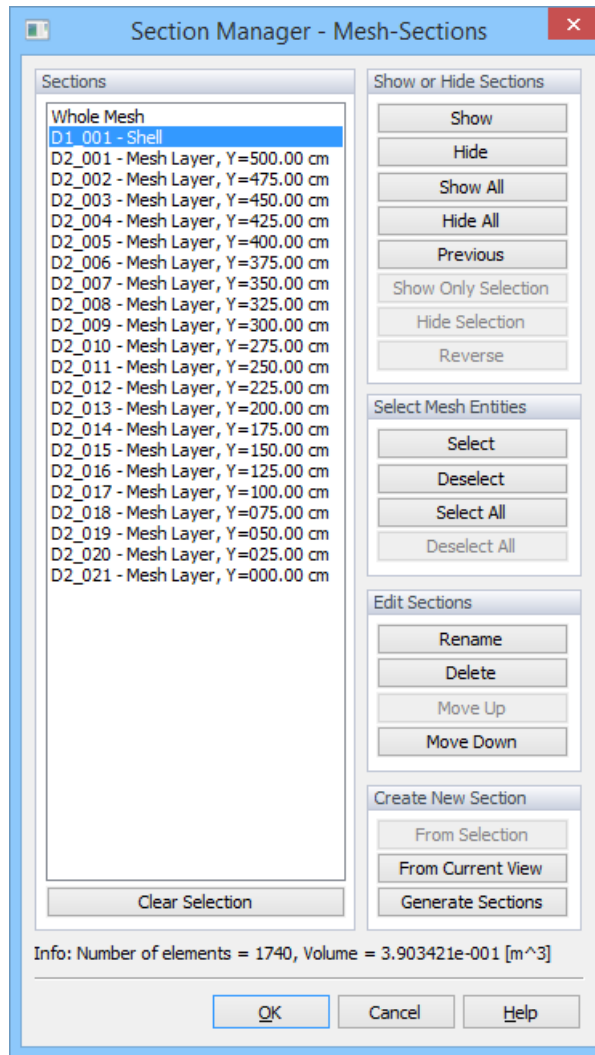


Figure 133. The FE-Mesh Sections dialog window.

The function "**Import FE-Mesh Section**" allows importing **FE-Mesh Sections** by reading their definition from a text file. The text file has the following format: The first three columns are the coordinates of the point, and the fourth is an index of the FE-Mesh Section (this Section will be created after the text file is read), into which the point belongs. An example of the text file (http://www.pc-progress.com/Images/Pgm_Hydrus3D/Test3_Sections.txt) can be downloaded from Tutorial 2.12 (<http://www.pc-progress.com/en/Default.aspx?h3d-tutorials>), which demonstrates the use of **FE-Mesh Sections**.

```
OBJECT=INDEXES_AT_POINTS
-1.200000e+000 -1.200000e+000 -7.450580e-009 2
-1.000000e+000 -1.200000e+000 -7.450580e-009 3
-8.500000e-001 -1.200000e+000 -7.450580e-009 3
-7.500000e-001 -1.200000e+000 -7.450580e-009 3
-6.700000e-001 -1.200000e+000 -7.450580e-009 3
-6.000000e-001 -1.200000e+000 -7.450580e-009 3
```

6. Domain Properties, Initial and Boundary Conditions

Initial and boundary conditions for both water flow and solute (heat) transport, and the spatial distribution of other parameters characterizing the flow domain (e.g., the spatial distribution of soil materials, hydraulic scaling factors, root-water uptake parameters, and possible hydraulic anisotropy) and/or observation nodes are specified in a graphical environment with the help of a mouse. The program automatically controls the logical correspondence between the water flow and solute transport boundary conditions.

Various spatially variable properties (e.g., material distribution, initial and boundary conditions) can be specified in Version 2.0 (or higher) of HYDRUS (Standard and Professional, not Lite) either

- a) directly on the finite element mesh (as done in Version 1.0), or
- b) on geometric objects (e.g., boundary curves, rectangles, circles, surfaces, volumes).

The main advantage of the latter approach is that when the FEM is changed, these properties are not automatically lost, but can be recalculated to the new FEM from their definition on Geometric Objects. Which option is used depends on the menu command *Edit->Properties and Conditions on FE-Mesh*. A similar button switch is also available at the end of the toolbar (), next to the Results button, and at the Edit Bar. The latter approach (i.e., on Geometric Objects) is described in detail below in Section 6.5.

6.1. Default Domain Properties

For rectangular two-dimensional domains and for layered three-dimensional domains, immediately after the finite element mesh is generated, one can specify the initial **Default Domain Properties** in the dialog window shown in Figure 134. Values listed in this window are initially assigned to each horizontal layer of the transport domain, but can later be modified graphically. The following variables are involved:

Code	Code of the boundary condition (0 for no flow, -1 for constant flux, +1 for constant head, -2 for unsaturated seepage face, +2 for saturated seepage face, -3 (-7, -8, -9) for variable flux, +3 (+7, +8, +9) for variable head, -4 for atmospheric, - 5 for tile drain, - 6 for free drainage)
h	Initial value of the pressure head [L]. The initial pressure head changes linearly between the first and last layer if one clicks on the command at the bottom of the dialog (<i>Linear interpolation of the pressure heads between the first and last layer</i>).
Q	Recharge flux, $[L^2T^{-1}]$ and $[L^3T^{-1}]$ for 2D and 3D applications, respectively. Since this variable is usually specified in individual nodes, it is uncommon to specify it here.
Mater	Material number
Roots	Root distribution
Axz	Scaling factor for the pressure head
Bxz	Scaling factor for the hydraulic conductivity
Dxz	Scaling factor for the water content
Temp	Initial temperature [K]
Conc	Initial concentration (of the equilibrium phase) $[ML^{-3}]$

Sorb Initial concentration of the nonequilibrium phase (kinetically sorbed [MM⁻¹] or of the immobile region [ML⁻³])

Values from each line are assigned to the entire layer within the FE-Mesh with the exception of Code (the boundary condition code), which is assigned only to boundary nodes. When multiple values are encountered within the single layer when initiating the table, the cell is left empty instead of displaying any particular value. Unless changed, this variable will not be assigned in a particular layer (after closing the dialog with OK), and original values will remain unchanged. The three commands (*Copy Sel.*, *Copy All*, and *Paste*, **MS Excel Import/Export**) facilitate the transfer of data from this HYDRUS dialog window to the Excel (or other) spreadsheet. The command “**Set Boundary Conditions for Solute Transport and Heat Transport for changed Codes:**” leads to assigning Cauchy boundary conditions for solute and heat transport to nodes where the Code was changed.

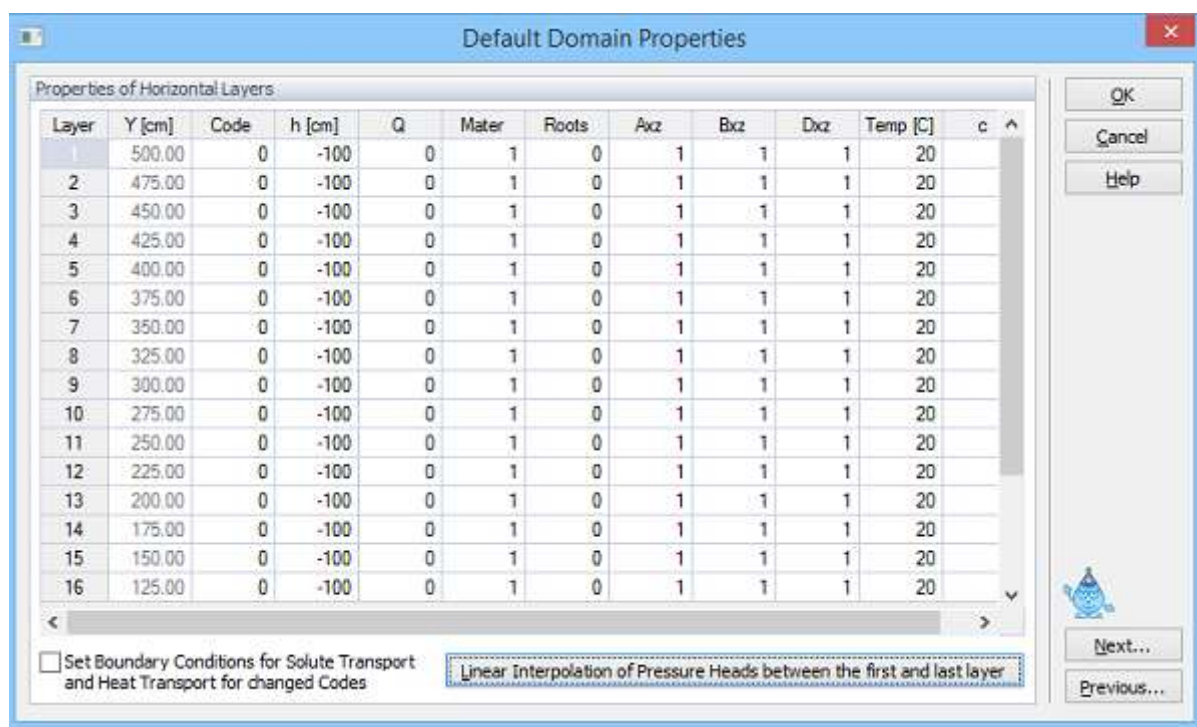


Figure 134. The Default Domain Properties dialog window.

6.2. Initial Conditions

After selecting nodes (using either the mouse in the View Window, selecting geometrical objects on the Data Tab of the Navigator Bar, selecting Sections on the Section Tab of the Navigator Bar, or selecting objects by the mouse in the View Window and using the Ctrl keyboard button) for which the initial condition is to be specified, and clicking on the command **Set Values** at the **Edit Bar** (on the right side of the view window), the **Water Flow Initial Condition** dialog window (Fig. 135) appears. Using this command, one can specify the initial conditions for water flow by defining the initial spatial distribution of the pressure head or water content over the flow domain. The decision of whether to use the pressure head or the water content initial

distribution is made in the main module of the [Iteration Criteria](#) dialog window (Fig. 18). One can specify:

- the same value to all selected nodes (*Same value for all nodes*),
- a distribution versus depth that is in hydrostatic equilibrium with the pressure head of the lowest point in the selected region (*Hydrostatic Equilibrium from the lowest located nodal point*),
- a distribution versus depth that is in hydrostatic equilibrium with the pressure head at the soil surface (*Hydrostatic Equilibrium from the domain top surface*),
- a *Linear distribution with depth*, and
- equal to the field capacity (see below).

When options a), b) or c) are selected, only one value of the pressure head needs to be specified. For option d), one needs to provide values of the pressure head (or water content) for the top and bottom of the selected domain. Option c) is currently available only for 2D-Simple, 3D-Simple, and 3D-Layered Geometries, and the vertical lines connecting different layers of FE nodes have to be vertical.

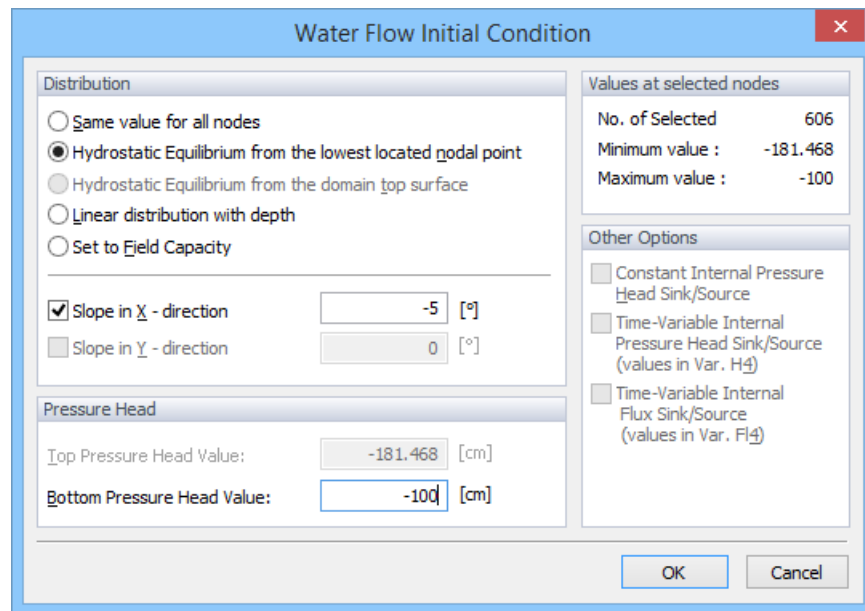


Figure 135. The Water Flow Initial Condition dialog window.

To simplify definition of the initial condition for problems that involve slopes, an option is provided to have pressure heads decrease in the x- and y- (the latter only for three-dimensional problems) directions (*Slope in X- direction* and *Slope in Y- direction*).

The right top part of the dialog window (*Values in selected nodes*) in Figure 135 provides information about the selected nodes, i.e., the number of selected nodes and the minimum and maximum values of the pressure head or water content.

If a certain node is selected that is not located on the boundary, this node can be declared an *Internal Pressure Head Sink/Source*. The pressure head at that node can then be kept constant or be time-variable during the simulation.

When the option "Set to Field Capacity" is selected, the initial pressure heads or water contents (depending on the selection made in the Iteration Criteria window, Fig. 18) is assigned to selected nodes as follows [Twarakavi *et al.*, 2009]:

$$S_{fc} = \frac{\theta_{fc} - \theta_r}{\theta_s - \theta_r} = n^{-0.60(2 + \log_{10}(K_s))}$$

where θ_{fc} and S_{fc} are the water content and saturation at field capacity, and θ , θ_s , n , and K_s are the soil hydraulic parameters for the *van Genuchten* [1980] model. Note that the water content at field capacity corresponds to the hydraulic conductivity of about 0.01 cm/d [Twarakavi *et al.*, 2009]. The initial pressure head at field capacity is calculated from the water content at field capacity using the *van Genuchten* [1980] retention curve model.

Similar but simpler dialog windows are used to specify initial values of the temperature and the liquid and adsorbed concentrations (e.g., **Temperature Distribution** dialog window, Fig. 136). The dialog window will then again provide information about the selected nodes (*Values in selected nodes*), i.e., the number of selected nodes and their minimum and maximum temperatures (concentrations). One can specify either constant value for all selected nodes or have the values change linearly with depth. When the box *Use top value for the entire selected region* is checked, the value in the *Top* box is assigned to all selected nodes.

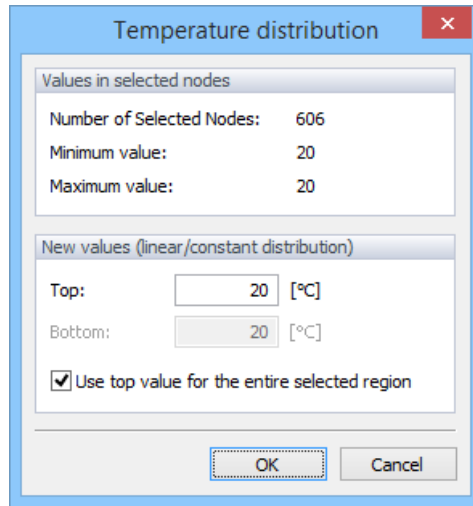


Figure 136. The Temperature distribution dialog window.

The initial conditions for the UNSATCHEM module are defined in terms of the Solution Composition numbers (integer), Exchange Species numbers, Solid Species numbers, and CO2 Concentrations (real). The composition numbers refer to different Solution Compositions, Exchange Species, and Solid Species defined in Figure 35.

6.3. Boundary Conditions

The specification of the boundary conditions is relatively straightforward. Users must first select from the **Navigator Bar** particular **Boundary Conditions** (i.e., water flow, solute transport, or heat transport) and then click on the **Edit Bar** on the particular boundary condition (e.g., constant head). They subsequently need to move the mouse to the selected position and click the left mouse button. Implementation of the boundary condition terminates with a repeated click of the left mouse button. The boundary nodes will acquire the same color as the corresponding type of the boundary condition. See the rules for specifying boundary conditions, as described in Chapter 8 of the Technical Manual [Šimůnek *et al.*, 2010]. Alternatively, users can first select boundary nodes and then assign desired boundary conditions by clicking at a particular boundary condition at the **Edit Bar**. Note that the Free Drainage and Deep Drainage boundary conditions cannot be specified simultaneously in one project. Similarly, when the Gradient Boundary Conditions is specified (see description below), the Time-Variable Flux 4 Boundary Condition is disabled.

In addition to system-dependent boundary conditions available in version 2.x (and higher) of HYDRUS-2D, several new options are available in HYDRUS. These new options are specified in the **Boundary Condition Options** dialog window (Fig. 137) that is called using the menu command *Edit->Boundary Conditions->Boundary Conditions Options* or from the **Edit Bar** for **Water Flow Boundary Conditions version** using the **BDRC Options** command. This dialog window has three tabs: a) **Time-Variable Head/Flux 1 BCs**, b) **Special Boundary Conditions**, and c) **Triggered Irrigation**.

6.3.1. Time-Variable Head/Flux 1 BCs

The options that are available on the first tab (**Time-Variable Head/Flux 1 BCs**, Fig. 137) apply to the first Time-Variable Head/Flux boundary condition. The following new options are available here:

- a) *Interpolate Time-Variable Pressure Head and Flux (1) boundary conditions in time:* While in version 2.0 of HYDRUS-2D, all boundary conditions (i.e., fluxes or pressure heads) changed in abrupt steps, the new version allows boundary pressure heads to change smoothly with time. Abrupt changes in the pressure heads lead to sudden changes in fluxes, while smoothly changing pressure heads provide smoothly changing fluxes. An example of such a boundary condition is the water level in a stream or furrow.
- b) *Switch the boundary condition from Time-Variable Pressure Head to "No Flux BC when Var-H.1.>99999":* While version 2.0 of HYDRUS-2D only allowed either time-variable pressure heads or time-variable fluxes on a particular part of the boundary, the new version allows boundary conditions to change from variable pressure heads to a zero flux and vice-versa. This boundary condition can be used, for example, for a disc permeameter where the specified head changes to a zero flux during time periods when the permeameter is re-supplied with water. The zero flux is initiated by specifying a value larger than 999999.

- c) *Switch the boundary condition from Time-Variable Pressure Head to "No Flux BC when the specified nodal pressure head is negative"*: When a time-variable pressure head boundary condition is specified along a boundary, then the specified value is assigned to the lowest nodal point of a particular boundary, while pressure heads at other nodes are adjusted based on the z-coordinate. When this option is selected, then nodes with calculated negative pressure heads are not associated with a Dirichlet boundary condition, but rather with a zero flux. A fluctuating water level in a stream or furrow is an example of this type of boundary condition. While positive pressure head values are below the water table, negative values occur above the water table.
- d) *Switch the boundary condition from Time-Variable Pressure Head to "Atmospheric BC when the specified nodal pressure head is negative"*: This is similar to c) except that an atmospheric boundary condition is assigned to nodes with negative calculated pressure heads.
- e) *Switch the boundary condition from Time-Variable Pressure Head to "Seepage Face BC when the specified nodal pressure head is negative"*: This is similar to c) except that a seepage face boundary condition is assigned to nodes with negative calculated pressure heads. Note that a Seepage Face boundary condition needs to be assigned to all boundary nodes, for which this option is to be used.
- f) *Treat the Time-Variable Flux boundary condition as the Atmospheric BC*: When this type of system-dependent boundary condition is selected, then HYDRUS treats the time-variable flux boundary conditions similarly to atmospheric fluxes. This means that pressure heads have two limiting values, with the maximum pressure head equal to h_{CritS} and the minimum pressure head equal to h_{CritA} . This is also true for Time-Variable Flux 2, 3, and 4 BCs.
- g) *Apply Atmospheric boundary condition to nonactive Seepage Face*: While in version 2.x of the code, the flux across the nonactive part of the seepage face was always equal to zero, the new version can apply atmospheric boundary conditions on a nonactive seepage face.
- h) *Consider snow accumulation at the soil surface when temperatures are negative*: When heat transport is simulated simultaneously with water flow and atmospheric boundary conditions, then snow accumulation on top of the soil surface can be simulated. The code then assumes that when the air temperature is below -2 C all precipitation is in the form of snow. When the air temperature is above +2 C all precipitation is in the form of liquid, while a linear transition is used between the two limiting temperatures (-2,2). The code further assumes that when the air temperature is above zero, the existing snow layer (if it exists) melts proportionally to the air temperature.

Boundary condition options a) through e) and g) can be used only with the first time-variable head condition.

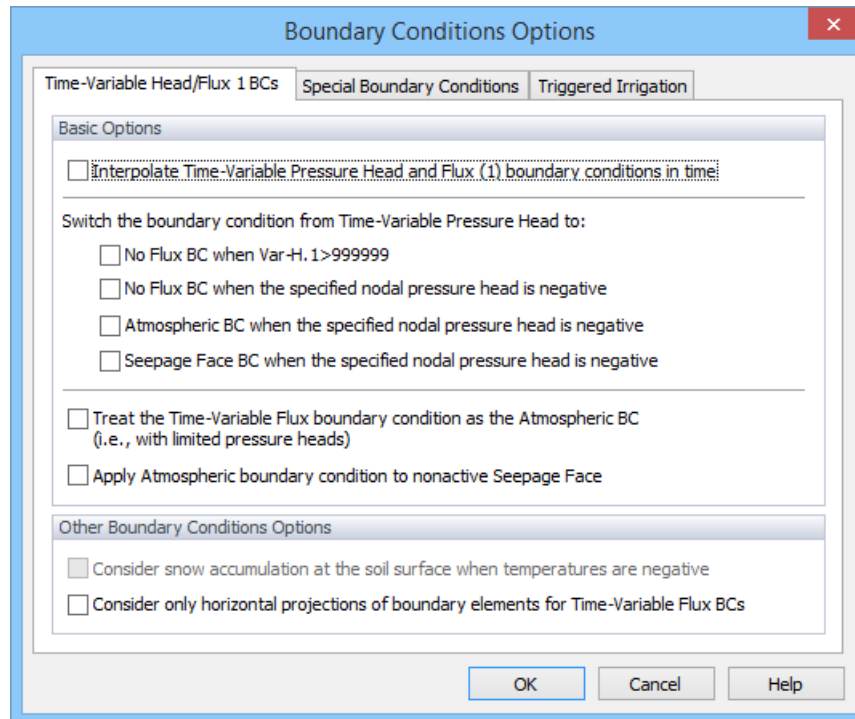


Figure 137. The Time-Variable Head/Flux 1 BCs tab of the Boundary Condition Options dialog window.

6.3.2. Special Boundary Conditions

The following **Special Boundary Conditions** (Fig. 138) can be selected from the second tab of the **Boundary Condition Options** dialog window:

1. Gradient Boundary Conditions
2. Subsurface Drip Characteristic Function
3. Surface Drip Irrigation with a Dynamic Evaluation of the Wetted Area
4. Seepage Face with a Specified Pressure Head

Gradient Type Boundary Condition

Version 1 of HYDRUS implements the **Gradient Type Boundary Condition** only as the **Free Drainage** boundary condition, or the unit gradient boundary condition. However, in many situations, one needs a non-unit gradient BC. For example, it is difficult to select appropriate boundary conditions for vertical boundaries for flow in a hill slope where the side-gradient is more or less parallel with the direction of the slope. In version 2 of HYDRUS, users can specify a gradient other than one (unit gradient). This option, i.e., non-unit gradient boundary condition, needs to be selected from the **Special Boundary Conditions** tab of the **Boundary Condition Options** dialog window. Gradients are positive for flow against a particular axis, i.e., from right to left (in the x -direction) and from back to front (in the y -direction), and should be used only (or mainly) on sides of the transport domain. In 3D, the gradient BC can be specified only in one direction (i.e., either in x - or y -direction).

Subsurface Drip Characteristic Function

The infiltration rate of water from a subsurface cavity (dripper) is affected by many factors, including the pressure in the cavity, its size and geometry, and the hydraulic properties of the surrounding soil [Lazarovitch *et al.*, 2005]. When a predetermined discharge of a subsurface source (e.g., a subsurface emitter) is larger than the soil infiltration capacity, the pressure head in the source outlet increases and becomes positive. The built-up pressure may significantly reduce the source discharge rate. A special system-dependent boundary condition for flow from subsurface sources that uses the drip characteristic function was implemented in HYDRUS (see the Technical Manual). This function has two variables, i.e., the nominal discharge (**Optimal Flux** in Fig. 138) of the source for the reference inlet pressure h_{in} (usually being 10 m) and the back pressure equal to zero, and an empirical constant (**Exponent** in Fig. 138) that reflects the flow characteristics of the emitter. Normally, $c = 0.5$ corresponds to a turbulent flow emitter and $c = 1$ to a laminar one. This option is currently available only for two-dimensional and axisymmetrical geometries.

Implementation: The user needs to specify the “**Time-Variable Flux 1**” boundary condition along the dripper boundary and h_{in} in the “**Var.H-1**” column of the “**Time Variable Boundary Conditions**” dialog window. A positive pressure indicates an irrigation period, and a negative pressure indicates a non-irrigation period.

Surface Drip Irrigation – Dynamic Evaluation of the Wetted Area

The radius of the wetted area for drip irrigation for transient conditions can be calculated in Hydrus as follows. The irrigation flux Q is applied to the single boundary node that represents the dripper with the Neumann (flux) boundary condition. If the pressure head required to accommodate the specified flux Q is larger than zero, the boundary condition in this particular node is changed into the Dirichlet (head) boundary condition with zero pressure head value, and the actual infiltration flux Q_a through this node is calculated. The excess flux ($Q - Q_a$) is then applied to the neighboring node, again with the specified Neumann boundary condition. This procedure is iteratively repeated until the entire irrigation flux Q is accounted for and the radius of the wetted area is obtained. Since the infiltration flux into the dry soil is larger for early times, the wetted area continuously increases as irrigation proceeds. This option is currently available only for two-dimensional and axisymmetrical geometries.

Implementation: The user needs to specify the “**Time-Variable Flux 1**” boundary condition at the surface boundary. The length of this boundary needs to be sufficient to accommodate the entire wetting zone. The drip discharge flux, Q , needs to be entered in the “**Var.FI-1**” column of the “**Time Variable Boundary Conditions**” dialog window. The user also needs to specify from which node of the **Time-Variable Flux 1** boundary irrigation starts. Irrigation can start in the left node of the boundary, and then the wetting zone will be spreading to the right (**From left to right**); it can also start in the right node of the boundary, and then the wetting zone will be spreading to the left (**From right to left**), or it can start in the arbitrary middle node of the boundary (**Center Node**) and spread in both direction (**From the center**).

Seepage Face with a Specified Pressure Head

This type of boundary condition is often applied to laboratory soil columns when the bottom of the soil column is exposed to the atmosphere (gravity drainage of a finite soil column). The condition assumes that the boundary flux will remain zero as long as the pressure head is negative. However, when the lower end of the soil profile becomes saturated, a zero pressure head is imposed at the lower boundary, and the outflow is calculated accordingly. This type of boundary condition is often used for lysimeters.

Users can specify a pressure head value other than zero (**Pressure Head**) for triggering flux across the seepage face (in several experimental settings, negative pressure can be applied at the bottom of laboratory columns or lysimeters).

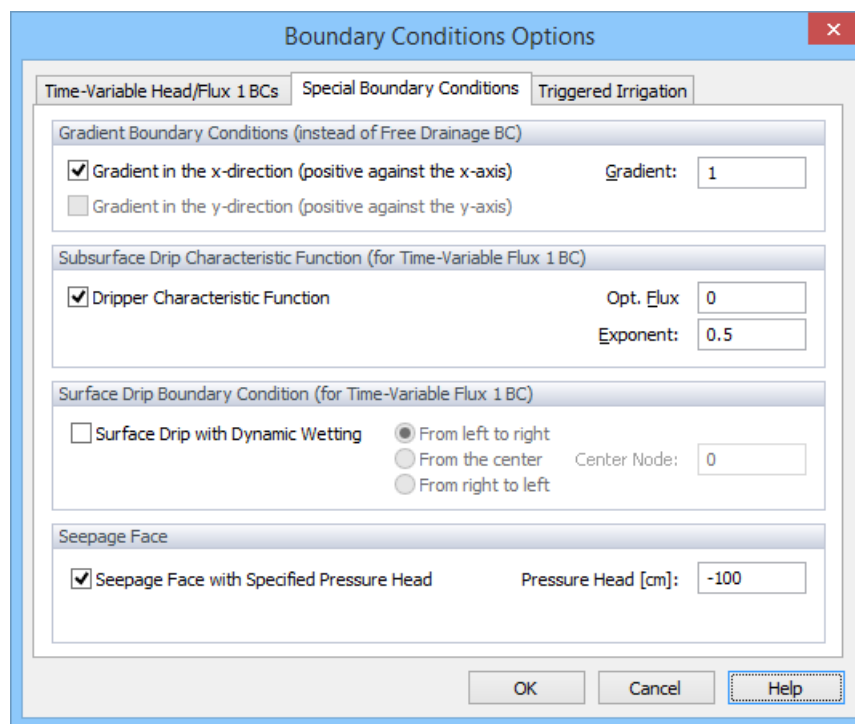


Figure 138. The Special Boundary Conditions tab of the Boundary Condition Options dialog window.

6.3.3. Triggered Irrigation

Triggered Irrigation can be specified on the third tab of the **Boundary Condition Options** dialog window (Fig. 139). Irrigation can be triggered by a user-specified “**Pressure Head Triggering Irrigation**” (input) reached in the selected “**Observation Node Triggering Irrigation**”. The irrigation starts after a user-specified **Lag Time** (input) at a user-specified **Irrigation Rate** or **Pressure Head** (input). The **Duration of Irrigation** has to be also specified.

This option is currently available only for two-dimensional and axisymmetrical geometries. An output file IRRIG.OUT is created when the triggered irrigation option is used containing information about irrigation scheduling and all triggered irrigation events (see Table 11.11 of the Technical Manual).

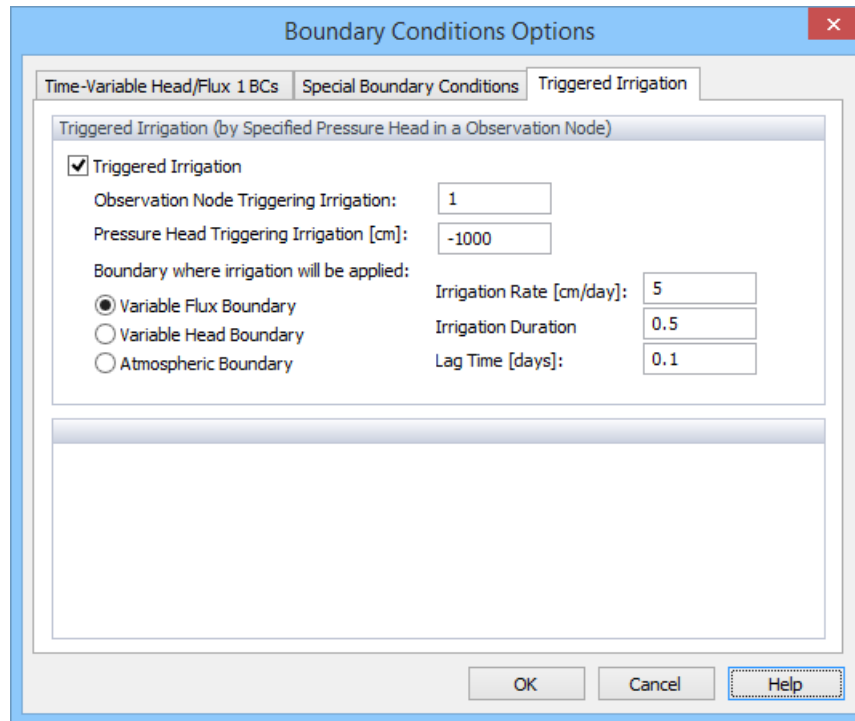


Figure 139. The Triggered Irrigation tab of the Boundary Condition Options dialog window.

6.3.4. Reservoir Boundary Condition

Version 3 of the two-dimensional module of HYDRUS (2D/3D) offers a new system-dependent boundary condition, further referred to as the **Reservoir Boundary Condition**. This option allows users to consider a reservoir that is external to the HYDRUS transport domain, while water can be added (injected) to or removed (pumped) from the reservoir. Flow into or out of the reservoir through its interface with the subsurface transport domain depends on the prevailing conditions in the transport domain (e.g., the position of the groundwater table) and external fluxes. Since mass balances of water and solute in the external reservoir are constantly being updated (based on all incoming and outgoing fluxes), the boundary conditions along the transport domain are dynamically adjusted depending upon the water level in the reservoir.

The **Reservoir** BC is implemented in HYDRUS (2D/3D) for three different geometries (Figure 1): a well, a furrow, and a wetland. While the furrow BC is implemented only for two-dimensional transport domains, the well and wetland BCs are implemented for both two-dimensional planar and axisymmetric transport domains.

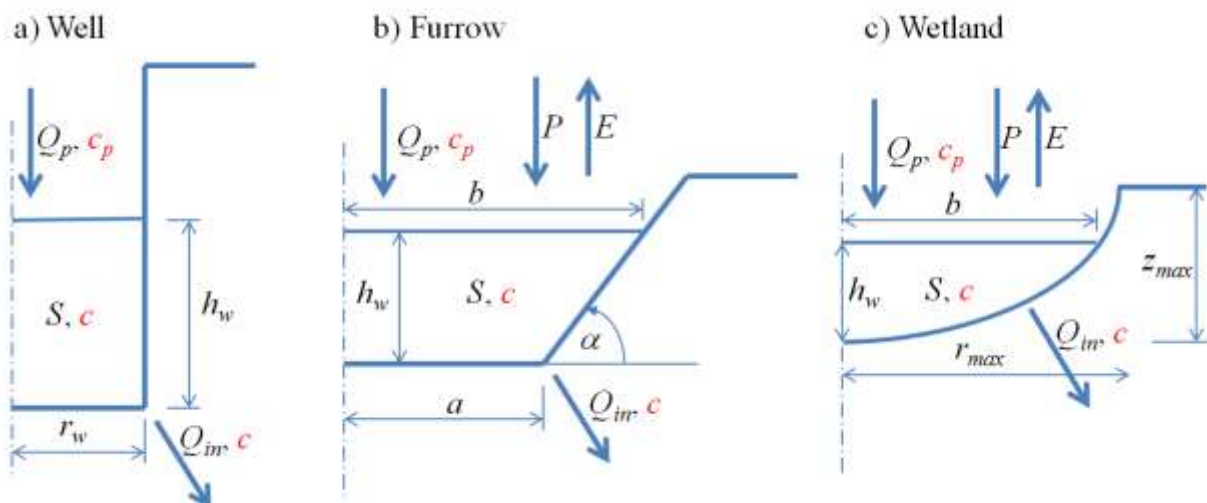


Figure 140. Three different types of the reservoir boundary condition: a well, a furrow, and a wetland. In the figure h_w is the water level in the reservoir [L], S is the volume of water in the reservoir ($[L^2]$ or $[L^3]$ for two-dimensional and axisymmetric systems, respectively), Q_p is the pumping rate (positive for removal of water, negative for adding water) ($[L^2T^{-1}]$ or $[L^3T^{-1}]$ for two-dimensional and axisymmetric systems, respectively), c is the solute concentration in reservoir water $[ML^{-3}]$, c_p is the solute concentration in injected water $[ML^{-3}]$, P and E refer to the precipitation and evaporation rates $[LT^{-1}]$, r_w is the radius of the well [L], a is the half-width of the furrow [L], α is the slope of the furrow side [-], r_{max} is the maximum width (radius) of the wetland [L], z_{max} is the maximum depth of the wetland [L], and b represents the width of the water table ($[L]$ or $[L^2]$ for two-dimensional and axisymmetric systems, respectively).

The parameters for the Reservoir Boundary Condition are specified using the **Reservoir Boundary Condition** Tab of the **Boundary Conditions Options** dialog window. Users have to first check the *Reservoir BC* check box and select the *Reservoir Type*, which can be either *Well (rectangular, cylindrical)*, *Furrow*, or *Wetland* (Figure 140). Users have then to provide information about the reservoir geometry (i.e., the *z-coordinate of the well (furrow, wetland) bottom*, *Well (Wetland) Radius or Half-Width of the Furrow Bottom*, the initial position of the water table in the reservoir (*Z-coordinate of the initial water level*), and *Pumping or Injection Rate*. When solute transport is considered, then the *Solute concentration initially in the reservoir water* needs to be specified as well. The *Pumping or Injection Rate* specified in this window is considered to be constant in time. When time-variable pumping or injection of water from/into the reservoir is to be simulated, this rate needs to be provided using the "Var.Fl.-1" column in the *Time-Variable Boundary Conditions* dialog window. Note that this rate is in units of $[L^2T^{-1}]$ or $[L^3T^{-1}]$ for two-dimensional or axisymmetrical applications. An output file WELL.OUT is created when the reservoir boundary condition is used containing information about fluxes into and from a reservoir (see Table 11.10 of the Technical Manual).

Boundary Conditions Options

Time-Variable Head/Flux 1 | Special BC | Triggered Irrigation | Reservoir Boundary Condition

Triggered Irrigation (by Specified Pressure Head in a Observation Node)

☒ Reservoir BC

Reservoir Type:

☒ Well (rectangular, cylindrical) ☐ Furrow ☐ Wetland

-2 Z-coordinate of the well bottom [cm]

0.25 Well radius [cm]

0 Not needed

0 Not needed

0.03 Pumping (+) or injection (-) rate [cm²/day]

-1.5 Z-coordinate of the initial water level [cm]

0 Solute concentration initially in the reservoir [M/L³]

0 Not needed

OK Cancel Help

Boundary Conditions Options

Time-Variable Head/Flux 1 | Special BC | Triggered Irrigation | Reservoir Boundary Condition

Triggered Irrigation (by Specified Pressure Head in a Observation Node)

☒ Reservoir BC

Reservoir Type:

☐ Well (rectangular, cylindrical) ☒ Furrow ☐ Wetland

85 Z-coordinate of the furrow bottom [cm]

15 Half-width of the furrow bottom [cm]

1 Tangent of the slope of the furrow wall (tan alpha [-])

0 Not needed

-60 Pumping (+) or injection (-) rate [cm²/day]

0 Z-coordinate of the initial water level [cm]

0 Solute concentration initially in the reservoir [M/L³]

95 Z-coordinate of the maximum water level that may be

OK Cancel Help

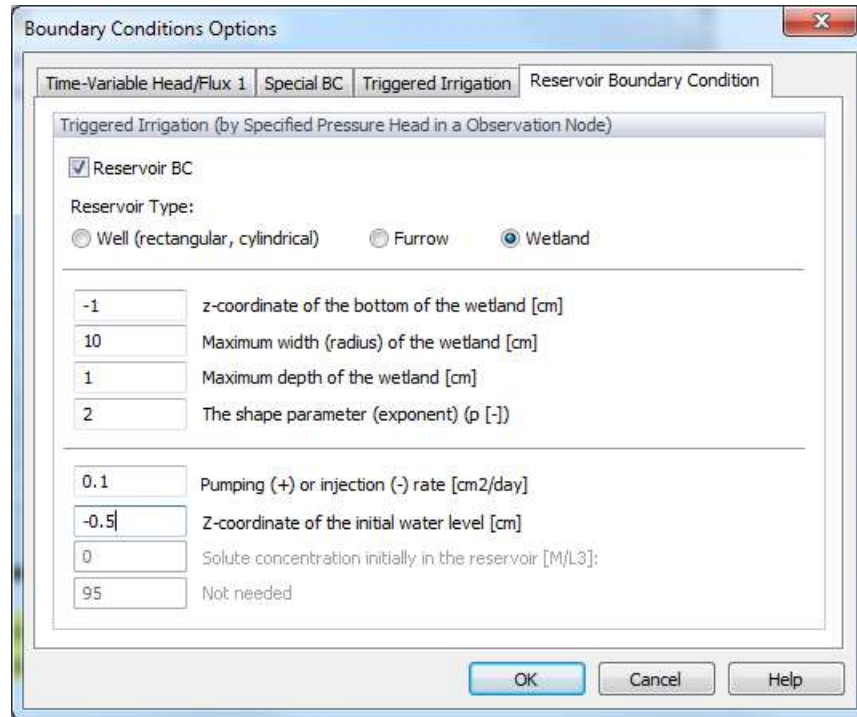


Figure 141. The Reservoir Boundary Condition tab for the Well (top), Furrow (middle), and Wetland (bottom) reservoir of the Boundary Conditions Options window.

Version 4 of HYDRUS extends the reservoir boundary condition also to three-dimensional applications for two types of geometries, i.e., a cylindrical well and a hexahedral reservoir (see the Technical manual for details).

6.4. Domain Properties

6.4.1. Domain Properties

Domain Properties are variables or parameters that may vary in space and are therefore defined either on Geometrical Objects or Finite Element Mesh. The table below lists **Domain Properties** recognized by HYDRUS.

Table 20. Domain properties.

Materials	Subsurface is usually composed of various material layers (horizons) that may have similar or dramatically different properties. Users must first define the Number of Materials needed to fully describe the subsurface in their project, then provide various parameters characterizing this material (e.g., Soil Hydraulic Properties and Solute Transport and Reaction Parameters), and finally describe the Spatial Distribution of Materials.
Roots	Roots , and correspondingly the root water uptake, are spatially distributed. There are usually more roots closer to the soil surface, and their number then decreases with depth. There are more roots closer to the trunk of the tree or a shrub and less further away. Users can either manually specify Spatial Distribution of Root Water Uptake or use predefined Root Distribution Analytical Functions.
Nodal Recharge	Nodes in the finite element mesh can be assigned either positive or negative Nodal Recharge , which may represent either sink or source of water in a particular node, respectively. These nodes can represent, for example, pumping or injecting wells.
Scaling Factors	The spatial distribution of soil hydraulic properties can also be described using the so-called Scaling Factors . These Scaling Factors, which can be specified for Pressure Head, Hydraulic Conductivity, and Water Content, then linearly transform the basic soil hydraulic functions. The spatial distribution of scaling factors can be defined either manually or they can be generated Stochastically .
Anisotropy	Hydraulic conductivity can have different values in different directions. For example, hydraulic conductivity may be significantly larger in the horizontal direction than in the vertical direction (likely due to the organization of soil particles). The Anisotropy is fully described by the Tensor of Anisotropy (angles between directions of anisotropy and spatial coordinates; and individual components of anisotropy).
Subregions	Subregions are parts of the transport domain, for which mass balances (for water, solutes, etc.) are evaluated and printed to the Balance.out output file. Their spatial distribution can correspond with the spatial distribution of Material Layers , but can also be different. One can, for example, request separate mass balances for the root zone and the rest of the transport domain (even when the domain is homogeneous or there are multiple soil horizons in the root zone).

Observation Nodes	Observation Nodes are selected finite elements nodes for which various output variables, such as pressure heads, water contents, temperatures, and concentrations, are reported at specified time intervals. Such information can then be used, for example, to compare HYDRUS predictions with measured data (e.g., pressure heads measured by tensiometers, water contents measured by TDR, etc.) or to calibrate the model against measured data.
Drains	A simplified way of representing Tile Drain .
Particles	Users can specify the initial positions of a set of hypothetical Particles (currently available only in two-dimensional applications), and the program then calculates trajectories and positions of these particles with time.

Parameters characterizing the flow domain (e.g., material distribution) are defined in a similar way as initial conditions (Section 6.2). Users must first select that part of the transport domain to which he/she wants to assign a particular value of the selected variable. It is possible to select the entire transport domain, part of it, or only individual nodes or elements. A particular part of the transport domain can be selected as follows: first, move the mouse to a selected position. The beginning and end of the selection operation are framed by clicking the left mouse button. The selected area is the rectangle defined by the two mouse positions when the left mouse button was clicked. Selection can alternatively (instead of using the rectangular selection) be made using a rhomboid (with the *Edit->Select->Select by Rhomboid* command), circle (*Edit->Select->Select by Circle*), or polygon (*Edit->Select->Select by Polygon*). When the selection is completed, users must click the **Set values** button and specify the value of a particular variable. The given value will then be assigned to the selected area. When material numbers are to be specified, users can do this directly by clicking on the color representing a particular material (at the **Edit Bar**). All variables are assigned to nodal points, except for those defining anisotropy angles, the first and second components of anisotropy, and subregion numbers, which are all assigned to elements.

6.4.2. Stochastic Distribution of Scaling Factors

Scaling Factors can be generated for two-dimensional applications using a random generator by clicking on the command *Edit->Domain Properties->Stochastic Distribution of S.F.* that calls the **Stochastic Distribution of Scaling Factors** dialog window (Fig. 142). Each scaling factor can be generated either independently of the other scaling factors or by assuming Miller-Miller similitude. In that case, the program generates hydraulic conductivity scaling factors and automatically calculates from their values the pressure head scaling factors.

Parameters for random generation of the scaling factors are specified in the **Stochastic Distribution of Scaling Factors** dialog window (Fig. 142). In this dialog, users need to specify whether the scaling factors are normally or log-normally distributed using the check box *Log-Normal Distribution*), and provide values for the standard deviation of a particular scaling factor, and correlation lengths in the x- and z-directions (if the scaling factors are spatially correlated).

6.5. Defining Properties on Geometric Objects

As described above, various spatially variable properties (e.g., material distribution, initial conditions, etc.) can be specified in Version 2.0 of HYDRUS (Standard and Professional, not Lite) either:

- directly on the **Finite Element Mesh** (FEM) (as done in Version 1.0), or
- on **Geometric Objects** (e.g., boundary curves, rectangles, circles, surfaces, solids) or **Geo Sections** (only in Version 2.0 and the Professional Version).

To be able to define properties on Geometric Objects, one needs to first enable this option (Edit domain properties, initial and boundary conditions on Geometric Objects) in the **Domain Type and Units** dialog window (see Figs. 6 or 7).

Which option is used depends on the menu command *Edit->Properties and Conditions on FE-Mesh* (disabled when the FE-Mesh does not exist). A similar button switch is also available at the end of the toolbar (), next to the Results button, and at the **Edit Bar**.

However, to be able to use this option (to specify properties on **Geo Sections**), the Transport Domain must be defined using (or divided into) a set of **Geometric Objects**, on which various properties can then be specified. An example of the transport domain divided into three components (or **Surfaces**) S2, S2, or S3 is shown in Figure 143.

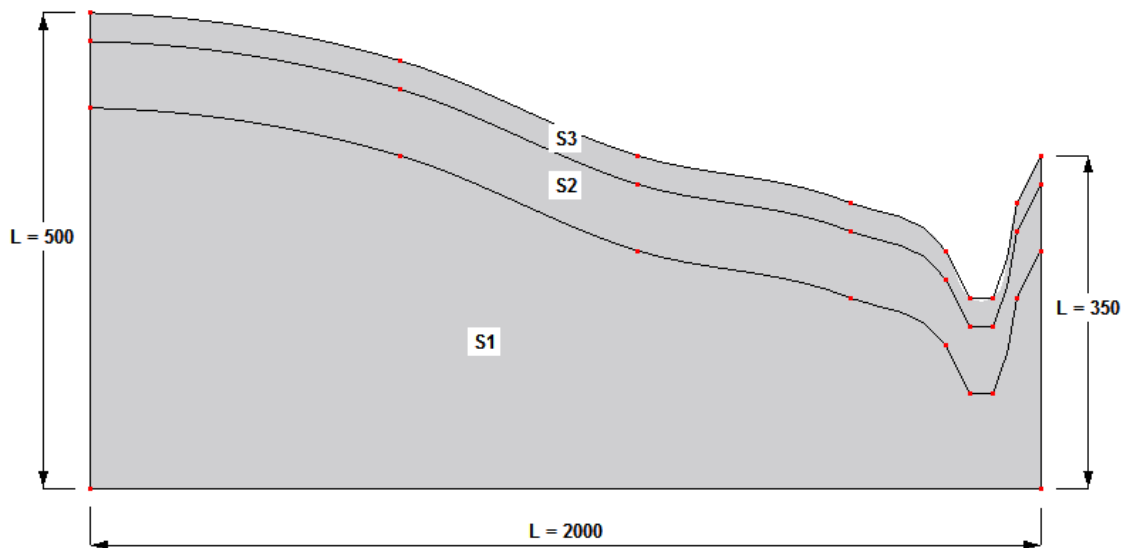


Figure 143. An example of the transport domain defined using three components S1, S2, and S3.

While for two-dimensional problems, the **Geo Sections** (displayed at the **Navigator Bar** at the **Section Tab**) need to be defined manually, for three-dimensional problems, they can also be generated automatically (see Section 8.1.8 what and how are these **Sections** generated). At the same time, when HYDRUS generates 3D objects, it also generates **Surfaces** belonging to each of

these objects. Some of these **Surfaces** are *Horizontal*, and some are *Vertical* (although these terms are only approximate). **Surfaces** can then be used to specify **Boundary Conditions**.

Vertical Surfaces are always created over the entire curve, which forms the boundary of the **Base Surface**. When the boundary of the **Base Surface** consists of several curves, then an independent *Vertical Surface* is created above each curve. Since the curves of the **Base Surface** can be arbitrarily divided, *Vertical Surfaces* can be created relatively freely.

While the text above in Section 6 refers to the first approach (specifying properties at FE-Mesh), the second approach (on Geo Objects) is briefly described below. While this latter approach can be used for all Domain Properties, and Initial and Boundary Conditions, we will demonstrate its use below on Material Distribution, for which it seems to be the most relevant. There are multiple commands that are common for most properties when defining Domain Properties, Boundary Conditions, and Initial Conditions on Geometric Objects. These commands are listed in the *Commands* part of the **Edit Bar** and are listed in Table 21.

Table 21. Definition of commands used to manipulate Property Objects.

Command	Description
New Property*	Creates a new Property Object. For some Properties, there is a list of available options, and the user needs to select from this list (e.g., water flow boundary conditions) or can extend this list (e.g., Materials). For others, the user needs to define values (e.g., scaling factors) or functional forms (e.g., initial conditions) of new Property Objects.
Set Property	Selects one particular Property from a list or Property Objects and assigns it to a selected Geo Object(s).
Clear Property	Clears a particular Property from selected Geometric Points. This command is used only for Properties that do not have a default Property (e.g., Nodal Recharge, Observation Nodes).
Clear All Properties	Clears all assigned Properties from geometric objects and assigns default properties where required (e.g., Materials) to the entire transport domain. Note that this command does not delete definitions of Properties (as done by the Delete All Properties command), which thus remain available in the data tree of the Navigator Bar.
Delete Property	Deletes a Property Object selected in the data tree of the Navigator Bar. This command is not used for Materials or Subregions, the number of which is specified elsewhere.
Delete All Properties	Deletes all Property Objects defined for a particular Property, except for a default Property (which is defined for those Properties where a default Property is needed). Similarly, as for the Delete Property commands, this command does not exist for Materials and Subregions.

Sort Properties	Calls a dialog window "Sort Property Objects", which displays all available Property Objects. Here, (the sequence of) the Property Objects can be arbitrarily rearranged.
Transfer to FE-Mesh	Transfers information about a particular Property defined on Geo Objects to the FE-Mesh. Note that this command is available only when information about a particular Property on Geo Objects and FE-Mesh does not correspond. This can occur, for example, when Property is defined (or refined) on FE-Mesh.
Edit Property	Recalls a dialog window with parameters of a particular Property to edit.

*Note that the word Property is used in place of a particular Property Object, such as Domain Property (e.g., Material, Observation Node), Boundary Condition, or Initial Condition.

6.5.1. Materials on Geometric Objects

Let's assign three different materials to three **Surfaces** in Figure 143. When only one material is defined (which is a default option in each new project), one needs to first define multiple materials (and/or their soil hydraulic properties). This can be done as usual using the Menu command *Edit->Flow and Transport Parameters->Water Flow Parameters->Soil Hydraulic Parameters*. The same dialog window (Fig. 20) can also be displayed by clicking on the **New Material** or **Edit Materials** commands on the **Edit Bar** (Fig. 144). Note that in Version 2.0 of HYDRUS, one can name materials.

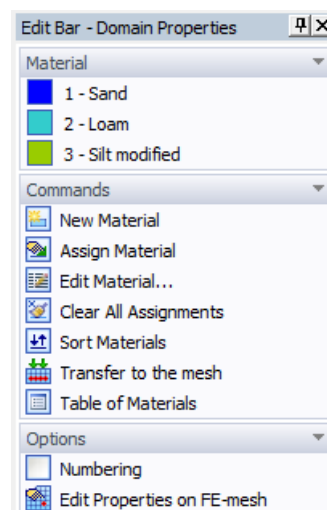


Figure 144. The upper part of the Edit Bar displaying defined materials and commands for various actions with materials.

There are three different ways of assigning materials to particular geometric objects (**Surfaces**):

- Click on a particular **Surface** (Geo Object) (to select it) and then on a **Material** (1, 2, or 3) in the **Materials** section of the **Edit Bar** to assign it.

- b) Click on a Material (1, 2, or 3) in the **Materials** section (to select it) of the **Edit Bar** and then on a particular **Surface** (to assign it).
- c) Click on the command **Set Material** in the **Commands** section of the **Edit Bar**, from the list box of the **Set Materials** window (Fig. 145) **Select Material to set**, click Assign to close the window, and click on a particular **Surface** to assign the selected material.

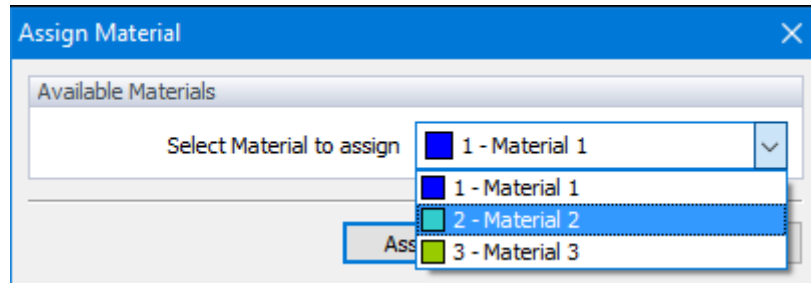


Figure 145. The Set Materials dialog window.

Note that nodes that are at the curve shared by two surfaces will be assigned material with a higher number. Color squares at nodes defining the **Geometry** (Fig. 146) indicate which material will be assigned to curves shared by two **Surfaces**.

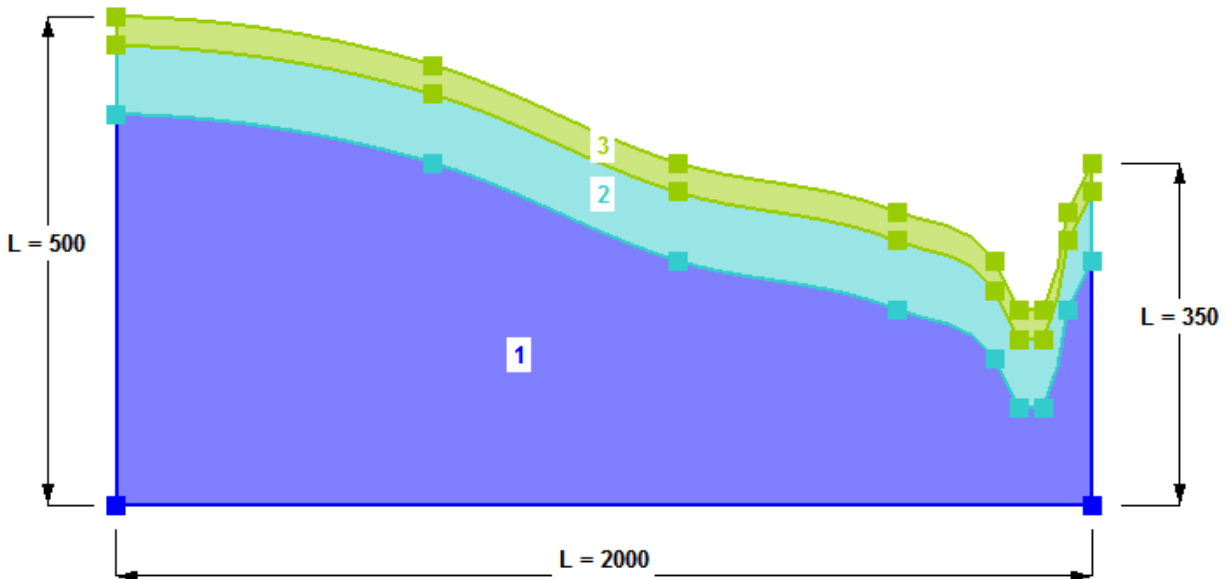


Figure 146. The transport domain with materials specified on geometric objects.

The sequence of materials (as well as other objects, such as Initial Conditions) can be reordered or sorted using the **Sort Materials** command on the **Edit Bar** and the **Sort Property Objects** dialog window (Fig. 147). In this dialog, the order of materials can be sorted using the **Top**, **Up**, **Down**, and **Bottom** command. While the sequence of materials can be sorted, colors representing the first, second, and other materials will remain the same.

Sorting can be done in two modes. When the **Auto-apply** check box is checked, any change done in the **Sort Property Object** window is immediately transferred to the transport domain and to the rest of the program. When this checkbox is unchecked, changes made in this dialog are transferred to the rest of the program only when the **Apply** command is clicked or after the window is closed using the **OK** button.

The command **Renumber All** can be used to renumber the **Property Objects**. This is useful when some previously defined Properties were deleted, and the numbering is no longer sequential.

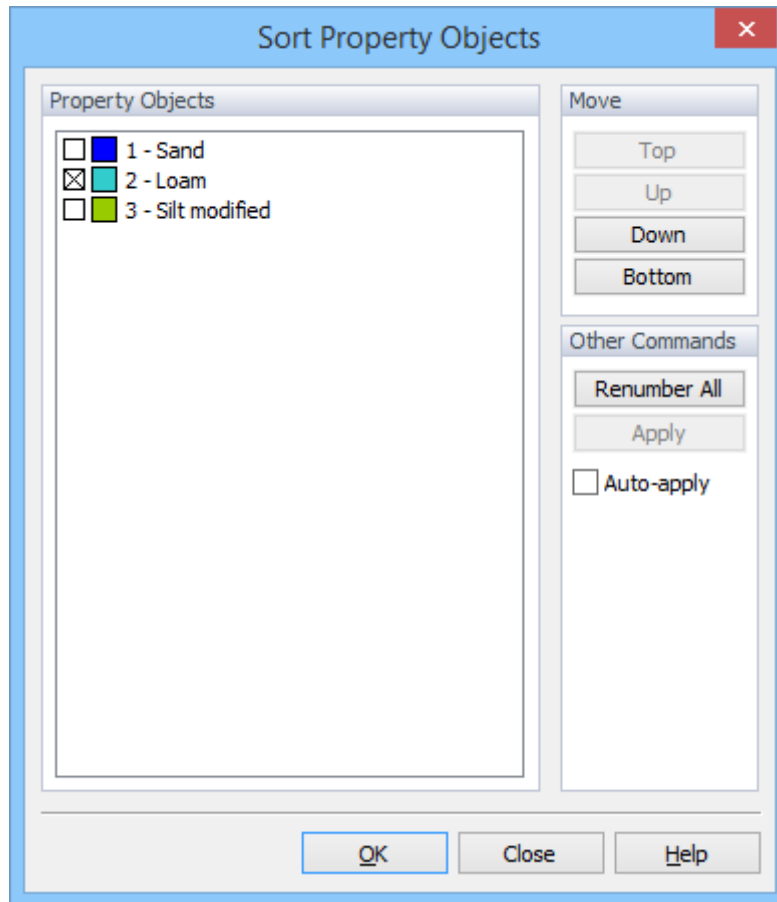


Figure 147. The Sort Property Objects dialog window.

A single click on any **Surface** will select this surface. A double click on any **Surface** will open a dialog for a Property assigned to a particular surface that is currently displayed, e.g., the **Edit Materials** dialog window (Fig. 148). In this dialog, one can change the **Name** of the material, its **Color** (the **Default** check box indicates whether the Color has been changed), **Assign** it to different **Surfaces** (indicated by their numbers), and register brief **Remarks** characterizing a particular material.

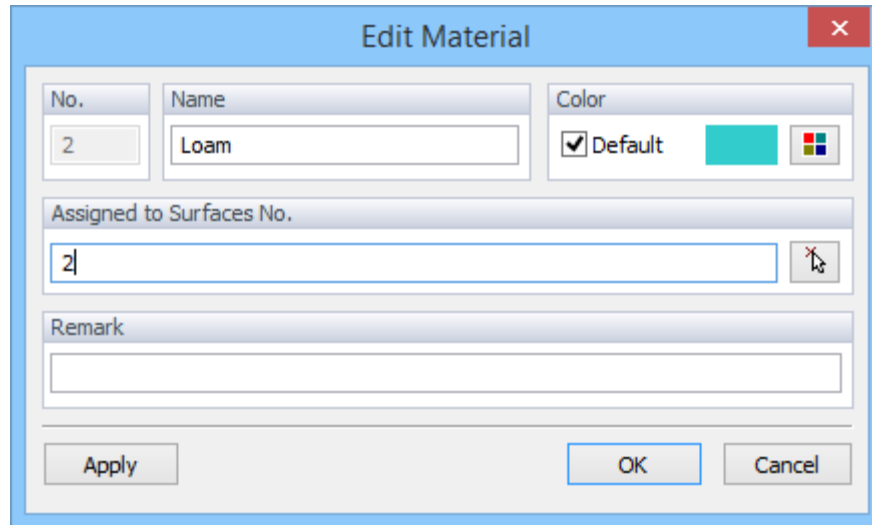


Figure 148. The Edit Materials dialog window.

Once the FE-Mesh exists, assigned properties (e.g., Materials) can be transferred on the FE Nodes (if it exists) using the **Edit Properties on FE-Mesh** (when FEM exists and a particular Property has not been yet edited on FEM) or the **Transfer to FE-Mesh** (Transfer to FE-mesh) (when a particular Property has already been edited on FEM) commands located on the **Edit Bar** (Fig. 144). Here the assignment of materials can be further edited, refined, and finalized. However, these changes cannot be transferred back to **Geometric Objects**. After changes have been made on FEM and thus Properties assigned on FEM and Geo Objects no longer correspond, the command **Transfer to FE-Mesh** can be used to synchronize the information in the two modes (from Geometric Objects to FEM) again.

The **Edit Bar** commands **Edit Properties on FE-Mesh** and **Edit Properties on Geo Objects** switches from one way of assigning properties (on Geo Objects) to another (on FEM).

A similar approach and similar commands can be used to assign other Domain Properties, and Initial and Boundary Conditions.

6.5.2. Observation Nodes on Geometric Objects

Observation Nodes are entered on Geometric Objects using either the Menu command *Insert->Domain Properties->Observation Nodes* or the **New Observation Node** command on the **Edit Bar**. The **New Observation Node** command can be used in the **Edit Properties on Geo Objects** mode to define observation nodes only on **Points** defining the **Geometry** (i.e., Points defining boundary curves). Observation nodes for any other location have to be specified on the FE-Mesh directly. The same is true also for Drains and Flowing Particles.

The **Edit Observation Node** window (Fig. 149) is displayed when double-clicking on an observation node in the **View** window (when working in the Properties on Geometric Objects mode) or an Observation Node item in the **Navigator Bar**. This window displays

- a) the **Name** of the observation node (note that the observation node can be renamed using a brief text, such as drain, tensiometer, TDR, etc.),
- b) indication whether it is **Defined at Geometric Node** or **FE-Mesh Node**, and
- c) a brief **Remark** (note).

Figure 149. The Observation Node dialog window.

6.5.3. Initial Conditions at Geometric Objects

Property Objects for Initial Conditions are defined or edited using the **New** or **Edit Pressure Head (Concentration) Initial Condition** dialog windows shown in Figure 150. Note that the parameters and values that are entered in these dialogs are the same as those entered in Figure 135 when defining Initial Conditions directly at the FE-Mesh. Here, one can additionally define the **Name** of the Initial Condition, the **Color** which represents it (either **Default** or selected), register a brief **Remark**, and select to which surfaces it is assigned to (**Assigned to Surfaces No:**).

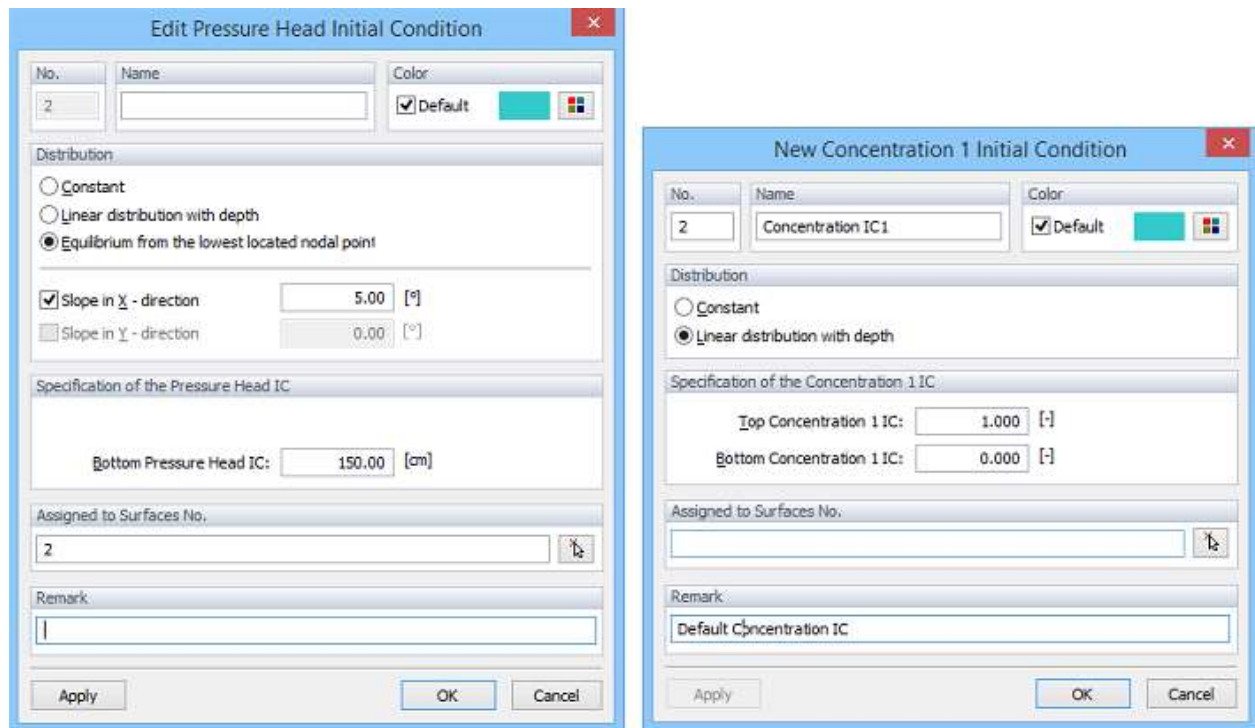


Figure 150. The Edit Pressure Head (left) and Concentration (right) Initial Conditions dialog window.

6.5.4. Boundary Conditions at Geometric Objects

New Property Objects for Boundary Conditions must be selected from existing boundary conditions used in HYDRUS. For example, for Water Flow Boundary Conditions, new Objects are selected from the list box **Boundary Condition Type** displayed in Figure 151. Similarly, as for other Properties, in this dialog, one can define **Name**, **Color**, register a **Remark**, assigned Boundary Condition at selected Boundary Curves, and, if needed, specify required parameters (e.g., for Deep Drainage BC).

Notes:

1. When the same pressure head initial (or boundary) condition involving either "Equilibrium from the lowest located point" or "A linear distribution" is chosen for multiple surfaces (or curves), then this condition is applied globally to all selected surfaces (e.g., a single point with the lowest z-coordinate is found for all selected surfaces).
2. The default solute and heat transport boundary conditions are the **Third-Type BCs**, which are listed right after the **No Flux BC**. This BC is by default assigned to all boundaries, to which the water flow BCs have been defined. Note that if you redefine this BC (e.g., change the Third-Type BC into the First-Type BC), the newly defined BC will be used as a default BC for solute and or heat transport.

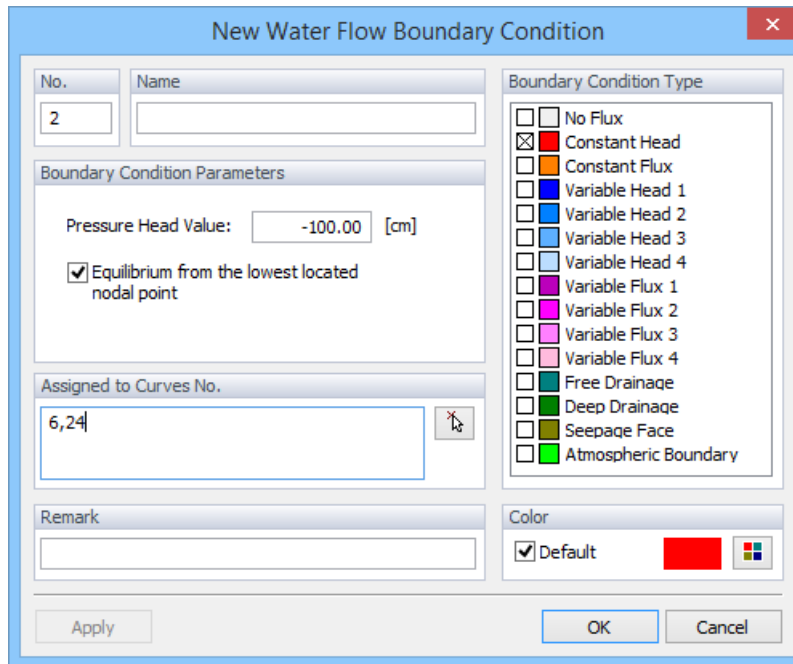


Figure 151. The Edit Water Flow Boundary Condition dialog window.

6.5.5. Additional Notes on Properties at Geometric Objects

- a) When the same pressure head initial (or boundary) condition involving either "Equilibrium from the lowest located point" or "A linear distribution" is chosen for multiple surfaces (or curves), then this condition is applied globally to all selected surfaces (e.g., a single point with the lowest z-coordinate is found for all selected surfaces).
- b) Nodes that are at the boundary line shared by two surfaces (or at the surface shared by two volumes) are assigned the property value with a higher number. The sequence in the list of properties can be adjusted using the command **Sort Property** (where Property is either Material, Scaling Factor, etc.) at the **Edit Bar** (Fig. 147).
- c) The option to assign Properties at Geometric Objects is not available for simple parametric (i.e., **Rectangular** or **Hexahedral**) Geometries available in the Lite Version of HYDRUS.
- d) **Name:** One can provide a **Name** for each newly defined **Property Object**. When the user does not define a **Name** for a **Property Object**, the GUI will automatically generate a generic name that is then used throughout the project (e.g., on the **Navigator** and **Edit Bars**).
- e) When different values are specified on Geometric Objects and FE-mesh, the warning **Different Values on FE-Mesh** is displayed in the Help section of the Edit Bar. A similar warning is also issued in such a case before calculations are started.
- f) All properties can be transferred from Geometric Objects to FE-Mesh using the menu command Edit->Transfer all Properties to FE-Mesh.

6.6. Import of Domain Properties and/or Initial and Boundary Conditions

Various domain properties and initial and boundary conditions can be imported either from existing HYDRUS projects and from data text files with values defined at specified locations.

6.6.1. Import Initial Condition from HYDRUS Projects

The initial condition can be imported from the results of previous calculations (from an existing HYDRUS project) using the Import command (*Edit->Initial Condition->Import* or *Insert->Initial Condition->Import*). After clicking on any of these two commands, an **Open** dialog window appears with **Files of type** preselected for HYDRUS applications (i.e., *.hyd5). One then needs to browse for the HYDRUS project from which the initial condition is to be imported. After selecting a particular project, the **Import Initial Conditions** dialog window appears (Fig. 152). This window provides information from which project the initial conditions will be imported (*Import data from Hydrus project*) and offers quantities that can be imported as initial conditions (*Select quantities to import*). Users must then also decide in the *Select Time Layer* part of the dialog if values for *The Last (Final) Time Layer* or for any intermediate time layer (using *Time Layer No.:* from the lower list box) are to be imported. *Time Layers* correspond with **Print Times** (Fig. 17) for which the output in the existing project was calculated.

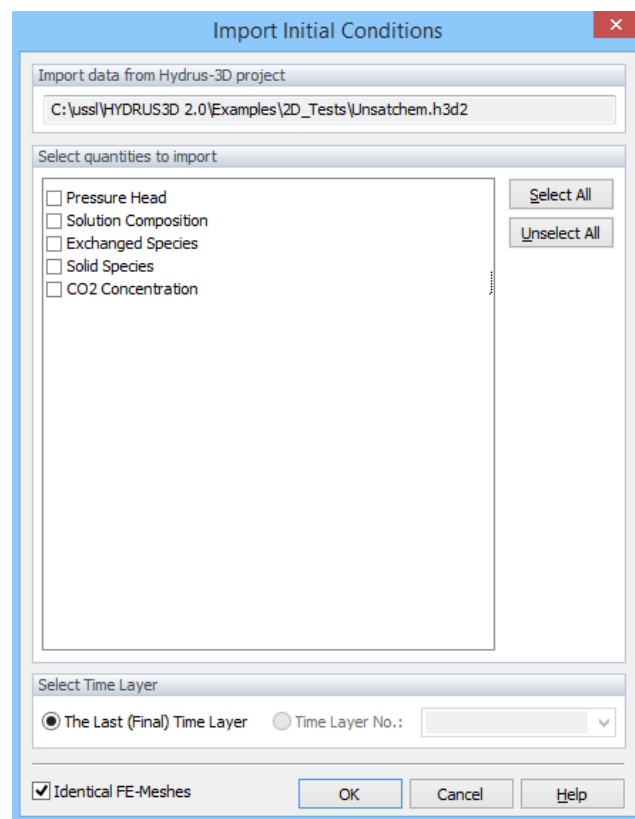


Figure 152. The Import Initial Condition dialog window.

Note: While in the previous HYDRUS versions, the import of results from previous calculations as initial conditions for the new simulation could be done only from a project that had an identical geometry and FE-Mesh discretization as the actual project, in newer HYDRUS versions (version 2.02 and later), the geometry may be slightly different (should not differ too much) and the FE-Mesh discretization can be different as well. Whether the FE-Meshes of the two projects are identical can be identified by the user (a check box *Identical FE-Meshes*) so that the code can simply transfer nodal values without the need to interpolate.

6.6.2. Import Data from HYDRUS Projects

Various other properties, such as Domain Properties, Initial Conditions, and Boundary Conditions, can be imported from an existing HYDRUS project using the Import command (*File->Import->Import Input Data from Another HYDRUS Project*). After clicking on this command, an **Open** dialog window appears with **Files of type** preselected for HYDRUS applications (i.e., *.hyd5). One then needs to browse for the HYDRUS project from which the initial condition is to be imported. After selecting a particular project, the **Import Selected Quantities** dialog window appears (Fig. 153). This window provides information from which project the initial conditions will be imported (*Import data from Hydrus project*) and offers quantities that can be imported as initial conditions (*Select quantities to import*). **Select All** or **Unselect all** commands can be used to make a selection.

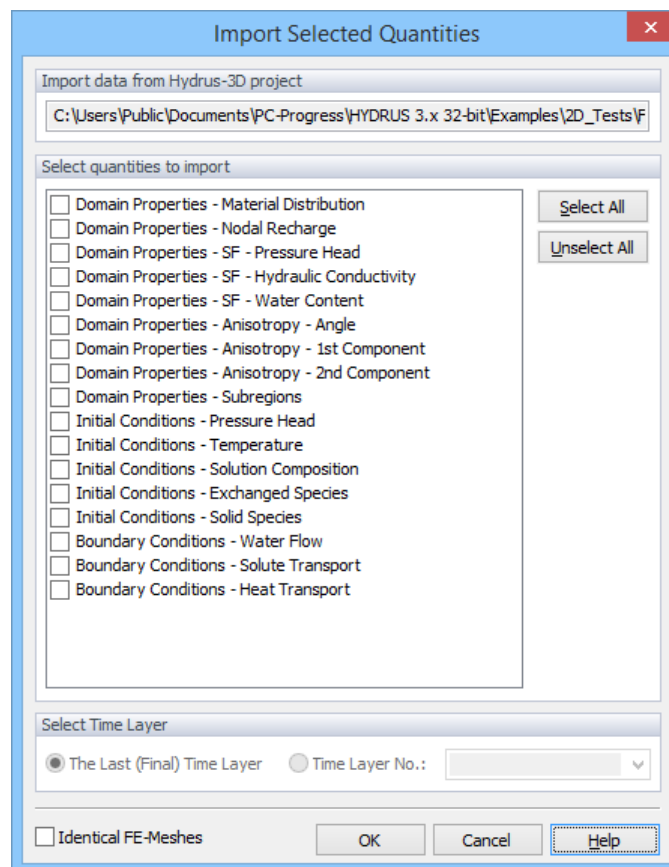


Figure 153. The Import Selected Quantities dialog window.

Warning: The import of selected quantities from another HYDRUS project can be done only from a project that has a similar geometry and FE-Mesh discretization as the actual project! Geometry cannot be significantly different! Users need to carefully check the results of the import if Geometries or FE mesh are different.

6.6.3. Import Data from a Text File

HYDRUS users often encounter a problem of defining a certain property, for which they have only limited information from multiple locations (such as the initial location of a contamination plume). A new function (*File->Import->Import Quantity defined by values at Scattered Points...*) was implemented in version 2.03 (and later) that allows users to import such information from a text file of a specified format. This function reads values defined in generally spaced points (for both 2D and 3D problems) and transfers them to the current FE-mesh using a linear interpolation of these values.

- a. Only input variables defined using real numbers (scalars) can be imported this way. Integer values specified in points (e.g., material numbers) can be imported differently – using FE-mesh Sections – see Tutorial 2.12 at <http://www.pc-progress.com/en/Default.aspx?h3d-tutorials>. It is not also possible to import output variables (results).
- b. The variable to be imported has to be displayed in the active **View** before the import process can be started.
- c. The values are transferred onto the current FE-mesh, which implies additional restrictions on quantities that can be imported this way. If the entire domain is displayed in the **View**, the values are transferred to all FE nodes of the domain. If only a certain part of the domain (FE-mesh Section) is displayed in the **View**, the values are transferred only to FE nodes of this Section.

Format of a text file (with spatial coordinates and property values):

- a. The input text file must have the following format (depending on the type of the transport domain of a project, to which data are imported):

For 3D Domains:

```
Column1 = x-coordinate [m]
Column2 = y-coordinate [m]
Column3 = z-coordinate [m]
Column4 = value [unit of the quantity displayed in the active view]
```

Example:

```
0.000000e+000  0.000000e+000  8.000000e-001  -3.000000e+001
0.000000e+000  0.000000e+000  0.000000e+000   5.000000e+001
3.000000e+000  0.000000e+000  0.000000e+000   5.000000e+001
...
```

For 2D-XY Domains:

```
Column1 = x-coordinate [m]
```

Column2 = y-coordinate [m]
Column3 = value [unit of the quantity displayed in the active view]

Example:

```
0.000000e+000  8.000000e-001 -3.000000e+001
0.000000e+000  0.000000e+000  5.000000e+001
3.000000e+000  0.000000e+000  5.000000e+001
...
```

For 2D-XZ Domains:

Expected format:

Column1 = x-coordinate [m]
Column2 = z-coordinate [m]
Column3 = value [unit of the quantity displayed in the active view]

Example:

```
0.000000e+000  8.000000e-001 -3.000000e+001
0.000000e+000  0.000000e+000  5.000000e+001
3.000000e+000  0.000000e+000  5.000000e+001
...
```

Other Formats:

In addition to the formats described above, one can also import values from a file generated using the function *File->Export->Export Current Quantity....* Although this file has a somewhat different format, HYDRUS will automatically detect that and loads the correct values from the block „TABLE_01: NODAL INFORMATION“.

- b. Data in columns can be entered in free format (a column width is not fixed); spaces, tabs, and semicolons can be used as column separators.
- c. Points in which values are defined should not overlap, nor should be very close to each other. The best way is to use points in a regular grid (2D or 3D), covering the entire computational domain.

The minimum number of points is 3 for 2D domains and 4 for 3D domains. The points must be linearly independent, i.e., they cannot lie in a straight line (2D) or in a plane (3D). The maximum number of points is not limited, but an excessive number of points (>10,000) may lead to extremely long calculation (linear interpolation of values for generally located nodes requires relatively complex geometric calculations) or to other problems.

Once the text file is read by the GUI, a dialog window "Import of Values from Scattered Points" shows up.

- a. This window first summarizes imported information in the top section "Imported Values" (i.e., the number of imported points, minimum and maximum values, and minimum and maximum x, y, and z coordinates, for points with given values).
- b. Users can then select whether or not
 - a *Linear interpolation of values* or
 - a *Linear interpolation/extrapolation of values* should be done when transferring values from *Scattered Points* to the *FE-Mesh Nodes*. Alternatively to linear interpolation, values can be
 - *Transferred* to FE-Mesh nodes *from the nearest points without interpolation/extrapolation*.

Note that when the *Linear interpolation of values* option is selected, linear interpolation is done only between locations with imported values, and a *Transfer of values from nearest points* is done in the rest of the domain (outside of the area/space with imported values, but within the transport domain).

- c. Users can also select the *Minimum* and *Maximum Values* that cannot be exceeded by interpolation (*Value Limited*).
- d. Finally, users can define the so-called *Clipping Box*. This is a part of the transport domain, defined by the minimum and maximum x, y, and z coordinates (X min, X max, Y min, Y max, Z min, Z max), for which a transfer of values from *Scattered Points* to *FE-Mesh Nodes* is done. There is no transfer of values outside of this box.

The actual transfer of values from *Scattered Points* to the *FE-Mesh Nodes* is done only after the button OK is clicked.

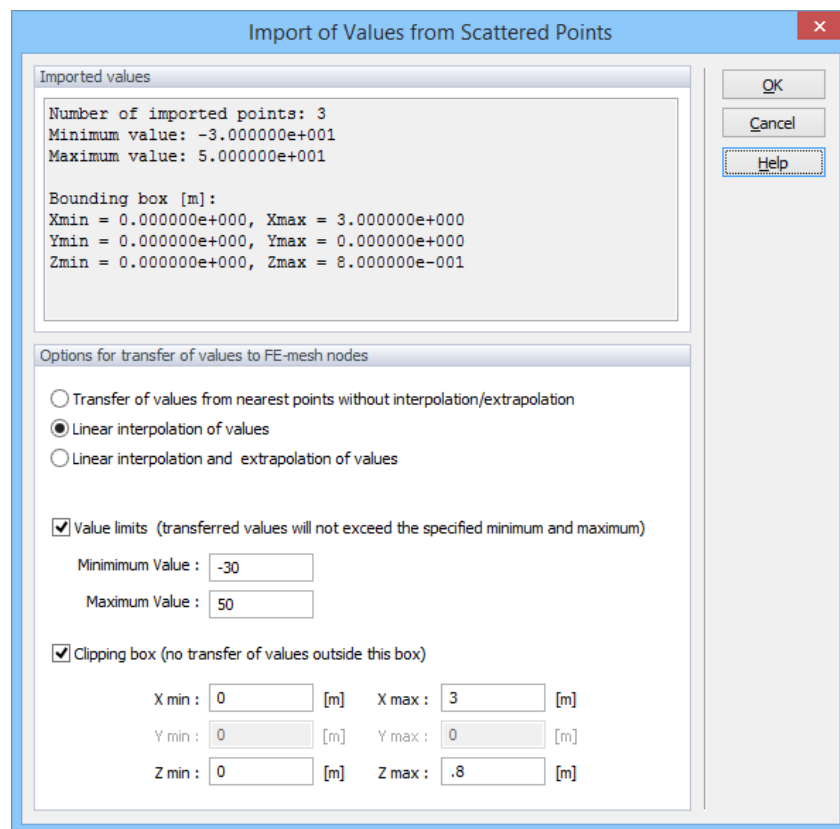


Figure 154. The Import of Values from Scattered Points dialog window.

When imported values (possibly available only in some part of the transport domain) are "linearly interpolated/extrapolated" to the rest of the transport domain, the calculated nodal values can be lower or higher (when extrapolated) than those measured (imported). If users want to prevent that, they have several options on how to proceed:

- f) They may specify additional import values for selected nodes in the transport domain or at the domain boundaries so that "interpolation" (rather than "extrapolation") is used in the entire transport domain. Extrapolation is used in the part of the domain where no imported values are located.

- g) They may constrain "interpolation/extrapolation" to only a certain part of the transport domain ("clipping box").
- h) They may specify what the minimum and maximum value could be ("Value Limits").

It is up to the users to select optimal import and interpolation options suitable for their purpose (also depending on an imported variable).

Note: For the maximum accuracy in the transfer of measured values to the finite element nodes, it is recommended to create FE nodes exactly in the points with measured values. This task depends on the type of the domain:

1. 3D-Layered Domain:

Here we recommend that you first import the projection of the points' locations to the **Base Surface**. Points obtained in this way will then become Internal Points of the Base Surface, and FE nodes generated in other layers above these base points will then be very close to locations with imported values, thereby increasing the accuracy of interpolated values. In practice, this can be done as follows (assuming that the Base Surface lies in the x - y plane and its $z = 0$):

- A. Make a copy of the file with coordinates of points with imported values and values themselves, prepared for the import of values, and delete the last column (values).
- B. In HYDRUS, use the command "File -> Import -> Import Points from Text File" and read points coordinates from this file.
- C. You will need to move imported points to the Base Surface. Select all imported points, press Alt + Enter, and, in the dialog for editing points, set $z=0$.

2. 3D-General Domain:

Here, it is possible to make the points with imported values to be directly part of the FE mesh as follows:

- A. Import the 3D points as described in item 1 above, but omit the projection to the Base Surface (item 1C above).
- B. Include the imported points into the Solids that form the Computational Domain as Integrated Points. Click on the Solid (either in View or Navigator), open the tab "Integrated Objects", and in the edit box "Points" insert a list of integrated points (it is possible to make a graphical selection).

Generated 3D FE-Mesh will then have some of its nodes located exactly in points with imported values, thereby achieving a higher accuracy when interpolating values to the rest of the FE-Mesh nodes.

3. 2D-General domain:

The procedure is the same as in item 2 above, except instead of 3D points, we have 2D points, which will be integrated into Surfaces.

4. 2D-Simple a 3D-Simple:

Here the situation is quite difficult because the locations of FE-Mesh nodes can be defined only using coordinates in the tables for generating structured FE-Mesh.

7. Graphical Output

Graphical output is divided into two main parts. In the first part, variables that change spatially throughout the transport domain are displayed by means of contour maps, isolines, isosurfaces, or isobands (**Results** on the **Data Tab** of the **Navigator Bar**, or *Options->Graph Type*). Additional information such as boundary fluxes and/or soil hydraulic properties are displayed using x-y graphs (**Results – Other Information** on the **Data Tab** of the **Navigator Bar**, or using the **Results Menu**).

7.1. Results

Results of a simulation for 2D/3D applications can be displayed by means of contour maps, isolines, isobands, isosurfaces, color points, color edges, spectral maps, and/or velocity vectors (*Graph Type* at the **View Tab** of the **Navigator Bar** or *Options->Graph Type->Isolines*), and/or by animation using both contour and spectral maps. The number of colors in the color spectrum, as well as the numerical increment between isolines, can be selected using the **Edit Isoband Value and Color Spectra** dialog window (Fig. 158). Contour and spectral maps may be drawn for the pressure head, water content, temperature, solute concentration (in the equilibrium or nonequilibrium phase), and/or velocity. Animation of these four variables is also possible (*Flow Animation* on the *Results* version of the **Edit Bar**, or using *Results->Time Layer->Animation*).

Graphs of all variables along the boundaries (*Boundary-Line Chart* on the *Results* version of the **Edit Bar**, or using *Results->Charts->Boundary Line*), as well as those along any selected cross-section (*Cross-Section Chart* on the *Results* version of the **Edit Bar** or *Results->Charts->Cross-Section*) can be readily obtained. The ability of charts displaying the distribution of various quantities along boundary-lines and cross-section lines has also been extended in Version 3. The GUI now allows the display of results at multiple time-layers simultaneously in one chart. This feature allows one to compare the values of a given quantity at different times very easily. Note that cross-section lines and charts now can also be applied to mesh slices created by the Clipper tool as described earlier and shown in Figure 169.

The entire finite element mesh, the boundary nodes, and the numbering of nodes, elements and/or edges can also be displayed (using the **Display Options** dialog window (Fig. 157), or *Options->Display Options->Edit*), together with isolines and spectral graphs. Users may zoom into a certain part of the transport domain and can enlarge or reduce the transport domain, among other features.

Flow animation is an alternative to displaying results at one particular time. Distributions during flow animation are displayed continuously at consecutive times, thereby visualizing the flow and transport process. Note, however, that display times are defined by the print time intervals specified in the input data file. This means that the print times must be at constant intervals so that the time scale of the flow animation will not be distorted. In other words, undistorted flow animation requires that the print time intervals be constant. The speed of the flow animation depends on the hardware being used, i.e., the speed of the microprocessor and graphical card.

7.1.1. Displayed Variables

Multiple variables can be displayed in the View window for 2D/3D applications. A comprehensive list of standard and alternative variables that can be displayed in the View window are summarized in Tables 22 and 23, respectively.

Table 22. Standard variables displayed in the View Window of the Results tab (Results - Graphical Display).

Variable	Description
Pressure Head	Pressure head h [L]; displayed always
Water Content	Water content θ [-] (or θ_m when the dual-porosity model is used); displayed always
Velocity	Values of Darcy's flux q [$L T^{-1}$]; displayed always
Velocity Vectors	Darcy's flux vectors q [$L T^{-1}$]; displayed always
Root Water Uptake	Root water uptake S [T^{-1}]; displayed when root water uptake is considered
Concentration i	Liquid phase concentration c [$M_c L_w^{-3}$]; displayed when solute transport in the standard module is simulated.
Sorbed Noneq. Conc. i	Concentration of kinetically sorbed solute s^k [$M_c M_s^{-1}$] ⁺ ; displayed when solute transport in the standard module is simulated and when the two-site sorption model is considered.
Immobile Conc. i	Concentration in the immobile water c_{im} [$M_c L_w^{-3}$]; displayed when solute transport in the standard module is simulated and mobile-immobile water or dual-porosity models are considered.
Temperature	Temperature T [$^{\circ}C$]; displayed when heat transport is simulated.
Unsatchem Variables	Major ions: Ca, Mg, Na, K, HCO ₃ , SO ₄ , Cl, tracer, sorbed Ca, sorbed Mg, sorbed Na, sorbed K, calcite, gypsum, dolomite, nesquehonite, hydromagnesite, sepiolite; displayed when the Unsatchem module is used.
Wetland Variables	Various variables used in the two constructed wetlands modules CW2D and CWM1 (see the Wetlands module manual for details).
Air-Water Interfacial Area	Air-Water Interfacial Area [$L^2 L^{-3}$] is displayed by the PFAS module.

⁺ Subscripts c , s , and w refer to the contaminant, soil, and water.

Table 23. Alternative variables that can be displayed in the View Window of the Results tab.

Variable	Description
Pressure Head	Standard display
Total Pressure Head	Total Pressure Head $H (=h+z)$ [L]; alternative display
Water Content	Standard display
Mobile Water Content	Water content in the mobile phase θ or θ_m [-]; default display
Immobile Water Content	Water content in the immobile phase q_{im} [-]; displayed when the dual-porosity model is used.
Total Water Content	Total water content $\theta (= \theta_m + \theta_{im})$; displayed when the dual-porosity model is used.
Velocity	Standard display
Total Value	Darcy's flux [LT^{-1}]; default display
x-component	x-component of the Darcy's flux q [LT^{-1}]
y-component	y-component of the Darcy's flux q [LT^{-1}]
z-component	z-component of the Darcy's flux q [LT^{-1}]
Concentration Options	
Liquid Equil. Phase Conc.	Liquid phase concentration c [$M_c L_w^{-3}$] ⁺ ; default display
Sorbed Equilibrium Conc.	The concentration of instantaneously sorbed solute s^e [$M_c M_s^{-1}$]
Sorbed Total Concentration	Sorbed concentration $s = s^e + s^k$ [$M_c M_s^{-1}$]
Gas Phase Concentration	Gas phase concentration g ($=K_{HC}$) [$M_c L_a^{-3}$]
Concentration on AWI	Concentration at the air-water interfacial area Γ [$M_c L^{-2}$]
Total Concentration	Total concentration mass S [$M_c L_s^{-3}$]
Sorbed Concentration Options	
Sorption Sites 1	Sorbed concentration on first kinetic sorption sites s_1^k [$M_c M_s^{-1}$]
Sorption Sites 2	Sorbed concentration on second kinetic sorption sites s_2^k [$M_c M_s^{-1}$]
Total Sorbed Conc.	Total sorbed concentration $s^k = s_1^k + s_2^k$ [$M_c M_s^{-1}$]

⁺ Subscripts c , s , a , and w refer to the contaminant, soil, air, and water.

Table 24. Definition of various concentration modes (for linear sorption model).

	Equilibrium model	Mobile-immobile model	Two-site sorption model	Two-kinetic sites model
Sorbed equilibrium concentration [M _c M _s ⁻¹]	$K_D c$	$K_D f c_m$	$f_e K_D c$	$K_D c$
Sorbed nonequil. concentration [M _c M _s ⁻¹]	-	$K_D (1-f) c_{im}$	s^k	$s_1^k + s_2^k$
Sorbed total concentration [M _c M _s ⁻¹]	$K_D c$	$K_D [f c_m + (1-f) c_{im}]$	$f_e K_D c + s^k$	$K_D c + s_1^k + s_2^k$
Gas-phase concentration [M _c L _a ⁻³]	$K_H c$	$K_H c$	$K_H c$	$K_H c$
Concentration on AWI, Γ [M _c L ⁻²]	$K_H c$	$K_H c$	$K_H c$	$K_H c$
Solute mass in the liquid phase, S_l [M _c L _s ⁻³]	$c \theta$	$c_m \theta_m + c_{im} \theta_{im}$	$c \theta$	$c \theta$
Solute mass in the solid phase, S_s [M _c L _s ⁻³]	$\rho K_D c$	$\rho K_D [f c_m + (1-f) c_{im}]$	$\rho (f_e K_D c + s^k)$	$\rho (s_1^k + s_2^k)$
Solute mass in the gas phase, S_g [M _c L _s ⁻³]	$K_H c a$	$K_H c a$	$K_H c a$	$K_H c a$
Solute mass on AWI, S_g [M _c L _s ⁻³]	$A_{aw} \Gamma$	$A_{aw} \Gamma$	$A_{aw} \Gamma$	$A_{aw} \Gamma$
Total concentration, S [M _c L _s ⁻³]	$S_l + S_s + S_g$	$S_l + S_s + S_g$	$S_l + S_s + S_g$	$S_l + S_s + S_g$

- a air content [L_a³L_s⁻³]
 A_{aw} air-water interfacial area [L_a²L_s⁻³]
 c liquid phase concentration [M_cL_w⁻³]
 c_m liquid phase concentration in the mobile phase [M_cL_w⁻³]
 c_{im} liquid phase concentration in the immobile phase [M_cL_w⁻³]
 θ water content [L_w³L_s⁻³]
 θ_m water content in the mobile phase [L_w³L_s⁻³]
 θ_{im} water content in the immobile phase [L_w³L_s⁻³]
 K_D distribution (sorption) coefficient [L_w³M_s⁻¹]
 K_H Henry's law constant [-]
 S_l solute mass in the liquid phase [M_cL_s⁻³]
 S_s solute mass in the solid phase [M_cL_s⁻³]

S_g	solute mass in the gas phase [$M_c L_s^{-3}$]
S	total concentration (solute mass), $S=S_l+S_s+S_g$ [$M_c L_s^{-3}$]
s	solid phase concentration [$M_c M_s^{-1}$]
s^k	solid phase concentration on kinetic sorption sites [$M_c M_s^{-1}$]
s_1^k	solid phase concentration on first kinetic sorption sites [$M_c M_s^{-1}$]
Γ	concentration on AWI [$M_c L^{-2}$]

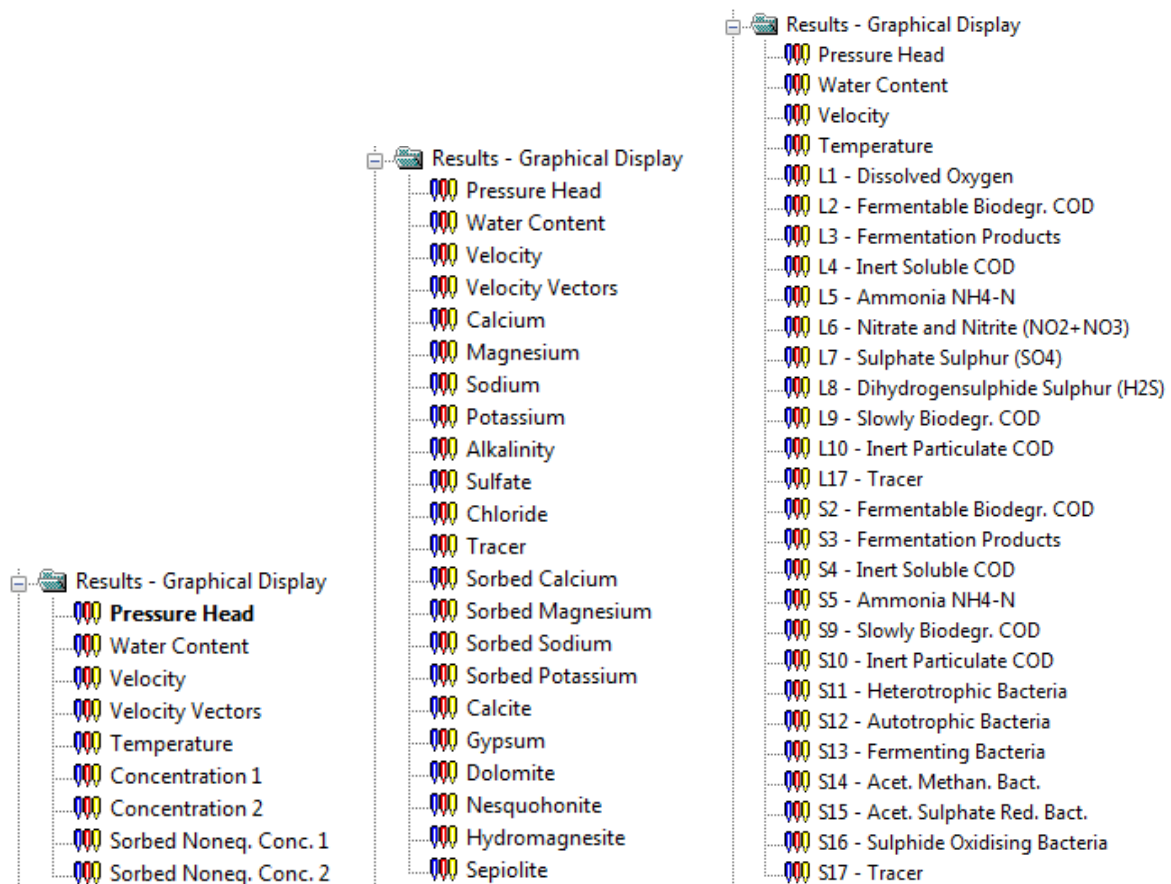


Figure 155. The "Results - Graphical Display" part of Data Tab of the Navigator Bar for the standard (left), Unsatchem (center), and Wetland (right) modules.

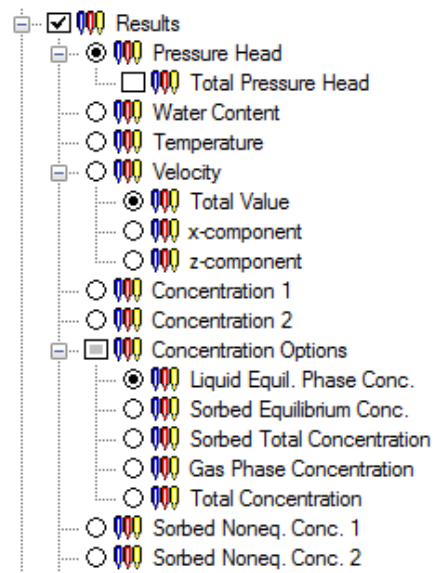


Figure 156. The "Results" part of the View Tab of the Navigator Bar displaying various alternative variables.

7.1.2. Display Options

The **Display Options** dialog window (Fig. 157) allows users to select

- how different objects from the **Category** list are to be displayed,
- what **colors** are to be used (colors can be redefined by clicking on the *Edit Color* command button),
- whether **lines** are displayed as solid, dotted, dashed, or dash-dotted (*Line Type*), and what *Thickness* should be used, and
- the position of **numbers** for various types of *numberings*, fonts for the numbers, and whether or not numbers are *Transparent*.

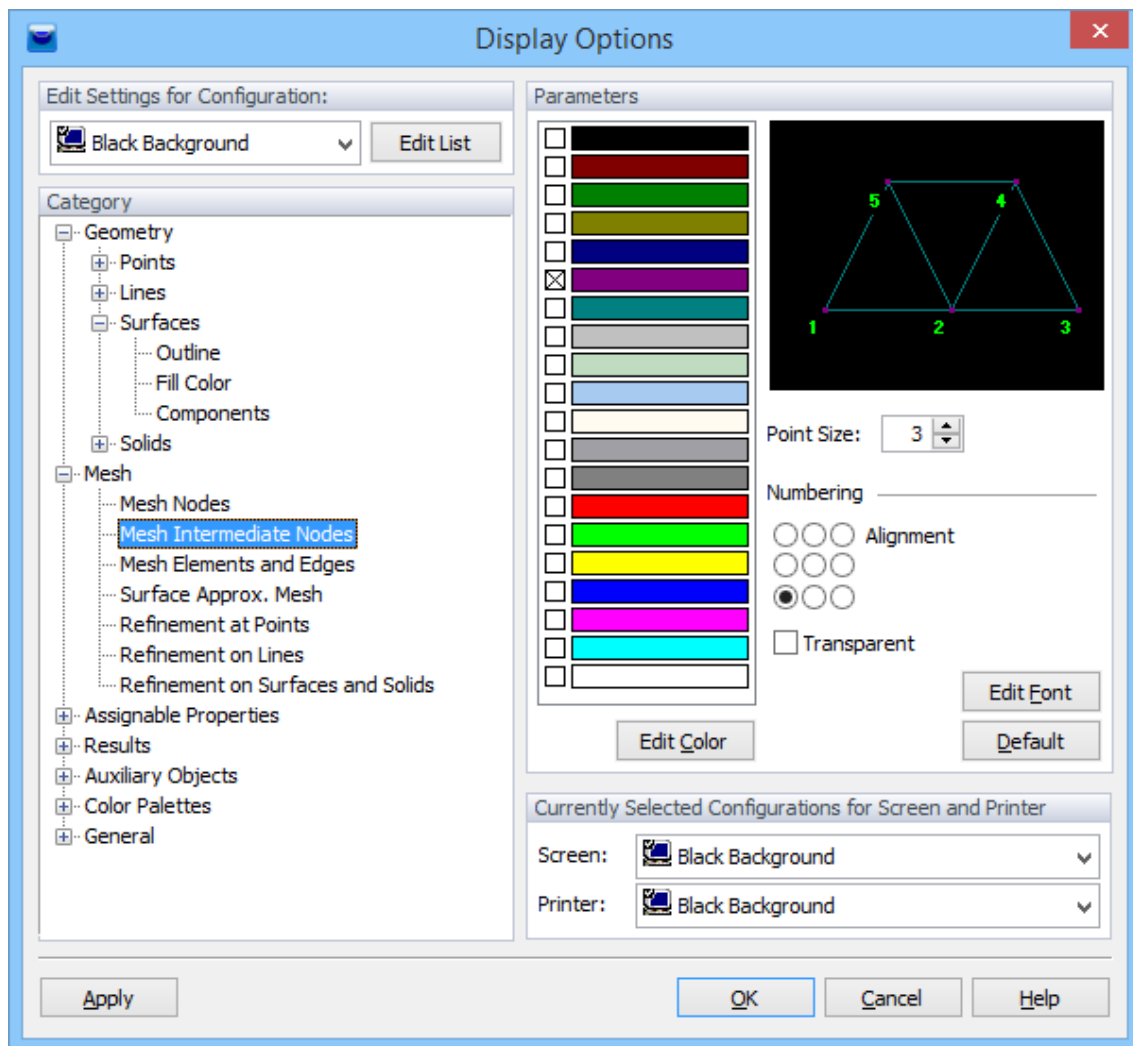


Figure 157. The Display Options dialog window.

7.1.3. Edit Isoband Value and Color Spectra

The **Edit Color Scale** dialog window (Fig. 158) (called by left-clicking the color scale display options of the **Results** version of the **Edit Bar**) allows users to define colors for the display of isobands isosurfaces, and color spectra, and values of particular isolines. The default scale always has 11 values, which corresponds to 11 colors for color contours and 12 colors for isolines. Values at the scale are calculated by evenly dividing the interval between the minimum and maximum of a particular variable. Numbers are formatted depending on units used to display a particular variable. When the number of displayed digits is insufficient, it is possible to use a scientific format (**E-format**). The E-format is then used also on the Edit Bar and for printing (only for a particular variable).

Note that switching from a regular format to the **E-format** also represents switching from the **Standard Scale** to the **Custom Scale** (see below), which is then kept for the display of the same variable at other times. Returning to the **Standard Scale** may be required to adjust the scale as needed to display a given variable at the new time.

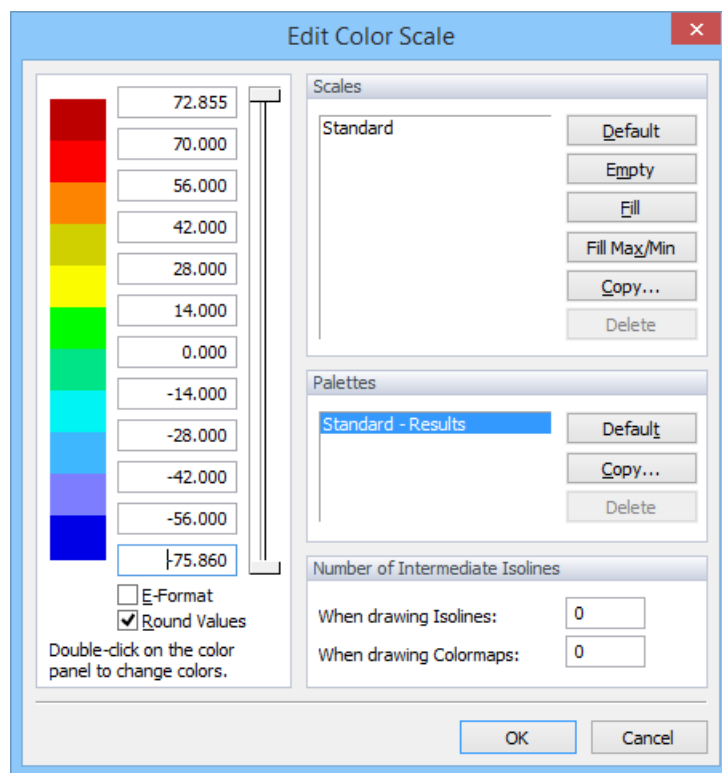


Figure 158. The Edit Color Scale dialog window.

Users can also define the **Color scale** (for contours and isolines). This can be done by simply changing the numbers in the edit boxes next to the colors. If the numbers are not in increasing or decreasing order, a warning will be issued. When modifying isoline scales, it is necessary to observe the rule that the difference between two adjacent values $d > (\max - \min) * \text{FLT_EPS}$,

where min and max are the minimum and maximum values from the value field of the currently displayed quantities, and $FLT_EPS = 1.192096e-07$. This condition is related to the precision of floating-point constants. If this condition is not met, users should switch the **Color Smoothing** option on.

The color scale numbers can be set by defining the first two (highest) numbers of the scale and then dragging the scale button down (Figure 159).

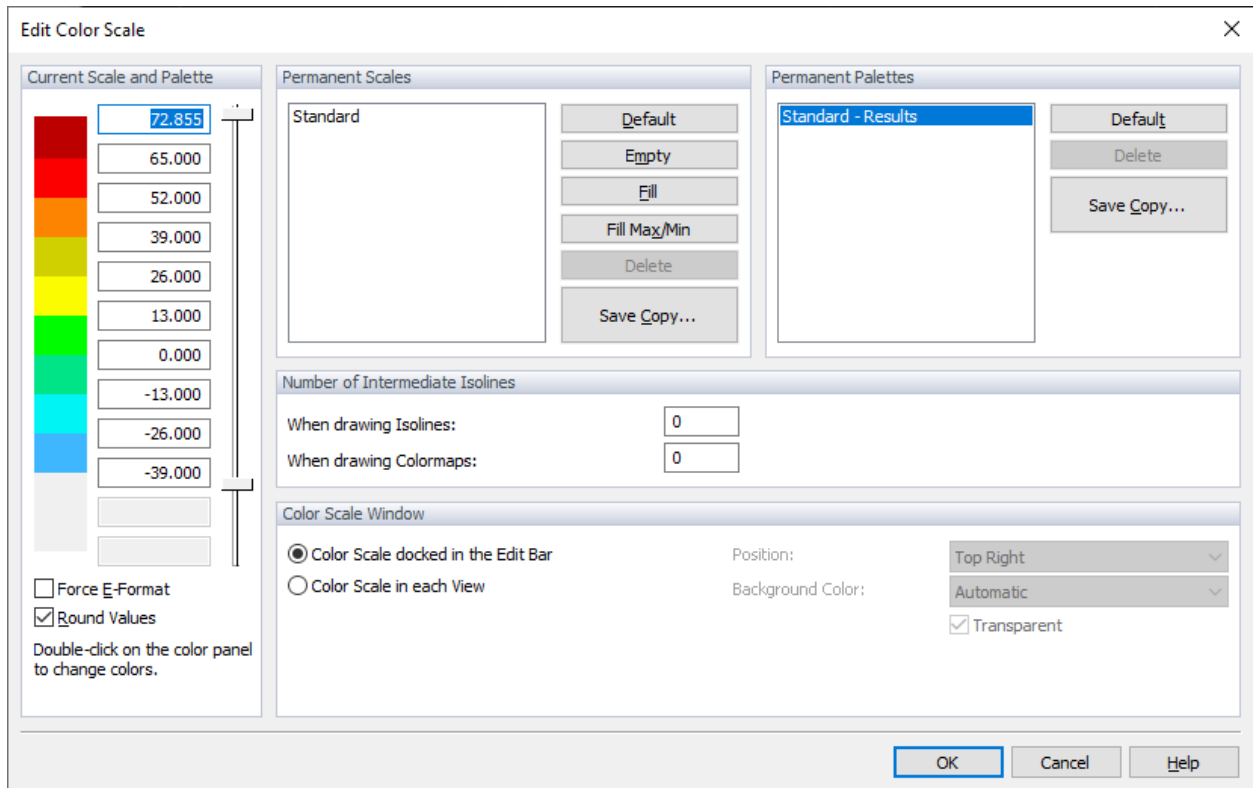


Figure 159. Setting values of the Color Scale.

Newly created **Color scales** can be saved (again locally or globally) and used later. Users need to specify only the maximum and minimum values (the top and bottom edit boxes); after clicking the **Fill** command, the program will calculate and fill (complete) the intermediate numbers by interpolation. A specified **Number of Intermediate Isolines** can be drawn between the main isolines using *When drawing Isolines* or *When drawing Color Contours*. This number is by default equal to zero. Five intermediate isolines are used in Figure 160. Version 3 also offers a new option for automatic numbering of isolines and displaying positions of minimum/maximum values of a current quantity. The **Color Scale** can be either docked on the Edit bar (the **Dock Color Scale in Edit bar** command) or displayed directly in the **View Window** (the **Display Color Scale in Each View** command).

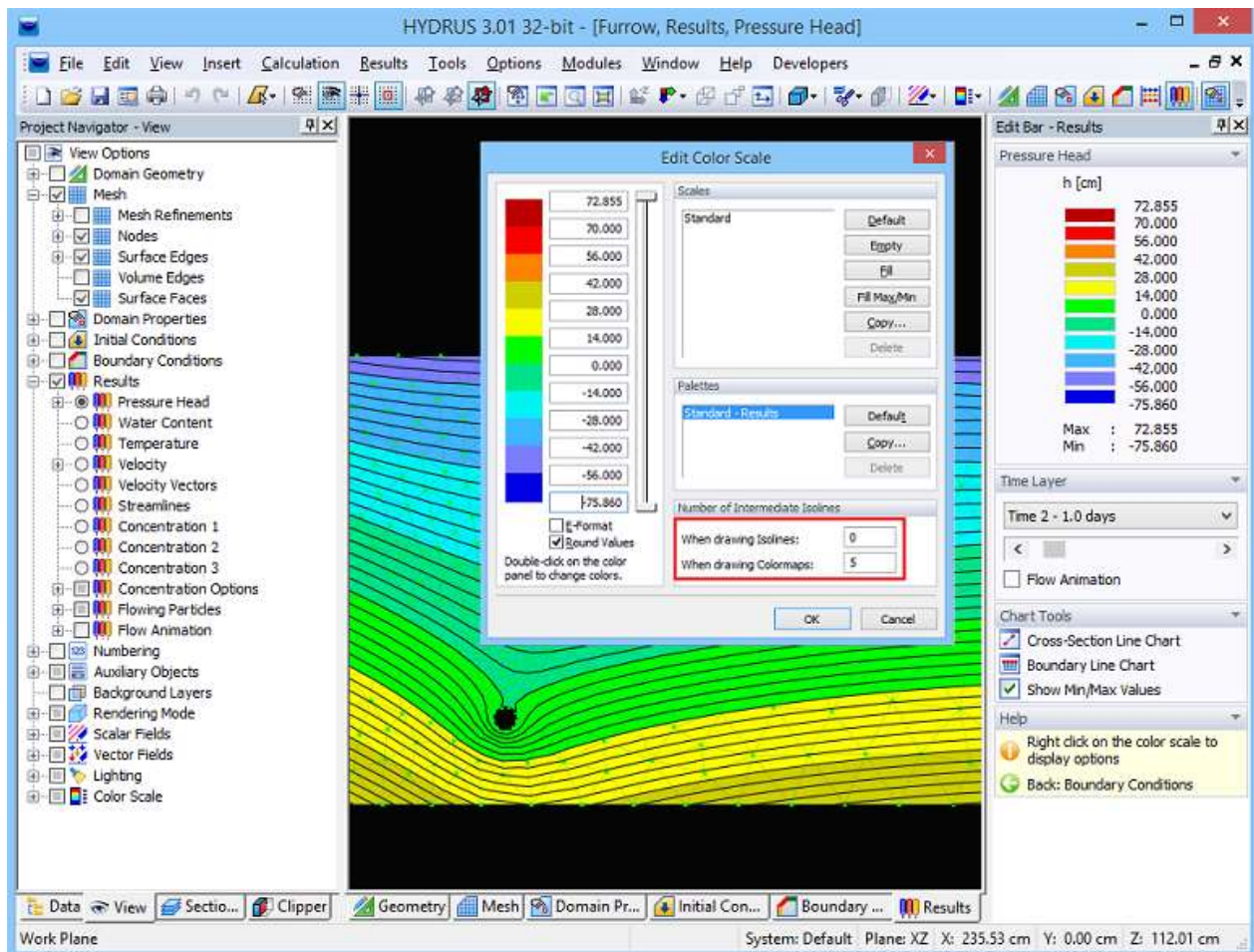


Figure 160. The use of intermediate isolines.

The minimum and maximum numbers of the scale are automatically adjusted to a particular problem and for a particular variable. By default, HYDRUS searches all output time levels of a particular project for the minimum and maximum values of a particular variable and then leaves the scale invariant in time between these two values. The scale, however, can also be automatically adjusted for each time level by specifying the minimum and maximum values for a particular variable and a particular print time when the option *Min/Max global in time* from the **Color Scale View Options** of the **View Tab** of the **Navigator Bar** is deselected. Similarly, the scale can be automatically adjusted for a particular layer of the FE-mesh (a section) (the minimum and maximum values for a particular variable and a particular section) when the option *Min/Max global in space* from the **Color Scale View Options** of the **View Tab** of the **Navigator Bar** is unselected.

After clicking on the color panel with the **left** mouse button, the **Color** dialog window (Fig. 161) appears, in which one can redefine colors to be used in displays. By default, a **Standard Palette** is used. If a Custom Scale exists for a displayed variable, colors for this scale will be displayed even when the **Standard Scale** was currently used (since the Standard Scale cannot be edited). Palettes with newly defined colors can be saved (Save Palette) under a new name and used for different purposes. The new palette can be saved locally and used with the given application or

globally and used for all HYDRUS applications. Users hence can, in this way, define different palettes for displaying water contents, pressure heads, concentrations, or temperatures. Since the Standard Palette cannot be changed, once any color is changed, the program will request to save a new scale under a new name. The changed colors will be used for all displayed variables (not only the actual one).

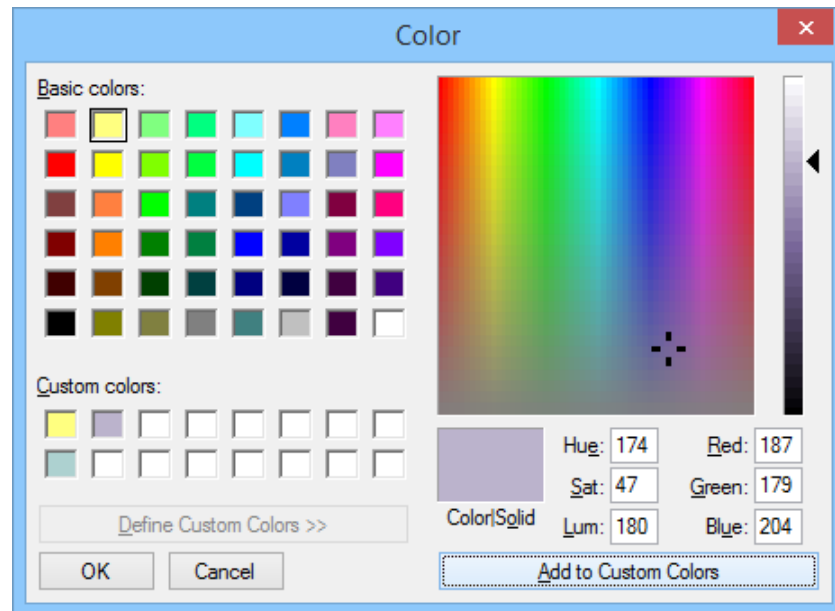


Figure 161. The Color dialog window.

Custom Scale

A user can define his/her own scale that is then remembered by the software and used for a particular variable in a given project. When one wants to use a certain scale also in other projects, he/she needs to save it using the **Save** command.

Other commands:

- **Default** – Sets the number of intervals to 11 and automatically fills values for the default scale
- **Empty** – Deletes all values (used with commands **Fill** and **Fill Max/Min**)
- **Fill** – Fills empty spaces between specified upper and lower values using linear interpolation
- **Fill Max-Min** – Similar to **Default**, except that this command does not set the number of values to 11 (it uses the number of values selected by a user)
- **Save** – Saves the Scale for use with other projects
- **Delete** – Deletes a selected **Custom Scale**

The number of values at the Scale cannot be increased; it can only be lowered (from 11) using a “slider“. By drawing a slider, one can also generate values at a Scale (see Figure 162):

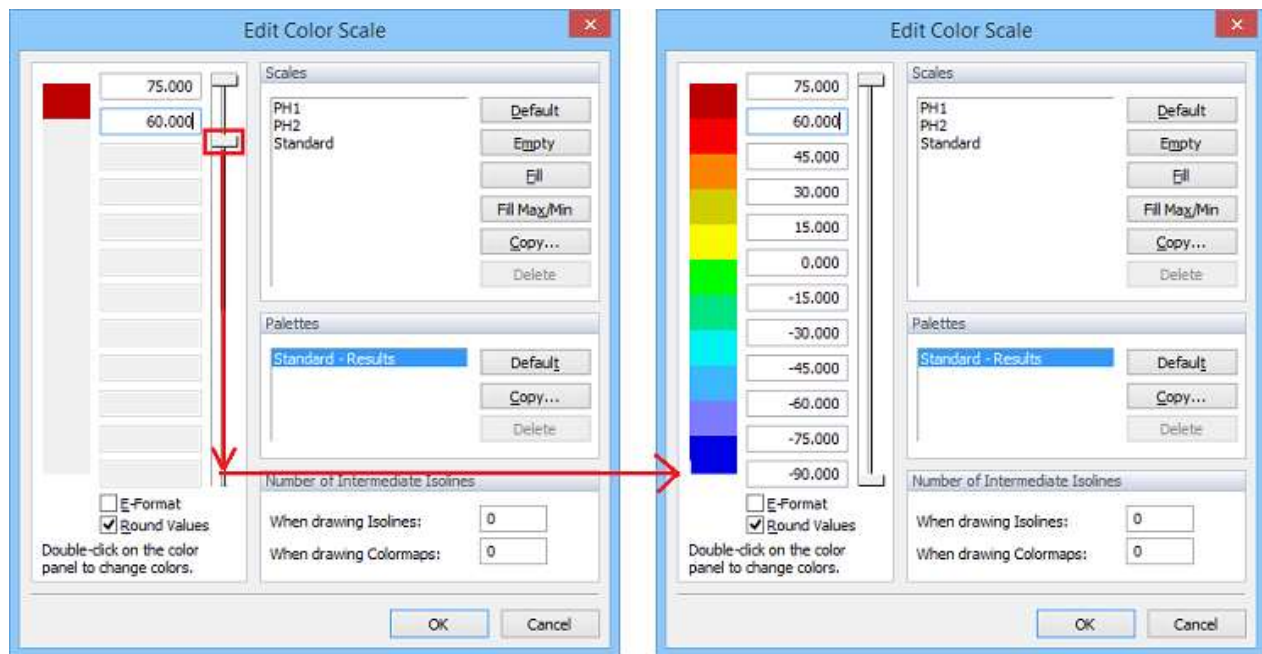


Figure 162. Adjusting scale in the Edit Isoband Value and Color Spectra dialog window.

When using a **Custom Scale**, the actual minimum or maximum of a displayed variable can be outside of the interval of the scale. Values outside of the interval of the scale are not displayed in the View window, resulting in empty spaces, as shown in the upper part of see Figure 163.

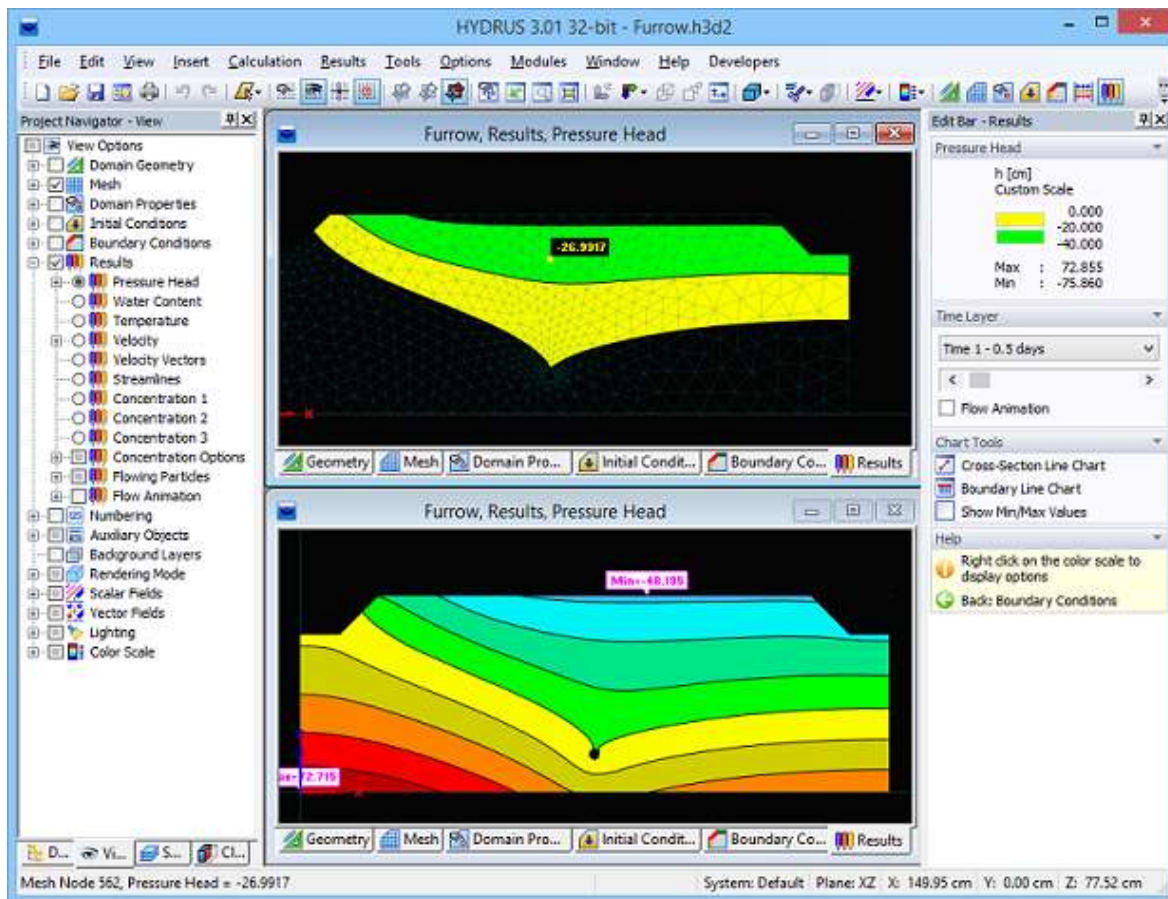


Figure 163. The use of the Custom Scale.

A **right** mouse button click on the Color Scale at the Edit Bar displays the menu for a fast change of various options related to scale.

- **Color Smoothing** – colors will change smoothly between particular iso-spectra corresponding to changes of the displayed variable (upper View at Figure 164).
- **Reverse Colors** – reverses colors in the color scale.
- **Min/Max global in Time** - the scale of a certain variable is defined by the minimum and maximum of all values from all time levels.
- **Min/Max global in Space** - the scale of a certain variable is defined by the minimum and maximum of all values over the entire transport domain.
- **Standard Scale** – uses the Standard Scale, while the Custom Scale for a given variable (if it exists) is remembered.
- **Custom Scale** – uses the Custom Scale if it exists. If it does not exist (default), this button is disabled. If one wants to use the Custom Scale, he/she needs to first create it in the **Edit Scale and Colors** dialog.
- **Edit Scale and Colors.**
- **Dock Color Scale in Edit bar** – docks the **Color Scale** on the Edit bar.
- **Display Color Scale in Each View** - displays the **Color Scale** in the **View Window**.

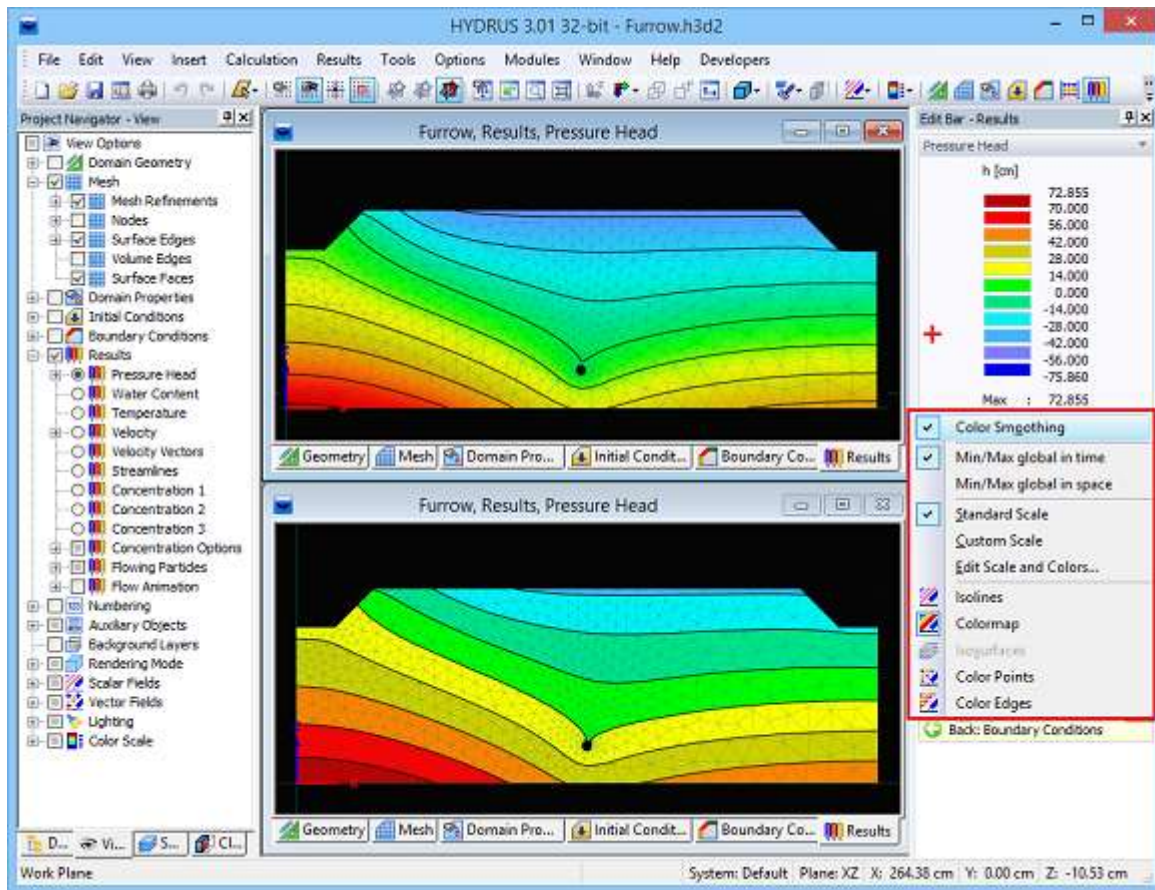


Figure 164. The color smoothing.

The values associated with individual isolines can be displayed using the checkbox on the Navigator Bar: Scalar Fields->Isolines->Display Values (see Figure 188). If one wants to add manually values to a particular point in the display, one can do that using the tool called Point Probes (see Section “4.7.6. Points Probes” and Fig. 105).

The *Separation Lines* between different *Contours* can be displayed (or hidden) using the checkbox on the Navigator Bar: Scalar Fields->Colormaps->Separation Lines.

7.1.4. Export Isolines

The **Export Isolines** command (File->Export->Export Isolines) saves coordinates of all currently displayed isolines (the *Isolines Graph Type* has to be selected) into a Project_Property_Isolines.txt text file (e.g., Furrow_Pressure_Head_Isolines.txt). Figure 165 displays an example of this file for the **Furrow** project. In the text file, a definition of each isoline is given first (e.g., Isoline 1, Value=-60.000, Segment 1), followed by the x and z coordinates of sequential points, in which the isoline crosses edges of finite elements. The **Export Isolines** command can be used, for example, to export coordinates of the groundwater table. In such a case, a custom scale with one single value ($h=0$) could be prepared and exported.

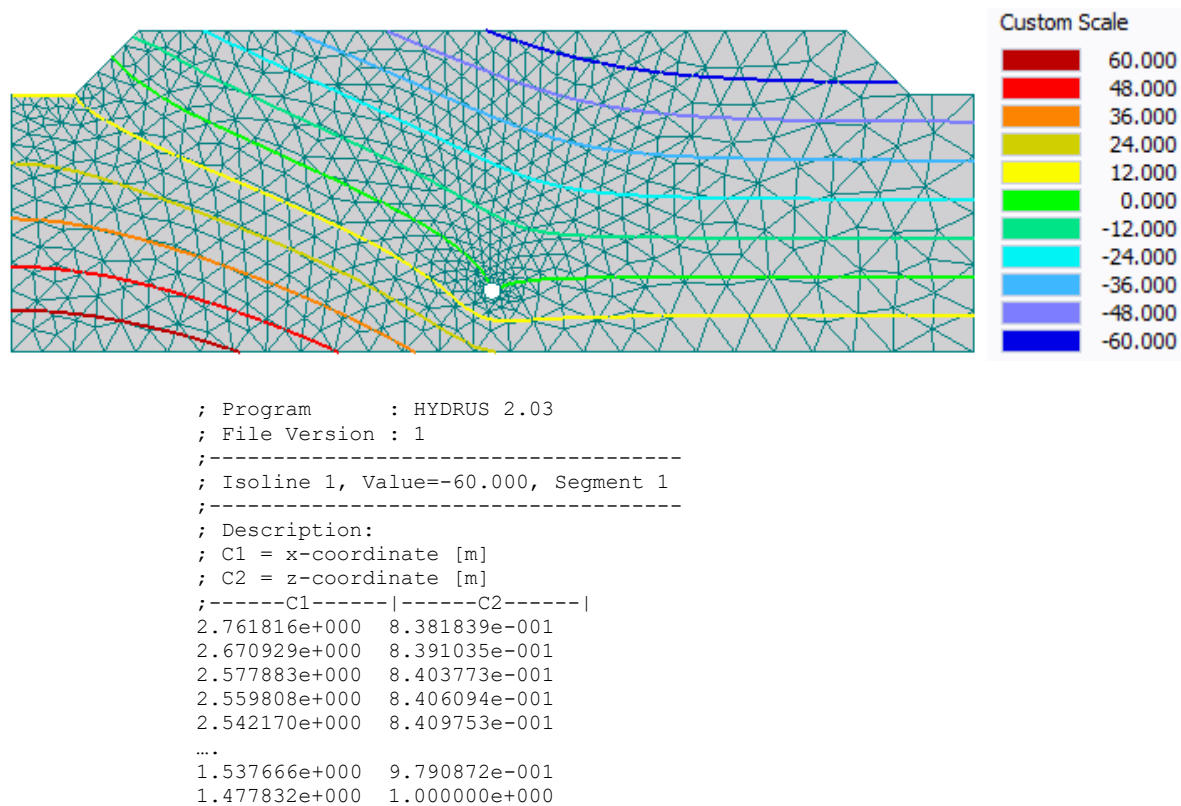


Figure 165. An example of the Project_Property_Isolines.txt text file (e.g., Furrow_Pressure Head_Isolines.txt; an excerpt) for the Furrow project (displayed in the top of the figure).

7.1.5. Streamlines

Previous Version 2 of HYDRUS (2D/3D) allowed one to show flowing particles, but only in two dimensions. Flowing particles are hypothetical objects that can be defined at any location of the transport domain by users, with the program then calculating trajectories and positions of these particles with time considering unretarded convective transport. The “flowing particles” feature is now available for both 2D and 3D projects.

A new feature of Version 3 is the calculation and display of streamlines for a given steady-state flow velocity field. Streamlines are one of the most commonly used graphical representations of CFD (computational flow dynamics) results in that they can display very clearly the flow direction, such as shown in Figure 166. The software now also has an option to run flow animations, i.e., the movement of particles along streamlines (Fig. 167). Users can save this animation as a video file and use in presentations of HYDRUS results.

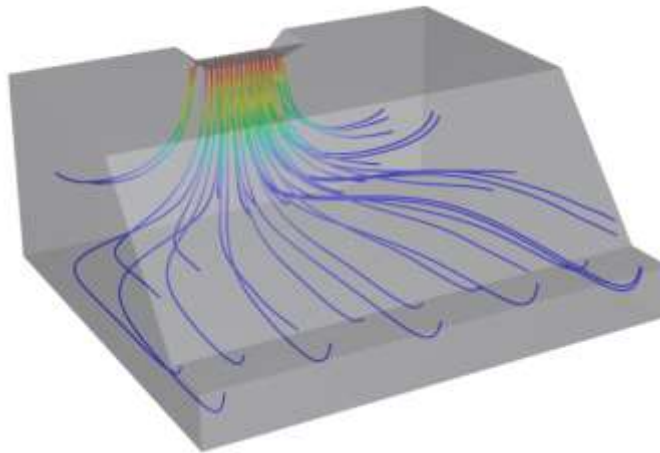


Figure 166. Example showing **3D Streamlines**. Streamlines can be calculated for a given time layer (i.e., steady-state flow) from a set of seed points. Seed point sources of several types can be set graphically.

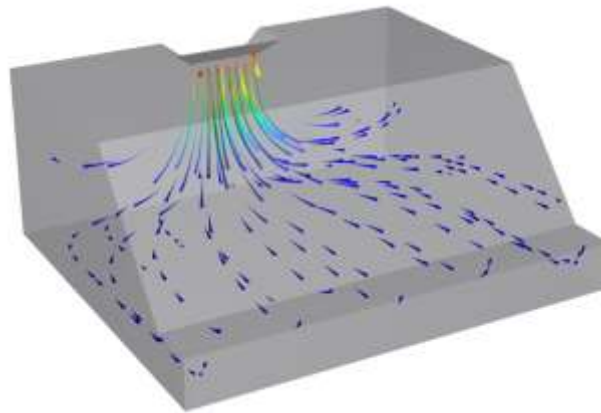


Figure 167. Example of **Particle Animation**. The movement of particles can be animated as flowing-lines or flowing-particles.

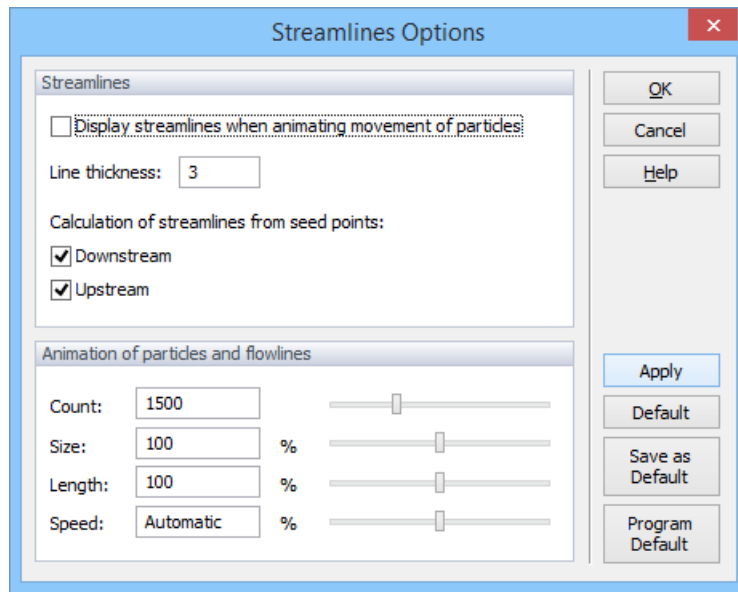


Figure 168. The Streamlines Options dialog window.

The Streamline Options are selected in the Streamlines Options dialog window (Fig. 168). In this window, users can select whether streamlines are displayed when the movement of particles is animated (*Display streamlines when animating the movement of particles*), the *Line thickness* of streamlines, whether the streamlines are calculated from the seep points "*Downstream*" or "*Upstream*", and the parameters for the *Animation of particles and flowlines*".

7.1.6. Clipper and Slicer

New graphical tools called “**Clipper**” and “**Slicer**” that can be used to cut or slice a 3D mesh is available in Version 3.0. Figures 169 and 170 show examples of these two applications. The **Clipper** and **Slicer** are controlled by a graphical tool called a Manipulator (see Figs. 169 and 172). Using this tool, the position and rotation of the plane can be defined. The **Clipper** has two modes, i.e., a **Plane** mode (Figs. 169 and 174) and a **Box** mode (Fig. 175).

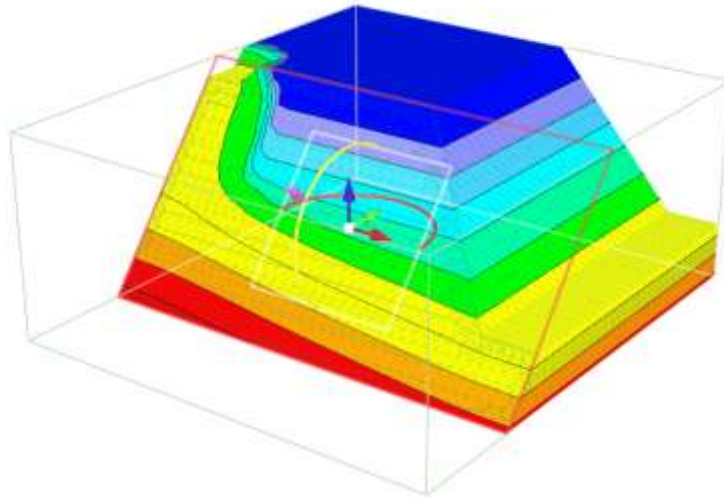


Figure 169. Example showing **3D Clipping**. When working with 3D models, the visible mesh (or geometric objects) can be clipped to view values inside the domain. The clipper is controlled by a graphical tool (a manipulator; see Fig. 169).

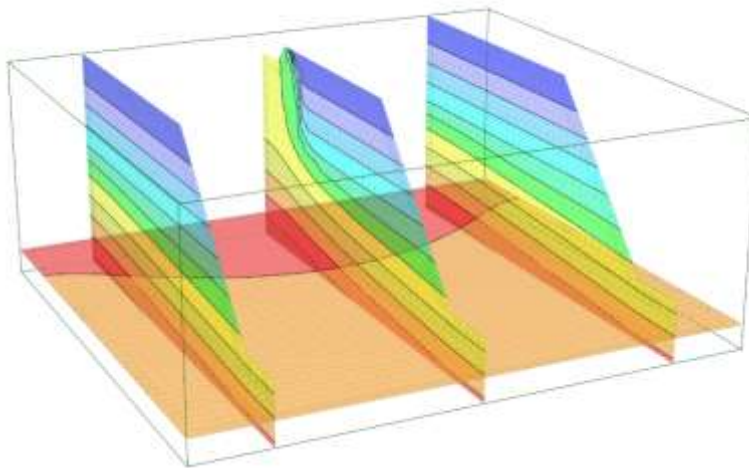


Figure 170. Example showing **3D Slicing**. The slicer is another tool for better visualization of 3D objects. The number of slices, their position, and rotation can be set either in a dialog or graphically (see Figs. 169 and 172).

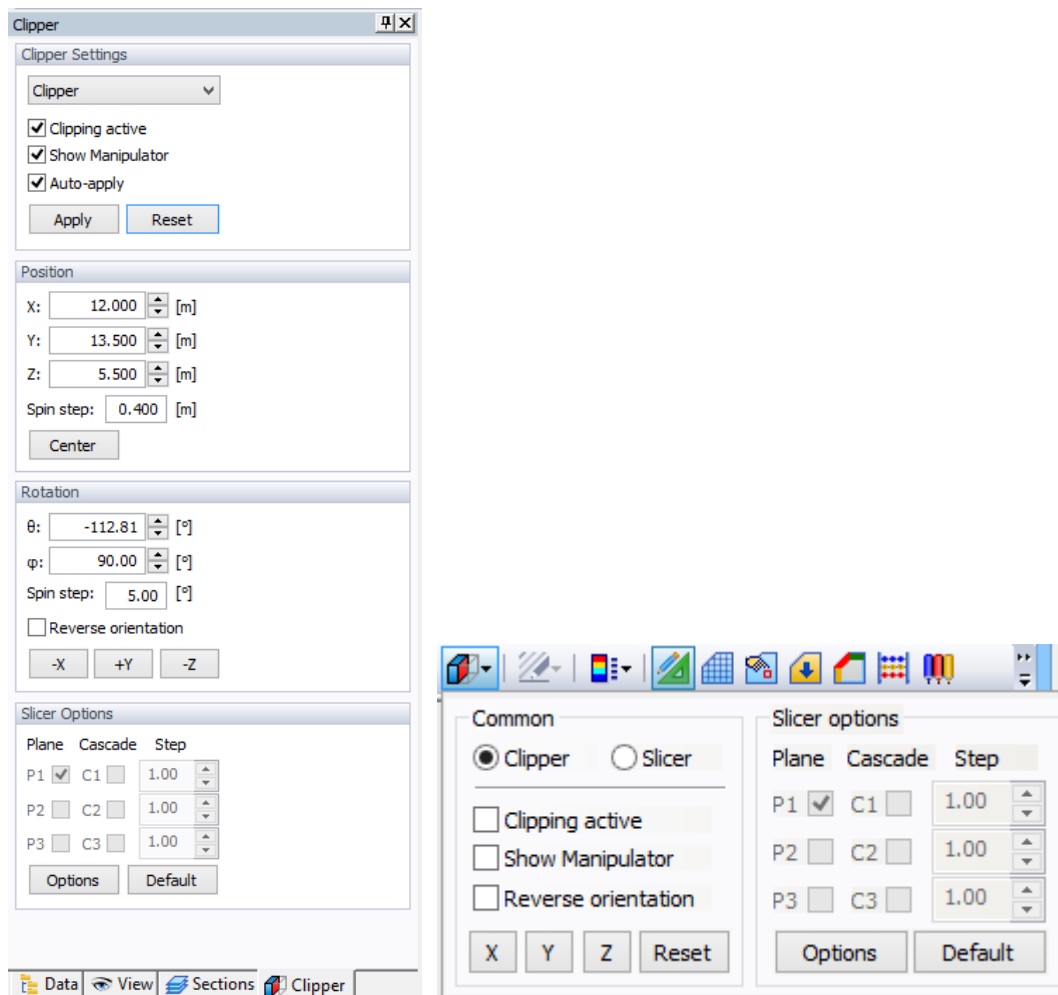


Figure 171. The Clipper Tab on the Edit bar (left) and the Clipper/Slicer setting dialog window activated from the toolbar.

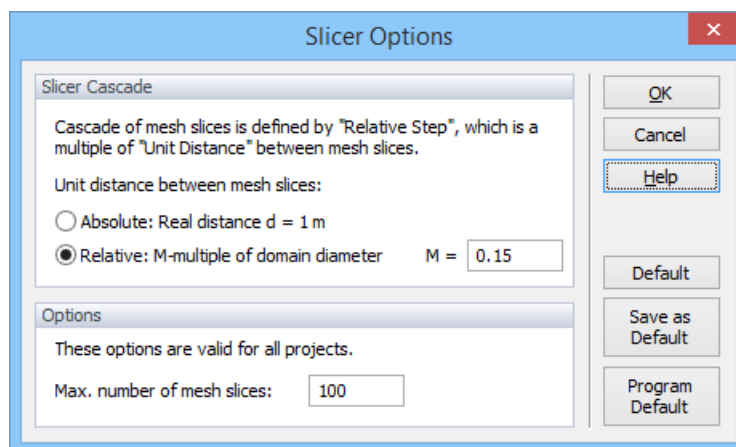


Figure 172. Slicer Options dialog window.

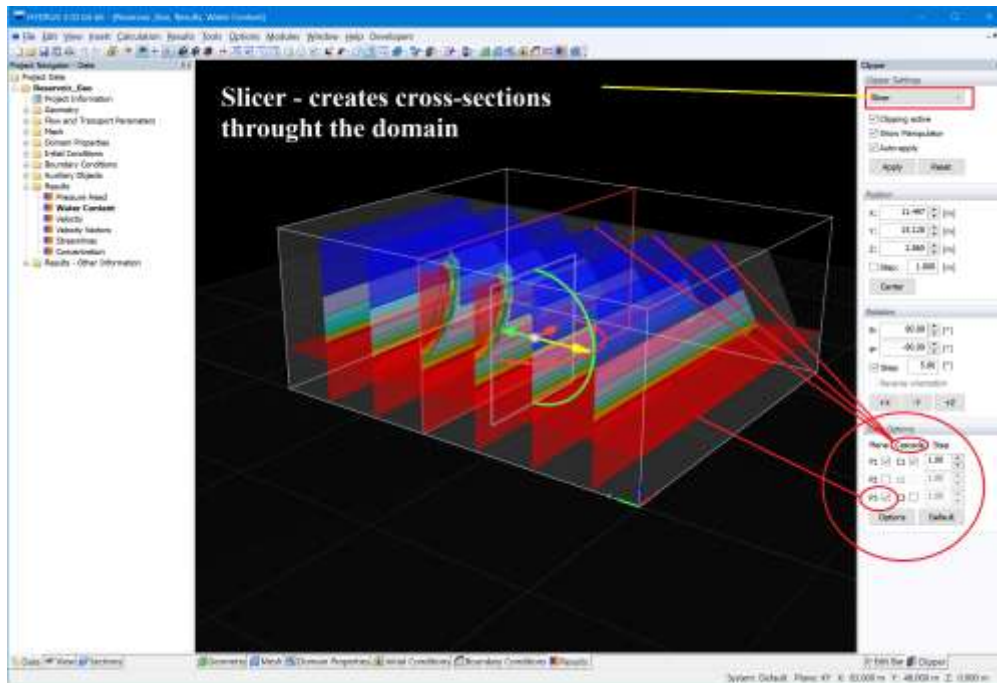


Figure 173. An example of the **Slicer** tool with 6 vertical and one horizontal cross-sectional planes.

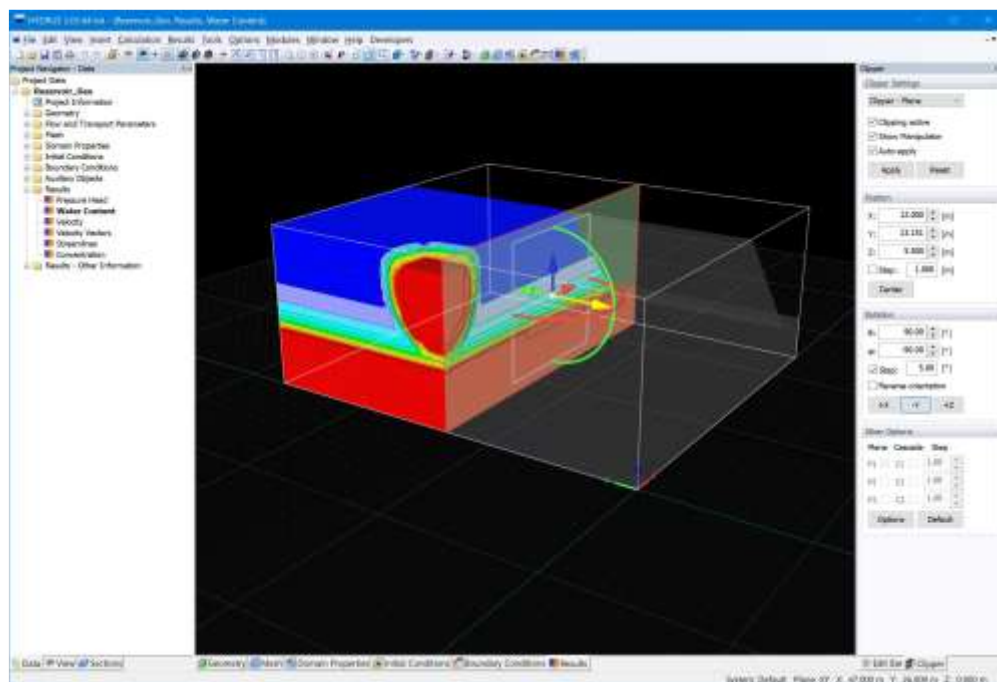


Figure 174. An example of the **Clipper Plane** tool with a displayed manipulator (defining the position and rotation of a display plane).

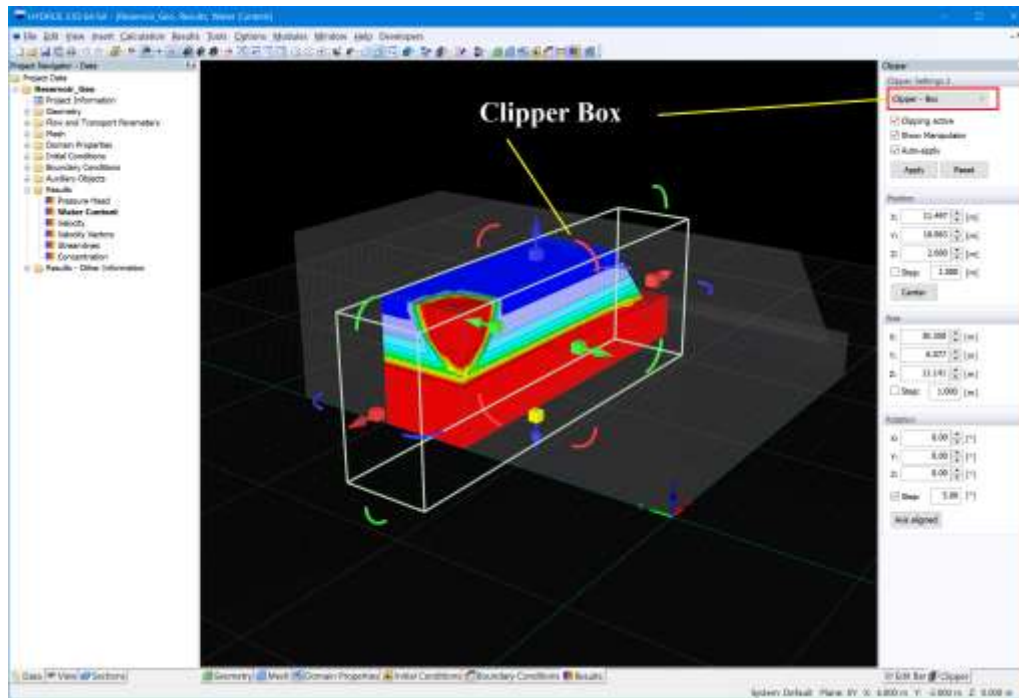


Figure 175. An example of the **Clipper Box** tool with a displayed manipulator (defining the position and rotation of the box).

7.1.7. Velocity Vectors

One of the variables that can be displayed spatially are **Velocity Vectors** (Darcian fluid flux densities). By default, velocity vectors are shown in all finite element nodes. All velocity vectors can be enlarged or reduced by using constant **Arrow Size** on the **Edit Bar**. The sizes of vectors can be either variable indicating the magnitude of fluxes by both the color and the size of the vectors, or uniform (*Uniform Size of Vectors*) when the magnitude of velocity vectors is indicated only by color.

However, the graphical display of velocity vectors for millions of mesh nodes is not only slow but usually also too complex for viewing. Version 3.0 of the GUI allows displaying velocity vectors either at mesh nodes or raster points, while the raster parameters (such as the density of points) are fully adjustable (Fig. 177). While **Raster** is a grid of points defining positions of velocity vectors, a **Raster Step** is a multiple of "Unit Distance" between raster points. Figure 176 shows an example of velocity vectors displayed at a Raster and Figure 177 shows how raster is defined.

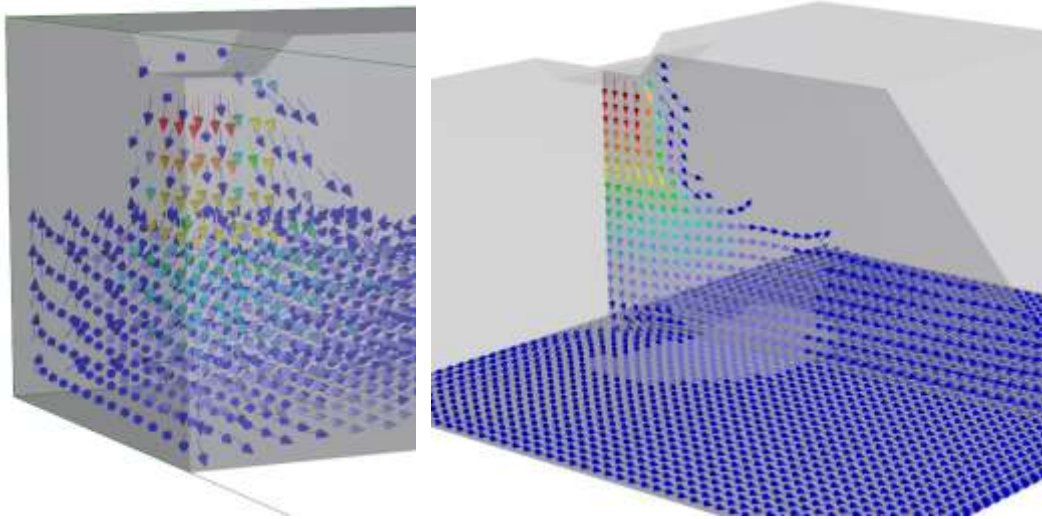


Figure 176. **Rasters for Vector Fields.** Vector fields can be displayed in mesh-independent rasters, i.e., regular 2D/3D grids with an arbitrary density of points. Rasters can also be used with the Clipper and Slicer.

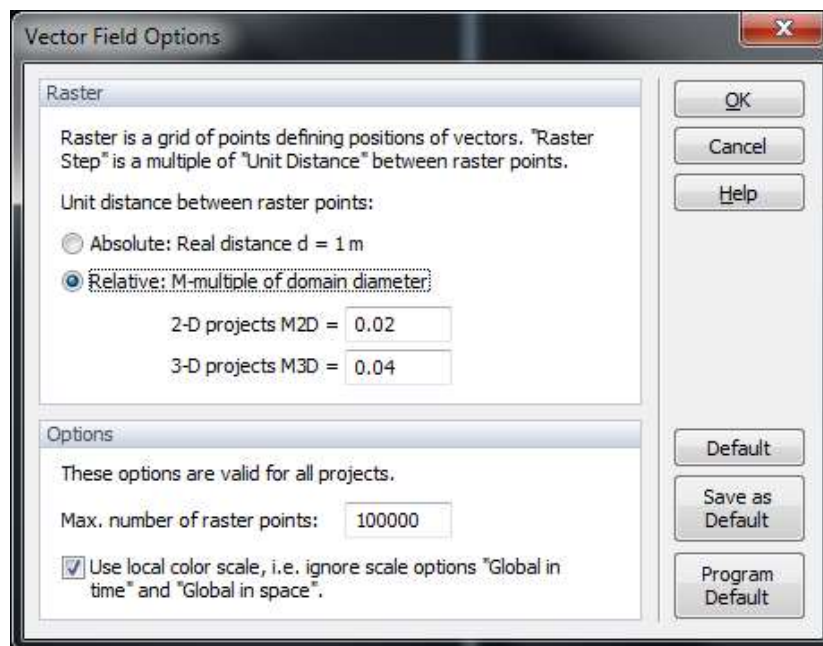


Figure 177. The Vector Field Options dialog window.

7.1.8. Export to ParaView

Although we believe that HYDRUS post-processing has all of the most important features needed for project execution, some users may require additional functions specific to their own needs. The new version of HYDRUS offers a robust solution by exporting all results to VTK files. VTK is a well-known open-source library intended for the visualization of scientific data. Exported HYDRUS results can then be opened in ParaView, such as illustrated in Figure 178, which is a free program based on VTK. Since both software products (VTK and ParaView) are open source, users have full control over the exported data and can implement any special post-processing as judged optimal for their application.

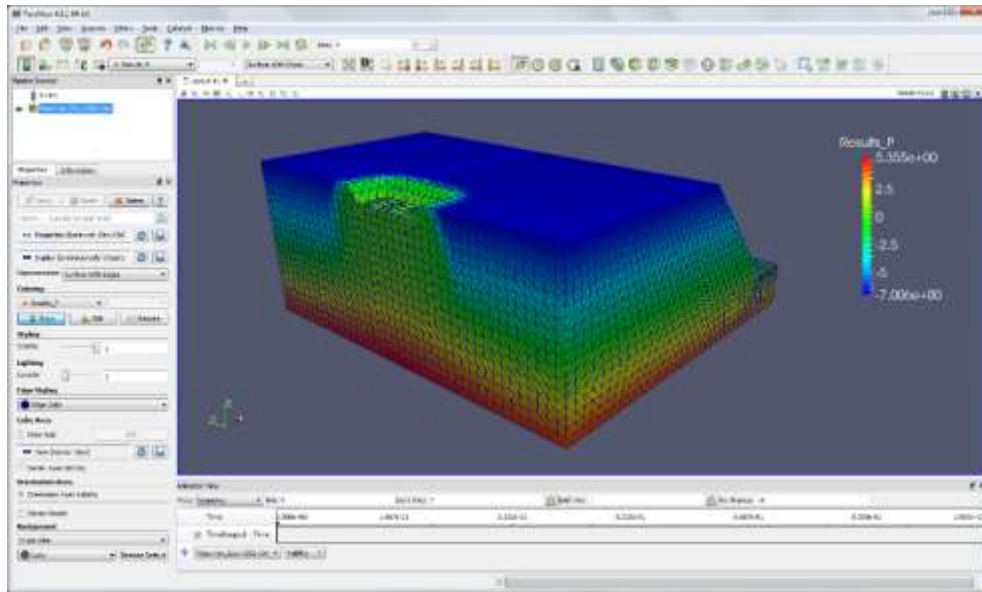


Figure 178. Example showing **Export to ParaView**. ParaView is an open-source, multi-platform data analysis and visualization application. New visualization options include custom post-processing based on scripting or plugin modules. Details are at www.paraview.org.

7.1.9. Display of 1D Results as z-t Surfaces

The results for one-dimensional applications can be displayed using the z-t surfaces (Fig. 179) (the command **Results as z-t surfaces** on the Edit Bar). The resulting graph will have the depth as a vertical axis and time as a horizontal axis. Since the graphical raster is defined by the Finite Element nodes and Print Times, the smoothness of this graph will depend mainly on the number of Print Times.

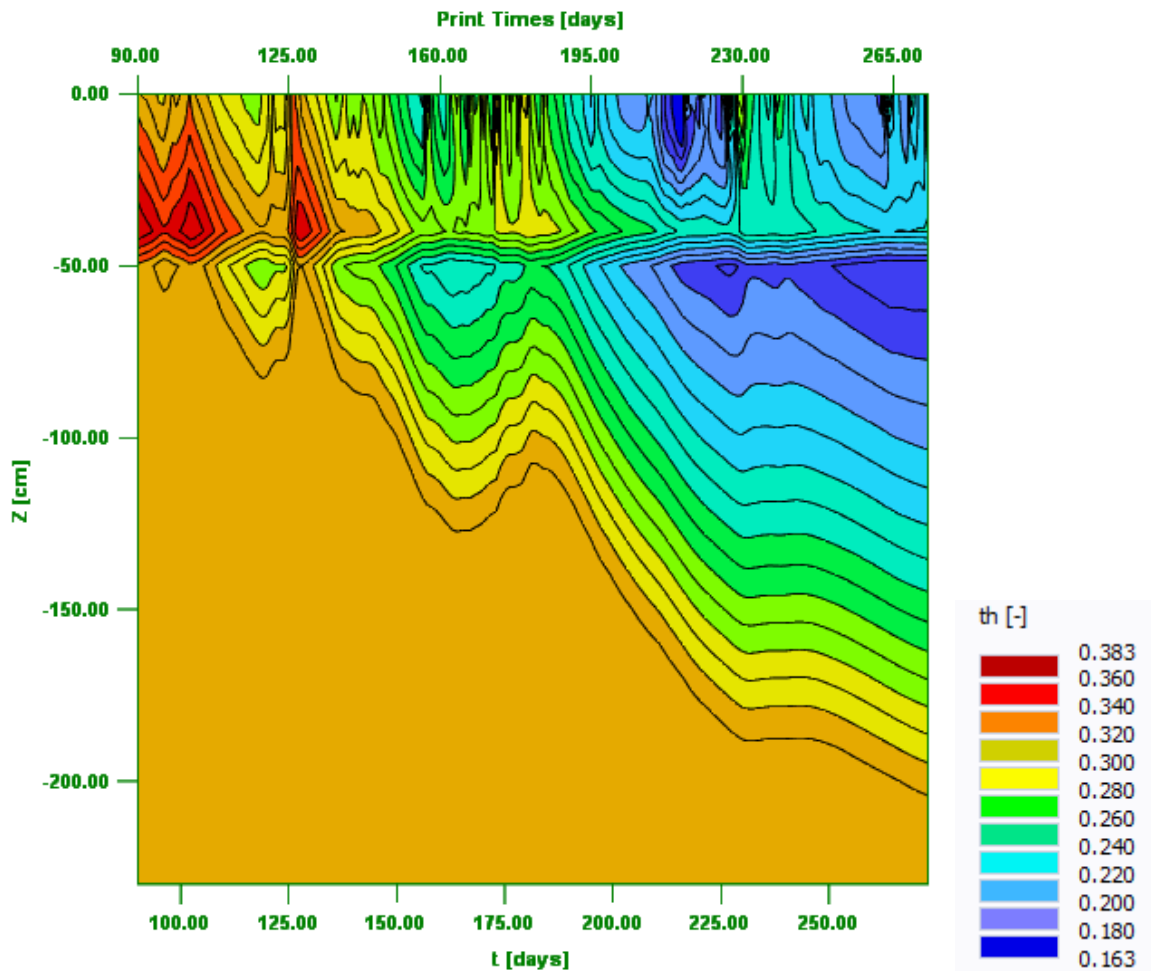


Figure 179. An example of the z-t surface for water contents for the two-layer Test2 example.

7.2. Convert to ASCII

The output files H.OUT, TH.OUT, CONCx.OUT, SORBx.OUT, TEMP.OUT, V.OUT, and AWIArea.out provide a binary output of specific variables. The user interface can convert these binary files into the ASCII files H.TXT, TH.TXT, CONCx.TXT, SORBx.TXT, TEMP.TXT, V.TXT, and AWIArea.txt using the **Convert to ASCII** dialog window (Fig. 180) (**Results – Other Information** on the **Data Tab** of the **Navigator Bar**, or *Results->Convert Output to ASCII*). The ASCII (text) files (e.g., h.txt, th.txt, v.txt) simply provide Print Time followed by a sequential list of values of a particular variable. These values are listed in the same order as Finite Element nodes. Coordinates for each FE node can be found in the MeshTria.txt file.

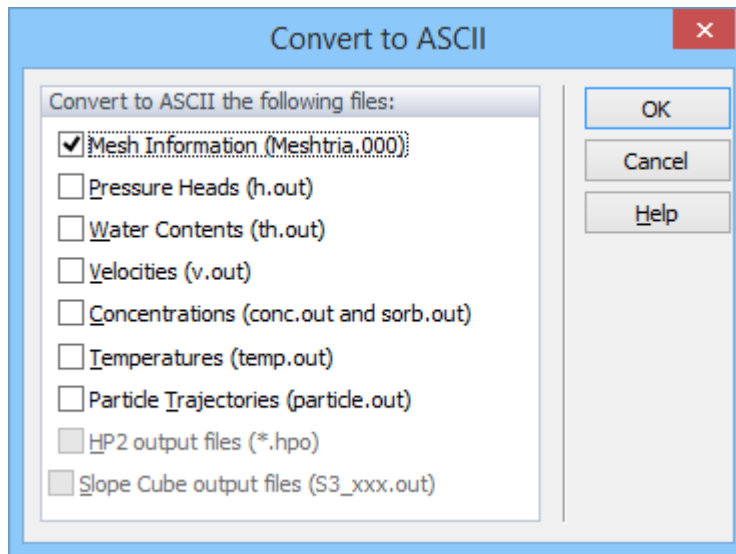


Figure 180. The Convert to ASCII dialog window.

7.3. Results – Other Information

Additional information, such as boundary fluxes and/or soil hydraulic properties, can be displayed using x-y graphs (**Results – Other Information** on the **Data Tab** of the **Navigator Bar**, or **Results Menu**, Fig. 181). Figure 181 shows the **x-y graph** dialog window that displays concentrations in observation nodes. Table 25 gives an overview of the different graph options that are possible. Two list boxes at the top of the **x-y graph** dialog window provide various combinations of graphs that are possible to display (Table 25). Browsing through various graphs is additionally also enabled using the *Previous* and *Next* commands. Double-clicking at various objects of the **x-y graph** (e.g., axis, title, captions, legend) will allow users to redefine them, i.e., to change their text, colors, or fonts. When the right mouse button is clicked above the graph, a pop-up menu will appear that will also allow users to redefine various objects of the **x-y graph**. One can, for example, change the text of both vertical and horizontal axis (*Axis->Title*) captions and titles (*Title*), their fonts, and colors; one can copy the content of the graph to the clipboard (*Copy*) for later paste in various other windows applications (e.g., MS Word, PowerPoint, or Excel), or one can change the thickness and colors of displayed lines. Many other modifications of the displayed **x-y graph** are possible. Data shown in the **x-y graph** can be exported into an ASCII file using the *Export* command. The **x-y graph** settings can be saved using the *Save* command. A selected variable can be displayed either for all or selected observation nodes.

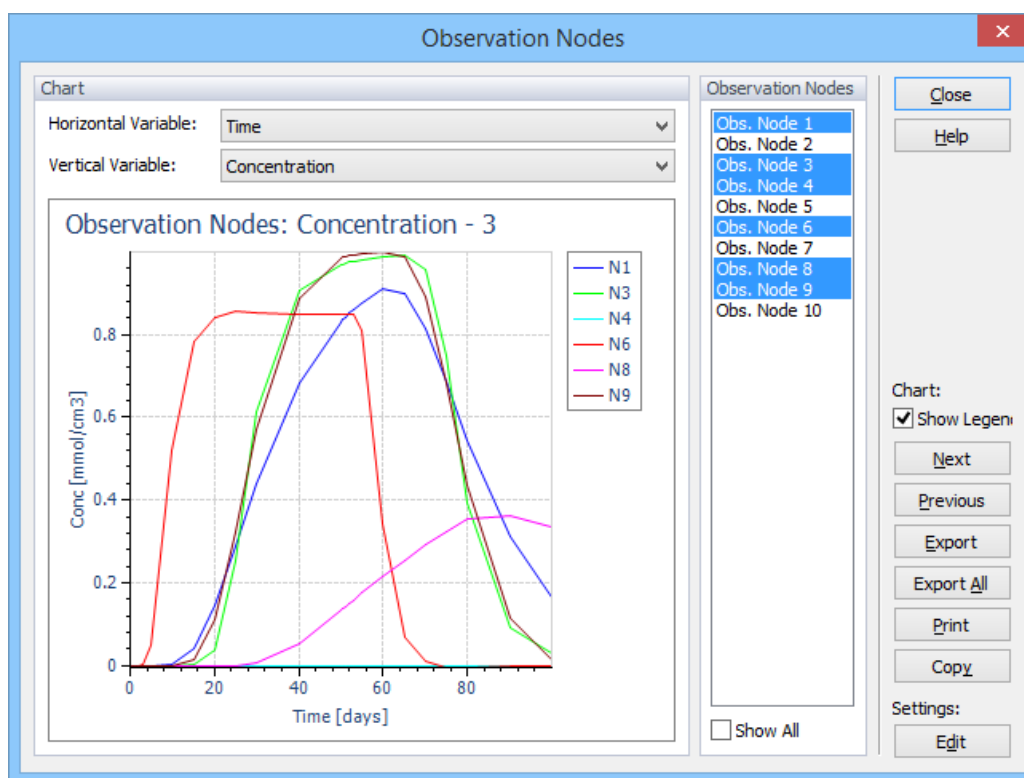


Figure 181. The x-y graph dialog window displaying concentrations in observation nodes.

Table 25. Graph options in the HYDRUS interface for 2D/3D applications.

Command	Horizontal Axis	Vertical Axis
Observation Points	Time	Pressure Head Water Content Temperature Concentration – x^+ Sorbed Concentration - x^+
Pressure Heads	Time	Atmospheric Boundary Head Root Zone Head Variable Boundary Head 1 Constant Boundary Head Seepage Face Head Drainage Boundary Head Free and Deep Drainage Boundary Head Variable Boundary Head 2 Variable Boundary Head 3 Variable Boundary Head 4 All Boundaries
Water Boundary Fluxes	Time	Potential Atmospheric Flux Potential Root Water Uptake Rate Actual Atmospheric Flux Actual Root Water Uptake Rate Variable Boundary Flux 1 Constant Boundary Flux Seepage Face Flux Drainage Boundary Flux Free and Deep Drainage Boundary Flux Variable Boundary Flux 2 Variable Boundary Flux 3 Variable Boundary Flux 4 All Atmospheric Fluxes All non-Atmospheric Fluxes Surface Runoff Infiltration Evaporation
Cumulative Water Boundary Fluxes	Time	Potential Atmospheric Flux Potential Root Water Uptake Rate Actual Atmospheric Flux Actual Root Water Uptake Rate Variable Boundary Flux 1 Constant Boundary Flux Seepage Face Flux Drainage Boundary Flux Free and Deep Drainage Boundary Flux Variable Boundary Flux 2 Variable Boundary Flux 3 Variable Boundary Flux 4 All Boundaries Fluxes Surface Runoff Infiltration Evaporation

Solute Fluxes ⁺	Time	Cumulative Zero-Order Reaction Cumulative First-Order Reaction Cumulative Root Solute Uptake Cumulative Non-Equil. Mass Transfer Cumulative Constant Boundary Solute Flux Cumulative Seepage Face Solute Flux Cumulative Variable Boundary 1 Solute Flux Cumulative Atmospheric Solute Flux Cumulative Drain Boundary Solute Flux Cum. Free/Deep Drainage Bound. Solute Flux Cumulative Variable Boundary 2 Solute Flux Cumulative Variable Boundary 3 Solute Flux Cumulative Variable Boundary 4 Solute Flux Constant Boundary Flux Seepage Face Flux Variable Boundary Flux 1 Actual Atmospheric Flux Drain Boundary Flux Free and Deep Drainage Boundary Flux Variable Boundary Flux 2 Variable Boundary Flux 3 Variable Boundary Flux 4 All Solute Cumulative Fluxes All Solute Fluxes
Soil Hydraulic Properties	Pressure Head Log Pressure Head Water Content	Water Content Soil Water Capacity Hydraulic Conductivity Log Hydraulic Conductivity Effective Water Content Pressure Head Log Pressure Head
Run-Time Information	Time Level Time	Time Step Number of Iterations Cumulative Number of Iterations Peclet Number Courant Number Number of Solute Iterations

⁺ This graph is given for each solute

The *x-y graphs* have only a limited capacity and can display only a certain number of data points and 20 lines. If a dataset to be displayed has more data points than allowed, then the automatic selection is made by the program (only each *n* data point is displayed), and a warning (*File is too big to be displayed entirely! Automatic selection has been made.*) is issued. If the number of observation nodes is larger than 20, only the first 20 observation nodes are displayed.

Table 26. Graph options in the HYDRUS interface for 1D applications.

Command	Horizontal Axis	Vertical Axis
Observation Points	Time	Pressure Head Water Content Temperature Concentration – x^+ All Concentrations
Observation Points*	Time	Ca, Mg, Na, K, Alk, Sulfate, Chloride, Tracer, EC, SAR
Profile Information	Pressure Head Water Content Hydraulic Conductivity Hydraulic Capacity Water Flux Root Water Uptake Temperature Concentration – x^+ Sorbed Concentration - x^+	Depth
Profile Information*	Solution Concentrations	Depth
Profile Information*	Solid Concentrations	Depth
Profile Information*	Chemical Information	Depth
Water Flow Information	Time	Potential Surface Flux Potential Root Water Uptake Actual Surface Flux Actual Root Water Uptake Bottom Flux Cum. Potential Surface Flux Cum. Potential Root Water Uptake Cum. Actual Surface Flux Cum. Actual Root Water Uptake Cum. Bottom Flux Surface Pressure Head Root Zone Pressure Head Bottom Pressure Head All Fluxes All Cumulative Fluxes All Pressure Heads Surface Run-Off Cum. Surface Run-Off Soil Water Storage Cum. Infiltration Cum. Evaporation Cum. Non-Equil. Water Transfer Snow Layer
Solute Transpor Information ⁺	Time	Surface Solute Flux Bottom Solute Flux Cumulative Surface Solute Flux Cumulative Bottom Solute Flux Cumulative Zero-Order Reaction

		Cumulative First-Order Reaction Surface Concentration Root Zone Concentration Bottom Concentration Root Solute Uptake Cumulative Root Solute Uptake Cum. Non-Equil. Mass Transfer All Solute Fluxes All Cumulative Solute Fluxes All Concentrations
Particle Tracking	Time	Depth
Soil Hydraulic Properties	Pressure Head Log Pressure Head Water Content	Water Content Soil Water Capacity Hydraulic Conductivity Log Hydraulic Conductivity Effective Water Content Pressure Head Log Pressure Head
Run-Time Information	Time Level Time	Time Step Number of Iterations Cumulative Number of Iterations Peclet Number Courant Number Number of Solute Iterations

+ This graph is given for each solute

* This graph is for the UnsatChem module.

When concentrations are displayed in the Basic Profile Information graph (Fig. 182) (in 1D applications), an additional list box appears (at the top right) allowing users to select various concentration modes, such as liquid phase concentrations, sorbed total concentrations, sorbed equilibrium concentrations, gas phase concentrations, and total concentrations.

Figure 183 shows the particle tracking graph, which displays trajectories of hypothetical particles that were initially in the soil profile or that were generated at the soil surface or the bottom of the soil profile. This graph include the **Statistics** button, which displays a window (Fig. 184) summarizing various particle statistics, such as the initial, final, and total number of particles, the number of particles released at the top and bottom of the profile, the start (when released) and end (when leaving the profile) day for each particle, and particle residence/travel time. Users can use this information to obtain a frequency distribution of particle travel times.

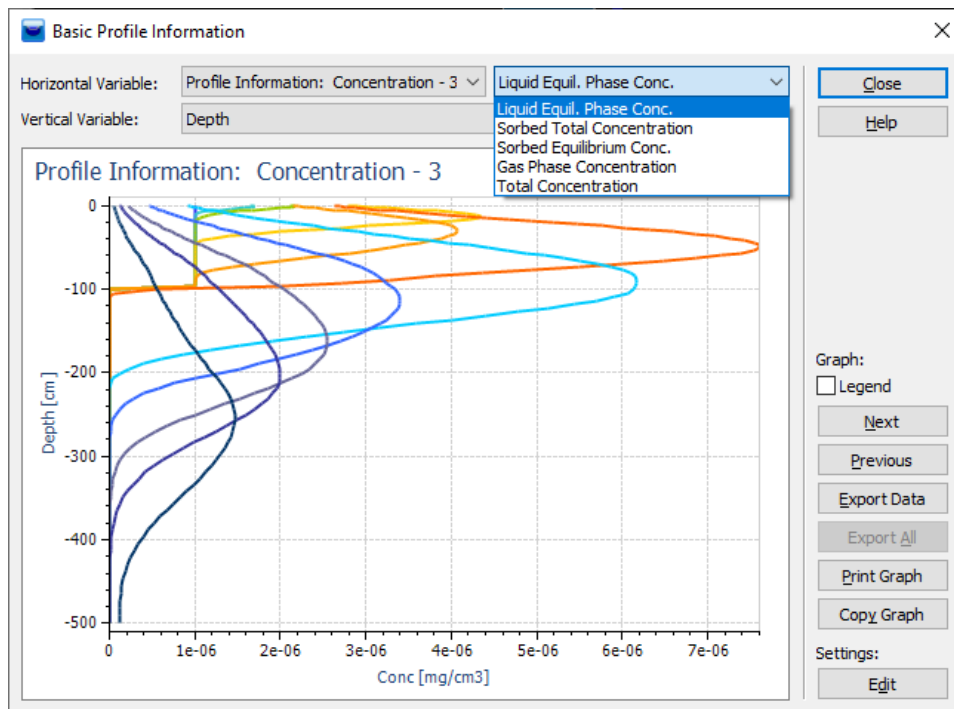


Figure 182. The Profile Information graph for concentrations.

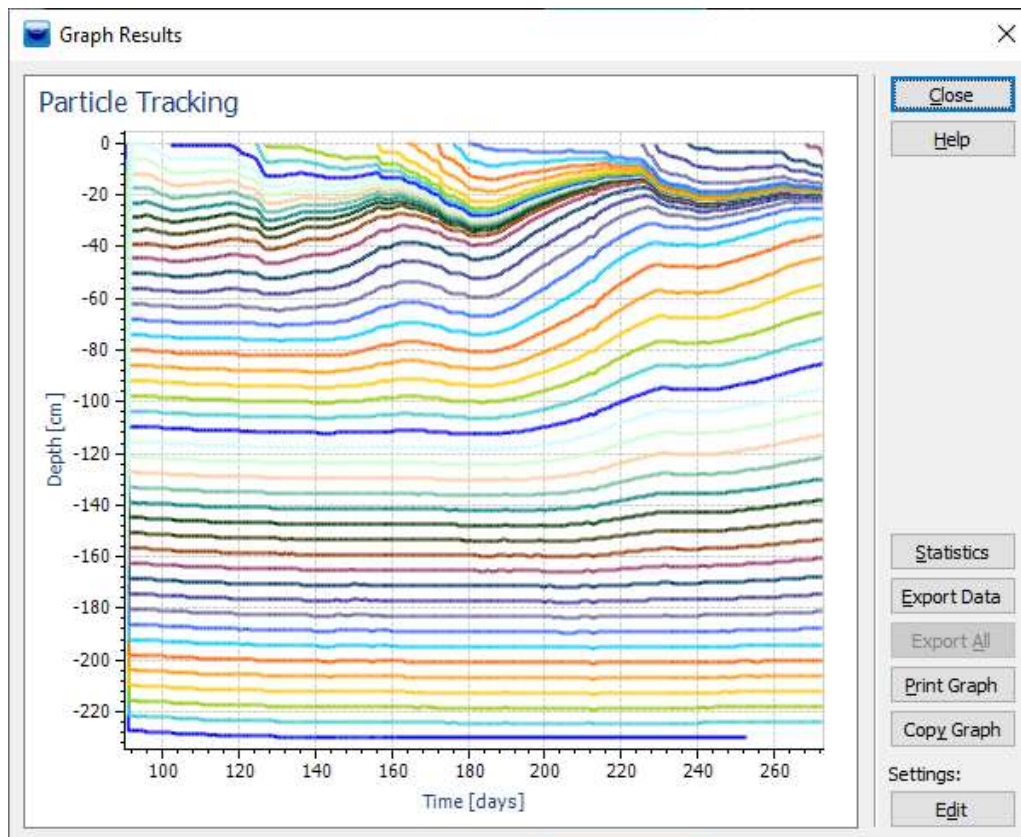


Figure 183. The graphical display of the Particle Tracking module results.

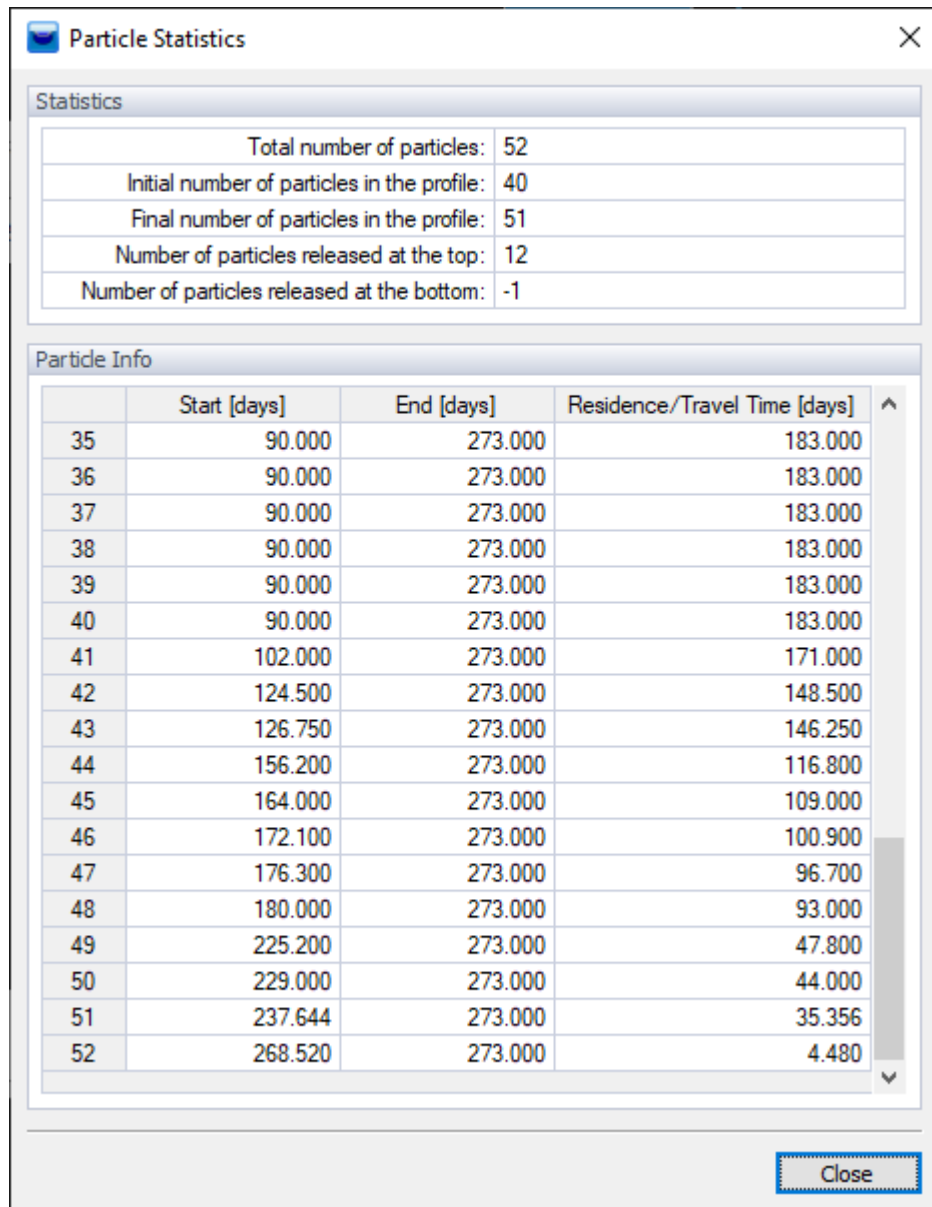


Figure 184. The particle statistics such as the start and end day, particle residence/travel time, the initial, final, and total number of particles, and the number of particles released at the top and bottom of the profile.

Additional text output is provided under the command *Mass Balance Information* on the **Data Tab** of the **Navigator Bar** (also at the **Results Menu**). This output gives the total amount of water, heat, and solute inside each specified subregion, and the inflow/outflow rates to/from that subregion, together with the mean pressure head (*hMean*), mean temperature (*TMean*), and the mean concentration (*cMean*) over each subregion (see Table 11.6 of the Technical Manual). Absolute and relative errors in the water and solute mass balances are also printed in this file. Output related to the inverse problem is provided under the command *Inverse Solution Results* on

the **Data Tab** of the **Navigator Bar**. The *Chemical Mass Balance information* (on the **Data Tab** of the **Navigator Bar** or at the **Results Menu**) is provided for the Unsatchem module. This file gives mass balances in different phases (liquid, sorbed, solid) for all major ions (i.e., Ca, Mg, Na, K, HCO₃, SO₄, and Cl).

The text dialog displaying *Mass Balance Information* or *Inverse Solution Results* had only a limited capacity in Version 1.x of HYDRUS. If the file to be displayed was larger than this capacity (when there are too many print times or a large number of data points in the inverse problem), a warning “*File is too big to be displayed entirely! Open it in any text editor.*” was given. Users, in such cases, needed to display the *Balance.out* or *Fit.out* files, respectively, directly using any text editor, such as *Notepad* or *WordPad*. Both files are located in the *Temporary Working Directory* (see Section 1). This capacity problem was overcome in Version 2 (and higher), and the dialog window now displays the button *Next* (or *Previous*), which allows browsing through larger text files.

8. Graphical User Interface Components

8.1. View Window

8.1.1. Scene and Viewing Commands

We will use here the term ‘**Scene**’ for the content of the **View** window. Four types of commands are available to change the display of the **Scene** in the **View** window.

a) Commands to define a required **Display of the Scene**.

Detailed information about particular commands is given in Section 8.4. In addition to those commands, it is always possible to adjust the **Display of the Scene** using the “mouse scroll wheel” as follows:

- Simultaneously holding the mouse scroll wheel and moving the mouse will move the **Scene** in the same direction as the mouse, i.e., to the left, right, up, or down.
- Simultaneously holding the **Ctrl** keyboard button and the mouse scroll wheel while moving the mouse rotates the **Scene** around the center of the displayed object (available only for three-dimensional objects).
- Simultaneously holding the **Shift** keyboard button and the mouse scroll wheel while moving the mouse leads to zooming in or out of the **Scene** from the center of the **View** window.
- Rotating the scroll wheel (up or down) while pointing the mouse to a particular point in the View window results in zooming (in or out) the **Scene** from this point.
- Simultaneously holding the right mouse button and the mouse scroll wheel while moving the mouse rotates the **Scene** around the center of the displayed object (available only for three-dimensional projects).

The above-described operations are available not only during selection (on existing transport domain), but also when defining basic geometric objects. This allows users to adjust the View window as needed without interrupting the process of graphically defining objects of the transport domain.

b) Commands to define the **Content of the Scene**.

In every view, one can independently specify what is to be displayed, e.g., a variable, the type of graph, or the numbering of objects. All possible options related to the **Content of the Scene** are located on the **Navigator Bar** of the **View Tab** (Section 8.2).

c) Displaying and/or hiding parts of complicated objects.

One often needs to display only some part of a complicated object while hiding the rest. For this purpose, one can use commands related to **Sections** (i.e., parts of the computational domain or FE-Mesh). Detailed information is given in Chapter 8.1.8 on **Sections**.

d) Colors, fonts, and types of lines.

One can define colors, the style, and thickness of lines, fonts for numbering, and other displaying options for almost all displayed/used objects. Separate default sets exist for the display for the screen and the printer. Users can create and save additional combinations of display options. Detailed information is provided in Chapter 7.1.1 on **Display Options**.

8.1.2. Grid and Work Plane

The **Grid and Work Plane** dialog window (Fig. 185) allows users to

- select a **Work Plane** (i.e., a plane in which users can specify various boundary objects, initial and boundary conditions, or other information),
- define the **Origin** of the coordinate system, and
- define the *Alignment Grid*. The **Grid** is defined by its *Origin*, the type (*Grid Type*) of the coordinate system involved (either *Cartesian* or *Polar*), and the *Grid Spacing*. The **Grid** can also be rotated to facilitate work, for example, when defining the domain for a hill slope problem.

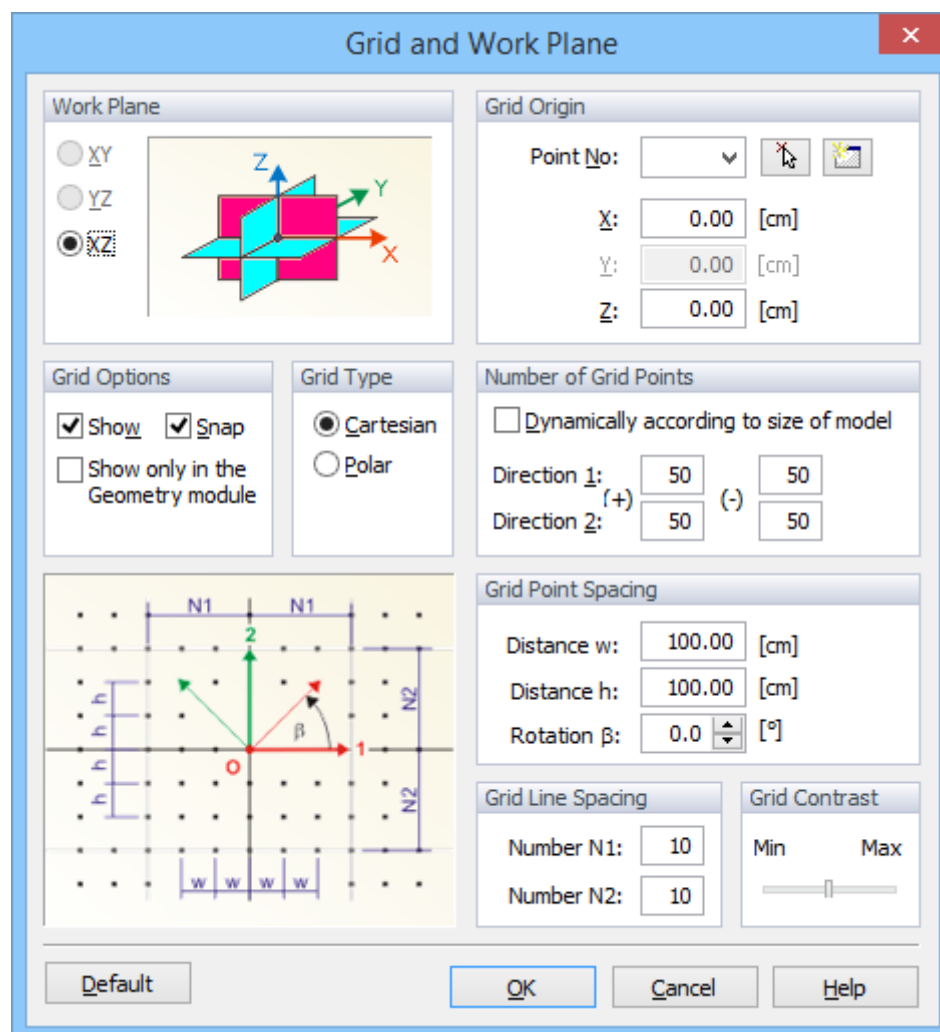


Figure 185. The Grid and Work Plane dialog window.

8.1.3. Stretching Factors

In many applications, one direction of the transport domain dominates the other direction (or the other two directions). To facilitate work in the graphical environment, HYDRUS allows stretching of the domain in one (or two) direction(s) using **Stretching Factors**. This is done using the **View Stretching Factors** dialog window (Fig. 186) that is called with the command *View->View Stretching*.

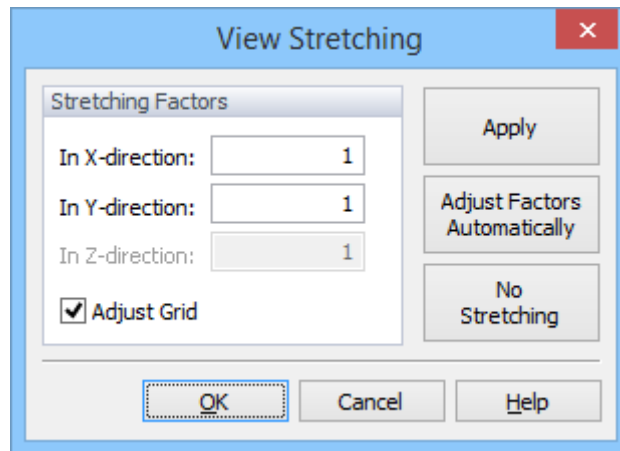


Figure 186. The View Stretching Factors dialog window.

Two options of View Stretching are available:

- a) **Strict Stretching** when all transport domain dimensions will be displayed as being the same. For example, a hexahedral of any dimensions will be displayed as a cube.
- b) **Mild Stretching**, which adjust view stretching only when large differences in dimensions in different directions exist. By default, there will be no view stretching when the largest dimension is five times larger than the smallest dimension.

A user should first select the **Method for Calculation of Stretching Factors** (either **Strict** or **Mild**), then click the command **Calculate Factors** (which will calculate stretching factors based on the method of stretching selected), and finally click the **Apply** command to update the **View Window**.

8.1.4. Rendering Model

Rendering serves to rapidly switch between displays of surfaces and solids. One can select the **Wire** and **Full Rendering** options. An advantage of **Wire Rendering** is mainly the speed of the display, while **Full Rendering** provides a more realistic display of three-dimensional objects.

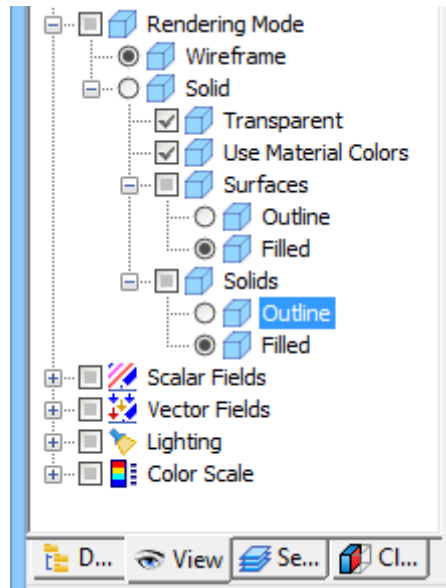


Figure 187. The Rendering part of the View Tab of the Navigator Bar.

The 3D graphics of Version 3 of HYDRUS was further improved by allowing the rendering to be smoother and faster. A transparent mode (object translucency) is now (in Version 3.0) available also for the graphical display of results. An example of this is shown in Figure 188.

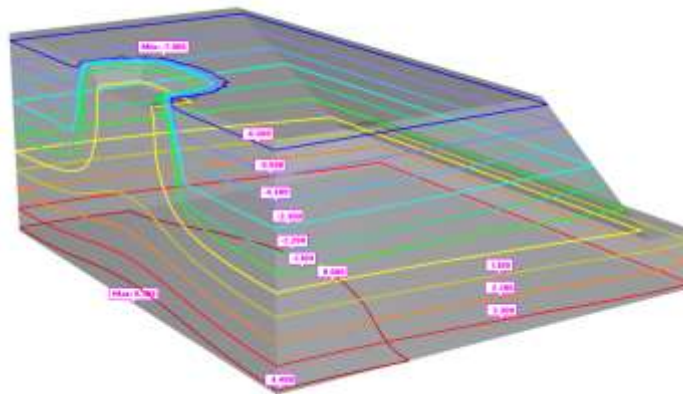


Figure 188. Example of the **Transparent mode** of the HYDRUS GUI. The Transparent mode is available for all types of graphical displays of scalar and vector fields. Isolines are automatically numbered, and min/max values of a particular variable in the transport domain are automatically identified.

8.1.5. Selection and Edit Commands

The **selection** of graphical objects is based on standards used in MS Office. An object is selected by clicking the left mouse button; a multiple selection is made by simultaneously holding the Shift button. A selection can be made using a rectangle (by clicking with the left mouse button outside of objects and holding the left mouse button while moving the mouse), rhomboid (see

Chapter 8.4. on **Toolbars** and **Tools**, with the *Edit->Select->Select by Rhomboid* command), circle (*Edit->Select->Select by Circle*) or polygon (*Edit->Select->Select by Polygon*).

In the Standard Selection Mode (*Edit->Select->Standard Selection Mode*), the status of the selected object is changed (selected or unselected) after its selection, i.e., the selection is toggled. If we want to only add or remove objects to or from existing selection (i.e., we want to prevent switching the status of selected objects (toggling)), respectively, it is possible to choose two special selection modes: “Add to Selection” (*Edit->Select->Add to Selection*) or “Remove from Selection”. (*Edit->Select-> Remove from Selection*). Both commands are accessible from the submenu *Edit->Select* or from the toolbar under the button “**Tools for Selection**”. Two special Selection Modes can also be activated by holding the “Left Ctrl” (*Add to Selection*) or “Right Ctrl” (*Remove from Selection*) keyboard buttons.

When the cursor (mouse) is moved above an object, information about that object appears on the status bar, and the object is temporarily highlighted; this process is referred to as **pre-selection**. Apart from selecting objects graphically, they can also be selected using their **Indices** or by means of **Sections**.

Double-clicking on selected objects or simultaneous holding the Alt+Enter buttons recalls dialogs for editing properties of particular objects. Most dialogs support **multiple editing**, i.e., if edit boxes with different values remain empty, the original values will not change. This feature allows, for example, Z-coordinates of multiple selected points to be changed while leaving the X- and Y-coordinates unchanged.

When different objects are selected simultaneously (e.g., points and curves), double-clicking causes a dialog window to appear from which objects can be selected for editing.

8.1.6. Pop-up Menus

Context-sensitive menus with useful commands for a particular object can be called from the **View** window when clicking the right mouse button. While the commands are also accessible from the main menu, right-clicking the mouse is much faster. Menus for multiple selections that may contain different types of objects operate in the same way. When the right mouse button is clicked, a default menu will appear when no object is close to the cursor.

When one clicks the right mouse button on the view window, the pop-up menu of Figure 189 will appear. This menu will allow users to

- a) select different views (*View*), i.e., Isometric, in X-direction, in Y-direction, in Z-direction, Reverse X-direction, Reverse Y-direction, Reverse Z-direction, or a perspective view.
- b) select *Numbering* (turns on and off the display of numbering for objects selected under *Numbering Options* on the **Navigator Bar**).
- c) go quickly to various *Numbering Options* (this command will bring the **Navigator Bar** to the View Tab on Numbering).
- d) switch *Full Rendering/Wire Rendering* (see 8.1.4).
- e) start the *Autorotate* function that will rotate the transport domain in the View window
- f) call the *Show Work Plane*, i.e., to show the axis, and the origin of the Work Plane

- g) call the **Set Grid and Work Plane** dialog window (Fig. 185) (*Set Grid and Work Plane*)
- h) select the *Coordinate System* (call the **List of Available Coordinate Systems** dialog window), and
- i) call the **Display Options** dialog window (Fig. 157).

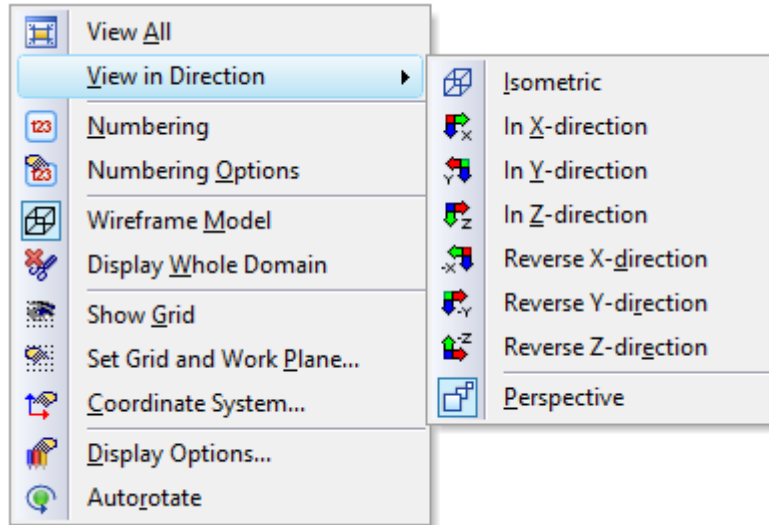


Figure 189. The Pop-up Menu from the View window.

8.1.7. Drag and Drop

By clicking and holding the left mouse button on selected objects in the **View** window, the **Drag and Drop** operation is started. This operation allows selected objects to be moved to a new location. Simultaneous holding the Ctrl keyboard button leads to the creation of a copy of the selected object. The copy can be moved into a different view or in a different open project. The operation terminates by holding the Esc button or by clicking the right mouse button. **Drag and Drop** can be used for most geometric objects, but also for auxiliary objects such as comments, labels, and bitmaps.

Holding the Shift button during the **Drag and Drop** operation leads to the movement of selected objects in a direction perpendicular to the current **Working Plane** (available only for three-dimensional objects).

8.1.8. Sections

Sections serve to divide complex objects (models) into simpler parts. Only the simpler parts are then displayed in the **View** window while the remaining parts are hidden. Two types of sections exist: those for geometric objects (**Geo Sections**) and those for the FE-Mesh (**FE-Mesh Sections**) (see also Section 5.7 and Table 19). New sections for both types can be created and named, a list of which is displayed on the **Section Tab** of the **Navigator Bar**. Clicking on the

Section of the **Navigator Bar** causes the **Section** to be displayed in the **View** window. Multiple **Sections** can be displayed simultaneously by holding the “Shift” button during the selection. Undesired (to be displayed) parts can be cut off and hidden from the **View** window using the **Cut with Rectangle** command. This leads to a temporary section that is remembered by the program and renewed after the project is closed and reopened. New **sections** can be named and listed in the **Navigator Bar** by using commands to create new sections. The simplest menu command is the **New Section from the View** command (alternatively, one can use the **Create New Section from Current View** command from the Edit Menu of the Sections Tab of the Navigator Bar), which creates a newly named **section** from currently displayed objects in the **View** window. The **New Section from Selection** menu command (alternatively, one can use the **Create New Section from Selected Objects** command from the Edit Menu of the Sections Tab of the Navigator Bar) creates a newly named section from currently selected objects or the FE-Mesh. The **Display Whole Domain (View All)** and **Display Whole FE-mesh** commands cause the entire computational domain or FE-Mesh to be displayed.

Geometric Sections can be created manually (as described above) or automatically. The automatically generated **Geo Sections** are generated as follows. An object above each part of the **Base Surface** (in the 3D-Layered Domain) forms a **Column**, which is divided into **Layers**, depending on how many vertical layers the domain is divided into. Each such **Layer** of each such **Column** then forms one **Object** (a **Domain Section**). When we have N **Columns** (that is, N parts in the **Base Surface**) and the domain is divided into M horizontal **Layers**, then the number of generated objects is $N*M$. At the same time, **Surfaces** belonging to each of these objects are also generated. Some of these **Surfaces** are *Horizontal*, and some are *Vertical* (although these terms are only approximate). **Surfaces** can then be used to specify **Boundary Conditions**.

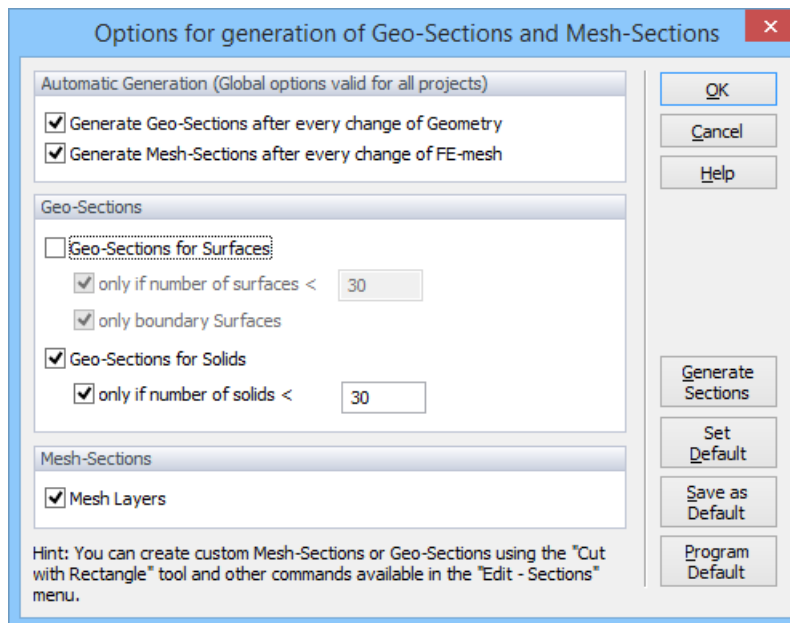


Figure 190. Options for Generation of Geo-Sections and FE-Mesh Sections dialog window.

Selected **Geo-Sections** and/or **FE-Mesh Sections** can be generated using the command **Generate Sections** in this dialog window (Fig. 190) obtained using the menu command *Edit-*

>*Sections->Generate Sections*. **Geo-Sections** can be generated either only for **Solids** or also for (Boundary and/or internal) **Surfaces**. Since working with **Geo-Sections** can be rather tedious when the number of **Surfaces** exceeds a certain limit, users can select this limit. The default setting (**Program Default**) is to generate **Geo-Sections** for up to 50 **Surfaces**. Note that the number of **Surfaces** can be prohibitively large for certain **3D-Layered Domains** with multiple internal lines and/or layers. Users can therefore choose to generate FE-Mesh Section only for **Boundary Surfaces**, which are useful when specifying the boundary conditions, and not for internal Surfaces. Users can change the default setting (**Program Default**), save it using the button **Save as Default**, and then recall it using the button **Set Default**. Note that different default settings can be saved for different types of domains.

Different **FE-Mesh Sections** are generated depending on the type of **Domain**. For the **3D-Layered Domains**, **FE-Mesh Sections** can be generated for the **Boundary Shell**, for each **Mesh Layer**, and for both automatically **Generated** and **User-Defined Geo-Sections**. For the **3D-General Domains**, **FE-Mesh Sections** can be generated for the **Boundary Shell**, and, again, for both automatically **Generated** and **User-Defined Geo-Sections**.

The **Section View** is the status of the display (in the View window) when only part of the transport domain is displayed (i.e., only one or few, but not all, Sections are displayed). The parts that are not displayed are still visible in the background (thin gray lines and/or surfaces), but are inactive and cannot be selected for various operations. The **Section View** can be canceled (and the entire domain displayed) using the menu command **Cancel Section View** or the popup menu command **Display Whole Domain**.

8.2. Navigator Bars

The **Navigator Bar** (Fig. 191) is, by default, located on the left side of the HYDRUS main window. A user can, however, move the **Navigator bar** to other positions. The **Navigator Bar** has three Tabs:

- A **Data Tab** to allow quick access to all input and output data. Input data include *Domain Geometry*, *Flow Parameters*, *FE-Mesh*, *Domain Properties*, *Initial* and *Boundary Conditions*, and *Auxiliary Objects*. Output data include various *Results*. Data are organized in a tree-like structure. Figure 191 shows *Data* with expanded *Domain Properties* on the left and *Results* in the middle.
- A **View Tab** (on the right of Figure 191) to specify what and how the information will be displayed in the *View window*, and
- A **Sections Tab** to show various Sections (not shown here and defined elsewhere).

View Options on the **View Tab** of the **Navigator Bar** mirror more or less the **Project Data**, i.e., **View Options** exists for *Domain Geometry*, *FE-Mesh*, *Domain Properties*, *Initial* and *Boundary Conditions*, and *Results*. Users can then select which objects (*Domain Geometry* objects, *Domain Properties* objects, *FE-Mesh* objects, such as *nodes*, *edges*, *triangles*, and *tetrahedrals*) are to be numbered (*Numbering*), display *Auxiliary Objects*, and initiate *Rendering* (*Outline*, *transparent*, *filled*). Users can also select the *Graph Type* (*Isolines*, *Isosurfaces*, *Contours* with or without *Separation Lines*, and *Color Edges*, *Color Points*, and *Velocity Vectors*) and *Color Scale* (either with or without *Min/Max global in time* or *Min/Max global in space*). Finally, *Lighting* can be turned on or off; the location of light sources can be shown (*Show Light Sources*), and the location of lights can be selected (*Light Switches*).

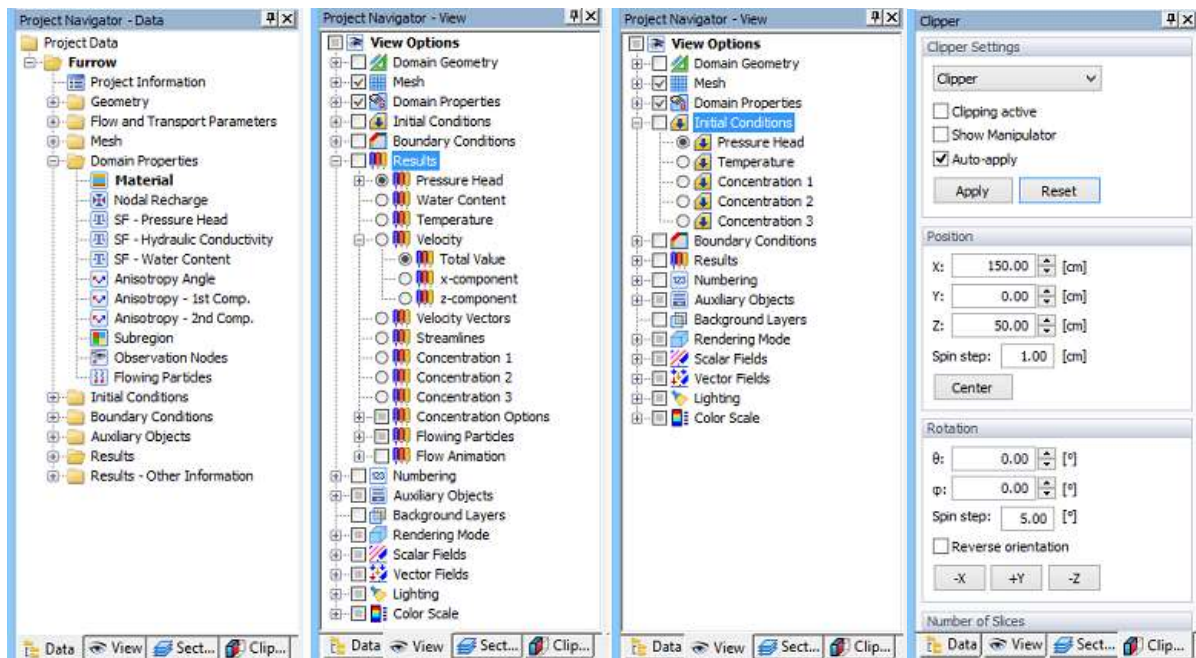


Figure 191. Selected Navigator Bars (Data Tab on the left, View Tabs in the middle, and Clipper Tab on the right).

8.3. Edit Bars

The **Edit Bar** is by default located on the right side of the HYDRUS main window. A user can, however, move the **Edit Bar** to other positions. The **Edit Bar** is very dynamic since it changes depending upon the process being carried out. Figure 192 shows the **Edit Bars** for different processes, i.e., for the Material Distribution in the *Domain Properties*, the Water Flow *Boundary Conditions*, the Pressure Head *Initial Conditions*, and the Water Content *Results*.

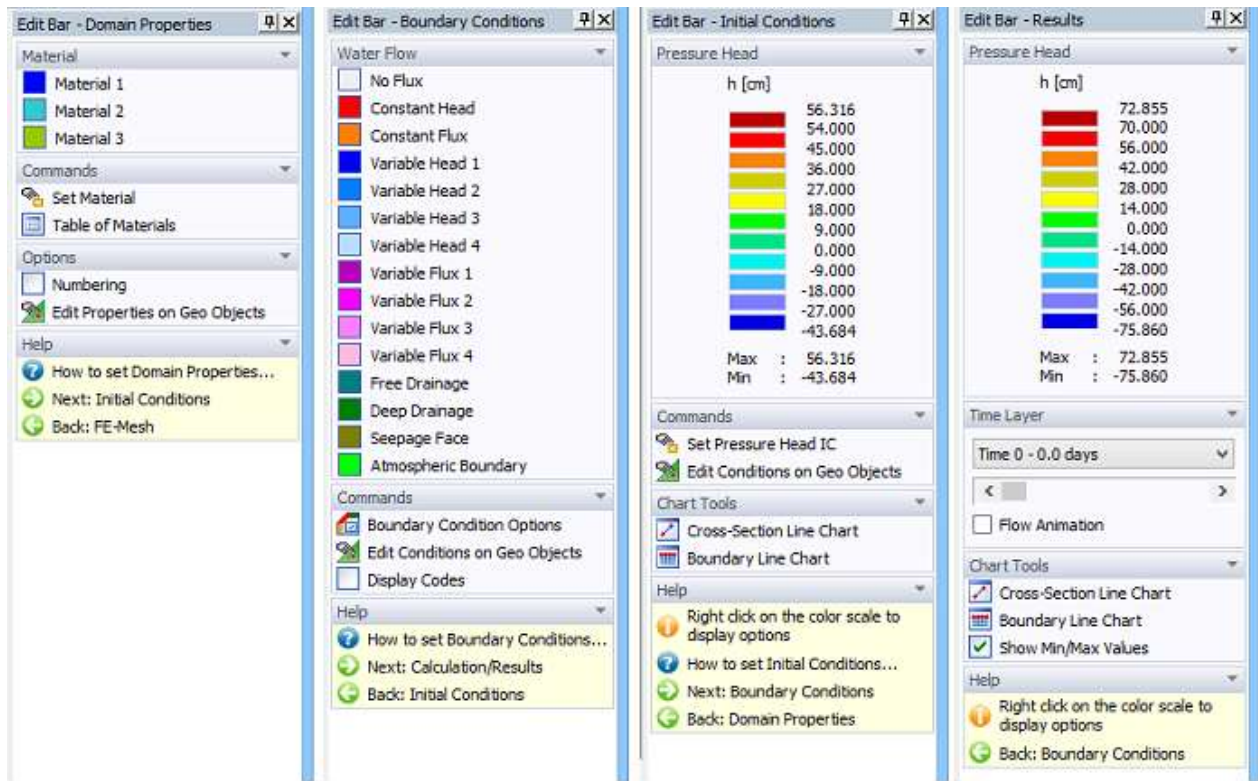


Figure 192. Selected Edit Bars (from left to right) for Material Distribution in Domain Properties, Water Flow Boundary Conditions, Pressure Head Initial Conditions, and Water Content Results.

As an example, the **Edit Bar** for **Domain Properties** and **Material Distribution** displays materials that can be assigned to selected nodes (in this case Materials 1, 2, and 3), the Command **Edit Materials** (which calls the **Water Flow Parameters** dialog window, Fig. 20), the command **Values by Pointer** (which displays the material number for a node closest to the cursor), and **Help**. The **Help** part of the **Edit Bar** usually contains help on a particular process (*How to ...*), and the direction of the data inputting process (next or backward).

The **Edit Bar** for **Boundary Conditions** and **Water Flow** displays the various boundary conditions that can be specified along boundaries of the transport domain, as well the command **Display Codes** (which displays boundary codes for all boundary nodes in the View window), the command **Codes by Pointer** (which displays boundary codes only for the node closest to the cursor), **Numbering Options** (which changes the **Navigator Bar** to the **View Tab** and **Numbering** option), **Boundary Conditions Options** (which allows additional system-dependent

boundary conditions for water flow, see the Technical manual and Fig. 137), and **Help** (which is similar as discussed above).

The **Edit Bar** for **Initial Conditions** and **Pressure Head - h** displays a color spectrum that is used to draw the initial conditions, and lists the minimum and maximum values that are used in the entire domain. This **Edit Bar** also includes:

- a) **Edit Commands: Set Values** and **Values by Pointer**. When nodes for which the initial conditions are to be specified are already selected, then the **Set Values** command calls the **Water Flow Initial Condition** dialog window (Fig. 135). When no nodes are selected, then clicking on the **Set Values** command causes a square cursor to appear, which may be used to select particular nodes, after which the **Water Flow Initial Condition** dialog window appears. The command **Values by Pointer** again displays the initial pressure head of the node closest to the cursor.
- b) Two **Chart Tools** commands: The **Cross-Section Chart** and the **Boundary-Line Chart**. The **Cross-Section Chart** command allows users to display a particular variable between any two points of the transport domain. The **Boundary-Line Chart** command allows users to display a particular variable between any two points on the boundary of the transport domain or along any line that is drawn along edges of finite elements within the transport domain. This line hence does not have to be straight but can turn in any direction along finite element edges.
- c) The **Help** commands as before.

The **Edit Bar** for **Results** and **Water Content** displays, similarly as for the initial conditions, a spectrum that is used to draw results, and the minimum and maximum values for the entire domain. This bar further includes:

- a) A **Time Layer** command to specify which time layers (corresponding to print times specified in the **Output Information** dialog window, Fig. 17) are to be displayed. Time layers can be chosen either from the list box or from a scroll bar. It is also possible to perform the animation of results by clicking on the **Flow Animation** check box.
- b) Two **Chart Tools** commands (**Cross-Section Chart** and **Boundary-Line Chart**), which have the same purpose as above for the initial condition. The last command (i.e., **Display Values at Nodes**) again causes the value of a particular variable (e.g., water content) of the node closest to the cursor to be displayed.
- c) The **Help** command. One useful feature of the **Help** command here is the *Right click on the Color Scale displays options* (a right-click displays the **Edit Color Scales** dialog window, Fig. 158). Right-clicking results in the display of the pop-up menu (Fig. 193) that allows users to choose different display options, such as *Color Smoothing*, *Isolines*, and *Isobands*. These options are defined in more detail below.

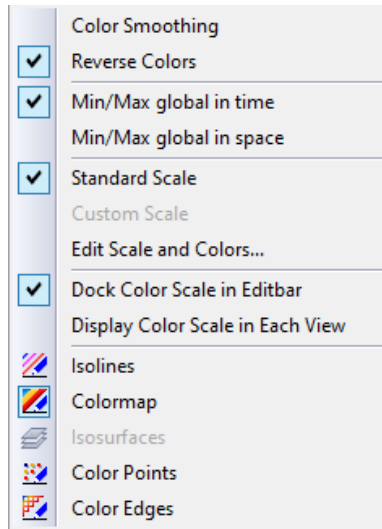


Figure 193. The Color Scale Display Options menu.

Color Smoothing	Colors are by default constant between isolines, but change abruptly at the isoline. Colors change gradually when this option is checked.
Reverse Colors	Users can reverse colors in the color scale (e.g., to display wet regions blue and dry regions red, or polluted regions red).
Min/Max Global in Time	The minimum and maximum values for the color spectrum are selected based on the minimum and maximum values of a certain variable during the entire simulation.
Min/Max Global in Space	The minimum and maximum values for the color spectrum are selected based on the minimum and maximum values of a certain variable in the entire transport domain (even when only part of the domain is displayed, e.g., one horizontal layer).
Standard Scale	Users can select between a standard or user-defined scale.
Custom Scale	Users can select between a standard or user-defined scale.
Edit Scale and Colors	Calls the Edit Isoband Value and Color Spectra dialog window (Fig. 158).
Dock Color Scale in Edit bar	Users can dock the Color Scale on the Edit bar.
Display Color Scale in Each View	The Color Scale can be displayed in the View Window .
Isolines	Displays a selected variable using isolines.
Colormap	Displays a selected variable using isobands (color spectrum).
Isosurfaces	Displays a selected variable using isosurfaces.
Color Points	Displays a selected variable using color points.
Color Edges	Displays a selected variable using color edges.
Velocity Vectors	Displays velocities using velocity vectors.

Figure 194 shows two more **Edit Bars**, i.e., those for *Domain Geometry* and *FE-Mesh*. The **Insert Object** of the **Domain Geometry Edit Bar** allows users to **Insert Objects** with which a transport domain is defined (i.e., points, lines, arcs, circles, splines, surfaces), as well as auxiliary

objects such as dimensions and comments. The **Edit Objects** part allows objects to be edited using various actions, such as *Move*, *Copy*, *Rotate*, and *Mirror*. This **Edit Bar** also provides **Help** on how to *Edit Domain Geometry* and to *Check Domain Definition*.

The **FE-Mesh Edit Bar** allows quick access to various commands needed for editing and generating the finite element mesh (**Edit FE-Mesh**), such as the *FE-Mesh Generator* (Fig. 117), *FE-Mesh Parameters* (Figs. 117 through 123), *Insert Mesh Refinement* (Fig. 125), *Delete All Refinements*, *Generate FE-Mesh*, *Delete FE-Mesh*, and *FE-Mesh Information* (Fig. 132). The **FE-Mesh Edit Bar** also allows users to generate the finite element mesh step by step (**FE-Mesh Advanced**), i.e., using individual steps such as *Fundamental Triangulation*, *Mesh Refinement*, *Delaunay Retriangulation*, *Convex Retriangulation*, and *Mesh Smoothing*. This **Edit Bar** additionally provides tools to work with **FE-Mesh Sections**, allows users to select how to make selections (**FE-Mesh Sections**) and **Help**.

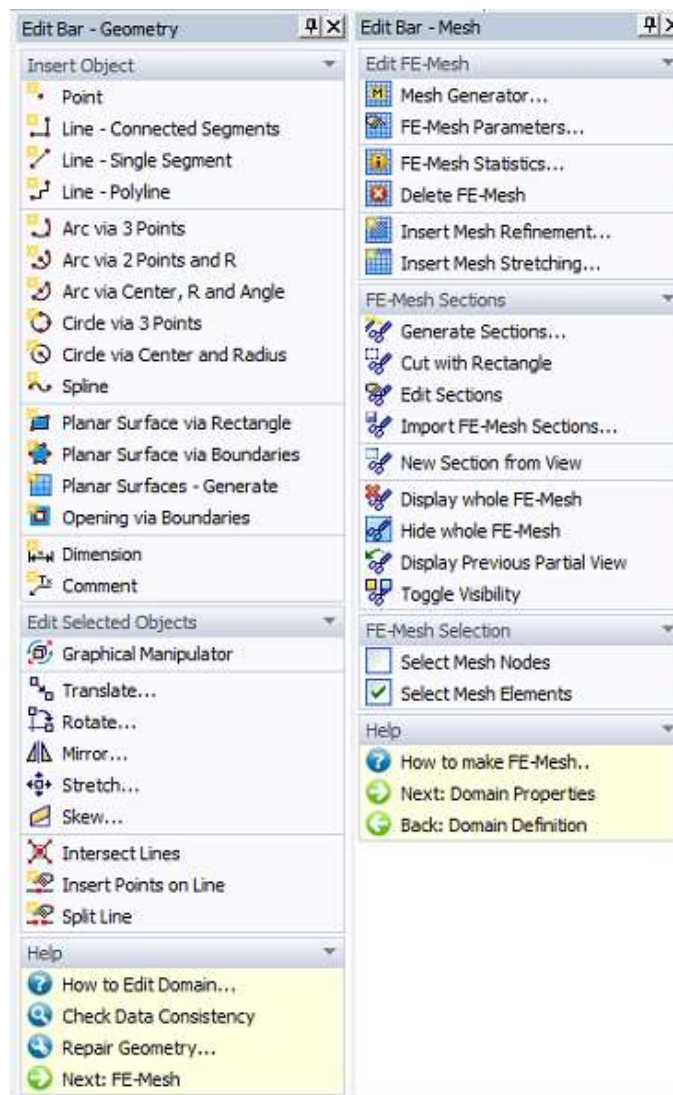


Figure 194. Selected Edit Bars (for Domain Geometry and FE-Mesh).

8.4. Toolbars

Users can use various **toolbars** that allow easy access to the most frequently used commands. These commands are grouped into two toolbars that can be displayed using the command *View->Customize Toolbars* (Fig. 195). Users can also create their own toolbars and customize them in various ways using the **Customize** dialog window (Fig. 195).

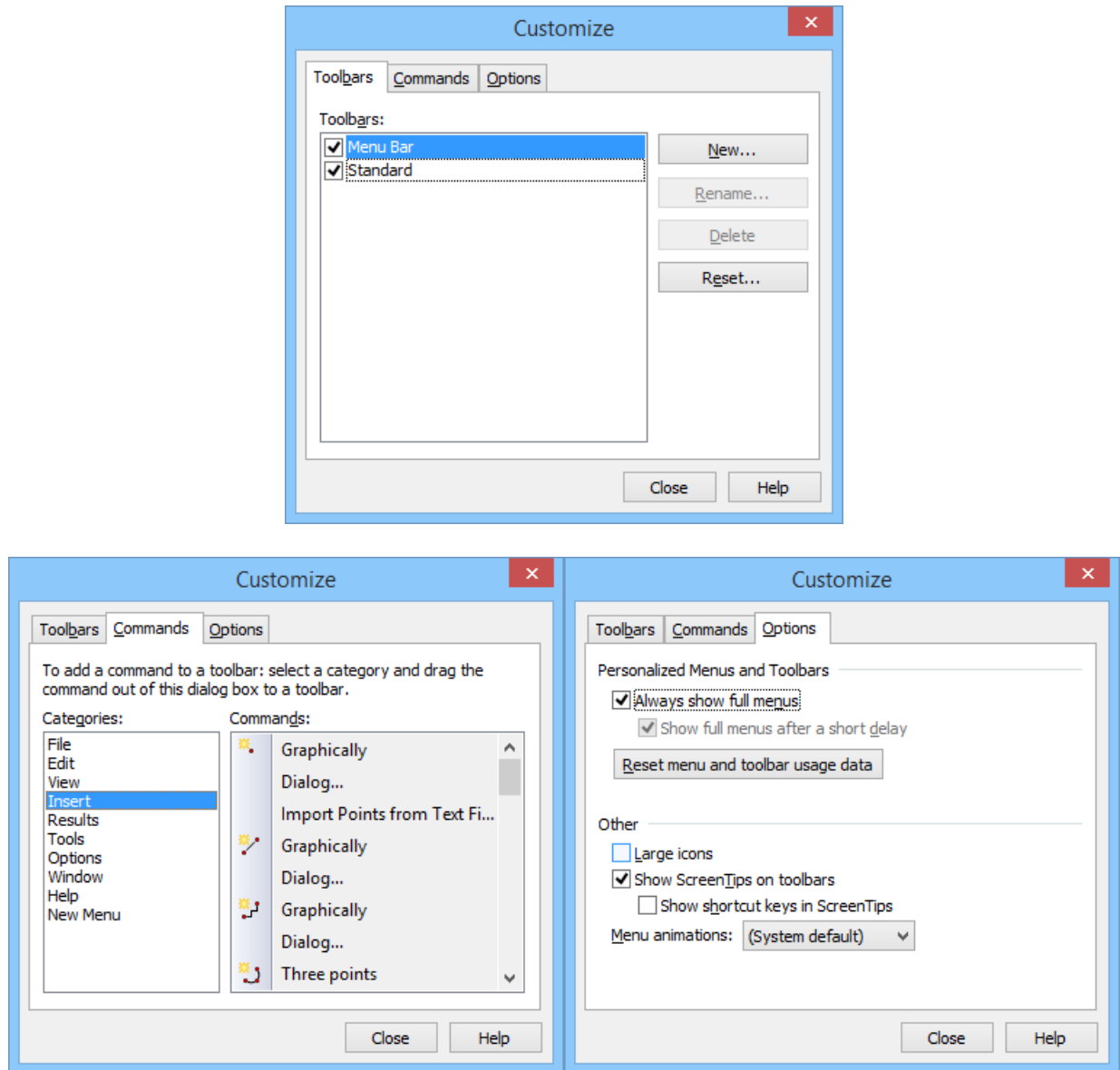


Figure 195. The Customize Toolbars dialog window (the Toolbars tab -top, the Commands tab - bottom left, and the Options tab - bottom right).

The default toolbars (i.e., **Standard Toolbar**, **Tools Toolbar**, **View Toolbar**, **GUI Toolbar**, and **Time Layer Toolbar**) are briefly summarized below (definitions in each case are from left to right).

a) Standard Toolbar:



New Project	Creates a new project.
Open a Project	Opens an existing project (represented by the <i>project_name.hyd5</i> file)
Save Project	Saves the input data of the current project specified in the main program module if the data were either newly created or changed during an application run.
Project Data Manager	Calls the project manager to manage data of existing projects; helps to locate, open, copy, delete, or rename the desired projects and their data (Figs. 2 and 3).
Print (Ctrl+P)	Prints the content of the View window.
Navigator Window	Displays or hides the Navigator Window.
Edit Bar	Displays or hides the Edit Bar.

b) Tools Toolbar:



Undo	Reverses the last edit actions.
Redo	Repeats the last edit actions.
Tools for Selection	Select by Rhomboid Selects objects using rhomboid. Select by Circle Selects objects using a circle. Select by Polygon Selects objects using a polygon. Add to Selection Add additional objects to the existing selection. Remove from Selection Remove objects from an existing selection. Standard Selection Mode
Grid and Work Plane Settings	Calls the Grid and Work Plane dialog window (Fig 185).
Show Grid	Shows a Work Plane (axis and origin of the grid) in the View window.
Set Grid Origin	Redefines the origin of the grid.
Snap to Grid	Mouse moves in steps given by the grid.
Set XY-Work Plane	Sets Work Plane to the XY plane.
Set YZ-Work Plane	Sets Work Plane to the YZ plane.
Set XZ-Work Plane	Sets Work Plane to the XZ plane.

c) View Toolbar:



Rotate View	Allows objects in the View windows to be rotated using the mouse while holding the left mouse button.
Scroll View	Allows moving (scrolling) of objects in the View window using the mouse while holding the left mouse button.
Zoom View	Allows zooming of objects in the View window using the mouse while holding the left mouse button.

Similar functions can be achieved by pressing various buttons on the keyboard. **Rotating** is achieved by holding simultaneously the **Ctrl** button on the keyboard and the left mouse button. **Scrolling** occurs by holding simultaneously the **Shift** button on the keyboard and the left mouse button. And finally, **zooming** is achieved by holding simultaneously the **Alt** button on the keyboard and the left mouse button.

Zoom by Rectangle	Zooms in on a certain part of the View window using a rectangle.
View All	Shows the default view of the View window.
Previous view	Shows the previous view of a certain part of the View window.
In Reverse Z-direction	Sets the view of the transport domain in the reverse Z-direction.
View Commands	Shows a pop-up menu with the following commands: <i>Isometric</i> <i>In X-direction</i> <i>In Y-direction</i> <i>In Z-direction</i> <i>In Reverse X-direction</i> <i>In Reverse Y-direction</i> <i>In Reverse Z-direction</i> <i>Perspective</i> <i>Default View</i>
Isometric View	Specifies the isometric view.
Perspective View	Specifies the perspective view.
View Stretching Factors	Calls the View Stretching Factors dialog window (Fig 186).
Rendering Commands	Displays a menu with three commands on how to display the transport domain (see 8.1.4): <i>Full Model</i> <i>Transparent Model</i> <i>Wire Model</i>
Sections Commands	Displays a menu with nine commands for editing sections: <i>Cut with Rectangle</i> <i>Cut with Indexes</i> <i>Create New Section from Selection</i> <i>Create New Section from Current View</i> <i>Display All</i> <i>Display Previous</i> <i>Hide Selection</i> <i>Display only Selection</i> <i>Display Reverse</i>

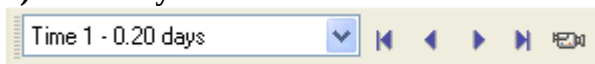
<i>Edit Section</i>	
Graph Type Commands	Displays a menu with five commands.
<i>Isolines</i>	Displays the spatial distribution of a certain variable by means of isolines.
<i>Colormap</i>	Displays the spatial distribution of a certain variable by means of color contours.
<i>Isosurfaces</i>	Displays the spatial distribution of a certain variable by means of isosurfaces.
<i>Color Points</i>	Displays the spatial distribution of a certain variable by means of color points.
<i>Color Edges</i>	Displays the spatial distribution of a certain variable by means of color edges.
<i>Velocity Vectors</i>	Displays Darcy velocity vectors.
Color Scale Options	Displays the menu with seven commands:
<i>Color Smoothing</i>	
<i>Reverse Colors</i>	
<i>Surface Lighting</i>	
<i>Min/Max Values Global in Time</i>	
<i>Min/Max Values Global in Space</i>	
<i>Standard Scale</i>	
<i>Custom Scale</i>	
<i>Edit Scale and Colors</i>	

d) GUI Toolbar:



View/Edit Domain Geometry	Sets the View window to View/Edit Domain Geometry mode.
View/Edit FE-Mesh	Sets the View window to View/Edit FE-Mesh mode.
View/Edit Domain Properties	Sets the View window to View/Edit Domain Properties mode, to edit materials.
View/Edit Initial Conditions	Sets the View window to View/Edit Initial Conditions mode, to edit pressure head initial conditions.
View/Edit Boundary Conditions	Sets the View window to View/Edit Boundary Conditions mode to edit water flow boundary conditions.
Execute Calculation	Executes a HYDRUS version 3.0 FORTRAN application.
View Results	Sets the View window to View Results mode to view the pressure head distribution.

e) Time Layer Toolbar:



List box of Time Layers	Displays a list box with Time Layers with available results.
First Time Layer	Displays the first-time layer.
Previous Time Layer	Displays the previous-time layer.
Next Time Layer	Displays the next-time layer.

Last Time Layer
Flow Animation

Displays the last-time layer.
Displays time layers of a particular variable consecutively and continuously.

8.5. HYDRUS Menus

The main window of HYDRUS contains a menu that has ten submenus, i.e., File, Edit, View (Fig. 196), Insert, Calculations, Results (Fig. 197), Tools, Options, Windows, and Help (Fig. 198). Table 27 lists the main groups, the main menu items, as well as the main submenu and submenu commands. Table 28 then provides brief descriptions of all menu commands.

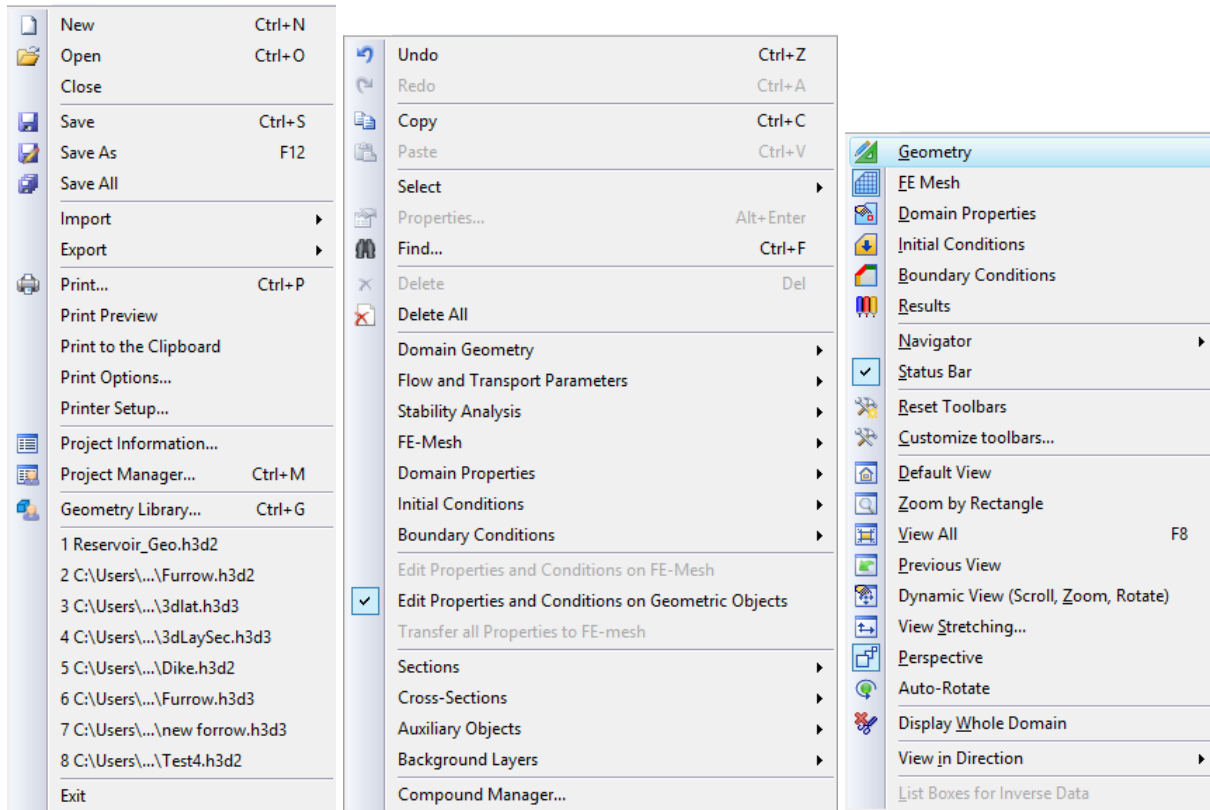


Figure 196. The HYDRUS Menus I (File, Edit, and View).

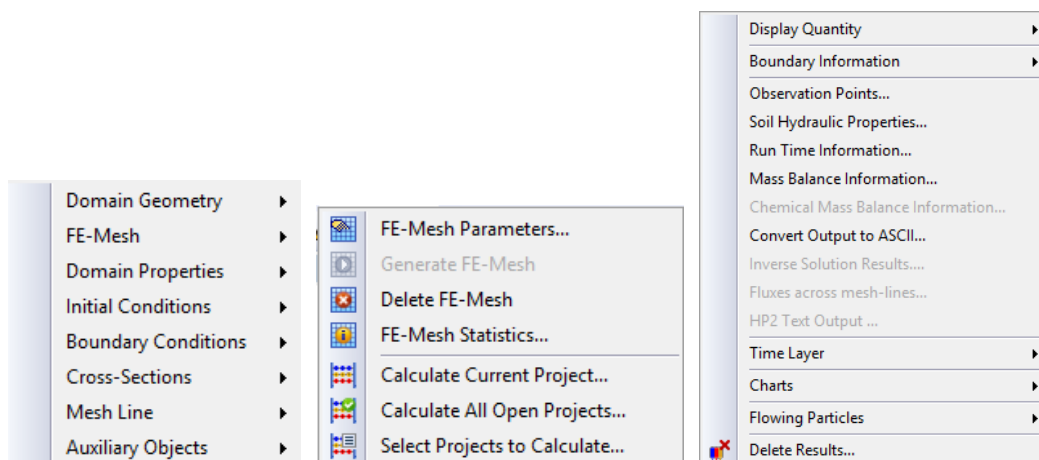


Figure 197. The HYDRUS Menus II (Insert, Calculations, and Results).

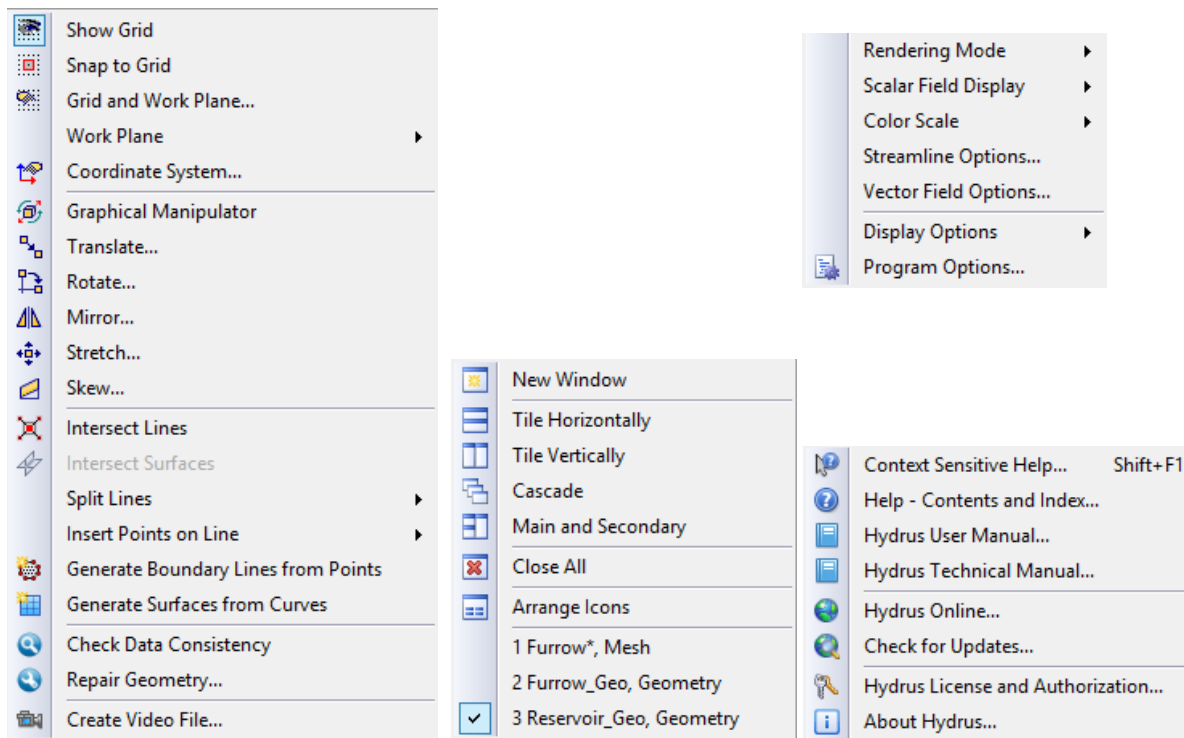


Figure 198. The HYDRUS Menus III (Tools, Options, Windows, and Help).

Table 27. HYDRUS menu commands (for 2D/3D projects).

Group	Menu	Submenu	Sub-Submenu
A File	New		
	Open		
	Close		
	Save		
	Save As		
	Save All		
	Project Information		
	Project Manager		
	Save as Project Template		
	Project Templates		
	Import	Import Input Data from another HYDRUS Project	
		Import Input Data from *.IN Files	
		Import Quantity defined by values at Scattered Points	
		Import Points from Text File	
		Import Geometry from Text File	
		Import Geometry from DXF File	
		Import Geometry from ESRI File	
		Import Background Layer	
		Import Data to ParSWMS	
	Export	Export Data for Hydrus Solver in Text Format	
		Export Geometry to Text File	
		Export Selected Geometrical Objects	
		Export FE-Mesh	
		Export Current Quantity	
		Export Isolines	
		Export Data to ParView	
		Export Data from ParSWMS	
		Save as Input for Modflow (only in 1D)	
	Print		
	Print Preview		
	Print to the Clipboard		
	Print Options		
	Print Setup		
	Recent Files		
	Exit		
B Edit	Undo		
	Redo		
	Copy		
	Paste		
	Select	Select by Rhomboid	
		Select by Circle	
		Select by Polygon	
		Add to Selection	
		Remove from Selection	
		Standard Selection Mode	

Properties		
Find		
Delete		
Delete All		
Domain Geometry	Domain Type and Units	
	Simple Domain	
	3D-Layered Domain	
	Delete 3D-Layered Domain	
	Points	
	Lines	
	Surfaces	
	Openings	
	Thickness Vectors	
	Solids	
Flow and Transport Parameters	Main Processes	
	Inverse Solution	
	Time Information	
	Output Information	
	HP2 Print Information	
	Water Flow Parameters	Iteration Criteria
		Hydraulic Properties Model
		Soil Hydraulic Parameters
		Anisotropy Tensors
	Solute Transport Parameters	General Information
		Solute Transport Parameters
		Solute Reaction Parameters
		Temperature Dependence
		Water Content Dependence
		UnsatChem Sol. Comp.
		UnsatChem Chem. Param.
		Constr. Wetlands Param. I
		Constr. Wetlands Param. II
		Surfactant Parameters
		Fumigant Application
		HP2 Components
		HP2 Definitions
	Heat Transport Parameters	
	Root Water Uptake	Root Water Uptake Models
		Pressure Head Reduction
		Osmotic Head Reduction
		Root Growth
		Dynamic Plant Uptake
	Variable Boundary Condition	
	Meteorological Parameters (only in 1D)	
	Meteorological Boundary Conditions (only in 1D)	
	Data for Inverse Solution	
	Data for Furrow Irrigation and Fertigation	
Stability Analysis	Slope Cube - Soil Stress Parameters	
FE-Mesh	Insert Mesh Refinement	
	Insert Mesh Stretching	
	Delete All Mesh Refinements	
	Delete All Mesh Stretchings	
	Remove Selected FE-Elements	

Domain Properties	Select Mesh Nodes	
	Select Mesh Elements	
	Material Distribution	
	Root Distribution	
	Nodal Recharge	
	Scaling Factor	Hydraulic Conductivity
		Pressure Head
		Water Content
	Local Anisotropy	Angle
		First Component
		Second Component
		Index
		Table of Anisotropy Tensors
	Subregions	
	Observation Nodes	Edit in View
Initial Conditions		Delete
		Clear All
	Drains	Edit in View
		Delete
		Clear All
		Drain Parameters
	Flowing Particles	Edit in View
		Delete
		Clear All
	Stochastic Distribution of S.F.	
Boundary Conditions	Subregions = Material Distribution	
	Nonequilibrium Conc. = a * Equil. Conc.	
	Parameters for Root Distribution	
	Delete All Domain Properties	
	Default Domain Parameters	
	Pressure Head/Water Content	
	Concentration	
	Nonequilibrium Concentration	
	Temperature	
	Import	
Mesh Sections and Geo Sections	Delete All Initial Conditions	
	Water Flow	
	Solute Transport	
	Heat Transport	
	Boundary Conditions Options	
	Delete All Boundary Conditions	
	Edit Properties and Conditions on FE-Mesh	
	Edit Properties and Conditions on Geometric Objects	
	Transfer all Properties to FE-Mesh	
	Edit Sections	
	Generate Sections	
	New Section from Selection	
	New Section from View	
	Display Whole Domain	
	Display Previous Section View	
	Display only Selection	
	Hide Selection	
	Toggle Visibility	
	Cut with Rectangle	

C View

	Cut with Rhomboid	
	Cut with Circle	
	Cut with Polygon	
	Cut with Indexes	
	Import FE-Mesh Sections	
Dimensions	Delete Selected	
	Delete All	
Comments	Edit	
	Delete Selected	
	Delete All	
Bitmaps	Edit	
	Delete Selected	
	Delete All	
Cross-Sections	Edit	
	Delete Selected	
	Delete All	
	Adjust Work Plane	
Point Probes	Current Probe Editor	Insert Points
		Clear Points
		Save Current Copy
	Edit Point Probes	
	Delete Selected Point Probes	
	Delete All Point Probes	
	Show All Probes	
	Show only Current Probe	
	Export Probe Values	
Line Probes	Edit	
	Delete Selected Line Probes	
	Delete All Line Probes	
Background Layers	Edit	
	Move	
	Rotate	
	Mirror	
	Stretch	
	Skew	
	Delete All	
Insert Fixed Points	Insert Fixed Point (only in 1D)	
	Delete Fixed Points (only in 1D)	
	Delete All Fixed Points (only in 1D)	
	Mesh Density at Fixed Points (only in 1D)	
Soil Profile Summary	(only in 1D)	
Geometry		
FE Mesh		
Domain Properties		
Initial Conditions		
Boundary Conditions		
Results		
Navigator	Data Tree	
	View Tree	
	Sections	

D Insert

	Edit Bar	
	Clipper Pane	
	Edit Bar Options	Show Icons with Text
		Allow Items to Appear as
		Icons Only
Status Bar		
Reset Toolbars		
Customize Toolbars		
Standard View		
View All		
Previous View		
View in Direction	Isometric	
	In X-direction	
	In Y-direction	
	In Z-direction	
	Reverse X-direction	
	Reverse Y-direction	
	Reverse Z-direction	
View Stretching		
Zoom by Rectangle		
Set View (Scroll, Zoom, Rotate)		
Perspective View		
Auto-Rotate		
Center of Rotation	Pick	
	Reset	
	Show/Hide	
Cancel Section View Mode		
Save Current View		
Edit Named Views		
Import/Export View Settings	Export View Transformation	
	Import View Transformation	
List Boxes for Inverse Data		
Domain Geometry	Points	Graphically
		Dialog
		Import Points from Text File
	Curves	Line
		Polyline
		Arc
		Circle
		Spline
	Surfaces	Rectangle Graphically
		Planar
		Quadrangle
		Rotary
		Pipe
		B-Spline
	Openings	Graphically
		Dialog
	Thickness Vectors	Graphically
		Dialog
	Solids	3D-Block Graphically
		3D-Layered Domain

		General Solid
FE-Mesh	Mesh Refinement - Graphically Insert Mesh Refinement - Dialog Insert Mesh Stretching	
Domain Properties	Material Distribution Root Distribution Nodal Recharge Scaling Factor	Hydraulic Conductivity Pressure Head Water Content
	Local Anisotropy	Angle First Component Second Component Index
	Subregions Observation Nodes Drains Flowing Particles	
Initial Conditions	Pressure Head/Water Content Concentration Nonequilibrium Concentration Temperature Import	
Boundary Conditions	Water Flow	No Flux Constant Head Constant Water Content Constant Flux Seepage Face Variable Head 1-4 Variable Flux 1-4 Gradient Boundary Free Drainage Deep Drainage Atmospheric Boundary
	Solute Transport	First-Type Third-Type Volatile Type
	Heat Transport	First-Type Third-Type
	Slope Cube	Free Displacement X-displacement Z-displacement XZ-displacement X-force Z-force XZ-force
Dimension		
Comment		
Bitmap		
Cross-Sections	Graphically Dialog	
Mesh Line	Graphically Dialog	
Point Probe		
Line Probe		
Background Layer		

E Calculation	FE-Mesh Parameters	
	Generate FE-Mesh	
	Advanced FE-Mesh Generation	Fundamental Triangulation
		Mesh Refinement
		Homogeneous Triangulation
		Check of Convexity
		Mesh Smoothing
	FE-Mesh Statistics	
	Delete FE-Mesh	
	Calculate Current Project	
F Results	Calculate All Open Projects	
	Select Projects to Calculate	
	Display Quantity	Pressure Heads
		Water Content
		Concentration
		Nonequilibrium Concentration
		Temperature
		Velocity
		Root Water Uptake
		Water Mass Transfer
		Solute Mass Transfer
		Dual-permeability Matrix
		Dual-permeability Fractures
	Boundary Information	Pressure Heads
		Boundary Fluxes
		Cumulative Fluxes
		Solute Fluxes
	Observation Points	Basic Information
		UnsatChem Information (only in 1D)
	Profile Information	Basic Information (only in 1D)
		Solution Concentrations (only in 1D)
		Solid Concentrations (only in 1D)
		Chemical Information (only in 1D)
		(only in 1D)
	Particle Tracking	
	Soil Hydraulic Properties	
	Run Time Information	
	Mass Balance Information	
	Chemical Mass Balance Information	
	Convert Output to ASCII	
	Inverse Solution Results	
	Meteorological Information	(only in 1D)
	Fluxes across Mesh Lines	
	HP2 Text Output	
	Cosmic-Ray Neutron Information	(only in 1D)
	Furrow Module	Stations
		Runoff
		Advance and Recession times
	DPU Module	DPU Solute Concentrations
		DPU Masses
		DPU Fluxes
	Time Layer	First
		Last
		Previous

G Tools

Graphs	Next Animation Cross-Section Line MeshLine Boundary Meshline Line Probe
Flowing Particles	Draw Particles Positions Draw Particles Trajectories
Streamlines	Show Manipulator or Seed Points Apply Changes Immediately Apply Changes Edit Seed Points Sources
Streamlines animation	
Delete Results	
Show Grid	
Snap to Grid	
Grid and Work Plane	
Work Plane	Set Origin Define XY Define YZ Define XZ
Coordinate System	
Graphical Manipulator	
Translate	
Rotate	
Mirror	
Stretch	
Skew	
Intersect Lines	
Intersect Surfaces	
Split Lines	Graphically n Points Distance Graphically n Points Distance
Insert Points on Line	
Extend Lines	
Extend Thickness Vectors	
Generate Boundary Lines from Points	
Generate Surfaces from Curves	
Check Data Consistency	
Repair Geometry	
Create Video File	
Display Options	Edit Default Import Export
Program Options	
Model Display	Solid Model Transparent Model Wire Frame Model Use Material Colors for Geo-Objects
Scalar Field Display	Isolines Colormaps

H Options

	Color Scale	Isosurfaces Color Points Color Edges Show Min/Max Values Color Smoothing Reverse Colors Min/Max Values Global in Time Min/Max Values Global in Space Standard Scale Custom Scale Edit Scale and Colors Dock Color Scale in Edit bar Display Color Scale in Each View
	Streamline Options Vector Field Options Clipper Options Transparency Options	
I Modules	Slope Stability - Classic	Input Parameters Open Slope Stability Module Printout Report and Results Delete Results Settings Slope Stability Help Slope Stability User's Manual
	Slope Stability - Cube	Slope Cube Stress Parameters Slope Cube Users Manual Slope Cube Tutorial
	Furrow	Furrow Parameters Furrow Manual
J Windows	New Window Tile Horizontally Tile Vertically Cascade Main and Secondary Close All Arrange Icons	
K Help	Context Sensitive Help Help – Contents and Index Hydrus User Manual Hydrus Technical Manual Hydrus Online Check for Updates Hydrus License and Authorization About Hydrus	

Table 28. Brief description of HYDRUS menu commands.

Group	Command	Brief description of the command
A	File	
	New	Creates a new project after the user provides required information (name and description) in the New Project dialog window (Fig. 4). The project will be located in the current Project Group.
	Open	Opens an existing project (represented by the <i>project_name.hyd5</i> file) using the Open dialog window, which a user uses to browse for the HYDRUS project.
	Close	Closes an open project.
	Save	Saves the input data of an actual project specified in the main program module if the data were either newly created or changed during an application run.
	Save As	Saves data of a particular project under a new project name using the Save As dialog window.
	Save All	Saves data of all projects.
	Project Information	Displays information about the current project (in the General Data dialog window (Fig. 4)).
	Project Manager	Calls the Project Manager (Figs. 2 and 3) to manage data of existing projects; helps to locate, open, copy, delete or rename the desired projects and their data.
	Save as Project Template	Saves the current project as a project template for future project initiation.
	Project Templates	Displays currently available Project Templates.
	Import	
	Import Input Data from another HYDRUS Project	Imports data from another project and interpolates properties when FE-Mesh grids are different.
	Import Input Data from *.IN Files	Imports input data from *.in files that may have been modified manually outside of the HYDRUS GUI.
	Import Quantity defined by values at Scattered Points	Imports various quantities (such as initial conditions) from a text file with values given for a series of locations.
	Import Points from Text File	Reads single point coordinates from a text file.
	Import Geometry from Text File	Reads definition of the entire geometry from a text file.
	Import Geometry from DXF File	Reads definition of the entire geometry from a DXF file.
	Import Geometry from ESRI File	Reads definition of the entire geometry from an ESRI file.
	Export Isolines	Exports spatial coordinates of isolines.
	Import Background Layer	Imports background layer as a template for defining the transport domain.
	Imports Data from ParSWMS	Imports output data created by ParSWMS on a supercomputer or cluster of computers and display them in HYDRUS GUI.
	Export	
	Export Data for Hydrus Solver in Text Format	Exports data for the HYDRUS solver into the working directory from which the computational module reads inputs and into which it writes outputs.
	Export Geometry to Text File	Writes a definition of the entire geometry to a text file.
	Export Selected Geometrical Objects	Writes a definition of the selected objects to a text file.
	Export FE-Mesh	Exports information about the FE-Mesh to a text file.

Export Current Quantity	Exports information about the currently displayed quantity (e.g., water content) into a text file.
Export Isolines	Exports spatial coordinates of isolines.
Export Data To ParView	Exports HYDRUS results to an external graphical package ParView.
Export Data to ParSWMS	ParSWMS is a parallelized version of SWMS-3D, which can be run on clusters or supercomputers. This command creates input files for ParSWMS from the HYDRUS project.
Save as Input for Modflow	Saves the current project in the format used by the HYDRUS package for Modflow
Print	Prints the content of the View window.
Print Preview	Previews the content of the View window before printing.
Print to the Clipboard	Copies the content of the View window to the clipboard for subsequent pasting into other software packages.
Print Options	Select various print options, such as print quality, text size, frame, and text content (Fig. 221).
Print Setup	Selects a printer and printer connection.
Recent Files	Displays recently opened projects.
Exit	Closes open projects and leaves the program. This command informs users before exiting the application whether or not the input data of open projects were changed during the application run. If changes did occur, users are given an option to save data before exiting the application.

B Edit

Undo	Reverses the last edit action.
Redo	Repeats the last edit action.
Copy	Copies a selected object.
Paste	Pastes a selected object.
Select	
Select by Rhomboid	Selects objects by means of a rhomboid.
Select by Circle	Selects objects by means of a circle.
Select by Polygon	Selects objects by means of a polygon.
Add to Selection	Add a new object to the existing selection
Remove from Selection	Remove objects from the existing selection
Standard Selection Mode	Selects objects by means of a quadrilateral.
Properties	Displays properties of a selected object.
Find	Finds an object.
Delete	Deletes a selected object.
Delete All	Deletes all objects.
Domain Geometry	
Domain Type and Units	Specifies whether the flow and transport problem occurs in a two- or three-dimensional transport domain and whether the domain is simple or complex using the Domain Type and Units dialog window (Fig. 6).
Simple Domain	Specifies parameters (dimensions and slopes) for simple rectangular or hexahedral transport domains using the Rectangular (Fig. 10) or Hexahedral Domain Definition (Fig. 11) dialog windows.
3D-Layered Domain	Calls Edit 3D-Layered Domain dialog window for editing the object.

Delete 3D-Layered Domain	Deletes 3D-Layered Domain.
Points	Edits selected points.
Lines	Edits selected lines using the Edit Curve dialog window (Fig. 60).
Surfaces	Edits selected surfaces.
Openings	Edits selected openings.
Thickness Vectors	Edits selected thickness vectors.
Solids	Edits solids.
Flow and Transport Parameters	
Main Processes	Selects the processes to be simulated, i.e., water flow, multiple solute transport, heat transport, and/or root water uptake (the Main Processes dialog window (Fig. 13)).
Inverse Solution	Selects the type of weighting of measured data, and whether soil hydraulic parameters, solute transport parameters, and/or heat transport parameters, are to be fitted (the Inverse Solution dialog window (Fig. 14)).
Time Information	Selects time units and gives the time discretization information (the Time Information dialog window (Fig. 16)).
Output Information	Specifies print options (The Output Information dialog window (Fig. 17)).
HP2 Print Information	Specifies print options for the HP2 modules.
Water Flow Parameters	
Iteration Criteria	Specifies iteration criteria for the solution precision and parameters for the time step control (The Iteration Criteria dialog window (Fig. 18)).
Hydraulic Properties Model	Selects the type of model used for the soil hydraulic properties and decides whether hysteresis is considered (the Soil Hydraulic Model dialog window (Fig. 19)).
Soil Hydraulic Parameters	Specifies parameters in the soil hydraulic model (the Water Flow Parameters dialog window (Fig. 20)).
Anisotropy Tensors	Defines anisotropy tensors for three-dimensional applications (the Tensors of Anisotropy dialog window (Fig. 23)).
Solute Transport Parameters	
General Information	Selects the time and spatial weighting schemes for the numerical solution of the solute transport equation; specifies the number of solutes to be considered (the Solute Transport dialog window (Fig. 28)).
Solute Transport Parameters	Specifies solute transport parameters (the Solute Transport Parameters dialog window (Fig. 30)).
Solute Reaction Parameters	Specifies solute reaction parameters (the Solute Reaction Parameters dialog window (Fig. 31)).
Temperature Dependence	Specifies parameters defining the temperature dependence of reaction and transport parameters (the Temperature-Dependent Solute Transport and Reaction Parameters dialog window shown in Figure 33).
Water Content Dependence	Specifies parameters defining the water content dependence of reaction parameters (the Water Content Dependent Solute Reaction Parameters dialog window shown in Figure 34).
UnsatChem Solution Composition	Specifies solution, adsorbed, and precipitated concentration combinations for the UNSATCHEM module (the Solution Compositions dialog window (Fig. 35)).
UnsatChem Chemical Parameters	Specifies various chemical parameters and selections for the UNSATCHEM module (the Chemical Parameters dialog window (Fig. 36)).

Constructed Wetlands Parameters I	Specifies parameters for constructed wetlands (the Constructed Wetland Model Parameters I dialog windows (Fig. 49)).
Constructed Wetlands Parameters II	Specifies parameters for constructed wetlands (the Constructed Wetland Model Parameters II dialog windows (Fig. 51)).
Surfactant Parameters	Parameters for surface tension and viscosity dependence of solution concentrations (i.e., for the PFAS module).
Fumigant Application	Allows additional application of a specified mass of a chemical into the transport domain (a specified location) at a specified time.
HP2 Components	Specifies the path to the thermodynamic database and components to be considered in PHREEQC calculations.
HP2 Definitions	Text editors for defining input for PHREEQC.
Heat Transport Parameters	Specifies heat transport parameters (the Heat Transport dialog window; Fig. 40).
Root Water Uptake	
Root Water Uptake Models	Selects the root water uptake stress response models for both salinity and water stress (the Root Water Uptake Model dialog window, Fig. 42).
Pressure Head Reduction	Specifies parameters in the root water uptake water stress response model (the Root Water Uptake Parameters dialog window; Fig. 43).
Osmotic Head Reduction	Specifies parameters in the root water uptake salinity stress response model (the Root Water Uptake Parameters dialog window; Fig. 44).
Root Growth	Specifies parameters for root growth.
Dynamic Plant Uptake	Parameters for the DPU module.
Variable Boundary Condition	Specifies time-dependent boundary conditions for all transport processes (the Time Variable Boundary Conditions dialog window; Fig. 48).
Meteorological Parameters	Specifies parameters for calculating potential ET using meteorological data (only in 1D).
Meteorological Data	Specifies time-dependent meteorological data such as incoming radiation, wind speed, temperature, humidity, etc.
Data for Inverse Solution	Specifies data for the inverse solution, their type, location, and associated weight (the Data for Inverse Solution dialog window; Fig. 15).
Data for Furrow Irrigation and Fertilization Parameters for the Furrow module.	
Stability Analysis	
Soil Cube - Soil Stress Parameters	Specifies soil stress parameters.
FE-Mesh	
FE-Mesh Generator	Selects the structured or unstructured finite element mesh generator (the Finite Element Mesh Generator dialog window).
FE-Mesh Parameters	Specifies either parameters of the Unstructured Finite Element Mesh Generator (the FE-Mesh Parameters dialog window; Figs. 117 through 123) or parameters of the structured mesh (the Rectangular Domain Discretization dialog window (Fig. 115) or the Hexahedral Domain Discretization dialog window (Fig. 116)).
Generate FE-Mesh	Generates unstructured finite element mesh.
FE-Mesh Statistics	Provides information about finite element mesh (the FE-Mesh Information dialog window (Fig. 132).
Delete FE-Mesh	Deletes unstructured finite element mesh.
Insert Mesh Refinement	Inserts new FE-mesh refinement using the FE-Mesh Refinement dialog window; Fig. 125).

Insert Mesh Stretching	Inserts new FE-mesh stretching using the FE-Mesh Stretching dialog window; Fig. 119).
Delete All Mesh Refinements	Deletes All Mesh Refinements
Delete All Mesh Stretchings	Deletes All Mesh Stretchings
Remove Selected FE-Elements	Removes selected finite elements from the finite element mesh. Note that this operation should not be performed when properties are specified on Geometric Objects.
Select Mesh Nodes	Selects FE-Mesh nodes. This command is usually used to select nodes that are then either used to define the new FE-Mesh Section or removed from the FE-Mesh.
Select Mesh Elements	Selects FE-Mesh elements (to perform similar operations as for selected mesh nodes).
Advanced FE-Mesh Generation	
Fundamental Triangulation	Performs triangulation of boundary nodes based on the Delaunay criterion.
Mesh Refinement	Inserts a new point in the center of all triangles that do not fulfill the smoothness criterion.
Homogeneous Retriangulation	Retriangulates mesh according to the Delaunay criterion.
Check of Convexity	Corrects possible errors that may appear during smoothing and retriangulating.
Mesh Smoothing	Smooths the mesh by solving a set of coupled elliptic equations using a recursive algorithm.
Domain Properties	
Material Distribution	Specifies the spatial distribution of soil materials.
Root Distribution	Specifies the spatial distribution of root water uptake.
Nodal Recharge	Specifies the spatial distribution of nodal recharge.
Scaling Factor	
Hydraulic Conductivity	Specifies the spatial distribution of hydraulic conductivity scaling factors.
Pressure Head	Specifies the spatial distribution of pressure head scaling factors.
Water Content	Specifies the spatial distribution of water content scaling factors.
Local Anisotropy	
Angle	Specifies the spatial distribution of the angle of local anisotropy.
First Component	Specifies the spatial distribution of the first component of local anisotropy.
Second Component	Specifies the spatial distribution of the second component of local anisotropy.
Index	Specifies the spatial distribution of the index that represents the local anisotropy tensor.
Table of Anisotropy Tensors	Displays the Anisotropy dialog window (Fig. 23).
Subregions	Specifies the spatial distribution of subregions for the mass balance calculations.
Observation Nodes	
Edit	Specifies observation nodes for output of the pressure head, water content, temperature, and concentration at each time step.
Delete	Deletes selected observation nodes.
Clear All	Deletes all observation nodes.
Drains	
Edit	Specifies nodal points representing tile drains.
Delete	Deletes selected tile drains.
Clear All	Deletes all tile drains.
Drain Parameters	Specifies drain parameters.

Flowing Particles

Edit	Specifies nodal points representing flowing particles.
Delete	Deletes selected flowing particles.
Clear All	Deletes all flowing particles.
Stochastic Distribution of S.F. Subregions = Material Distribution	Generates a stochastic distribution of scaling factors. Makes the subregions for mass balance calculations similar to those for the soil materials.
Nonequilibrium Conc. = a * Equil. Conc.	Specifies that nonequilibrium concentrations (i.e., kinetically sorbed concentrations or concentrations in the immobile water) are a multiple of the liquid phase concentrations.
Parameters for Root Distribution Delete All Domain Properties	Specifies parameters for the spatial distribution of root water uptake. Command used when defining properties on Geometric Objects. Deletes all defined domain properties and assigns default values.
Default Domain Parameters	Specifies default domain properties that are constant for the same depths (the Default Domain Properties dialog window; Fig. 134).

Initial Conditions

Pressure Head/Water Content Concentration	Specifies the initial condition for water flow. Specifies the initial condition for solute transport (equilibrium concentrations).
Nonequilibrium Concentration	Specifies the initial condition for solute transport (nonequilibrium concentrations).
Temperature	Specifies the initial condition for heat transport.
Import	Imports the initial condition from previous simulations for water flow and solute and heat transport.
Delete All Initial Conditions	Command used when defining Initial Conditions on Geometric Objects. Deletes all defined Initial Conditions and assigns default values.

Boundary Conditions

Water Flow	Specifies boundary conditions for water flow.
Solute Transport	Specifies boundary conditions for solute transport.
Heat Transport	Specifies boundary conditions for heat transport.
Boundary Conditions Options	Specifies additional system-dependent water flow boundary conditions.
Deletes All Boundary Conditions	Clears all boundary conditions and assigns a No Flow boundary condition on all boundaries
Edit Properties and Conditions on FE-Mesh	Selects that spatially variable properties (e.g., materials, initial conditions) are assigned directly to the FE-Mesh rather than to Geometric Objects
Edit Properties and Conditions on Geometric Objects	Selects that spatially variable properties (e.g., materials, initial conditions) are assigned to Geometric Objects
Transfer all Properties to FE-Mesh	Transfer all properties (e.g., materials, initial conditions) from Geometric Objects to FE-Mesh

Mesh Sections and Geo Sections

Edit Sections	Calls the FE-Mesh Section dialog (Fig. 133). HYDRUS recognizes two different definitions of Sections – one for geometric objects and one for the FE-mesh. A different dialog appears when called from the “Domain Geometry” part of the program. In all other cases, the FE-mesh Section dialog appears.
Generate Sections	Generates Geo-Sections and FE-Mesh Sections.
New Section from Selection	Creates a new section from currently selected objects/FE-Mesh
New Section from View	Creates a new section from currently displayed objects/FE-Mesh
Display Whole Domain	Displays all objects or entire FE-Mesh
Display Previous Section View	Displays a previously displayed view (sections)

Hide Selection	Hides selected elements.
Display only Selection	Displays only currently selected objects/FE-Mesh
Toggle Visibility	Hides currently displayed objects/FE-Mesh and displays currently hidden objects/FE-Mesh
Cut with Rectangle	Displays objects/FE-mesh nodes within a rectangle and hides all the others
Cut with Rhomboid	Displays objects/FE-mesh nodes within a rhomboid and hides all the others
Cut with Circle	Displays objects/FE-mesh nodes within a circle and hides all the others
Cut with Polygon	Displays objects/FE-mesh nodes within a polygon and hides all the others
Cut with Indexes	Displays objects with given indexes and hides all the others
Import FE-Mesh Sections	Import FE-Mesh Sections
Dimensions	
Delete Selected	Deletes selected dimensions
Delete All	Deletes all dimensions
Comments	
Edit	Edits a comment
Delete Selected	Deletes selected comments
Delete All	Deletes all comments
Cross-Sections	
Edit	Edits a cross-section
Delete Selected	Deletes selected cross-sections
Delete All	Deletes all cross-sections
Auto-Adjust Work Plane	Adjusts Work Plane
Point Probes	
Insert Points	Inserts coordinates of Point Probes
Clear Points	Deletes Point Probes
Save Current Copy	Saves current Point Probes under a group name
Edit Point Probes	Edits coordinates of Point Probes
Delete All Point Probes	Deletes all Point Probes
Show All Probes	Displays all Point Probes in the View window
Show Only Current Probe	Displays selected Point Probes in the View window
Export Probe Values	Exports values at Point Probes
Line Probes	
Edit	Edits coordinates of Line Probes
Delete Selected Line Probes	Deletes Selected Line Probes
Delete All Line Probes	Deletes all Line Probes
Background Layers	Geometric objects that are imported to HYDRUS and are used as templates for defining HYDRUS geometries
Edit	Edits a selected Background Layer
Move	Moves a selected Background Layer
Rotate	Rotates a selected Background Layer
Mirror	Mirrors a selected Background Layer
Stretch	Stretches a selected Background Layer
Skew	Skews a selected Background Layer
Delete All	Deletes all Background Layers
Insert Fixed Points	Inserts fix points into the soil profile. The fixed points are used to adjust FE discretization (only in 1D).
Insert Fixed Point	Inserts a fixed point (only in 1D)
Delete Fixed Points	Deletes fixed points (only in 1D)

Delete All Fixed Points	Deletes all fixed points (only in 1D)
Mesh Density at Fixed Points	Assigns FE-Mesh density at fixed points (only in 1D)
C View	
Geometry	Sets the View window to View/Edit Domain Geometry mode.
FE Mesh	Sets the View window to View/Edit FE-Mesh mode.
Domain Properties	Sets the View window to View/Edit Domain Properties mode to edit materials.
Initial Conditions	Sets the View window to View/Edit Initial Conditions mode to edit pressure head initial conditions.
Boundary Conditions	Sets the View window to View/Edit Boundary Conditions mode to edit water flow boundary conditions.
Results	Sets the View window to View Results mode to view pressure head distribution.
Navigator	Displays or hides the Navigator window.
Status Bar	Displays or hides the Status Bar.
Reset Toolbars	Reset toolbars.
Customize Toolbars	Customizes toolbars (the Customize Toolbars dialog window, Fig. 195).
Standard View	Sets a default viewing direction (in 3D) and performs the “View All” command
View All	Changes a scroll position and a zoom factor so that all currently displayed objects are visible in the View Window. This command does not change the viewing direction.
Previous View	Shows the previous view on a certain part of the View window.
View in Direction	
Isometric	Sets isometric view.
In X-direction	Sets the view of the transport domain in the X-direction.
In Y-direction	Sets the view of the transport domain in the Y-direction.
In Z-direction	Sets the view of the transport domain in the Z-direction.
Reverse X-direction	Sets the view of the transport domain in the reverse X-direction.
Reverse Y-direction	Sets the view of the transport domain in the reverse Y-direction.
Reverse Z-direction	Sets the view of the transport domain in the reverse Z-direction.
View Stretching	Calls the View Stretching Factors dialog window (Fig. 186) and adjust stretching factors.
Zoom by Rectangle	Zooms in on a certain part of the View window using a rectangle.
Set View (Scroll, Zoom, Rotate)	Sets the View windows so that dynamic actions can be carried out with a cursor. Moving the cursor while holding the left mouse button allows the object to be displayed in a different part of the View window. Pressing the Shift button on the keyboard allow zooming actions around the cursor.
Perspective View	Sets perspective view.
Auto-Rotate	Starts <i>Autorotate</i> function that will rotate the transport domain in the View window.
Display Whole Domain	Cancels the Section View and displays the entire transport domain.
Center of Rotation	
Pick	Selects graphically (using a mouse) the Center of Rotation.
Reset	Resets the Center of Rotation previously manually selected to the default Center of Rotation (center of the domain).
Show/Hide	Shows or hides the Center of Rotation from the View window.
Cancel Section View Mode	Cancel the current display mode and displays the entire domain.

Save Current View	Saves the definition of the current view
Edit Named Views	Edits Named Views
Import/Export View Settings	
Export View Transformation	Export information describing camera settings (angle of view and zoom).
Import View Transformation	Export information describing camera settings.
List Boxes for Inverse Data	Shows text information in the inverse data list (the Data for Inverse Solution dialog window; Fig. 15).
D Insert	
Domain Geometry	
Points	
Graphically	Inserts single points graphically.
Dialog	Inserts single points numerically (the Edit Point dialog window without the FE-Mesh tab; Fig. 58).
Lines	
Line	Inserts a line either graphically or numerically (the Edit Curve dialog window without the FE-Mesh tab; Fig. 60).
Polyline	Inserts a polyline either graphically or numerically (the Edit Curve dialog window without the FE-Mesh tab; Fig. 60).
Arc	Inserts an arc either graphically or numerically.
Circle	Inserts a circle either graphically or numerically.
Spline	Inserts a spline either graphically or numerically (the Edit Curve dialog window without the FE-Mesh tab; Fig. 60).
Surfaces	Inserts a surface either graphically or numerically.
Planar Surface	Inserts a planar surface either graphically or numerically.
Quadrangle Surface	Inserts a Quadrangle surface either graphically or numerically.
Rotary Surface	Inserts a Rotary surface either graphically or numerically.
Pipe Surface	Inserts a Pipe surface either graphically or numerically.
B-Spline Surface	Inserts a B-Spline surface either graphically or numerically.
Openings	Inserts an opening either graphically or numerically.
Thicknesses	Inserts thicknesses either graphically or numerically.
Solids	Inserts solids either graphically or numerically.
3D-Layered Domain	Inserts Layered solids either graphically or numerically.
General Solid	Inserts General solids either graphically or numerically.
FE-Mesh Refinement	
Insert Mesh Refinement - Graphically	Inserts new FE-mesh refinement graphically (the FE-Mesh refinement dialog window; Fig. 125).
Insert Mesh Refinement - Dialog	Defines new FE-mesh refinement graphically (the FE-Mesh refinement dialog window; Fig. 125).
Domain Properties	
Material Distribution	Specifies the spatial distribution of soil materials.
Root Distribution	Specifies the spatial distribution of root water uptake.
Nodal Recharge	Specifies the spatial distribution of nodal recharge.
Scaling Factor	
Hydraulic Conductivity	Specifies the spatial distribution of the hydraulic conductivity scaling factors.
Pressure Head	Specifies the spatial distribution of the pressure head scaling factors.
Water Content	Specifies the spatial distribution of the water content scaling factors.
Local Anisotropy	

Angle	Specifies the spatial distribution of the angle of local anisotropy (for two-dimensional applications).
First Component	Specifies the spatial distribution of the first component of local anisotropy (for two-dimensional applications).
Second Component	Specifies the spatial distribution of the second component of local anisotropy (for two-dimensional applications).
Index	Specifies the spatial distribution of anisotropy tensors (for three-dimensional applications).
Subregions	Specifies the spatial distribution of subregions for mass balance calculations.
Observation Nodes	Specifies observation nodes for the output of the pressure head, water content, temperature, and concentration at each time step.
Drains	Specifies nodal points representing tile drains.
Flowing Particles	Specifies nodal points representing flowing particles.
Initial Conditions	
Pressure Head/Water Content	Specifies the initial condition for water flow.
Concentration	Specifies the initial condition for solute transport.
Nonequilibrium Concentration	Specifies the initial condition for nonequilibrium solute transport.
Temperature	Specifies the initial condition for heat transport.
Import	Imports initial conditions for water flow, solute transport, and/or heat transport.
Boundary Conditions	
Water Flow	
No Flux	Specifies a no-flux boundary condition along a selected part of the boundary.
Constant Head	Specifies a constant pressure head boundary condition along a selected part of the boundary.
Constant Flux	Specifies a constant flux boundary condition along a selected part of the boundary. Flux is positive for inflow.
Seepage Face	Specifies a seepage face boundary condition along a selected part of the boundary.
Variable Head 1-4	Specifies a variable pressure head boundary condition along a selected part of the boundary.
Variable Flux 1-4	Specifies a variable flux boundary condition along a selected part of the boundary. Flux values are negative for inflow.
Free Drainage	Specifies a free drainage boundary condition along a selected part of the boundary.
Deep Drainage	Specifies a deep drainage boundary condition along a selected part of the boundary.
Atmospheric Boundary	Specifies an atmospheric boundary condition along a selected part of the boundary.
Solute Transport	
First-Type	Specifies a first-type boundary condition for solute transport along a selected part of the boundary.
Third-Type	Specifies a third-type boundary condition for solute transport along a selected part of the boundary.
Volatile Type	Specifies a volatile-type boundary condition for solute transport along a selected part of the boundary.
Heat Transport	
First-Type	Specifies a first-type boundary condition for heat transport along a selected part of the boundary.
Third-Type	Specifies a third-type boundary condition for heat transport along a selected part of the boundary.

Slope Cube

Free Displacement	Specified Free Displacement boundary condition for the Slope Cube soil stability module
X-displacement	Specified X-displacement boundary condition for the Slope Cube soil stability module
Z-displacement	Specified Z-displacement boundary condition for the Slope Cube soil stability module
XZ-displacement	Specified XZ-displacement boundary condition for the Slope Cube soil stability module
X-force	Specified X-force boundary condition for the Slope Cube soil stability module
Z-force	Specified Z-force boundary condition for the Slope Cube soil stability module
XZ-force	Specified XZ-force boundary condition for the Slope Cube soil stability module

Cross-Sections

Graphically	Inserts a cross-section graphically.
Dialog	Inserts a cross-section using the dialog window.

Mesh Line

Graphically	Inserts a mesh line graphically.
Dialog	Inserts a mesh line using the dialog window.

Auxiliary Objects

Dimension	Inserts auxiliary object (dimensions).
Comment	Inserts auxiliary object (comment).
Bitmap	Inserts auxiliary object (bitmap).
Background Layer	Inserts auxiliary object (background layer).

E Calculation

FE-Mesh Parameters	Specifies either parameters of the Unstructured Finite Element Mesh Generator (the FE-Mesh Parameters dialog window; Figs. 117 through 123) or parameters of the structured mesh (the Rectangular Domain Discretization dialog window (Fig. 115) or the Hexahedral Domain Discretization dialog window (Fig. 116)). Generates the unstructured finite element mesh.
Generate FE-Mesh	
Advanced FE-Mesh Generation	
Fundamental Triangulation	Performs triangulation of boundary nodes based on the Delaunay criterion.
Mesh Refinement	Inserts a new point in the center of all triangles that do not fulfill the smoothness criterion.
Retriangulation	Retriangulates mesh according to Delaunay criterion.
Check of Convexity	Corrects possible errors which may appear during smoothing and retriangulating.
Mesh Smoothing	Smooths the mesh by solving a set of coupled elliptic equations using a recursive algorithm.
FE-Mesh Statistics	Provides information about the finite element mesh (the FE-Mesh Information dialog window (Fig. 132).
Delete FE-Mesh	Deletes the unstructured finite element mesh.
Calculate Current Project	Carries out calculations for the currently active project.
Calculate Current Project	Carries out calculations for all currently open projects.
Select Projects to Calculate	Opens the Project Manager to select projects to be calculated.

F**Results****Display Quantity**

Pressure Head

Displays results in terms of pressure heads.

Water Content

Displays results in terms of water contents.

Velocity

Displays results in terms of velocities.

Concentration

Displays results in terms of concentrations

Nonequilibrium Concentration

Displays results in terms of nonequilibrium concentrations (kinetically sorbed or in the immobile water)

Temperature

Displays results in terms of temperatures

Boundary Information

Pressure Heads

Graphical presentation of pressure heads at different boundaries and in the root zone.

Boundary Fluxes

Graphical presentation of potential and actual boundary water fluxes at different boundaries.

Cumulative Fluxes

Graphical presentation of potential and actual cumulative boundary water fluxes.

Solute Fluxes

Graphical presentation of actual and cumulative boundary solute fluxes.

Observation Points

Graphical presentation of changes in water content, pressure head, temperature, and/or solute and sorbed concentration at specified observation nodes.

Profile Information

Basic Information

(only in 1D)

Displays basic variables versus depth (only in 1D).

Solution Concentrations

Displays solution concentrations versus depth for the UnsatChem module (only in 1D)

Solid Concentrations

Displays solid and exchange concentrations versus depth for the UnsatChem module (only in 1D)

Chemical Information

Displays chemical variables (e.g., pH, SAR) versus depth for the UnsatChem module (only in 1D)

Particle Tracking

Displays particles as they travel through the soil profile (only in 1D)

Soil Hydraulic Properties

Graphical presentation of the soil hydraulic properties.

Run Time Information

Graphical presentation of information about the number of iterations, time step, and Peclet and Courant numbers.

Mass Balance Information

Displays mass balance information and mean profile properties.

Chemical Mass Balance Information

Displays chemical mass balance information.

Convert Output to ASCII

Convert binary input and output files into ASCII files.

Inverse Solution Results

Displays information about the inverse solution.

Meteorological Information

Displays meteorological fluxes and information (only in 1D)

Fluxes across Mesh-Lines

Displays actual and cumulative, water and solute fluxes across selected mesh-lines in 2D or mesh-surfaces in 3D.

HP2 Text Output

Displays the PHREEQC.out text output file.

Cosmic-Ray Neutron Information

Displays results for the Cosmic Module (only in 1D)

Furrow Module

Stations

Displays furrow water depths, infiltration rates, cumulative infiltration rates, concentrations, and solute infiltration rates at individual furrow stations.

Runoff

Displays actual and cumulative, water and solute fluxes at the outflow from the furrow.

Advance and Recession times

Displays advance and recession times.

DPU Module

DPU Solute Concentrations

Displays solute concentrations for the DPU module.

DPU Masses	Displays solute masses for the DPU module.
DPU Fluxes	Displays solute fluxes for the DPU module.
Time Layer	
First	Displays a particular variable at the first-time layer.
Last	Displays a particular variable at the last-time layer.
Previous	Displays a particular variable at the previous time layer.
Next	Displays a particular variable at the next time layer.
Animation	Displays time layers of a particular variable consecutively and continuously.
Graphs	
Cross-Section Line	Displays the values of a particular variable along an arbitrary cross-section.
Mesh Line	Displays the values of a particular variable along a selected mesh line.
Boundary Line	Displays the values of a particular variable along a certain part of a boundary.
Line Probe	Displays the values of a particular variable along a line probe.
Flowing Particles	
Draw Particles Positions	Draws positions of flowing particles.
Draw Particles Trajectories	Draws trajectories of flowing particles.
Streamlines	
Show Manipulator or Seed Points	Display the Manipulator tool and Seed Points.
Apply Changes Immediately	???
Apply Changes	???
Edit Seed Point Sources	Edits locations of Seed Points.
Delete Results	Deletes all output results.
G Tools	
Show Grid	Shows or hides the grid.
Snap to Grid	Specifies whether or not the mouse should move in steps defined by the grid.
Grid and Work Plane	Calls the Grid and Work Plane dialog window (Fig 185).
Define Work Plane	
Set Origin	Redefines origin of the grid.
Define XY	Sets Work Plane to the XY plane.
Define YZ	Sets Work Plane to the YZ plane.
Define XZ	Sets Work Plane to the XZ plane.
Coordinate System	Selects coordinate system
Graphical Manipulator	???
Translate	Moves or copies a selected object.
Rotate	Rotates a selected object.
Mirror	Mirrors a selected object.
Stretch	Stretches a selected object.
Skew	Skews a selected object.
Intersect Lines	Finds the intercept of two lines and insert an interception point on the lines.
Intersect Surfaces	Finds the curve that is created by the intercept of two surfaces.
Split Lines	Splits lines.
Insert Points on Line	Inserts points on a line.

Extend Lines
 Extend Thickness Vectors
 Check Geometry
 Repair Geometry
 Generate Domain Surfaces
 Create Video File

Extends selected lines.
 Extends selected thickness vectors.
 Checks geometry for consistency.
 Repairs geometry if inconsistent
 Attempts to generate Domain Surface if they were not specified.
 Allows users to save flow animation in a video file.

H Options

Display Options

Edit

Edits display options in the **Display Options** dialog window (Fig 157).

Default

Sets display options to their default values.

Import

Reads display options from a file.

Export

Saves display options to a file.

Program Options

Displays program options information (the **Program Options** dialog window has two tabs, one related to **Graphics** (Fig. 199) and one to **Program** itself (Fig. 200)).

Model Display

Solid Model

Displays the transport domain as a solid object.

Transparent Model

Displays the transport domain as a transparent object.

Wire Frame Model

Displays the transport domain as a wired object

Use Material Colors for Geo-Objects

???

Scalar Field Display

Isolines

Displays the spatial distribution of a particular variable by means of isolines.

Colormaps

Displays the spatial distribution of a particular variable by means of isobands.

IsoSurfaces

Displays the spatial distribution of a particular variable by means of isosurfaces.

Color Points

Color Points Displays the spatial distribution of a particular variable by means of color points.

Color Edges

Displays the spatial distribution of a particular variable by means of color edges.

Show Mix/Max Values

Display values of property minimum and maximum

Color Scale

Color Smoothing

Changes color from abrupt to gradual at isolines.

Min/Max Values Global in Time

Selects minimal and maximal values for the color scale either for the entire time duration or only for a selected time layer.

Min/Max Values Global in Space

Selects minimal and maximal values for the color scale either for the entire transport domain or only for the displayed part of the domain.

Standard Scale

Selects a standard color scale for the display of a particular variable.

Custom Scale

Selects a custom color scale for the display of a particular variable.

Edit Scale

Calls the **Edit Isoband Value and Color Spectra** dialog window (Fig. 158).

Streamline Options

Selects options for displaying streamlines (Fig. 168)

Vectors Field Options

Selects options for displaying Darcy velocity vectors.

Clipper Options

Selects options for the Slicer display.

I Modules

Slope Stability

Input Parameters

Contains basic input parameters of the **Slope Stability** module.

Open Slope Stability Module	Opens the add-on Slope Stability module, which carries out required slope stability calculations.
Printout Report and Results	Produces a standard Report that summarizes results obtained by the Slope Stability module.
Delete Results	Deletes results calculated by the Slope Stability module.
Settings	Sets the global parameters for the Slope Stability module
Slope Stability Help	Displays help information for the Slope Stability module
Slope Stability User's Manual	Displays a PDF version of the Slope Stability module User Manual.
Slope Cube	
Slope Cube Stress Parameters	Specifies stress parameters for the Slope Cube module.
Slope Cube Users Manual	Opens Slope Cube Users Manual.
Slope Cube Tutorial	Opens Slope Cube Tutorial.
Furrow	
Furrow Parameters	Specifies stress parameters for the Slope Cube module.
Furrow Users Manual	Opens Slope Cube Users Manual.
J Windows	
New Window	Open a new View window.
Main and Secondary	Displays open View windows as main and secondary windows.
Tile Horizontally	Tiles open View windows horizontally.
Tile Vertically	Tiles open View windows vertically.
Cascade	Cascades open View windows.
Close All	Closes all open View windows.
Arrange Icons	Arranges minimized windows as icons at the bottom of the View window.
K Help	
Context Sensitive Help	Help for various objects of GUI.
Help – Contents and Index	Displays help information.
Hydrus User Manual	Displays a PDF version of the HYDRUS User Manual.
Hydrus Technical Manual	Displays a PDF version of the HYDRUS Technical Manual.
Hydrus Online	Launches Internet Explorer Browser and opens the HYDRUS web page.
Check for Updates	Displays a window that informs the user about the latest version of the program and, and if available, recommends an update. If prompted, it launches an Internet Explorer Browser and opens the "Program Updates and Upgrades" page of the HYDRUS web page, from which an upgrade can be downloaded.
Hydrus License and Activation	Displays the Hydrus license and activation information (the HYDRUS License and Activation dialog window; Fig. 203).
About Hydrus	Displays the version and authors of the HYDRUS application.

8.6. Input Tables in HYDRUS

Tables (e.g., in the "*Water Flow Parameters*" (Fig. 20) or the "*Time-Variable Boundary Conditions*" (Fig. 48) windows) are compatible with various standard spreadsheet software (e.g., MS Excel). Input data can be prepared in such software (e.g., MS Excel) and then copied into various input tables of HYDRUS. One can use keyboard keys **Ctrl+C** to *Copy* a content selected cells (in Excel) into the clipboard and **Ctrl+V** to *Paste* it into the HYDRUS table.

8.7. New Features in Version 3.0 of GUI

The GUI of Version 3 of HYDRUS (2D/3D) now includes a significant number of major new features (Šimůnek et al., 2018), as well as a large number of smaller corrections and improvements. Although the external look has been preserved and is similar to Version 2, Version 3 internally uses the latest software development tools and libraries, which is critical to ensure compatibility with new Windows operating systems and the development of more efficient software in the future. This section provides a brief overview of the most important improvements and extensions.

One important objective of the new version was to increase the performance and capacity of the GUI. The limit of Version 2 of HYDRUS (about 1 million finite elements) was extended by almost an order to 10 million finite elements. The extension was achieved by overall optimization of the code and developing a 64-bit version of HYDRUS, which can now use all physical memory available on modern PCs. This feature permitted a considerable increase in the size of HYDRUS simulations, with the main limiting factor now being the speed of the calculation module(s).

We further replaced many old HYDRUS (2D/3D) software components for charts and tables in Version 3 with new components, which also included fixing some known errors. Now all dialogs containing charts or tables are resizable, thus making entering and viewing data more comfortable. The GUI also supports Unicode and can now correctly display special characters such as Greek symbols. Although manipulating graphical objects in HYDRUS, in general, was relatively easy thanks to drag-and-drop features, some operations (such as rotations) had to be defined numerically in a dialog box. Version 3 offers a new graphical tool called "Manipulator" for more user-friendly transformations of selected objects in two or three dimensions.

We also improved several features related to Mesh-sections, 3D mesh clipping and slicing. The optimization of a GUI for work with relatively large FE meshes required certain changes in using mesh-sections. While mesh-sections are still fully supported, the program by default does not generate as many mesh-sections as in Version 2.

9. Miscellaneous Information

9.1. Program Options

The **Program Options** dialog window has four tabs, one related to **Graphics** (Fig. 199), one to **Program Options** (Fig. 200), one to **FE-Mesh** (Fig. 201), and one to **Files and Directories** (Fig. 202).

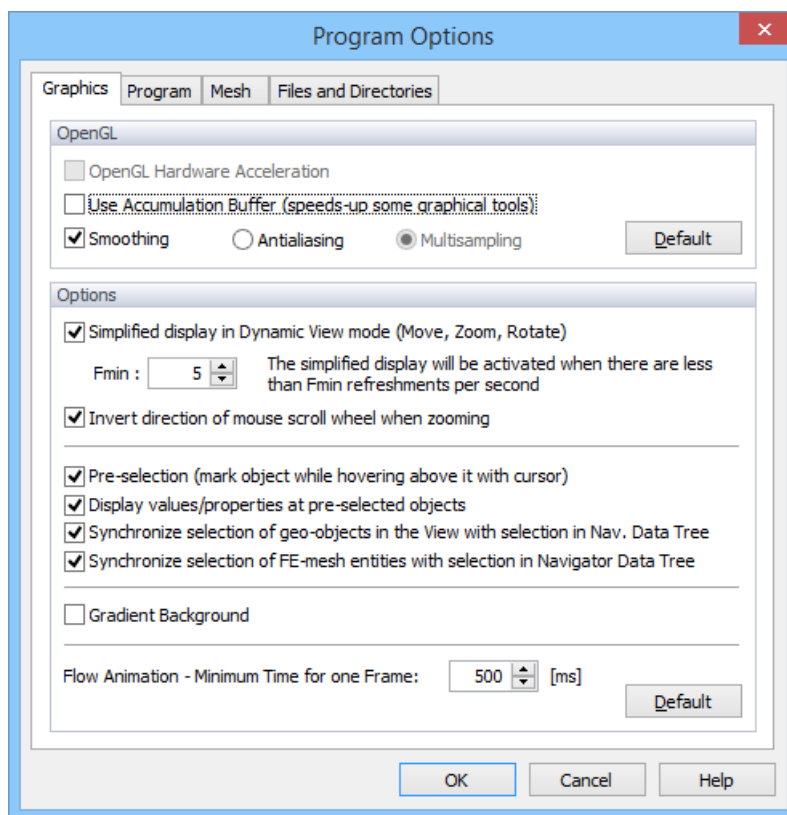


Figure 199. The Program Options dialog window (the Graphics Tab).

In the top part of the **Graphics** Tab (Fig. 199) (*OpenGL*) one can turn on or off the *OpenGL Hardware Acceleration* (*OpenGL* is a library of functions developed by Silicon Graphics Inc. for handling graphical objects), and select the speed for *OpenGL optimization*.

In the bottom part of the **Graphics** Tab (*Options*) one can select

- Simplified display in Move modus*
- whether to *Invert direction of mouse scroll wheel when zooming*
- whether or not an object is selected when the cursor hovers above it (*Pre-selection (Mark object while hovering above it with cursor)*),
- whether or not values and properties are displayed numerically when the cursor is close to a selected object (*Display values/properties at pre-selected objects*),
- a different background (*Gradient Background*) (visually more effective background is displayed, which may be useful for presentations), and

- f) minimum time for one frame during flow animation.

Simplified Display Mode: When the graphics (View Window update) is too slow, this option accelerates it during dynamic rotating, moving, or zooming. When rotating the model, only its simplified version is drawn, which results in a faster display of the model. When rotating is finished, the full model is displayed again. This option is initiated only when the number of “refreshments” per second falls below the specified number.

When the checkbox "**Synchronize selection in the Navigator and Views**" is checked, clicking on any object on the **Navigator Bar** leads to its automatic selection in Views. When this checkbox is not checked, one can select an object by clicking on it with the right mouse button at the **Navigator Bar** and using the **Select** command from the popup menu.

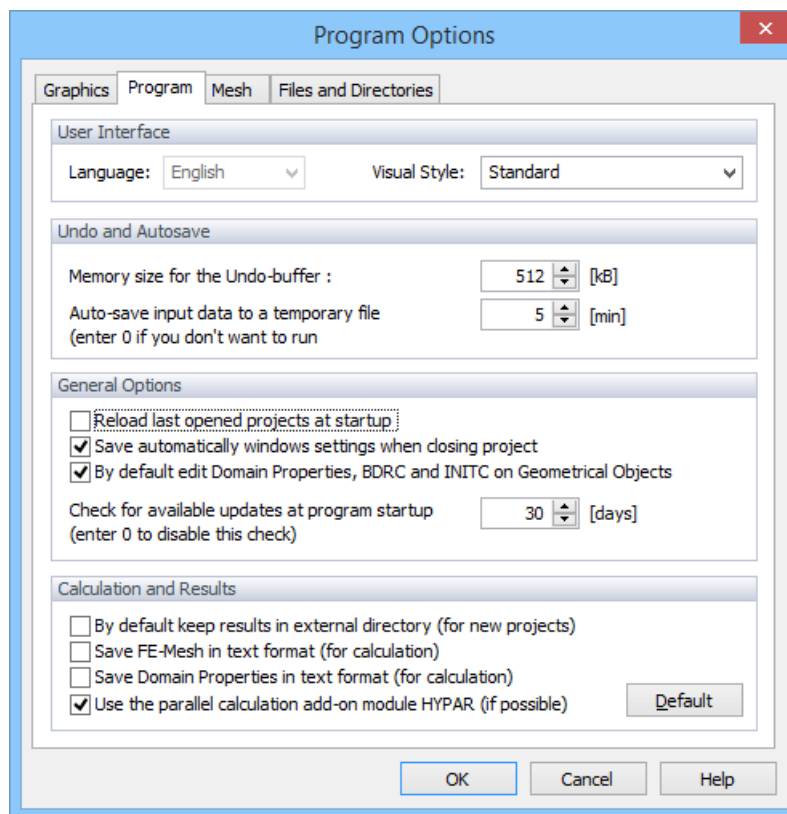


Figure 200. The Program Options dialog window (the Program Options Tab).

In the **Undo and Autosave** part of the **Program Options** Tab (Fig. 200) one can

- select a time interval for *Auto-save*
- specify *Memory size for the Undo buffer*, and

In the **General Options** part of the **Program Options** Tab one can

- specify whether or not the program *Reloads last opened projects at startup*
- specify whether or not the program should *Save automatically windows settings on close project*

- c) select whether *Domain properties, and boundary and initial conditions are edited by default on Geometrical objects* or finite element mesh.
- d) select how often (every *nn* days) the program should "*Check for available updates at Hydrus startup*" at the Hydrus website. This check can be disabled by entering zero (0). Note that customers who own a HYDRUS license are entitled to free **updates** of the purchased version within the next two years.

In the **Calculation and Results** part of the **Program Options** Tab one can

- a) specify whether the results are to be kept in an external directory (*By default keep results in an external directory*),
- b) select whether the FE-Mesh is to be saved in text format (*Save FE-Mesh in text format*),
- c) select whether or not Domain Properties are to be saved in text format (*Save Domain Properties in text format*).
- d) Select whether the parallelized version, i.e., the **HyPar module** (see Section 9.8), of the standard computational module (h2d_calc.exe and h3d_calc.exe) is to be used (*Use Parallel Calculation Module*).

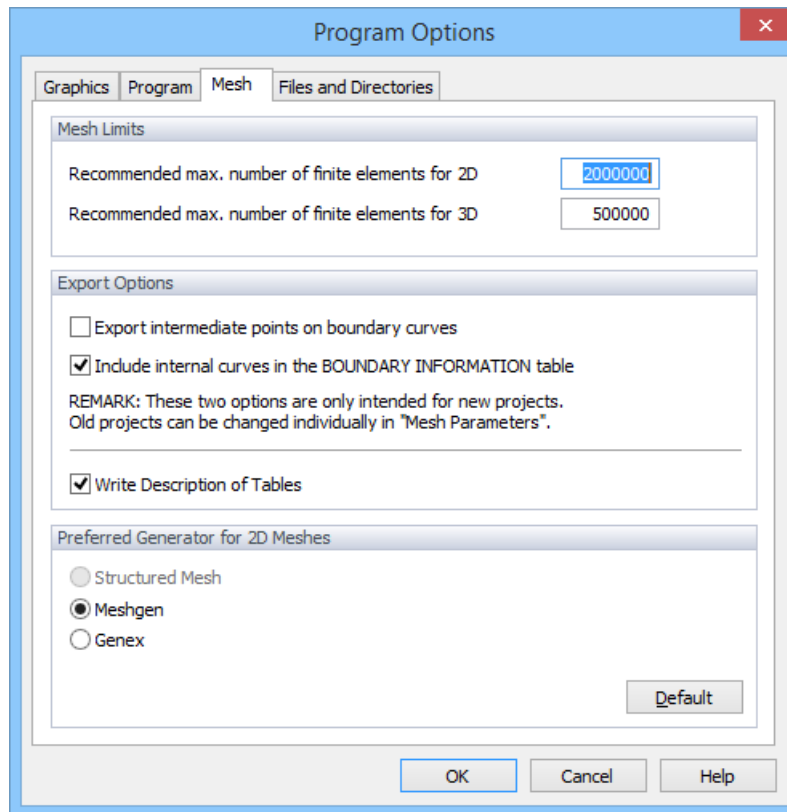


Figure 201. The Program Options dialog window (the FE-Mesh Tab).

In the **Mesh Limits** part of the **FE-Mesh** Tab (Fig. 201) one can

- a) specify the *Recommended maximum number of finite elements for 2D projects*,
- b) specify the *Recommended maximum number of finite elements for 3D projects*.

In the **Export Options** part of the **FE-Mesh** Tab one can select various export options, such as

- a) whether to *Export intermediate points on boundary curves*,
- b) whether to *Include internal curves in Boundary Information Table*, and
- c) whether to *Write Description Tables*.

Finally, in the **Preferred Generator for 2D Meshes** part of the **FE-Mesh** Tab, one can select whether to use the MESHGEN (default) or Genex program.

In the **Files and Directories** Tab (Fig. 202) (*Options*) one can specify locations of various HYDRUS files and the file having information about display options:

- Directory for HYDRUS Settings and Authorization Files
- Working Directory for Temporary Files
- Default Directory for HYDRUS Projects
- Configuration file for display options
- Directory for Thermodynamic Databases (for the HP2 program)

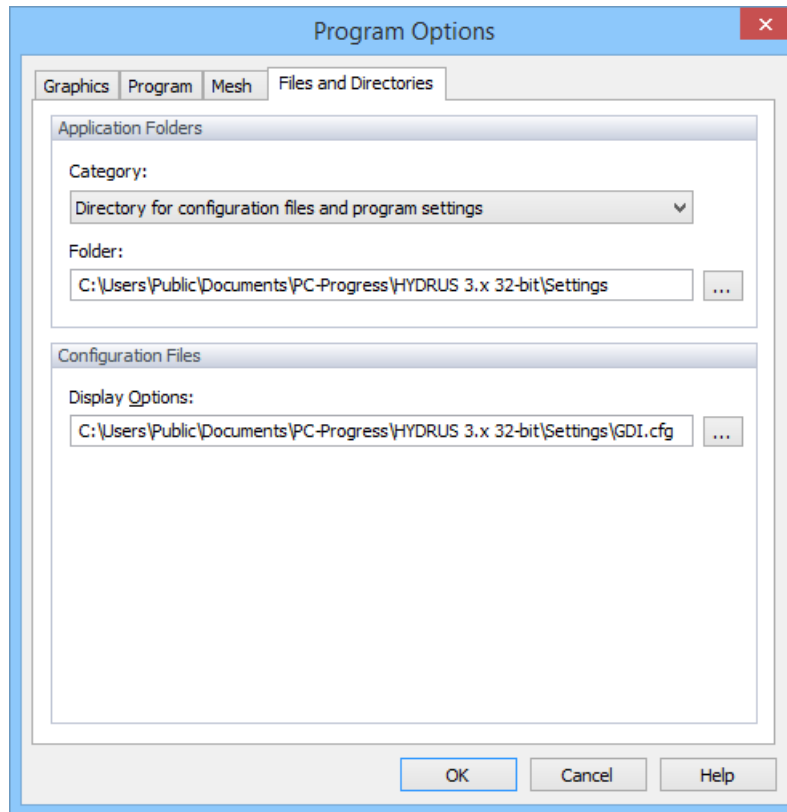


Figure 202. The Program Options dialog window (the Files and Directories Tab).

9.2. HYDRUS License and Activation

HYDRUS is protected either by a **Software Lock** that is based on information about the hardware on which it is run or, starting with version 2.02, using a **Hardware Key (HASP)**. Starting with version 2.02, the software key can be used to authorize only separate computers, while a **Hardware Key** is required for the network or server installations designated for remote access (see Section 9.2.5). Without activation, HYDRUS works as a demo version - you can run it but you will not be able to run calculations and save your data. A customer using a **Software Lock** can choose to **Activate HYDRUS by E-mail** with the help of the HYDRUS support or directly **On-line** (an internet connection is required). Using the **Online** activation system, customers can themselves manage their HYDRUS license, i.e., installation, de-installation, and/or reinstallation of HYDRUS. The HYDRUS software package is activated (using the Software Lock) using the **HYDRUS Authorization Status** dialog window (Fig. 203) that is called using the command *Help->Hydrus License and Activation*.

9.2.1. Brief Description of HYDRUS Activation Using a Software Lock

A. On-Line Activation (recommended)

- To activate online you need to know your **License Number** (four digits) and the **Activation Key** (hexadecimal, 32 characters). You should receive both numbers from the HYDRUS distributor from whom you purchased the license for HYDRUS or from HYDRUS customer support support@pc-progress.cz.
- Enter both numbers into the **Online Activation** dialogue window (Fig. 207).
- After clicking the **Activate Now** command, HYDRUS establishes a connection over the Internet with the license server and performs its activation.

B. Activation by E-Mail (when encountering problems with on-line activation)

The activation process by email consists of generating two request codes that need to be sent to the HYDRUS distributor together with information about the license, customer, and workplace. Based on this information, the HYDRUS distributor will generate a corresponding activation code and send it back to the HYDRUS user. Different HYDRUS functions will be activated after inserting the activation code depending upon the type of purchased license.

- In the dialog window **Activation by E-mail** (Fig. 222), generate **Request Codes**.
- Send the **Request Codes** by email to support@pc-progress.cz or to the HYDRUS distributor, from whom you purchased the license for HYDRUS.
- After that, you will receive by email the **Activation Code**, which you enter into the dialog window **Activation by E-mail (Step 3 Tab, Fig. 213)**, and activate HYDRUS.

9.2.2. Detailed Description of HYDRUS Activation Using a Software Lock

The **HYDRUS Authorization Status** dialog window (Fig. 203) displays information about **Authorization Status**, **Last Activation**, and **License Information**, such as **License Number**, **Computer ID**, **Workplace**, and **License Owner**. **Authorization Status** information includes information about

- a) **Status**, which can be either *Not Authorized* or *Authorization OK*,

- b) **Level** of authorization, which can be either *2D-Lite*, *2D-Standard*, *3D-Lite*, *3D-Standard*, or *3D-Professional*,
- c) whether or not the **Authorization is Time-Limited** (if yes, then the *Expiration Time* is given), and
- d) whether or not the **Network Installation** is active (if yes, then the *Number of Clients* is given)

All this information is displayed as read-only text that is filled in during the first activation of the software. The button “**Send Authorization Report**” is used when resolving problems with software activation.

Figure 203. The HYDRUS Authorization Status dialog window (Tab Status).

For the commands in this dialog window to be active (e.g., **Activate by E-mail** or **Activate on-line**), HYDRUS needs to be run with administrator privileges. That means that you need to be logged as an **Administrator** (or as a user belonging to the "Administrators" group) when making changes to the authorization. To run HYDRUS as administrator under Windows Vista or Windows 7 operating systems, click on the HYDRUS icon on your desktop using the right mouse button and

select **"Run as Administrator"** from the popup menu. Warning displayed in Figure 204 is issued when attempting to make changes to the **Authorization Status** while not running HYDRUS with administrator privileges.

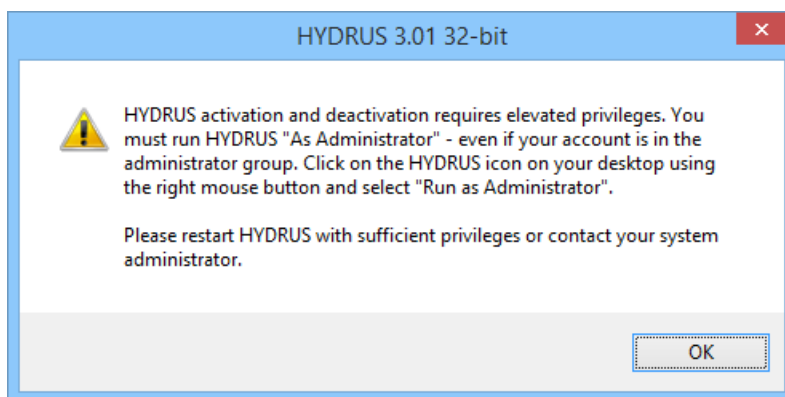


Figure 204. Warning issued when attempting to make changes to the Authorization Status while not running HYDRUS with administrator privileges.

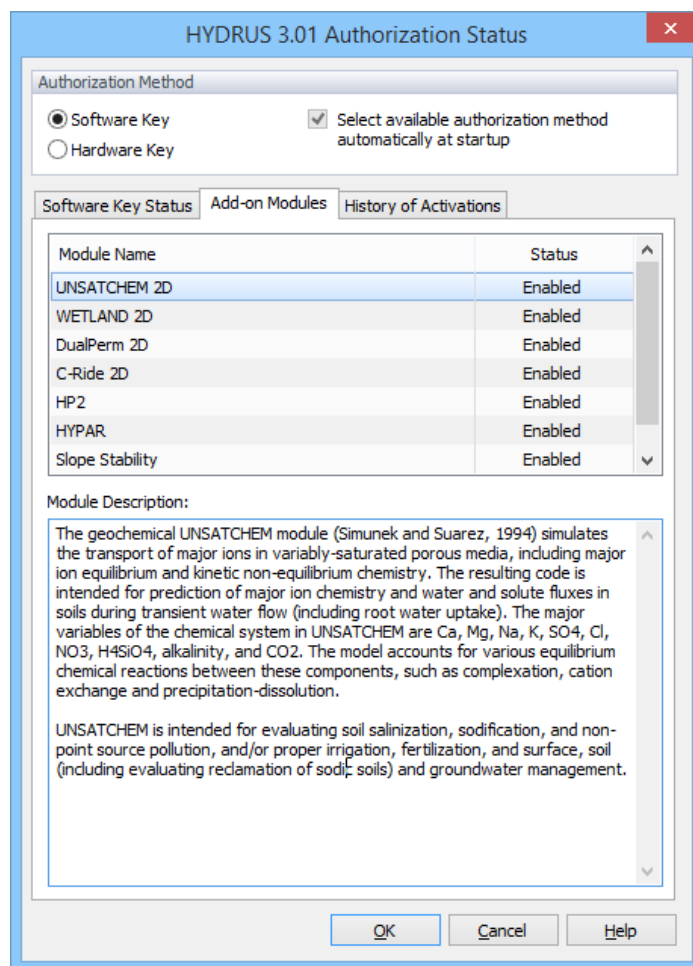


Figure 205. The HYDRUS Authorization Status dialog window (Tab Add-on Modules).

The second Tab of the **HYDRUS Authorization Status** window, i.e., the **Add-in Modules** Tab list additional HYDRUS modules (e.g., Unsatchem, Wetland, DualPerm, C-Ride, or HP2) that are currently available and activated. At the top of the Tab, there is an indication, which **Authorization Method** (either of Software Key or a Hardware Key) is used.

The third Tab of the **HYDRUS Authorization Status** window, i.e., the **History of Activation** Tab reports recent actions related to HYDRUS activation.

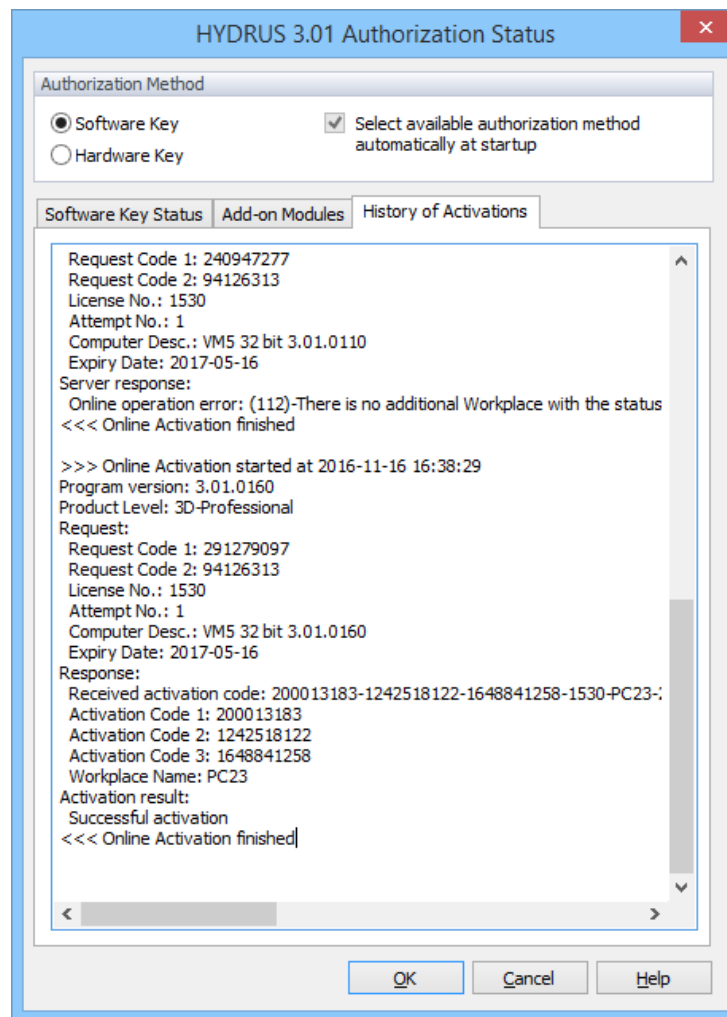


Figure 206. The HYDRUS Authorization Status dialog window (Tab History of Activation).

9.2.2.1. On-Line Activation

Online activation is the fastest and most convenient way to activate HYDRUS. The **Online Activation** window (Fig. 207) appears after clicking on the **Activate on-line** button on the **HYDRUS Activation Status** window. Here you need to enter information about the **License Number** and the appropriate **Activation Key** that you received, together with an invoice from

the HYDRUS Customer Support. This **Activation Key** is used for all Workplaces of a particular license. For special purposes, different **Activation Keys** can be generated for individual Workplaces (e.g., when a particular Workplace has authorization for a different HYDRUS Level or a specific HYDRUS module).

In the section **Specify the required authorization level**, select the required **HYDRUS Level to Activate** (i.e., *2D-Lite*, *2D-Standard*, *3D-Lite*, *3D-Standard*, or *3D-Professional*; please note that this Level has to correspond with the purchased Level) and the Type of License to activate (e.g., **Time-Limited Authorization** with the *Expiration Date*, or the **Network Installation** with the *Number of Clients*). If no checkbox is selected, a **Time-Unlimited Single User License** is authorized. With regard to a possible loss of authorization due to failure of hardware, it is recommended to choose a shorter period of validity (default is 0.5 years). An item **Computer Description** serves for the future identification of a particular computer in the electronic licensing system and is usually characterized by a user or its location (e.g., John - Laptop, Harry - Lab 001).

The screenshot shows the 'Online Activation' dialog box. It is divided into three main sections. The first section, 'Enter Password', contains a 'License Number' field with the value '1530' and an empty 'Activation Key' field. The second section, 'Specify the required authorization level and expiration date', includes a dropdown menu for 'Select HYDRUS Level to activate' set to '3D-Standard'. Below this are two checkboxes: 'Time-limited Authorization' (checked) and 'Network Installation' (unchecked). The 'Time-limited Authorization' section has an 'Expiry Date' dropdown set to '5/28/2017' and a 'Number of Clients' field set to '0'. The third section, 'Computer Description (to identify this computer in the future)', has a 'Computer Description' field with the text 'VM5 32 bit'. At the bottom of the dialog are three buttons: 'Activate Now', 'Close', and 'Help'.

Figure 207. The Online Activation dialog window.

After clicking on the **Activate Now** button, you will be asked to confirm all specified parameters (Fig. 208) (note that you may be prompted by your firewall to allow communication between your computer and the license server of PC Progress). At this point, all specified information will be verified against the data of our electronic licensing system, and if confirmed, the actual activation of HYDRUS will occur. This communication applies only to data entered in the **Online Activation** window, and no other information stored on your PC is transferred. In case of unsuccessful activation, an error message is displayed explaining the problem. After correcting the problem, you can use the **Activate Now** command again.

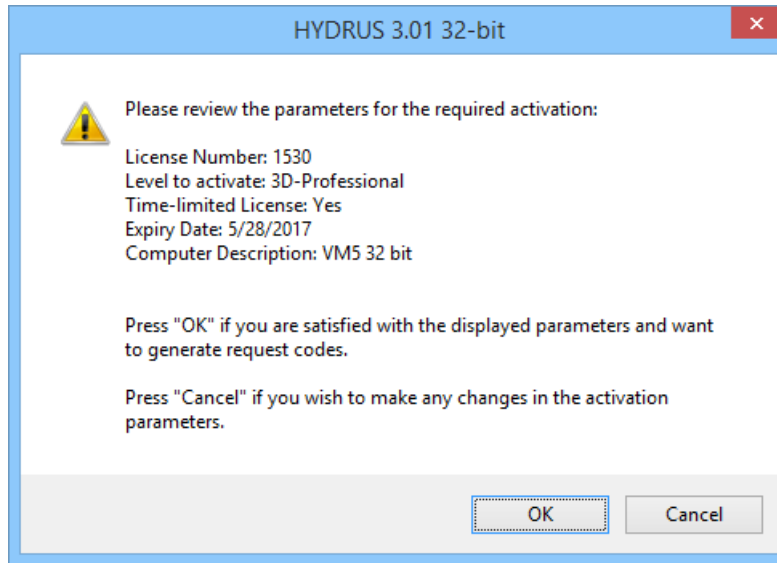


Figure 208. Window requesting confirmation of entered parameters.

Prior to the expiration (**Expiry Day**) of the **Time-Limited Authorization**, the user will be alerted about it, and the license can be easily repeatedly extended using the **Extend Activation** function.

9.2.2.2. *Activation by E-mail*

For this option, the user is guided through a three-step form (three Tabs of the **Activation by E-mail** dialog window, Fig. 222). During the first two steps, he/she prepares information needed to obtain HYDRUS Authorization and emails it to the HYDRUS distributor. In the third step, the user enters the **Activation Code** that he receives by e-mail on the third Tab (**Step 3**) of the **Activation by E-mail** and activates HYDRUS.

The first step is to fill in information about the license (**License Number**), the name of the license owner (**Customer**), and a description of the Workspace (**WP Description**). This last item (i.e., **WP Description**) serves for future identification of a particular computer in the electronic licensing system and is usually characterized by a user or its location (e.g., John - Laptop, Harry - Lab 001).

In the section **Required Authorization** select the required **HYDRUS Level to Activate** (i.e., *2D-Lite*, *2D-Standard*, *3D-Lite*, *3D-Standard*, or *3D-Professional*; please note that this Level has to correspond with the purchased Level) and the Type of License to activate (e.g., **Time-Limited Authorization** with the *Expiration Date*, or the **Network Installation** with the *Number of Clients*). If no checkbox is selected, a **Time-Unlimited Single User License** is authorized. With regard to a possible loss of authorization due to failure of hardware, it is recommended to choose a shorter period of validity (default is 0.5 years).

Activation by E-mail

Step 1

License Information

License Number: 1530

Customer: PC-Progress

Enter your HYDRUS license number and/or name and address of the institution that purchased the license.

Workplace Description

WP Description: VM5 32 bit

Enter a text to identify this workplace or computer

Required Authorization

Select HYDRUS Level to activate: 3D-Professional

☒ Time-limited Authorization ☐ Network Installation

Expiry Date: 5/28/2017 Number of Clients: 0

Next Step

Generate Request Codes Regenerate Request Codes

Cancel Help

Figure 209. The Activation by E-mail dialog window (Tab Step 1).

After clicking on the **Generate Request Codes** button on the **Step 1** Tab of the **Activation by E-mail** window (Fig. 222), the user is prompted to confirm all entered information (Fig. 208), and then the **Step 2** Tab (Fig. 210) appears.

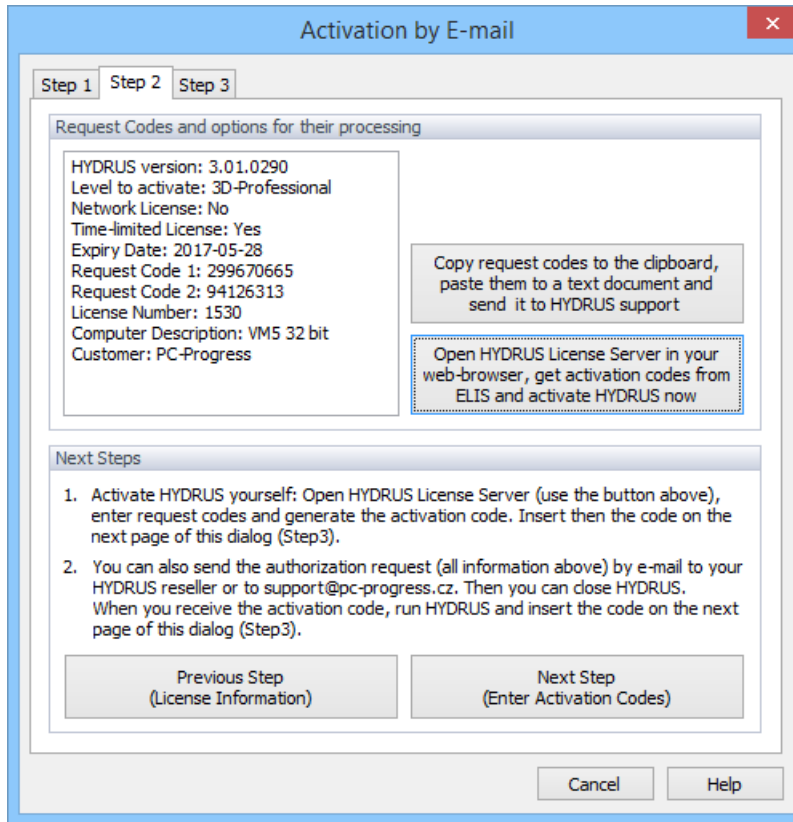


Figure 210. The Activation by E-mail dialog window (Tab Step 2).

Information entered during **Step 1** (on Tab Step 1) is summarized in the **Authorization Request Codes** section of the **Step 2** Tab. This information can be copied to the clipboard using the **Copy to Clipboard** button and then sent by email to the HYDRUS support or other HYDRUS distributors. The command **Send Request Codes by E-mail** will attempt to start the emailing program (e.g., Microsoft Outlook) directly and copy there automatically an email address of the HYDRUS support (support@pc-progress.cz) and all required information (see an example of such email displayed in Outlook in Fig. 211).

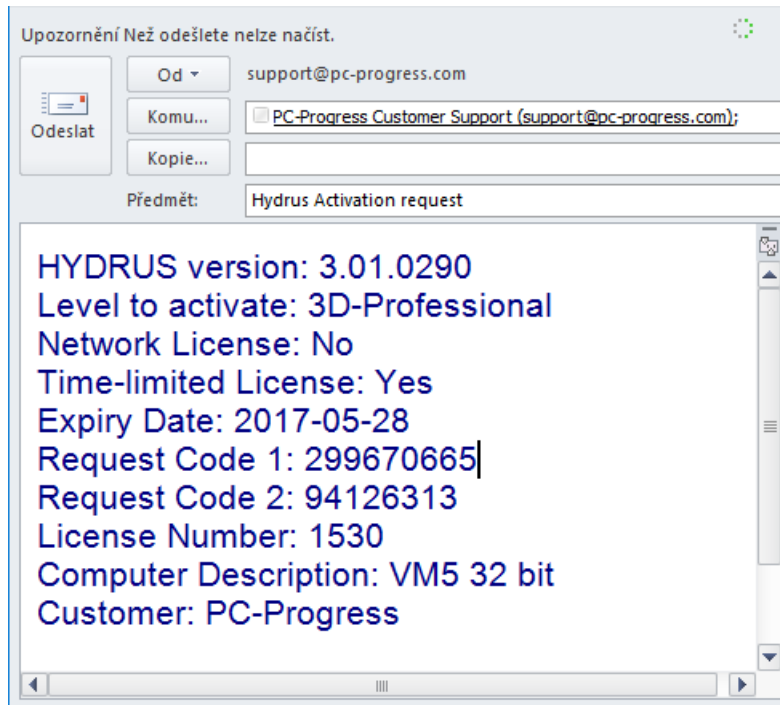


Figure 211. An email with the HYDRUS Activation Request in Outlook.

On the basis of this information, the HYDRUS support or other resellers will promptly email back the **Activation Code**.

Notes on Request Codes

1. Request Code 1 is a randomly generated number that can be used for a single activation. After the activation (either successful or unsuccessful), this number is changed, and therefore, the same number cannot be used repeatedly even for the same computer.
2. Request Code 2 (Computer ID) is a number that uniquely characterizes the hardware of a computer or a computer network (for the network license). This number should be constant for a particular computer unless there is a change of hardware. If this number changes, the authorization system will evaluate the license as invalid. It is thus necessary before the change of hardware (e.g., a change of the motherboard) or reinstallation of the operating system (Windows) to deactivate HYDRUS since HYDRUS will need to be reactivated after hardware changes are completed.
3. There are only three attempts available to activate HYDRUS with a particular request and activation codes. If wrong activation codes are inserted during the first three attempts, HYDRUS issues a warning. After the third attempt with wrong activation codes, the Request Code 1 is changed, and new activation codes need to be requested.
4. We recommend using standard functions Copy & Paste when inserting activation codes to minimize the risk of inserting wrong numbers.

When starting unauthorized HYDRUS again, the user is informed that request codes have recently been generated and if he/she wants to enter the **Activation Code** and activate HYDRUS (Fig. 212). It is important not to regenerate request codes at this time as the **Activation Code** would then not be active any more since one of the request codes would be changed.

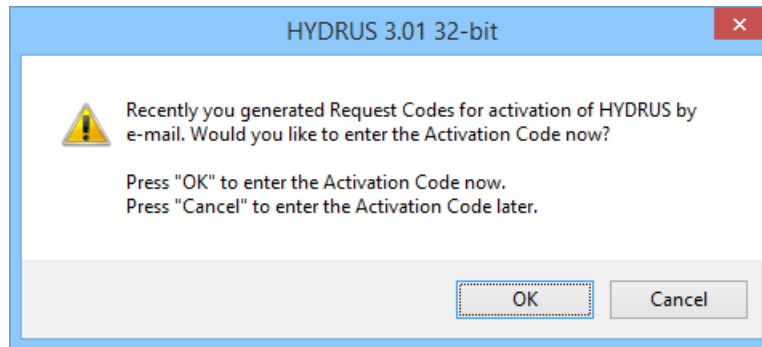


Figure 212. Window inquiring if the user wants to enter the Activation Code.

After receiving the **Activation Code**, enter this code on the **Step 3** Tab of the **Activation by E-mail** dialog window (Fig. 213) and click on the **Activate Now** button. You should receive a confirmation that the authorization process was successful (Fig. 214).

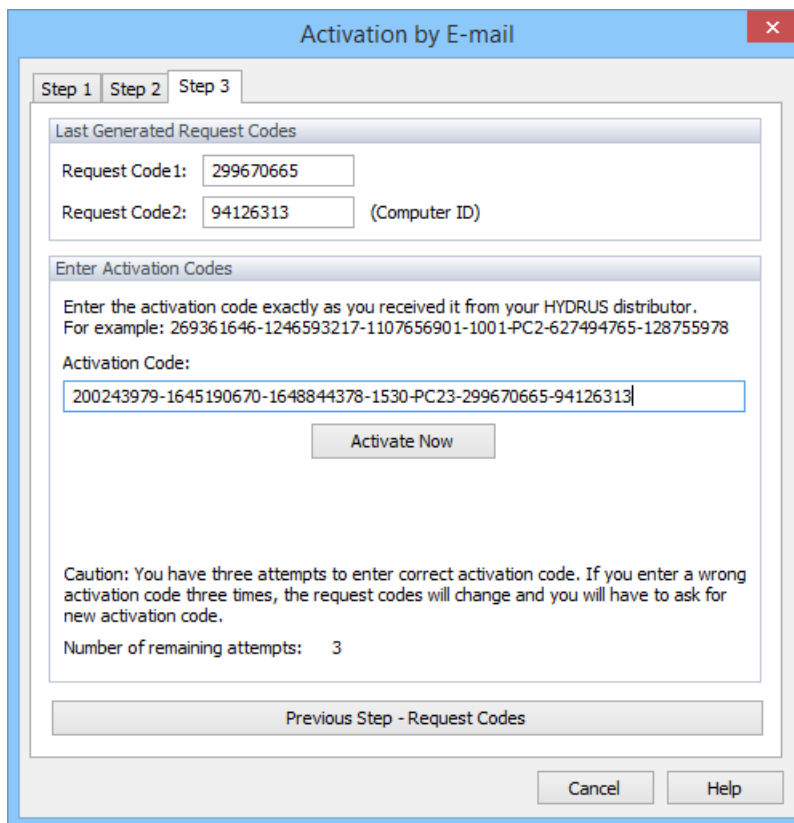


Figure 213. The Activation by E-mail dialog window (Tab Step 3).

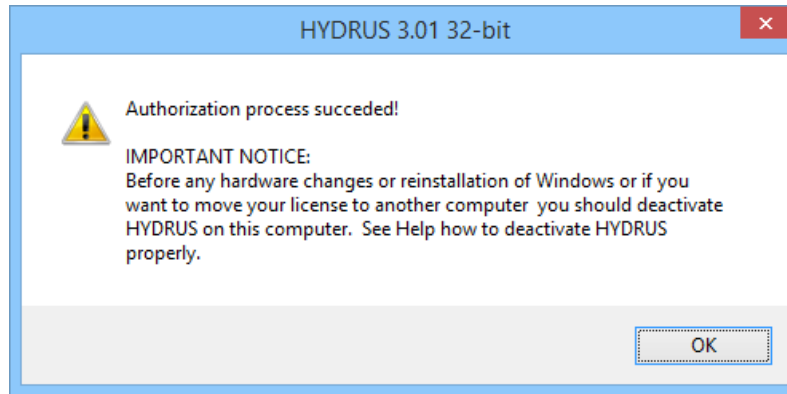
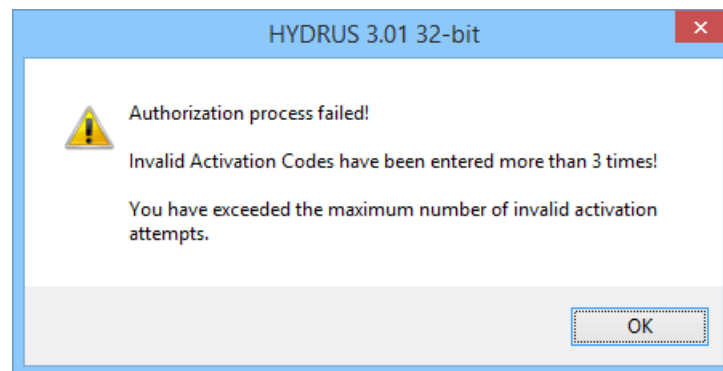


Figure 214. Window confirming successful HYDRUS authorization.

Note that the **Request Code** and a **Computer ID** are displayed in the upper part of the **Step 3** Tab. Remember that your Request Code and Computer ID are hardware-dependent. After upgrading your hardware (e.g., BIOS, hard drives), you will very likely have to request a new **Activation Code**. You are eligible to obtain those codes for free (although subject to some limitations - ask for details).

When the activation fails three times (likely due to incorrectly entered information), the request keys will change, and windows shown in Figure 215 will be displayed, providing instructions on how to proceed further. The user will be requested to send a report to the HYDRUS support so that the cause of the problem can be analyzed.



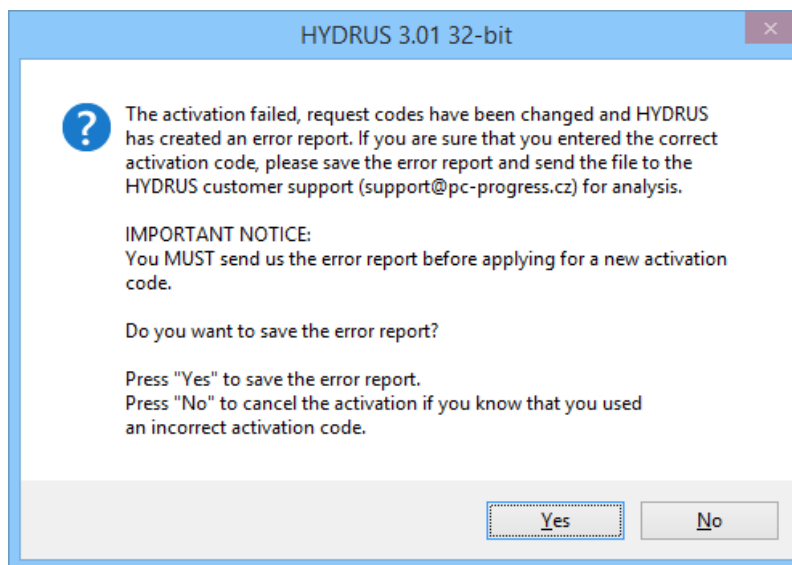


Figure 215. Window reporting a failure of HYDRUS authorization.

9.2.3. Reinstallation, Moving to another Computer

With a "single-user" license, you are eligible to install and use HYDRUS on two computers (for example, a computer in your office and your notebook). If you reinstall HYDRUS on an activated computer or if you install a newer HYDRUS version, then your previous authorization will remain active.

Deactivation of HYDRUS and/or Reinstallation to another computer

Users should deactivate HYDRUS before a) any hardware change (motherboard, hard-drives, graphic card, BIOS, etc.), b) reinstallation of the Windows OS, c) reformatting the hard-drive with HYDRUS, d) changing the network path to HYDRUS (applies to the network installation), and e) moving HYDRUS license to another computer. The HYDRUS software package is deactivated using the **HYDRUS Authorization Status** dialog window (Fig. 203), which is called using the command *Help->Hydrus License and Activation*. Similarly, as for HYDRUS activation, you can deactivate HYDRUS either by email (the command *Deactivate by E-mail*) or online (the command *Deactivate on-line*).

9.2.3.1. On-Line Deactivation

After clicking on the command *Deactivate on-line* in the **HYDRUS Authorization Status** dialog window (Fig. 203), in the **Online Deactivation** window (Fig. 216), enter the **Activation Key** and press the button **Deactivate Now**. You should receive a warning that this action will deactivate HYDRUS, and after clicking Yes, the confirmation that HYDRUS has been successfully deactivated on your computer (Fig. 217).

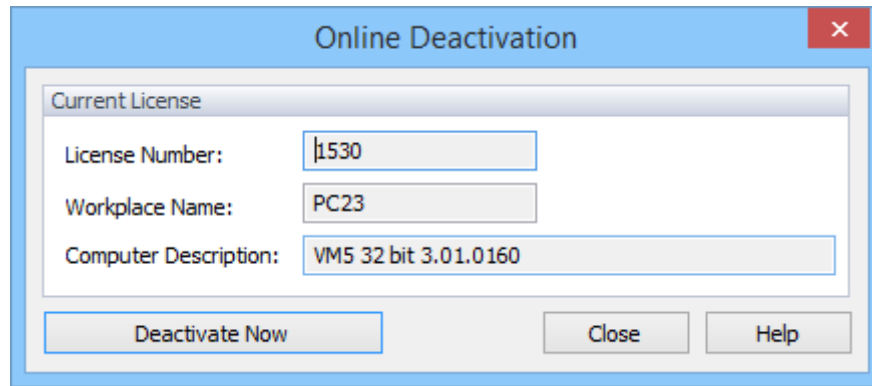


Figure 216. The Online Deactivation dialog window.

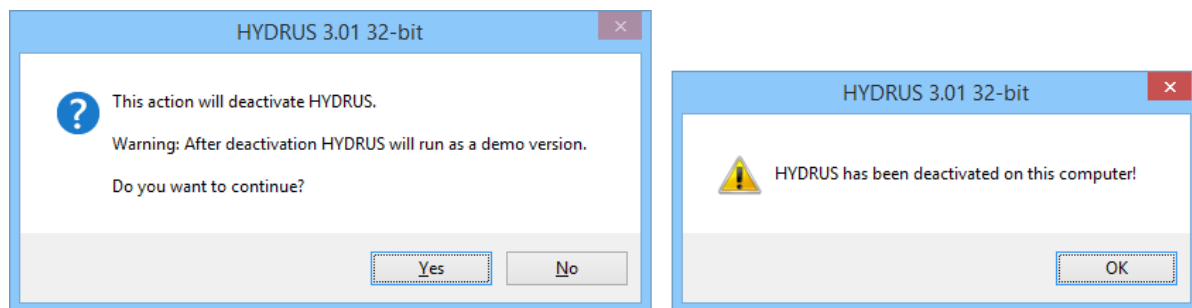


Figure 217. Window confirming successful online deactivation of HYDRUS.

9.2.3.2. Deactivation by Email

After clicking on the command *Deactivate by E-mail* in the **HYDRUS Authorization Status** dialog window (Fig. 203), in the **HYDRUS Deactivation** window (Fig. 218), press the button **Deactivate HYDRUS Now**. You should receive a series of warnings that this action will deactivate HYDRUS, and after clicking Yes, the confirmation that HYDRUS has been successfully deactivated on your computer (Fig. 219). The **Deactivation Code** will then appear in the **HYDRUS Deactivation** window (Fig. 218). This code can be copied to the clipboard using the **Copy to Clipboard** button and then sent by email to the HYDRUS support or other HYDRUS distributors. The command **Send Deactivation Code by E-mail** will attempt to start an emailing program (e.g., Microsoft Outlook) directly and copy there automatically an email address of the HYDRUS support (support@pc-progress.cz) and all required information (see an example of such email displayed in Outlook in Fig. 211).

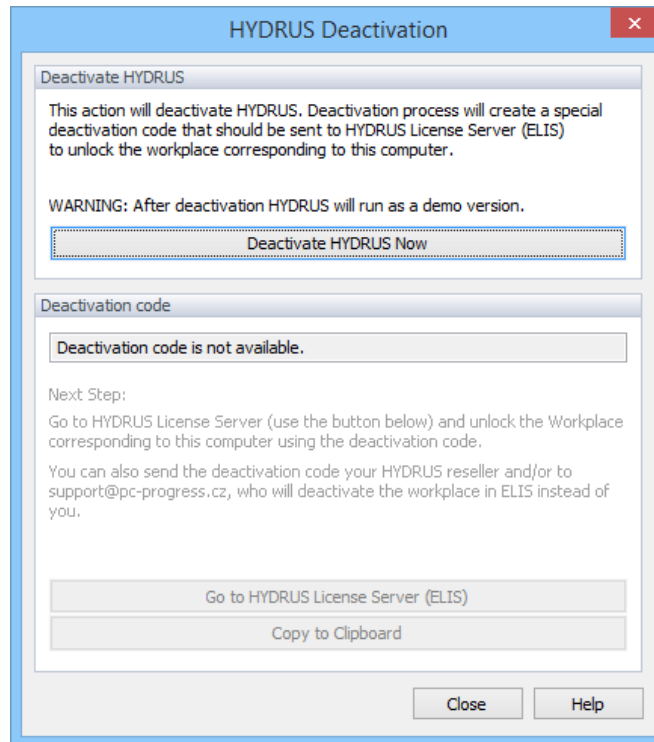


Figure 218. The HYDRUS Deactivation dialog window.

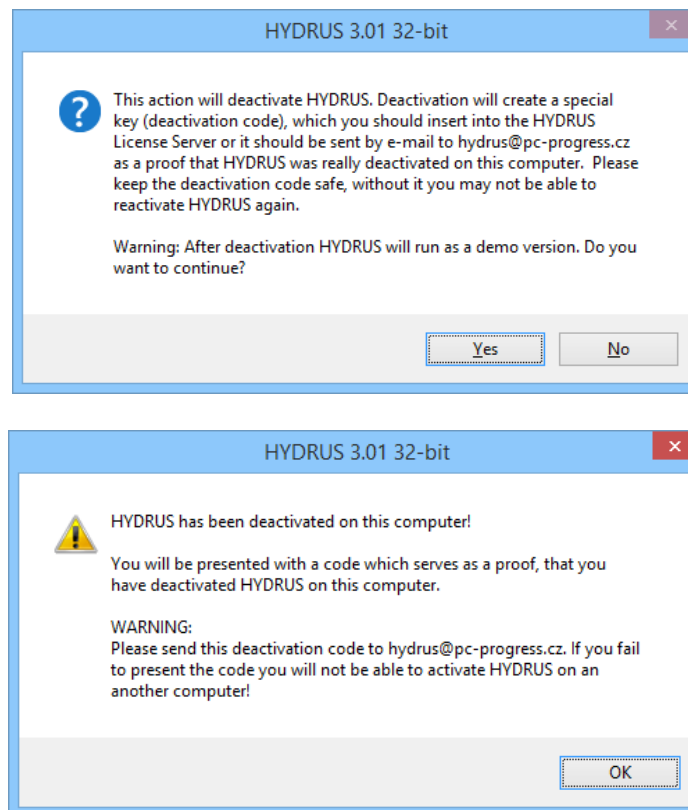


Figure 219. Window confirming the successful deactivation of HYDRUS by email.

9.2.4. Extending Activation

Prior to the expiration (**Expiry Day**) of the **Time-Limited Authorization**, the user will be alerted about it, and the license can be easily repeatedly extended using the **Extend Activation On-Line** button. This button will appear instead of the **Activate on-line** button on the **Status** Tab of the **HYDRUS Authorization Status** window (Fig. 203). To extend the activation, you will need again the **Activation Key** (either for the entire license or for a particular Workspace).

9.2.5. Hardware Key

Starting with Version 2.02, the network authorization of the HYDRUS program can be done either as in previous versions using the software key (activation) or newly using a **Hardware Key (HASP)**. The software key can be used to authorize only separate computers, while a **Hardware Key** is required for the network or server installations designated for remote access.

A **Hardware Key (HASP)**, also called a "**dongle**", is a software copy protection device that plugs into the USB port of the computer. Upon startup, the application looks for the key and will run only if the key contains the appropriate code. Hardware keys are very effective copy-protection devices, because they cannot be duplicated by the user.

1. The HASP for HYDRUS is sent (by PC Progress) by mail, and its use is very simple. You just connect it to the computer via the USB port, and HYDRUS is then immediately authorized. The HYDRUS software then does not require any further activation.
2. Although the drivers for the HASP should normally be installed automatically when it is connected to the USB (Windows operating system and Plug-and-play should take care of that), we still recommend installing the drivers at the same time when the Hydrus software is installed (during the HYDRUS installation). In one of the dialog windows that appears during installation, there is a special check-box "**Install the hardware-key driver**" (Fig. 220), which needs to be checked - see the picture below:

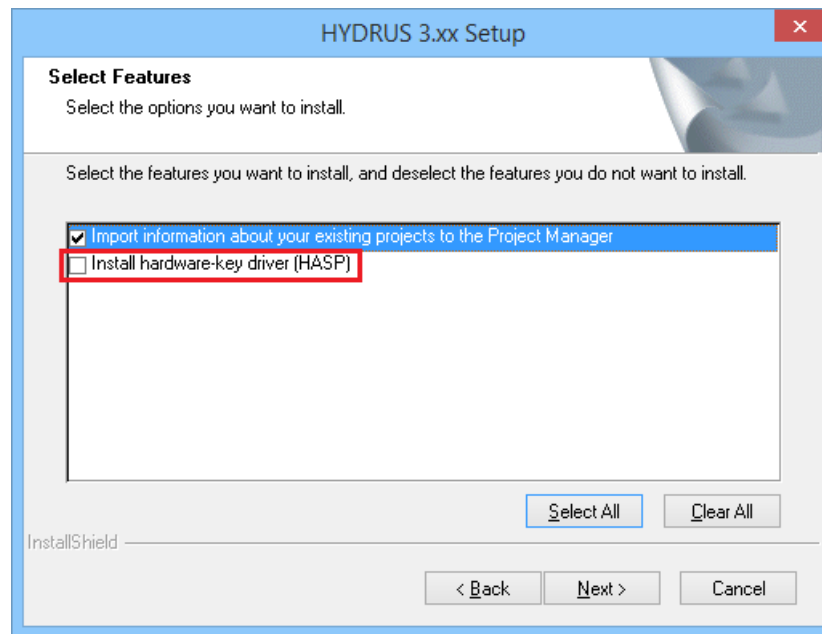


Figure 220. The HYDRUS 2.xx Setup window with a choice to install the hardware-key driver.

Advantages of HASP:

- Proven solutions by SafeNet, verified by hundreds of installations and users.
- No activation of the software (e.g., HYDRUS) is needed. Activation of the program brings some disadvantages, such as that the program can be activated only on the allowed number of computers, and the activation is always time-limited (up to 1 year) and needs to be repeatedly renewed. Under certain circumstances, the activation code may not be immediately available, and users have to wait till they get it (e.g., activation by e-mail). The hardware key (dongle) gives users assurance that the program can be easily installed and used, for example, on a new computer.
- The program (e.g., HYDRUS) can be used on multiple computers (e.g., desktop and laptop) only by transferring a small USB key.
- Easier and safer installation of a network version. The network installation using a software key (activation) is somewhat more complicated, and some network administrators have complained about its lack of flexibility. The use of HASP eliminates these problems.

9.3. Print Options Dialog Window

The **Print Options** dialog window contains four tabs (Fig. 221). In the **General Tab** a user selects whether the content of the View window (*Picture*) is to be printed with or without a **Legend**, **Page Orientation** (Portrait or Landscape), and **Page Margins**. In the **Picture Tab**, users further select **Print Quality** (the Standard print quality, which can be changed by users, is 5,000*5,000 pixels), whether the **Frame** is to be printed in black or color (**Colors and Frame**), and **Text Size**. In the **Color Scale Tab**, users select **Orientation** of the **Color Scale**, its **Position**, **Alignment**, and **Size**. Finally, in the **Legend Tab**, users select what texts (**Legend Rows**) are to be printed, with what **Font**, and how far from the picture. Users can use a predefined text or can write their own.

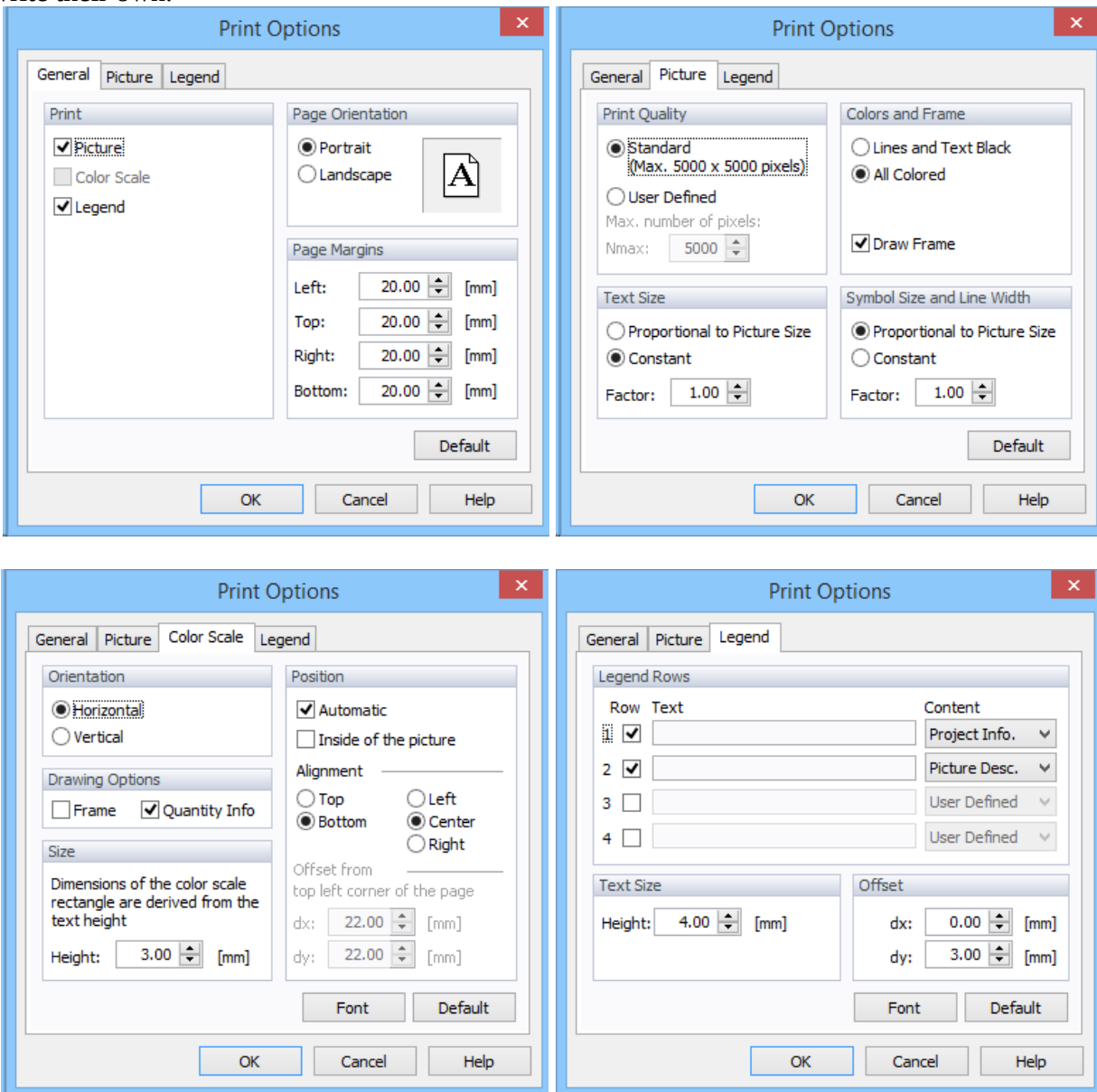
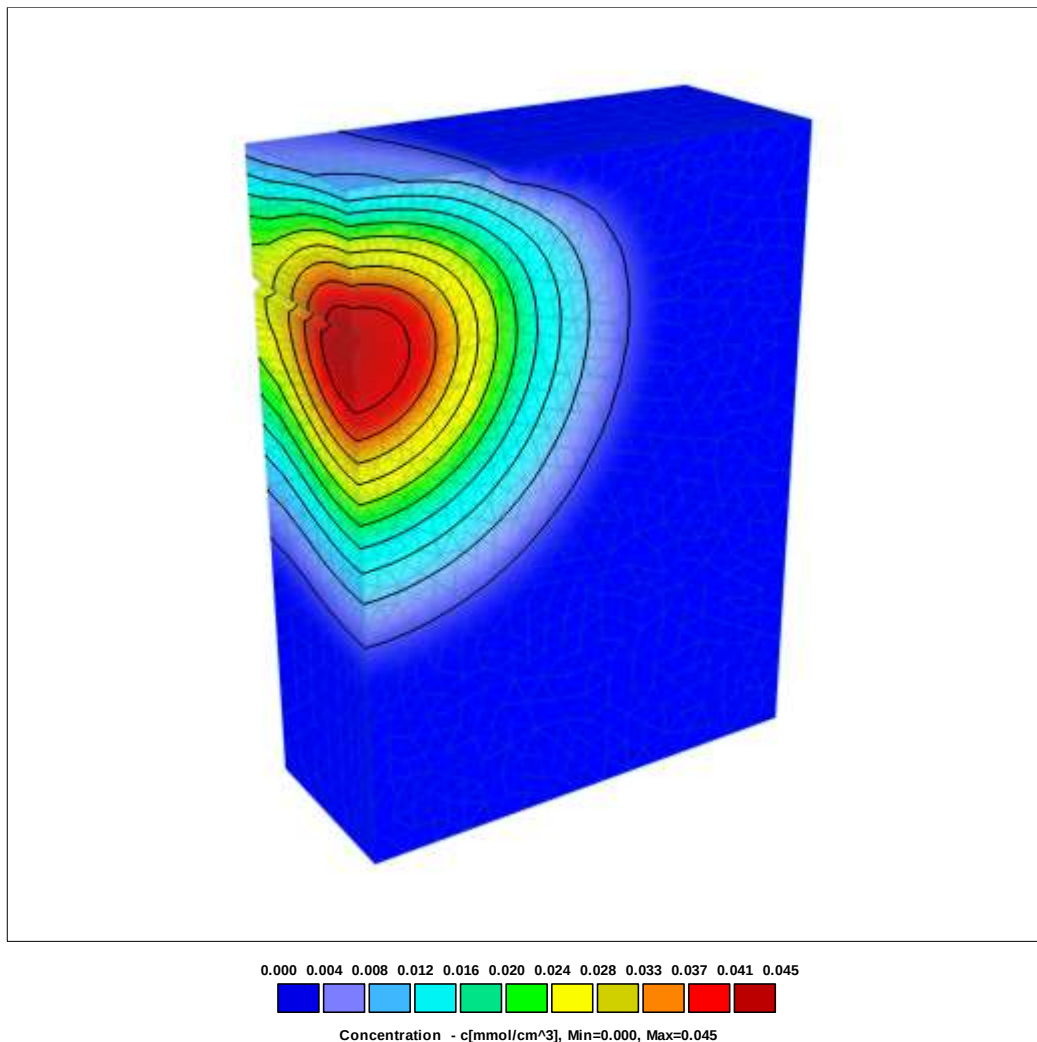


Figure 221. The General, Picture, and Legend tabs of the Print Options dialog window.

9.4. Print Preview and Copy to the Clipboard Commands

The result of commands **Print Preview** and **Copy to the Clipboard** is shown in Figure 222. The **Print Preview** command displays the content of the **View Window** on the screen as it would appear in printed form, while the **Copy to the Clipboard** command copies the same content to a metafile (enhanced metafile, EMF, http://en.wikipedia.org/wiki/Windows_Metafile) in the Clipboard for subsequent pasting into other software packages, such as Word, PowerPoint, etc. Additional content of the metafile (in addition to the content in the View Window, such as the text of the legend) is defined using the **Print Options** window. The metafile contains the bitmap (the resolution of this bitmap (max 6000x6000 pixels) can be specified in the Print Options window) with the graphics displayed in the View Window and additional vector objects (e.g., texts and/or numbering).



Project 3DFumig6 - 3D, Finite res., Heat Tr., Tarp, Tarp removal, part untarped
Results, Concentration, Time 6 - 1.50 days

Figure 222. Result of commands Print Preview or Copy to the Clipboard.

9.5. Coordinate systems

The **Coordinate System** used for the transport domain definition can be selected from the **List of Available Coordinate Systems** dialog window (Fig. 223, top) called by the *Tools->Coordinate System* command. **Cartesian**, **Cylindrical**, and **Spherical** systems are available. The **Cartesian** coordinate system is selected by default. A **New Coordinate System** can be defined using the dialog window of the same name (Fig. 223, bottom).

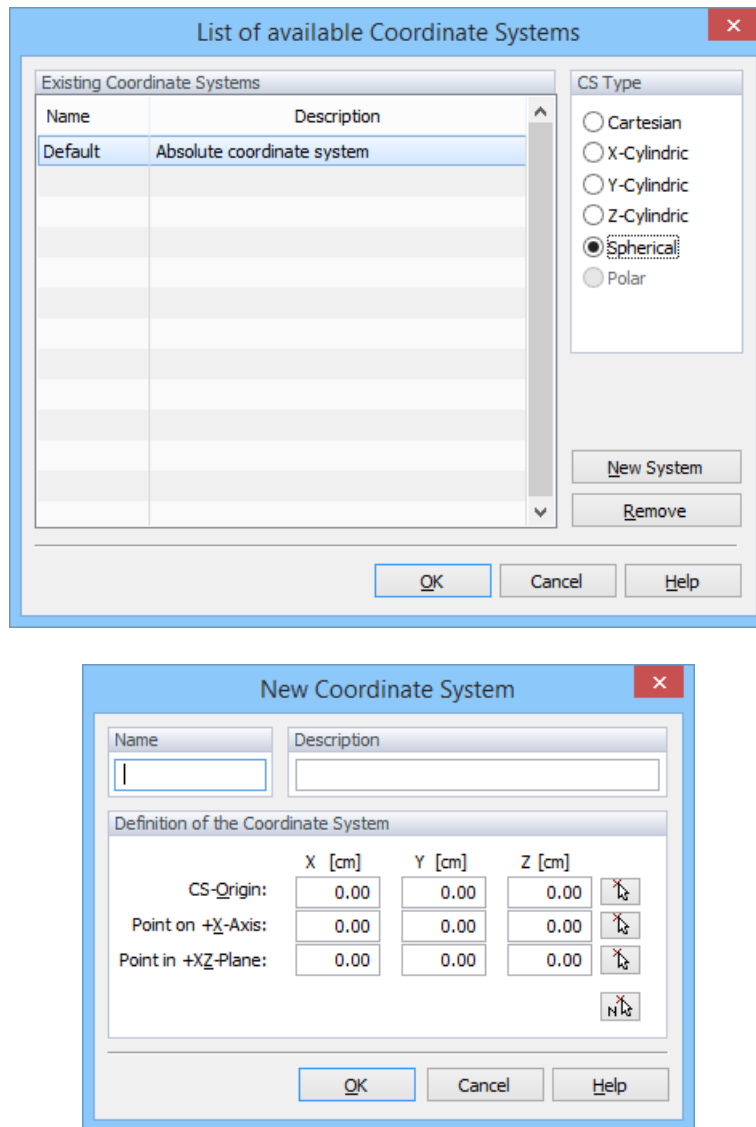


Figure 223. The Coordinate Systems dialog windows.

9.6. DOS Window During Calculations

During the calculations, a different type of information can be written to the screen. The following information may be written to the screen depending upon the problem:

Time	Time
T-Level	Time level
ItW	Number of iterations to solve the water flow problem at a certain time step
ItC	Number of iterations to solve the solute transport problem at a certain time step
ItCum	Cumulative number of iterations
CumAtmBC	Cumulative flux across the atmospheric boundary
CumConst	Cumulative flux across the boundary having a constant flux or pressure head
CumDrain	Cumulative flux across the boundary having a time-variable flux or pressure head
CumRootUp	Cumulative actual root water uptake
CumCh0	Cumulative zero-order production in the domain (solute transport)
CumCh1	Cumulative first-order degradation in the domain (solute transport)
CumChS	Cumulative solute flux across the boundary having a time-variable flux or pressure head
hAtm	The average pressure head at the atmospheric boundary
hConst	The average pressure head at the boundary having a constant flux or pressure head
hDrain	The average pressure head at the boundary having a time-variable flux or pressure head
hRoot	The average pressure head in the root zone
hSeep	The average pressure head at the boundary with the seepage face
vConstBC	Flux across the boundary having a constant flux or pressure head
vSeep	Flux across the boundary having a seepage face

9.7. Running Computational Modules Outside of GUI or in a Batch

Computational modules (e.g., h2d_calc.exe, h2d_clci.exe, h3d_calc.exe) can be run either directly from GUI or by clicking on any of them in the folder in which HYDRUS is installed. When these modules are run from GUI, GUI will send them as a parameter the path to the folder in which the input and output files are located (the working folder, the path to which is displayed in the project manager (h1d) or in the project information dialog (h3d)). When the program does not receive a path as a parameter, it will look for the text file called Level_01.dir that needs to be located in the same folder as the computational module. This file can be written using any text editor, such as Notepad. This file must have one line, which provides the path to the folder in which the input and output files are located.

Example of the “Level_01.dir” file:

```
c:\program files\pc-progress\hydrus3d\mydirect\run1
```

For the input files to be available in the Working Folder, the Working Folder needs to be either 'Permanent' (see the Project Information dialog) or the HYDRUS GUI needs to be opened when the Working Folder is 'Temporary'. In each case, the text input files need to be created using the menu command File->Import and Export->Export Data for HYDRUS Solver in Text Format.

HYDRUS (2D/3D) allows users to select multiple projects and run them simultaneously using the “Calculate All Open Projects” or “Select Projects to Calculate”. To run several projects sequentially is more complex. One needs to prepare a batch file (e.g., run.bat) and files describing paths (e.g., path1, path2, etc) to project folders (to be run) in advance. One needs to copy these files into the program folder (e.g., c:\program files\ussl\hydrus3d). Additionally, the check box "Hit Enter at the End?" in the Output Information window has to be unchecked for all projects to be run sequentially.

Example of the “run.bat” file:

```
copy path1 level_01.dir
h2d_calc
copy path2 level_01.dir
h2d_calc
```

Example of the “Path1” file:

```
c:\program files\ussl\hydrus3d\mydirect\run1
```

Example of the “Path2” file:

```
c:\program files\ussl\hydrus3d\mydirect\run2
```

9.8. The HyPar Module, a parallelized version

HyPar is a parallelized version of the standard two-dimensional and three-dimensional HYDRUS computational modules (h2d_calc.exe and h3d_calc.exe). HyPar uses parallel programming tools and techniques to take advantage of multiple cores and to accelerate calculations on multi-core processor computers. HyPar currently supports only calculations in the direct mode (does not support the inverse mode), and it does not support any add-on modules (e.g., HP2, UnsatChem, Wetland, and/or C-Ride). The HyPar module is initialized on the **Program** Tab of the Program Options dialog window (Fig. 200).

The name **HYPAR (HyPar)** is an acronym for "Hydrus Parallelized". The term, which has been suggested by Rien, is also intended to indicate a "Hyper" action when multiple cores of a PC processor work in unison like 'a bunch of bees'. The results of the speedup of the HyPar module compared to the standard modules are presented in (Table 29).

Table 29. A comparison of the HyPar module to standard computational modules.

System	Info
Computer	HP Elite 7300 Series MT
Operating System	W7/64
Processor	Intel(R) Core(TM) i7-2600 CPU @ 3.40 GHz
Number of cores	8

2D Tests:

Project Name	Processes	Number of Elements	Standard Module	HyPar Module	Ratio
2DWater1	2D WF	20 k	8.36 s	6.12 s	0.73
2DWater1s	2D WF, ST	20 k	13.83 s	8.08 s	0.58
2DWater2	2D WF	200 k	310.24 s	169.45 s	0.55
2DWater2s	2D WF, ST	200 k	508.79 s	262.87 s	0.52
2DWater3	2D WF	1,000 k	3134.9 s	1666.2 s	0.53
2DWater3s	2D WF, ST	1,000 k	7296.0 s	3549.2 s	0.49

WF - Water Flow; ST - Solute Transport

3D Tests:

Project Name	Processes	Number of Elements	Standard Module	HyPar Module	Ratio
3DWater1	3D WF	20 k	15.88 s	5.78 s	0.36
3DWater1s	3D WF, ST	20 k	32.24 s	12.19 s	0.38
3DWater2	3D WF	200 k	211.41 s	87.07 s	0.41
3DWater2s	3D WF, ST	200 k	502.0 s	194.33 s	0.39
3DWater3	3D WF	1,000 k	1554.3 s	689.71 s	0.44
3DWater3s	3D WF, ST	1,000 k	7078.0 s	2427.4 s	0.34

9.9. Video Files

Users can save the flow animation using the **Create Video File** command (Tools->Create Video File). This command calls the **Create Video File** dialog window (Fig. 224), in which a user needs to specify where the *Video File* should be saved and under what name, type of the video file [a) Cinepac Codec by Radius, b) Microsoft Video 1, c) Intel Indeo Video 4.5, d) Intel Indeo Video 5.10, e) Microsoft MPEG-4 Video Codec V1, and f) Microsoft MPEG-4 Video Codec V2] and its *Quality*, and finally whether the recording is carried out at *Real Time* (i.e., the video will run at the same speed as HYDRUS animation) or only when frames in the View Window change (only changes in View Window are recorded). Additional options (such as Smoothness, Data Rate (i.e., kilobits per second)) are available for each particular video format. OpenGL acceleration should be disabled when problems occur when creating a Video File.

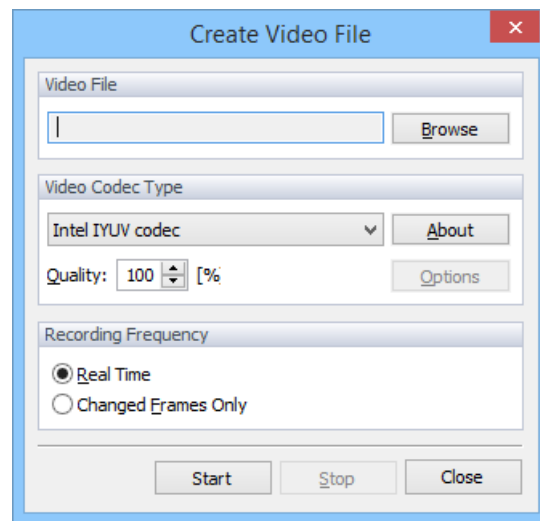


Figure 224. The Create Video File dialog window.

Animation files (*.avi) created by the HYDRUS command **Create Video File** can be displayed using standard video software, such as the **Windows Media Player**. Animation files can also be inserted directly into PowerPoint presentations using the menu command "**Insert->Movie->Movie from File ...**" and selecting whether animation starts **Automatically** or **When Clicked**. Animation can then be stopped and restarted using additional mouse clicks.

Notes on Video Editing:

1. Video records only change in View. Thus, if nothing changes in the View window, only the first picture is recorded. When one records animation of flow or transport, then while the View window is redrawn, each change is recorded. Similarly, one could record video for any other manipulation of the View, which requires its redrawing (e.g., rotation of the model).

2. If the option "Real-Time" is on, each recorded View has an assigned time, which elapsed between redrawing of the View window. This means that the video is then played at approximately the same rate as redrawing of the View window.
3. If the option "Changed Frames Only" is on, then changes in the View window are stored regardless of the actual time elapsed in redrawing the View. For example, if some changes in redrawing of view take place quickly, followed by a pause, and again fast changes, in the resulting video, all changes will be played back with a constant time delay. The current version of HYDRUS does not have an option of allowing to set a time interval between recorded frames. It is entirely possible that one can edit Video recordings created by HYDRUS using some public domain programs for editing videos. We currently do not have any experience with that and cannot make any recommendations.

9.10. About HYDRUS

This window displays the program version (the Program Tab), authors of the HYDRUS application (the Authors Tab), and the License agreement (the License Agreement Tab). The Program Tab additionally displays other software products (such as mesh generators) that are used in HYDRUS.

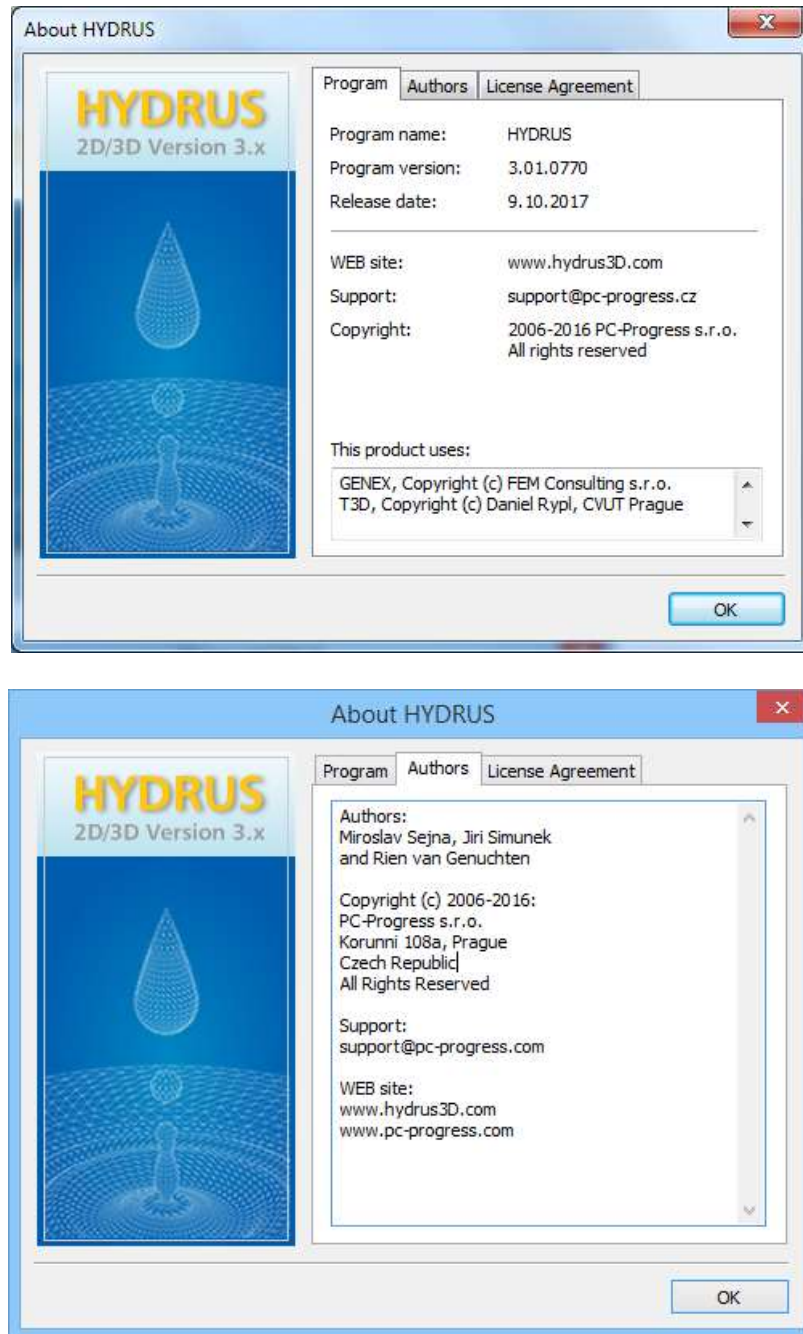


Figure 225. The About HYDRUS dialog window (the Program tab (top) and the Authors tab (bottom)).

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