

# Using Cerity NDS for Chemical QA/QC for Highly Customized Applications

**Technical Overview** 

## Authors

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# Abstract

Agilent Technologies' Cerity NDS for Chemical QA/QC provides the programming tools required to develop highly specialized custom user interfaces, manipulate sample runs, monitor the GC status, and obtain sample data for further processing outside of Cerity. This functionality is provided through external calls. These calls are documented in the Cerity Programmatic Interface and an example Visual Basic program.

Fully functional application programs developed by Agilent using these calls are reviewed in this article. Included in these applications are an OLE Process Control (OPC) communication program, a program that sends selected results data to a Comma Separated Value (CSV) file, and a Sample Stream Selection Program.

## Introduction

The Cerity Programmatic Interface allows programmers to create customized pre- and post-run applications that can communicate with Agilent Technologies' Cerity NDS for Chemical QA/QC. Applications developed using the Programmatic Interface can obtain the instrument status, enter samples into the Worklist, set the sample priority within the Worklist, run the Worklist, and stop/abort the Worklist. Applications developed using the example Visual Basic program can obtain results data for use in highly customized reports, including trend analysis.

This technical overview discusses key elements of the programmatic interface and the example Visual Basic (VB) program and reviews the following applications that Agilent has developed using these:

- A fully functional Stream Select Program that controls multiple Valco Instruments Co., Inc. stream selection valves and directs the correct sample stream to the GC for analysis
- The Cerity Chemical CSV file generation program, which allows users to configure specific GC information for export to a CSV file
- The Cerity Chemical OPC communication program, which allows users to configure specific GC information for export to an OPC compliant process control system



#### **The Cerity Programmatic Interface**

The programmatic interface for Cerity NDS for Chemical QA/QC offers an ActiveX interface through which user-written software can enter and run samples, obtain results of analyses, and monitor instrument status.

The programmatic interface is implemented using the Component Object Model (COM). Any programming language that supports COM should be usable. For VB, version 6 service pack 6 is required. To access the functionality described herein, the ActiveX server, "AgCerityChem.dll," must be installed and registered on the user's system. It is also assumed that the user has installed and "setup" Cerity with suitable instruments and methods (this is done using the ConnectAdmin function and method editing capabilities of the Cerity user interface). Once these steps are completed, the user can create a VB project and include in the project a reference to AgCerityChem (to link the VB project).

The programmatic interface allows the user to develop a custom user interface that runs routine samples and that is optimized for your particular needs.

The programmatic interface software contains complete documentation and an example VB program, with source code for those wishing to develop their own application. By examining the source code, a visual basic programmer sees how to extract data for processing and storage outside of Cerity.

To obtain a copy of the programmatic interface software, it is necessary to sign a Confidential Disclosure Agreement. Contact Agilent Technologies, Chemical Analysis Solutions marketing for additional information.

#### The Example Visual Basic Program

This example program demonstrates how to access the sample results via a post analysis program. Programmers can examine the documented VB source code to see how to obtain results or data from Cerity for use in a custom application. It also serves as an excellent starting point for developing customer calculations and / or reports. The source contains markers to show where to insert custom code. The source for this program is included on the Cerity CD. This program was used as the starting point for the CSV and OPC applications discussed below.

When installed, this program runs as a post run program in Cerity and displays the results of the analysis in a separate window, as shown in Figure 1.

This program requires VB version 6 with VB service pack 6. Documentation included with Cerity explains how to set up and use the program.

#### **The Stream Selection Program**

Created for users needing to analyze multiple sample streams using a single GC, the Cerity stream selection and switching program allows control of up to two Valco multi-stream selection valves.

There are two parts to the program, both of which are delivered in a single executable file.

The first part of the program allows for the configuration of the streams to be analyzed. See a hypothetical configuration in Figure 2. For each valve that is connected to the PC via the serial ports, the user enters the name of the streams that are switched by the valve. These stream names will be the sample names that are used in the data system; therefore, the stream can be associated with a particular sample analysis. Also, a wildcard can be used to take advantage of the data system's sample auto-numbering capability. The "\*" shown in the configuration for "valve 2, stream 1" in Figure 2 indicates that any sample name starting with "Benzene" will switch "valve 2, stream 1."

The second part of the configuration allows the user to enter a purge time. When the stream selection valve is switched, the program will wait for the designated time before control is returned to Cerity. This allows the GC sample input line of the previous runs sample to be flushed before the next sample is taken. The valves are switched by the run time part of the stream selection program.

To configure the Cerity method, the stream selection program is set up as a pre-run program. See Figure 3.

When a run is made from the data system, the stream selection program looks at the name of the

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3	1	1	5.57184	4022625155	5.46791666666671	1 5.66791666666	715 Peak9		
4	1	4		0		D	0 Peak@5.572		
		1			1	1	1	1	
port Errors					Somple 1	lote			
o report erro	rs found.				Check out t	nis note			
ethod Infor	mation -				Instrume	nt Information			
ethod Name:		Tim1			GC Descr	GC Description: HP6850GC - US1111104			
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Figure 1. Visual Basic example program output.

sample that is being run. Then, if a match for the sample name is found in the stream selection configuration, the valve is switched to the configured stream. After waiting the designated purge time, the program returns to the data system, allowing the run to start.

The pre-run program option to "wait for program completion" must be selected in order for the Stream Selection Program to work properly.

## **Custom CSV File Generation Program**

The Cerity Chemical custom CSV file generation program allows users to configure specific GC information (Figure 4) to send to a CSV file at the end of an analysis (post-run). The Post-run program option to 'wait for program completion' must be selected in order for the CSV program to run properly.

Users select the GC, method, and sample for which they want to collect CSV information. Therefore, users can collect information that is generic for a method or specific for each sample run.

Stream Selection Configuration						
Stream Selection						
Purge Time: 22 sec						
Valve:	1	2				
Stream	Stream	n Name				
1	Benzene*		<b></b>			
2	Propylene					
3	Pentane					
4	Tebuconazole	e				
5	DDT					
6	Tdd					
7						
8			•			
Se	lect	)one				

Figure 2. The Cerity Stream Selection screen.

A wildcard has been provided to allow the users to take advantage of Cerity's sample auto-numbering capability. The "\*" shown in the sample name "Repo\*" in Figure 4 indicates that any sample starting with "Repo" being analyzed by the method "RepoTest" on GC "Benzene (D4492) HP6850GC US11111104" will have the configured Cerity information placed in a CSV file post-run.

When a run is made from Cerity, the instrument, method, and sample names are checked against the configuration. If a match is found, the configured information is retrieved and placed in the CSV file. The CSV file is identified by the instrument serial number, the method name, and the sample name (US11111104-repotest-repo). In this manner, users can generate many different CSV files for many different applications and still have a way to individually identify each one.

When the first analysis is performed, the CSV program will create the file, write the header in the first row, and enter the information from the first sample in the second row. In subsequent analysis, the information from the sample is appended to the next row in the CSV file.

🗆 Ag	ilent Cerity - Method: First Connection						
Eile y	∠iew <u>C</u> onfigure <u>H</u> elp 						
Sample	Method Filter:         Show all methods           Method         Instrument         Time Stamp         Description           First Connection         6890A         6/2/2003 3:44:23 PM         (Uploaded from instrument when first 'discovered'.)						
ment	First Connection 6850B 6/2/2003 3:44:24 PM (Uploaded from instrument when first discovered.)   First Connection 6850A 6/11/2003 7:44:06 AM (Uploaded from instrument when first discovered.)						
Instru	General Acquisition Analysis Uutput IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	Edit Masks					
* pou	Method Instructions File: Method Description: [Uploaded from instrument when first 'discovered'.]	Browse					
s Met	Run Programs ✓ Pre-Run Program C:\Program Files\Agilent\TestTool.exe Browse ✓ Wait For Comple	etion					
roces	Post-Run Program     C:\Program Files\Agilent\CustomCSV.exe     Browse     Image: Wait For Complete	etion					
Rep	Method: First Connection						
	(Uploaded from instrument when first 'discovered'.)						
	Create Save Save As Cancel Print	Help					
<b>Ð</b> •	ouble Click to Show Message History 7/17/20	003 12:12:11 PM					

Figure 3. Screen view in Method setup, illustrating Pre- and Post-Run options.

🖗 Cerity CSV Configuration								
CSV Configuration Storage Configure CSV								
Analysis Qualifiers								
GC	-		Benzene (D4492)	HP6850G0	CUS11111104	-		
			· · ·	_				
Me	etho	d Name	repotest	Sam	ple Name   repo*			
	rity	Informa	ation					
	inty				Cority Information			
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	Meti	hod			Peak Height			
	Mine	collanoo			Peak Area			
IY.	miai	Cellaneor	13		Peak Width			
	Run				Peak Amount	•		
0	Sarr	nple		•		•		
C 6	W 1.	nformati						
CS	SV I	nformati	ion —					
- CS	SV I	nformati	ion Cerity Information	n	Column Head	ler 🔺		
- CS	3 <b>V I</b> 1	nformati Injection	ion Cerity Information Date/Time	n	Column Head Date/Time	ler 🔺		
- CS	1 2	nformati Injection Benzene	ion Cerity Information Date/Time 9. Retention Time	n	Column Head Date/Time RT	ler		
- CS	3 I	nformati Injection Benzene Benzene	ion Cerity Information Date/Time 9.Retention Time 9.Peak Amount	n	Column Head Date/Time RT Amount	ler		
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Figure 4. The Cerity CSV Configuration screen.

#### Cerity Chemical OLE for Process Control (OPC) Communications

Agilent Technologies' OPC Communications for Cerity NDS for Chemical QA/QC is a newly developed software package that allows smooth and seamless integration of pre-selected gas chromatographic output data into a plant's process control system using the dialog box shown in Figure 5.

First, users select a GC and the OPC server that they want to use. This OPC server can be on the same PC as Cerity or on a remote PC where the process controller is located. Then users specify the instrument, method, and the samples for OPC configuration. By allowing this level of configuration, the user can configure OPC information that is generic for a method or specific for each sample run. A wildcard has been provided to allow the user to take advantage of Cerity's sample autonumbering capability. The "\*" shown in the sample name "NITest\*"in Figure 5 indicates that any sample starting with "NITest" being analyzed by the method "TestOPC" will have the configured Cerity information transferred to the OPC server.

The OPC information is sent to the OPC server by the run time part of Cerity Chemical OPC communications program. In the Cerity method, the Cerity Chemical OPC communications program is set up as a post-run program.

The post-run program option "wait for program completion" must be selected in order to the OPC Communications program to run properly.

When a run is made from Cerity, the instrument, method, and the sample name are checked against the configuration. If a match is found, the configured information is retrieved and sent to the designated OPC server. After the information is transferred, program control is returned to Cerity.

#### Summary

The Cerity Programmatic Interface and the example Visual Basic program allow users to create customized pre- and post-run programs to run in conjunction with Agilent Technologies' Cerity NDS for Chemical QA/QC.

Three applications have been written by Agilent using this feature:

- A Custom CSV file generation program, which allows users to configure specific GC information to send to a CSV file at the end of an analysis
- The Chemical OPC Communications program, which allows users to configure specific GC information to send to an OPC compliant process control system
- A pre-run Sample Stream Selection Program, which allows users to analyze multiple sample streams using one GC and a Valco multi-stream selection valve.

#### For More Information

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OPC Configuration Storage       Configure OPC       Find OPC Servers         Communications       OPC Server       OPC Server Computer:         National Instruments.OPCLabVIEW.6       OPC Server Computer:         Solution Sony    Analysis Qualifiers          Method Name       TestOPC       Sample Name         Peak       Cerity Information         Peak       Sample Name         Method       Sample Comments         Sample       Sample Comments         Run       Sample Comments         Sample       Sample Comments         Sample       OPC Tag         1       Current Date/Time         2       Operator Name       OPCTest ReportTime         3       Method Name       OPCTest SampleName         4       Sample Name       OPCTest SampleName         5       Pentane.Retention Time       OPCTest.PentaneAmount         6       Pentane.Retention Time       OPCTest.PentaneAmount         7       Benzene.Retention Time       OPCTest.PentaneAmount	Serity OPC Configuration					x
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Figure 5. The Cerity OPC Configuration screen.

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