Discoverant SimApi User Guide

1. Introduction

This document is the user guide for the *Discoverant SimApi* from Umetrics.

The SimApi uses ODBC to connect to an Accelrys Discoverant server. For an important list of requirements for this SimApi, see 1.2 below. For more information about Discoverant, see the Accelrys web site.

For a detailed list of changes in different versions of this SimApi, see the *Version Info.txt* file that comes with the installation.

This SimApi can be used by SIMCA-online, SIMCA-Batch On-Line, SIMCA-4000, or SIMCA.

For more information on available SimApis, see www.umetrics.com/simapi.

1.1 Features

This SimApi implements;

- Configurable set of AG_PATHs to expose through the SimApi (optional).
- Read current and historical continuous / process data (AG_C_DATA).
- Read batch data (used for batch conditions and local centering in SIMCA-online) (AG_D_DATA).
- Read discrete data, i.e. IPC or lab data (AG_R_DATA).
- Read batch information / batch node.

The following two items are currently *not* supported

- Write back of process or batch data through the SimApi.
- Phase information from batch data are not available from the batch node. Phase tags needs to exist in the AG_C_DATA or in another data source with process data. This means the batch node cannot be used in phase conditions in SIMCA-online to determine when phases execute.

A note on nomenclature;

- Continuous data, AG_C_DATA corresponds to what Umetrics calls process data.
- Discrete data, AG_D_DATA corresponds to what Umetrics calls batch data.
- Replicate data, AG_R_DATA corresponds to what Umetrics calls discrete data.

The nomenclature for Discoverant will be used throughout this document.

1.1.1 AG_D_DATA

There are two ways to configure how discrete data will be read. One simple way where no configuration is needed and one way where each AG path is configured with a specific tag names the start time- and the stop time columns.
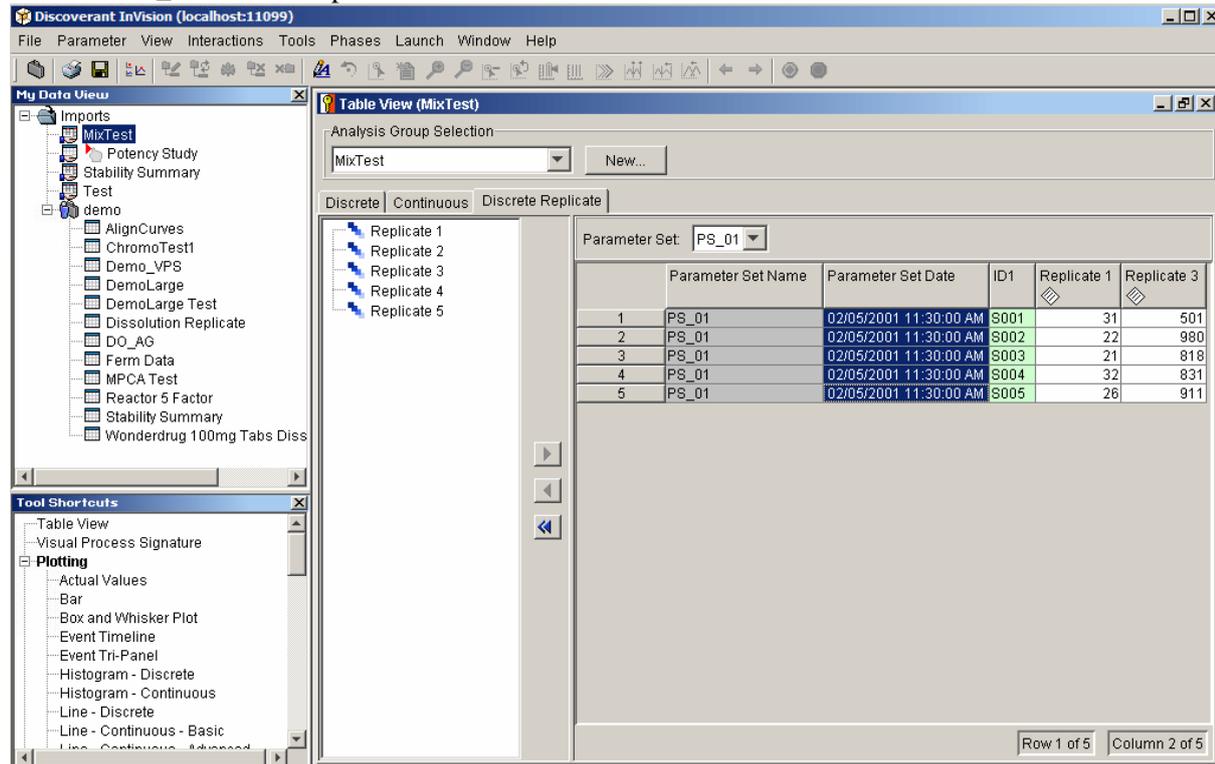
1. Simplest way, no configuration is required. All AG paths are loaded and default column name is used for start and stop time, see section 2.4 for further details.

2. Each AG path is configured against a specific start and stop time column in the XML file, see 1.5 and 2.4. This should be used when the default values for the start and stop time columns don't apply for the specific AG path. Note that when AG paths are configured in this section only the configured AG paths will be exposed through the SimApi.

1.1.2 AG_R_DATA

There are two ways to configure how replicate data is read. One simple way where no configuration is needed and one way where each discrete tag is configured with a "group by" tag so that an average of multiple samples for the same age/maturity/time-point can be returned as read value.

1. Simplest way, no configuration is needed. However this assumes that there is only one sample per age/maturity/time-point. It also assumes that all replicate tags that will be used from one AG path have the same number of values. The reason for this is because there are no time points for the replicate values in Discoverant to align data against.

   The following example from Discoverant shows two discrete tags, *Replicate 1* and *Replicate 3* for batch *PS_01* in the AG path *MixTest*.
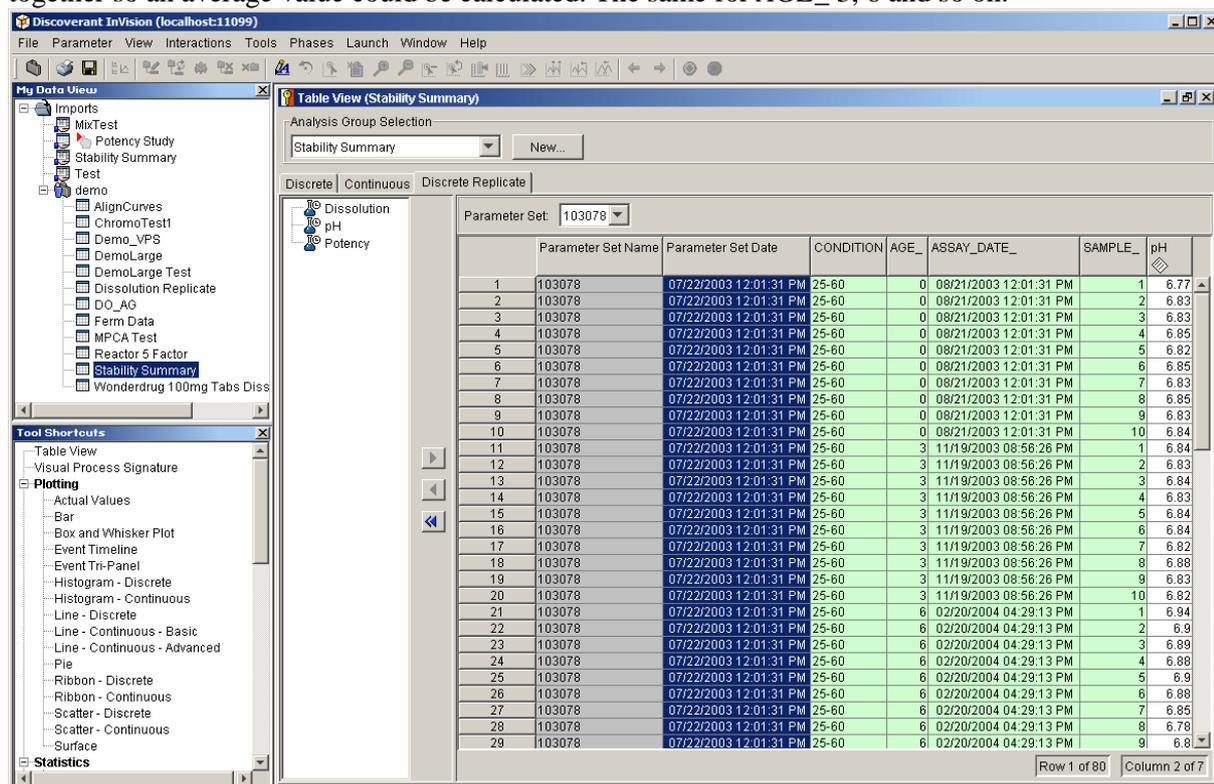

2. Each replicate tag is configured in the enclosed XML file, see 1.5 and 2.4. This should be used when there are more than one data sample per age/maturity/time-point. When this is used an average value of all samples for a certain age/maturity/time-point is used. In order for this to work a replicate id number needs to be configured for the concerned replicate tag so that the SimApi can group all samples belonging to a certain age/maturity/time-point. See example below.

   The following example from Discoverant shows one discrete tag, *pH* for batch *103078* in the AG path *Stability Summary*. Here we can see there are ten samples for each age/maturity/time-point. In this case we would configure the discrete tag *pH* to be grouped by *AGE_*, i.e. replicate id number *2*. This would mean that all samples with *AGE_* 0 would be grouped

together so an average value could be calculated. The same for *AGE_* 3, 6 and so on.

1.2 Prerequisites

In order for the Discoverant SimApi to work, you must first install ODBC drivers for Discoverant.

Obtain the Discoverant setup program from Accelrys, and when installing select to install the *ODBC Client*. After the installation a system data source (DSN) will have to be setup in ODBC Data Sources in Windows. This DSN should be specified in the configuration (XML) file of the Discoverant SimApi (see below).

1.2.1 The Discoverant Server

The Discoverant server version 4.3 must have the hot fix from December 2013. Otherwise the SimApi will not be able to read data from different AG paths.

In order for the SimApi to be able to read data correctly there can only be one analysis group per unit operation. The reason for this is because how the SimApi requests data compared to how data is structured in Discoverant.

1.3 Installation

Run the Discoverant SimApi setup program to install the SimApi on the computer where you want to use it. After installing, you need to set up the SimApi as described below.

1.4 Troubleshooting

Make sure you have installed and configure the Discoverant ODBC client. Test it with another Discoverant client on the same computer that you want to use the SimApi on.

Use the SimApi log file and the SIMCA-online server log files to determine what is happening. See http://www.umetrics.com/KBArticle?ArticleID=742 for more information.

Also see the SIMCA-online technical guide for more information on SimApi troubleshooting, including issues that can occur when trying to use a 32-bit SimApi on a 64-bit windows computer.

1.5 Configuration file and log file locations

The SimApi stores its settings in a XML settings file in the *Program Data* directory:

Window Vista and later: C:\ProgramData\Umetrics\SimApi

Windows XP: C:\Documents and Settings\All Users\Application Data\Umetrics\SimApi

This folder also contains the log file that the SimApi writes. This log file is useful for troubleshooting.

2. Setting up

In order for SIMCA or SIMCA-online to be able to use the SimApi you need to configure it as described here.

2.1 Setting up the SimApi for use in SIMCA

Start SIMCA-import by *File->New Regular Project->New Batch Project*. If the database import wizard is not opened automatically, open it from *File->New Spreadsheet->From Database*. Click on *Add data source*.
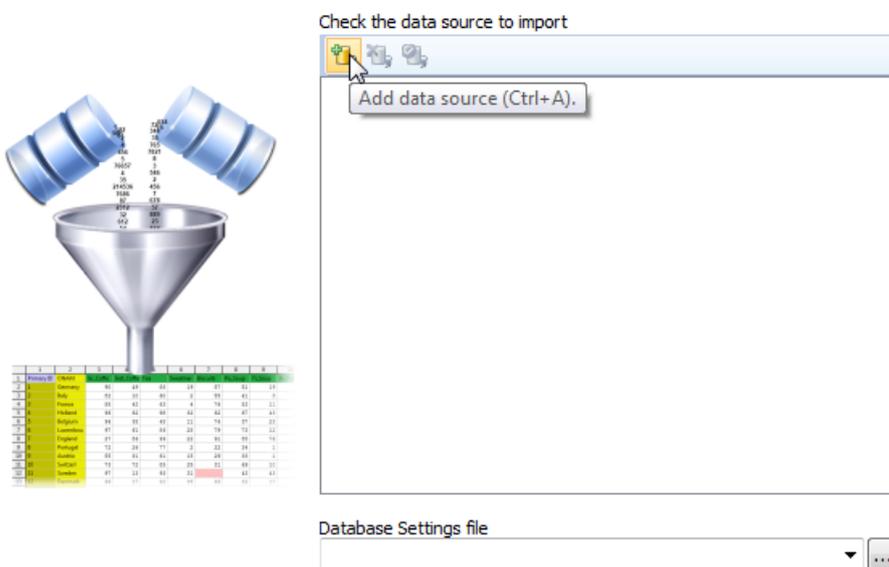
Select *SimApi* as connection type, find the installed DiscoverantSimApi.dll. Continue to 2.3 below.

2.2 Setting up the SimApi for use in SIMCA-online

Start the SIMCA-online Server Options utility from the start menu. Go to the SimApi tab and click *Add...*
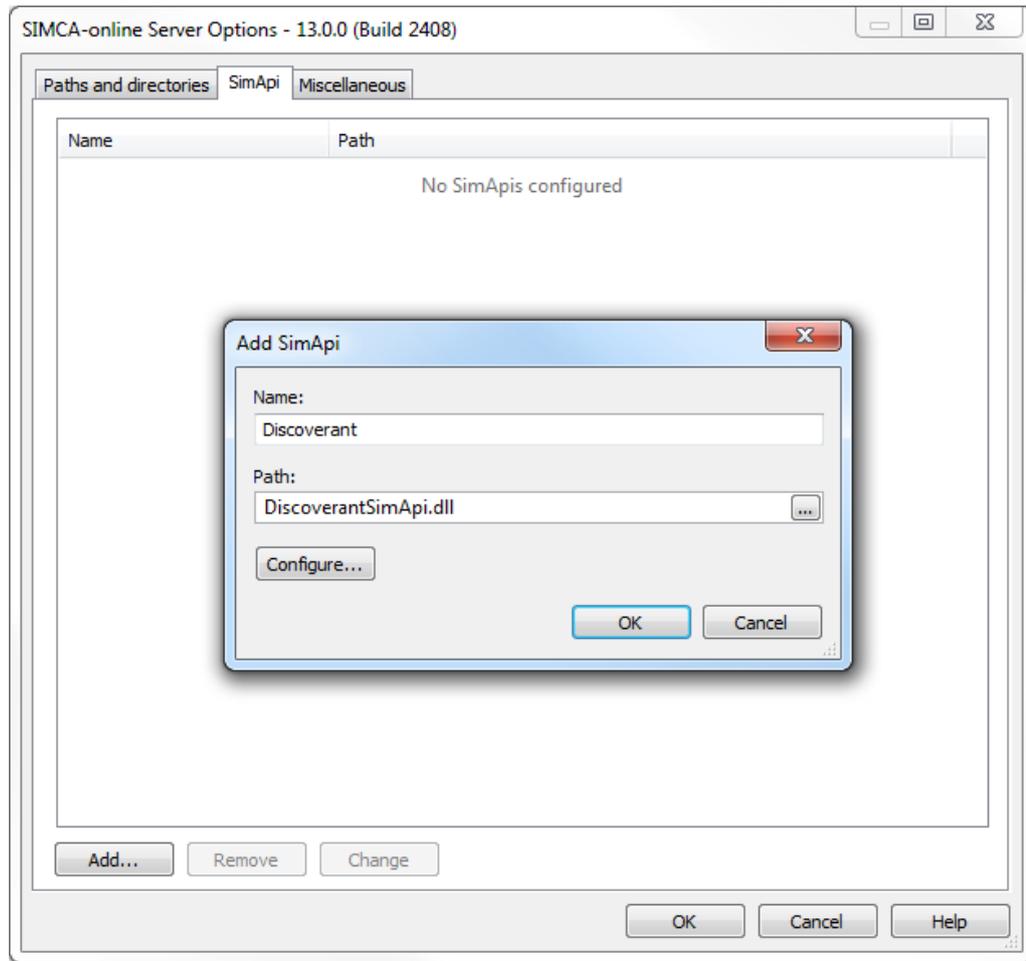
Enter a name to use for the SimApi in SIMCA-online, for example Discoverant, and then click the …-button to browse to and select the DiscoverantSimApi.dll. Click the *Configure* button and the Opc configuration dialog is opened. This is described in the next section.

2.3 Discoverant SimApi Configuration

In the configuration dialog you can provide the user name and password that will be used to connect to Discoverant. The information is stored in encrypted form. If you leave user name and password empty, the SimApi will connect as the process that calls the SimApi (meaning offline SIMCA or in the case of SIMCA-online the account configured to run the SIMCA-online server in the services control panel).
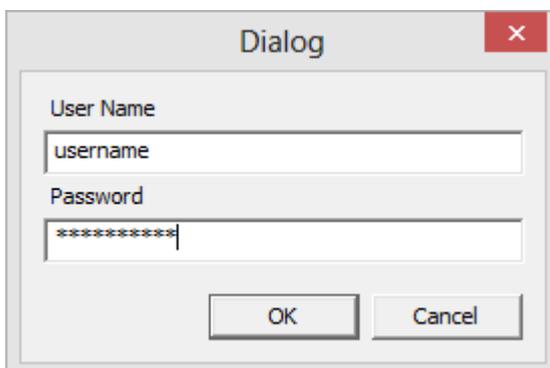
In addition there are some settings that need to be manually set in the XML-file which is described next.

2.4 The XML Configuration File

Below the available settings in the XML file are shown. Some of the settings are made using the graphical interface above, but others have to be made by hand in the file. These settings are marked bold below, and described in the sub sections.

2.4.1 Log File Specific Settings

- **LogFileSize** − The maximum allowed size of the log file before the file is truncated
- **LogLevel** − An integer from 0 to 4. The higher the value the more information is printed to the log file (log level 3 = information).

2.4.2 Connection Specific Settings

- **DSN** − The Data Source Name that has been setup by Discoverant in the Windows *ODBC Data Sources* control panel program
- **Credentials** − Encrypted information about user name and password as entered in the graphical configuration utility.
- **QueryTimeout** − The time, in seconds, before a query or connection to the database will timeout and fail. The default is 20.
- **StartTimeField** − The name of the field/column in the AG path that contains the start time for batch. This setting is used for all AG paths that contains batch information, if different AG paths have different start time fields use the **agpaths** setting below to configure this for each AG path.
- **StopTimeField** − The name of the field/column in the AG path that contains the stop time for batch. This setting is used for all AG paths that contains batch information, if different AG paths have different stop time fields use the **agpaths** setting below to configure this for each AG path.
- **agpaths** − One or more AG_PATHs to expose through the SimApi. One <agpath> element (row in the example below) for each AG path. The name of the AG path and the start and stop time fields are configured for each element. The following is an example with two configured AG paths:

  ```
  <agpaths>
      <agpath Name="Imports:\Test" StartTimeField="Parameter Set Date" StopTimeField="Stop" />
      <agpath Name="Imports:\umetrics\MixTest" StartTimeField="Start" StopTimeField="Stop" />
  </agpaths>
  ```

  Note that when AG paths are configured in this section no AG paths are read from the AG_MANIFEST, only the configured AG paths will be exposed through the SimApi.
- **discretetags** − All discrete tags that are grouped by a replicate id needs to be configured here. One row (<discretetag> element) for each discrete tag. The name of the discrete tag and the AG path it belongs to and by which replicate id it should be grouped by are configured for each row. The following is an example with two configured discrete tags:

  ```
  <discretetags>
      <discretetag Name="pH" AGPath="Imports:\Test" GroupBy="1" />
      <discretetag Name="Dissolution" AGPath="Imports:\Test" GroupBy="2" />
  </ discretetags >
  ```

3. Support

See http://www.umetrics.com/support