OPUS

Spectroscopy Software

Version 6

User Manual

PROCESS

BRUKER

Table of Contents

1 Introduction

The process control software OPUS PROCESS mainly aims to provide a comprehensive standard software for customers dealing with process control, allows stand-alone setups, the integration into already existing process control systems, as well as easily adapts new hardware interfaces. In general, high flexibility is and will be needed to control special analyzing programs, last but not least to comprehensively meet future requirements in this respect. With OPUS PROCESS, however, the user can also minimize the complexity of process control systems.

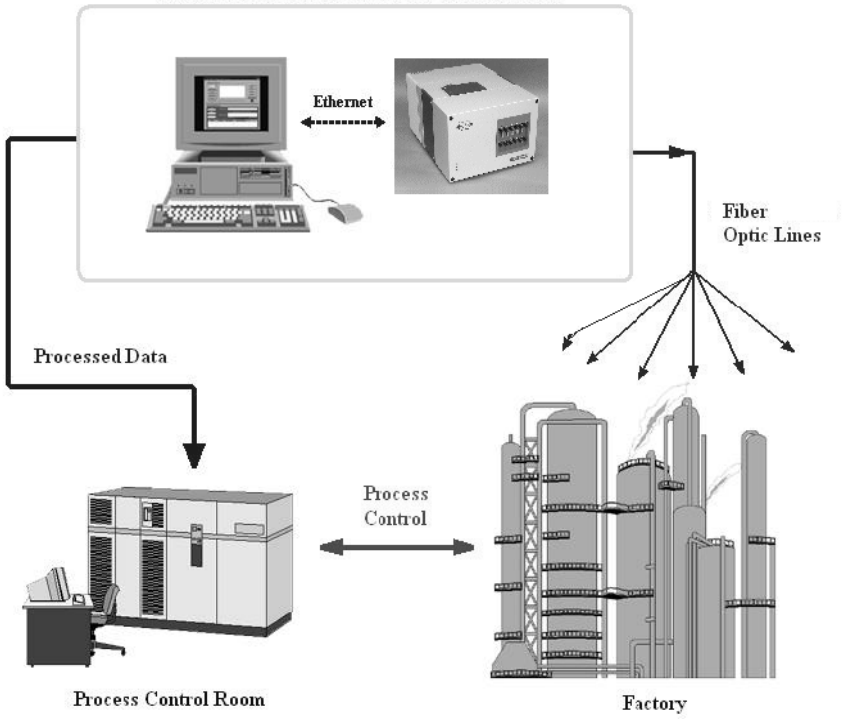


Figure 1: Process Control Setup

Measurements in a process environment frequently aim to perform quantitative analyses of chemical substances. Bruker FT spectrometers are designed to measure various components at different measuring points, using several probes. Normally, the analysis absorption spectrum will first be measured and then analyzed, e.g. by using OPUS QUANT. The quantitative evaluation of the single components forms the basis for the final process data results.

Figure 1 shows a typical process control environment, in which the spectrometer performs measurements at different positions. The data processed will be evaluated and transferred to a process control system while the resulting measurement data can be used to control the complete process.

OPUS PROCESS is an integrated software for data acquisition, data processing and data export, which supports different communication methods with process control systems.

OPC, the software interface used, can communicate with many different external components. For the basic and more detailed OPC protocol features, see appendix A.

2 Features

2.1 General

This chapter describes the basic system features of OPUS PROCESS:

- Cyclic measurement
- Control at runtime
- Data evaluation

OPUS PROCESS allows to measure sample spectra from one or more measurement spectrometer channels. A large number of options is available for processing the raw data acquired by the spectrometer.

The setup enables to define the settings and analyses to be performed on each measurement position.

The data evaluation is performed by using QUANT and/or IDENT which are separate program packages, not automatically integrated in OPUS PROCESS. After performing the analysis, the results will be transferred to the corresponding output interfaces.

In addition to these basic functions several interfaces can be addressed to different input/output modules. Consequently, this enables an easy integration into an existing process control system.

The following features summarize the basic OPUS PROCESS concept, and give you an idea of the program design:

- User-friendly setup browser
- Measurement scenario (all parameters stored in a single file)
- Graphical real-time display of the measurement data
- Complete multitasking even during cyclic measurements
- Measurement control in message queue
- Instrument diagnostic status and maintenance demands
- Editing non-active measurement scenarios during an active cycle
- Switching scenario during an active cycle
- Several log file formats
- External triggering of background measurement scripts and macros
- Spectral evaluations using IDENT, Conformity Test, QUANT 1 and QUANT 2 software packages etc.
- Combination of qualitative and quantitative analysis
- Easy installation and parameterization of communication interfaces via OPC

2.2 Scenario

The basic OPUS PROCESS concept is the measurement scenario which defines the measurement parameters, methods for data evaluation and output interface definitions. All process settings are defined during setup and stored in a single file. The complete cycle with all the different sampling points/measurement accessories and measuring times is stored in the form of a script.

A long-term monitoring of a chemical reactor may require to change the parameters of the actual measurement routine. In OPUS PROCESS this is accomplished by selecting different measurement scenarios. If this concerns several components or parameters, the process control system only has to select a new (pre-defined) scenario. This single command may be sufficient to automatically change the entire system setup (e.g. the measurement channel selected, method, priority etc.).

2.3 Scenario Browser

The setup of all process instructions is designed to perform user-friendly. For this purpose, the multi-level scenario browser, which is similar to an explorer, and appropriate dialog boxes allow to define measurements and evaluations as well as to create a scenario within the scope of the process software. Depending on the methods and channels selected the corresponding parameters required will be enabled only in the respective dialog. All other dialogs will not be considered.

The process control system selects the requested scenario by its file name. Special parameters (e.g. measurement time) of an active scenario will not be changed separately. Instead, a change of the measurement conditions is achieved by selecting a new scenario, i.e. an existing scenario is loaded and relevant parameters are modified before saving the modified scenario by a different file name.

2.4 External Control

In particular, a process control system can externally monitor the measurements by running a specific measurement at a particular time or by selecting a completely new scenario. As a result, the process control system can change all tasks at runtime, e.g:

1) A scenario defines which components have to be measured and how often the analyses are to be cyclically repeated.
2) Evaluation parameters of a component will be triggered by switching to a different scenario.
3) Special reference measurements at any probe can directly be started.
4) Certain important calibration measurements will be stored separately, if required.

OPC is the standardized communication interface used in OPUS PROCESS (see appendix A). Even if the process data of one OPC server will change, OPUS tasks can still be run.

2.5 Measurements

Repeated measurements are permitted at one or more sampling points/ measurement accessories. These measurements are periodically entered into a measurement list as previously defined in the scenario. The measurements are repeated as long as the maximum number of repetitions is achieved, or as long as they are aborted by the process control system or the operator.

Cyclic measurements and measurements performed by the process control system or the user are commonly routed in a message queue. Measurements resulting from external triggers or direct user interaction have high priority, i.e. they will be started immediately after the running measurement has finished. Therefore, the measurements with low priority are pushed down until the high-priority measurements have been finished. The same applies to manually started measurements or process control systems initiated, where the measurements will be processed according to the FIFO principle (first-in-first-out). Measurements with high priority are never cyclically repeated.

2.6 Hardware Installation

On the basis of the general OPC interface, OPUS PROCESS can work with various different hardware interfaces. For any further details about the installation of a particular interface card, refer to the hardware manual supplied.

2.7 Experiment Definition, QUANT and IDENT Method Files

OPUS PROCESS mostly uses measurement experiment definitions (XPM files), QUANT methods etc. These files are to be prepared first by using the usual OPUS functions, e.g. QUANT or IDENT setup.

Note: If you define a scenario, make sure that the defined measurement experiment parameters are identical to those used to generate the QUANT and/or IDENT methods. You can select all components stored in a QUANT method.

If you have updated the OPUS version, it is recommended to load and re-save experiment measurement files created by the previous OPUS version, before using them in OPUS PROCESS. This is achieved by loading and saving the XPM files by using the OPUS *Advanced Measurement* command in the *Measure* menu.

2.8 Registration

OPUS PROCESS will be installed with the OPUS standard software. To be able to use OPUS PROCESS by OPUS you may need a new license key. If you update your license, make sure that you enter the correct serial number and licence key by the *Register OPUS* command in the *Setup* menu.

2.9 Multitasking

Due to the multitasking functions in OPUS interactive measurements are possible, regardless of the kind of process scenarios running in the background. This is mainly useful if, e.g., additional spectra are required for calibration or correction. These measurements are completely independent and not any information has to be exchanged with the process control system. The measurement and evaluation results can be displayed in a separate window in OPUS.

2.10 Process Probes/Flow Cells

Usually, probes/flow cells are mounted at different locations within the process system. The process measurements are initiated by the control system and the instrument returns the analysis results, status or possible errors. By means of a multiplexer it is possible to observe 6 different measurement points. In addition to these types of analysis, the control system might also request different measurements at the process probes/flow cells, e.g. calibration measurements. The cyclic process measurements as well as the reaction to special external signaling are both defined in the scenario.

2.11 References

To generate absorption spectra a background or reference spectrum is required. In this case the spectrum measured does not depend on the spectrometer or probe/flow cell. As the background spectrum may temporarily vary, OPUS PROCESS enables to measure such spectrum interactively or via a trigger sent by the control system.

2.12 Runtime Module

The process runtime module executes a scenario which contains all the information about the process control, measurements and evaluations.

This module includes a graphical user interface with real-time data display and trend charts as well as the entire internal process communication.

Even the OPUS OPC server is part of the runtime package. This interface enables the access to all channels defined during setup.

2.13 User Rights

OPUS provides several levels of access rights for each user. OPUS PROCESS distinguishes between different user groups and their rights assigned by the *User Settings* command in the OPUS *Setup* menu:

a) Administrators are allowed to execute cyclic and reference measurements. They can also modify all parameters within a scenario.
b) Users who are allowed to execute cyclic and reference measurements, but cannot modify the parameters of a scenario set up their workspace without the setup process icon.
c) Users who are only allowed to perform cyclic measurements should not have the right to change parameters. To ensure this you have to deactivate the *Change Parameters* check box on the *Rights* tab of the *User Settings* command in the *Setup* menu.

2.14 OPC Interface

OPUS PROCESS can integrate the OPC interface both as server and client.

2.14.1 OPC as client

OPUS PROCESS queries data from other OPC servers. In this case OPUS is the process control system which gets data. These data can be displayed in OPUS, stored and processed. See also appendix A.

2.14.2 OPC as server

OPUS PROCESS provides data which can be read by a client.

- OPUS server name: *OPUSOPCSvr*
- When starting OPUS two OPC items are displayed by default:
  - *OPUSCommand* (for advanced programming)
  - *OPUSStatus* (refers to the instrument status)
- When starting a script additional items are hierarchically displayed according to the scenario name.

3 Process Setup

3.1 General

OPUS PROCESS is a measurement and evaluation software. The basic requirement is to execute cyclic measurements, evaluate spectra measured and export data recorded. Instrument-specific parameters, such as measurement probes/flow cells, measurement experiment files and QUANT methods are selected and defined by the administrator using the *Setup Process* command from the *Measure* menu. These parameters must be defined before any kind of scenario can be run.

This chapter exemplifies an easy type of setup. The following steps have to be observed to be able to use OPUS PROCESS successfully:

1) Define the number of measurement positions and components to be evaluated. Make sure that for each measurement value or component
   - measurement experiment files and
   - QUANT or IDENT files

   are available.
2) Optionally, set up the communication by means of a process control system.
3) Optionally, define how to react on external triggering.

If you define the process setup for the first time, you do not need to specify the communication parameters as OPUS PROCESS will automatically generate items for all data defined in its standard OPC server. The aim is to set up a cyclic measurement, define a QUANT evaluation and display the results in real-time.

To define the routine select the *Setup Process* command from the *Measure* menu. The result is stored as one single file which is called *measurement scenario* in the following and defines the current instrument setup and the corresponding analytical method used at a dedicated measurement port/probe.

3.2 Basic Setup

To define a scenario select the *Setup Process* command in the *Measure* menu. The *Basic Process Setup* dialog on the *Scenario*.obs* level opens:

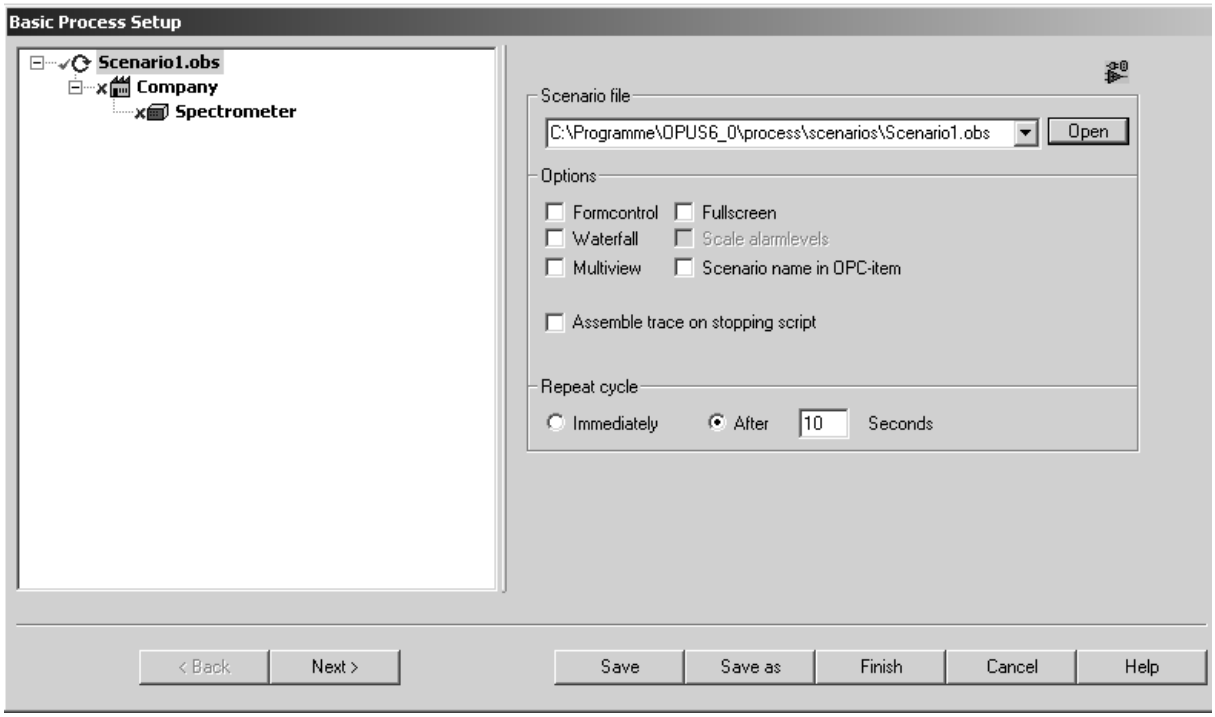


Figure 2: Basic Process Setup

Define the file path used to store the scenario and type in an appropriate file name.

Note: You can use any path, except <*OPUS Path*>*Process*.

Leave all the display options unchecked. Activate the *After* option button for the repeat cycle and enter, e.g., *10* into the *Seconds* entry field. Click on the *Next* button to continue.

You do not need to fill in the entry fields on the *Company* level. The data on the *Spectrometer* level will automatically be generated by OPUS. Therefore, the entry fields are disabled. For further details on these two levels see chapter 6.2.1 and 6.2.2.

3.3 Measurement Experiment

Apart from the measurement channel, file names and saving options all measurement parameters are read from a measurement experiment file. As data channels are assigned to a specific measuring point, you first have to define this measuring point. Therefore, right click on the *Spectrometer* level and select the *Add Measuring Point* command from the pop-up menu.

Clicking on the *New Measuring Point* sub-level opens the following dialog:

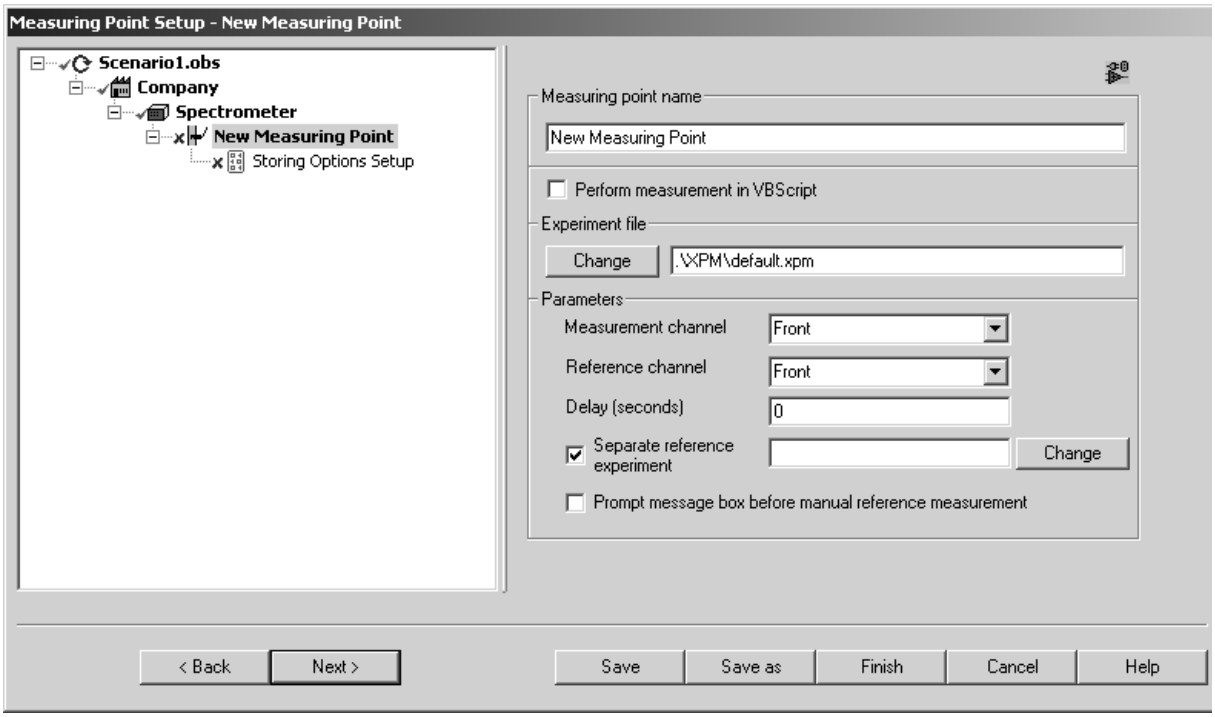


Figure 3: Measuring Point Setup

Make sure that you define a unique name for the measuring point. By default, the *New Measuring Point* name is displayed.

3.3.1 Experiment File

An measurement experiment file (XPM) is the file used by OPUS to configure the instrument and to perform a measurement. All relevant measurement parameters are contained in the XPM file, including measurement position, number of scans for reference and sample measurement, wavelength range, spectral resolution and further detailed parameters for the measurement and Fourier transformation.

OPUS PROCESS measurements are based on these XPM files. To determine the port and parameters to be able to perform the requested measurement you have to create at least one XPM file.

In addition, it is recommended to store the XPM files in a central directory to facilitate the setup. If you have not yet defined your experiment file, select the *Advanced Measurement* command in the *Measure* menu and define all necessary parameters, especially on the *Optics* tab. Click on the *Advanced* tab and save the XPM file by using the *Save* button.

Specify the path and file name of the experiment file to be used by OPUS PROCESS for this channel. If you click on the *Change* button, a file selection box opens which you can use to select the experiment file for this particular channel.

The experiment file selected must have been manually configured in OPUS. Before using the experiment file in OPUS PROCESS it is recommended to test it in OPUS by a single measurement. This ensures that the spectrum is generated by using the parameters desired.

3.3.2 Parameters

The options included in the channel drop-down lists depend on the spectrometer type. In general, this list contains all the sample compartments and/or fiber-optic ports available to the respective spectrometer. To simplify this example, the same measurement setup is used for both sample and reference channel.

The *Delay (seconds)* entry field refers to the delay before measurement, which allows to specify individual queue times for each channel.

3.4 Storing Options Setup

Whenever you define a measuring point the *Storing Options Setup* level is automatically displayed in the browser window. The corresponding dialog shows some additional measurement-related parameters. You can e.g. define where to store the files measured.

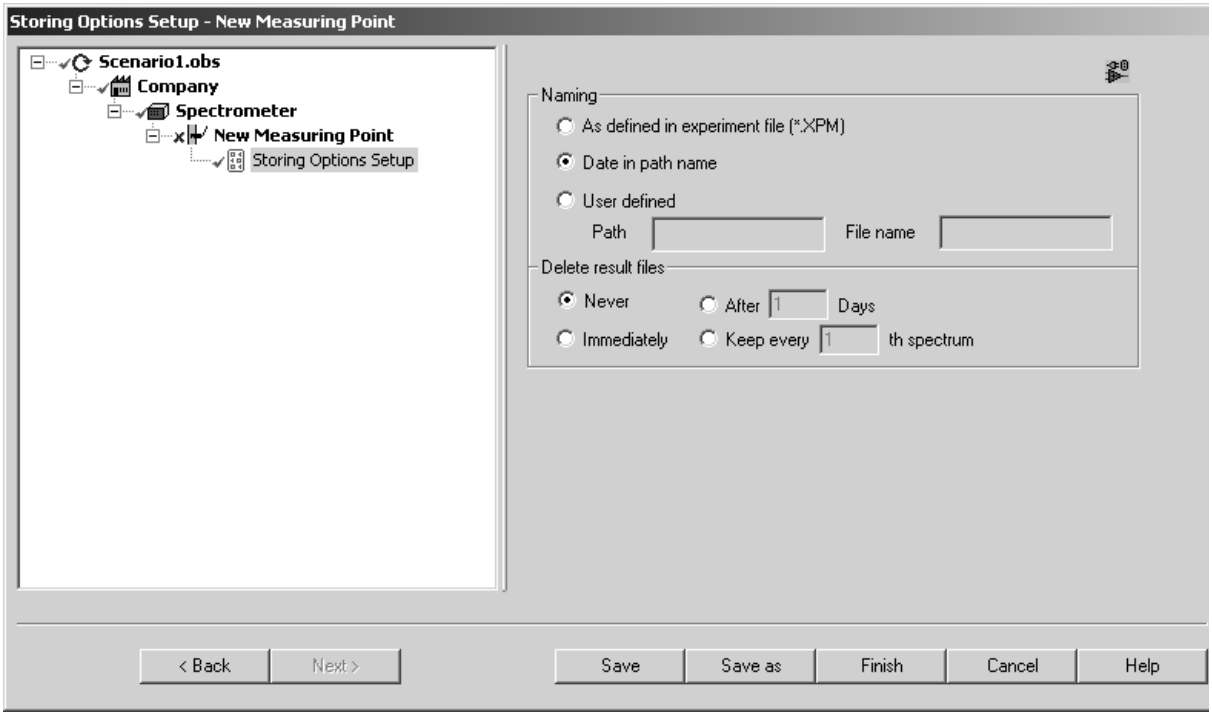


Figure 4: Storing Options Setup

The example in figure 4 indicates that the files will be named by the measurement date in the path name. The result files will not be deleted, even after the evaluations have been performed. This means that after a long process run many files will be stored which have to be deleted manually.

3.5 Channel Setup

Right click on the *New Measuring Point* level and select the *Add Data Channel* command from the pop-up menu. The *New Data Channel* sub-level will be displayed in the browser window.

Clicking on the *New Data Channel* sub-level opens the following dialog:

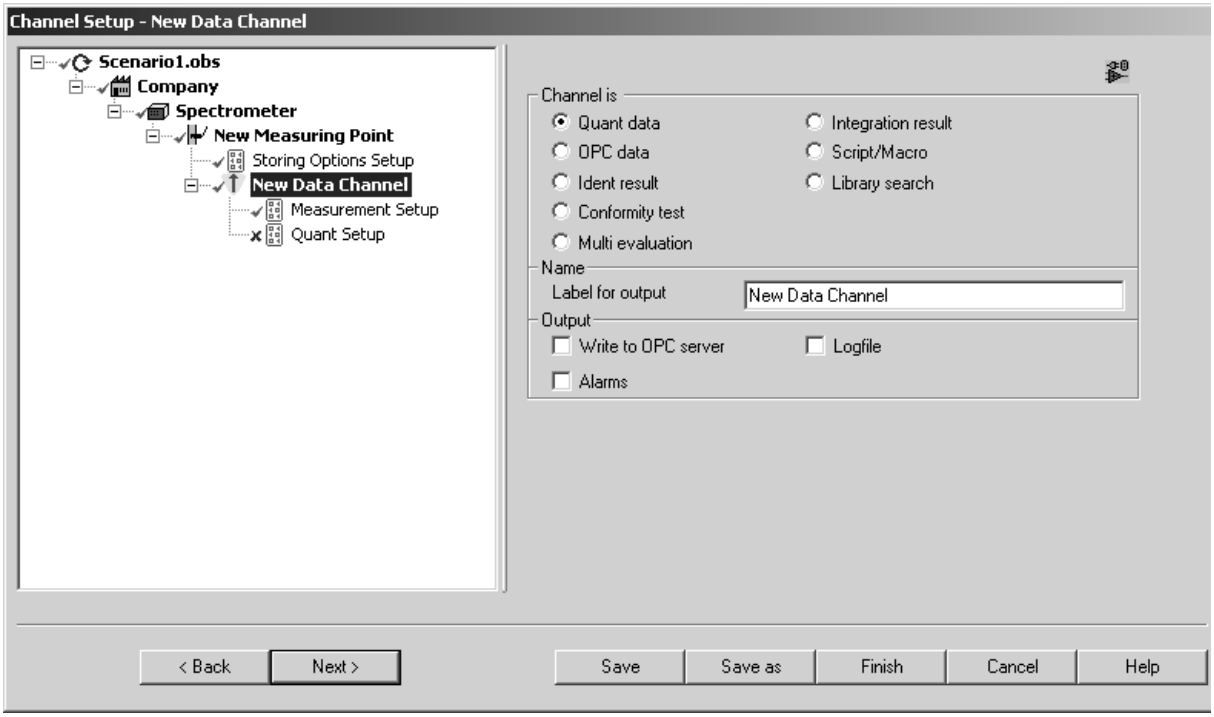


Figure 5: Channel Setup

Define the specific type of data for each channel. In this example select a measurement with a subsequent evaluation. Neither a special script nor macro or OPC communication are required. Activate the *Quant data* option button.

No log file is needed. The data will not be written to an OPC server for special output. Therefore, do not activate the *Write to OPC server* and *Logfile* check box. The *Alarms* check box do not have to be activated, as not any notifications are necessary if a certain limit is exceeded.

Enter the *Label for output* manually. If you do not enter any name, *New Data Channel* is assigned by default. As the *Quant data* option button has been activated click on the *Quant Setup* level to continue with the QUANT settings.

3.6 QUANT Setup

The *QUANT Setup* dialog (figure 6) defines the current evaluation settings for the spectra acquired.

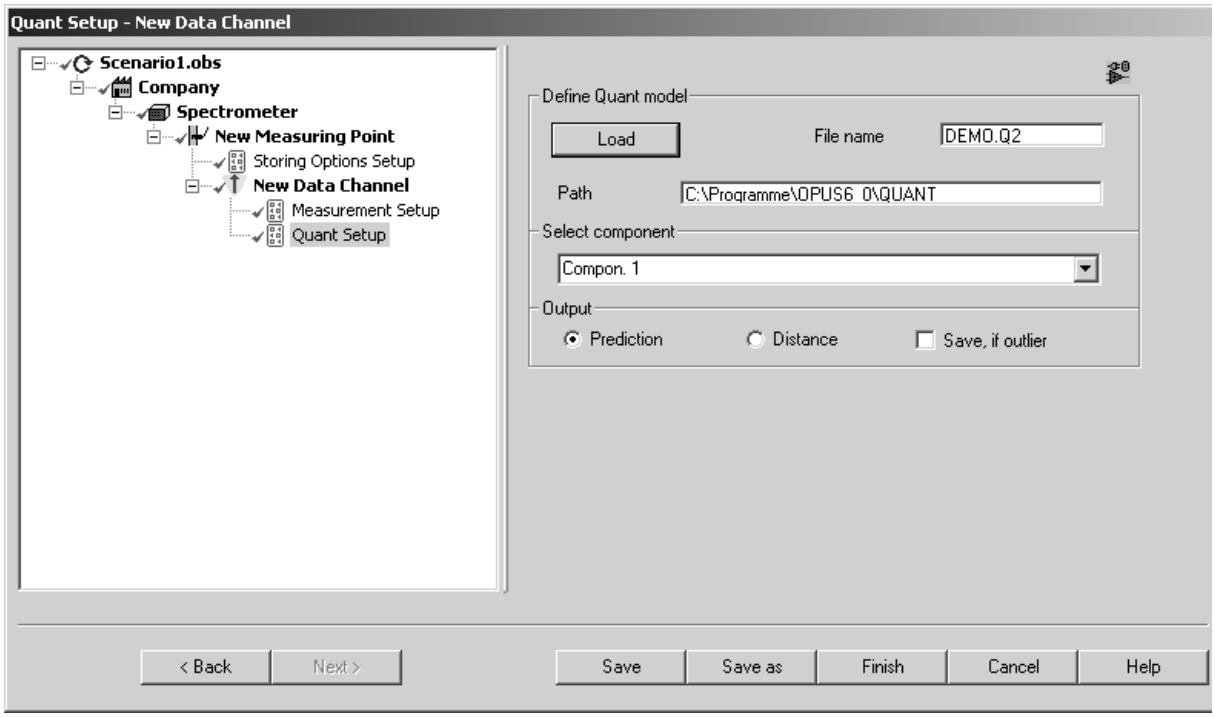


Figure 6: QUANT Setup

OPUS PROCESS allows to perform both IDENT and QUANT analyses on spectra acquired. Both IDENT and QUANT analyses require method files which have to be generated in advance. If no method files are available, you can only acquire and store spectral data files, but you cannot perform any analysis on these data files.

Click on the *Load* button. The normal file selection box opens. Select the directory in which the QUANT methods have been stored. If you load a method file, the *Select Component* drop-down list automatically displays the components stored in this method. Use this drop-down list to select the correct component for the evaluation.

Activate the *Prediction* option button as output. Finally, click on the *Finish* button to complete the setup process. The parameters will be stored in the scenario file.

4 Process Start

4.1 Selecting a Scenario

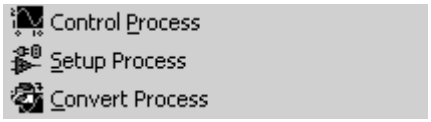


Figure 7: OPUS PROCESS menu items

The OPUS *Measure* menu also includes the *Control Process* command. Select this command to start a scenario. The following dialog opens:

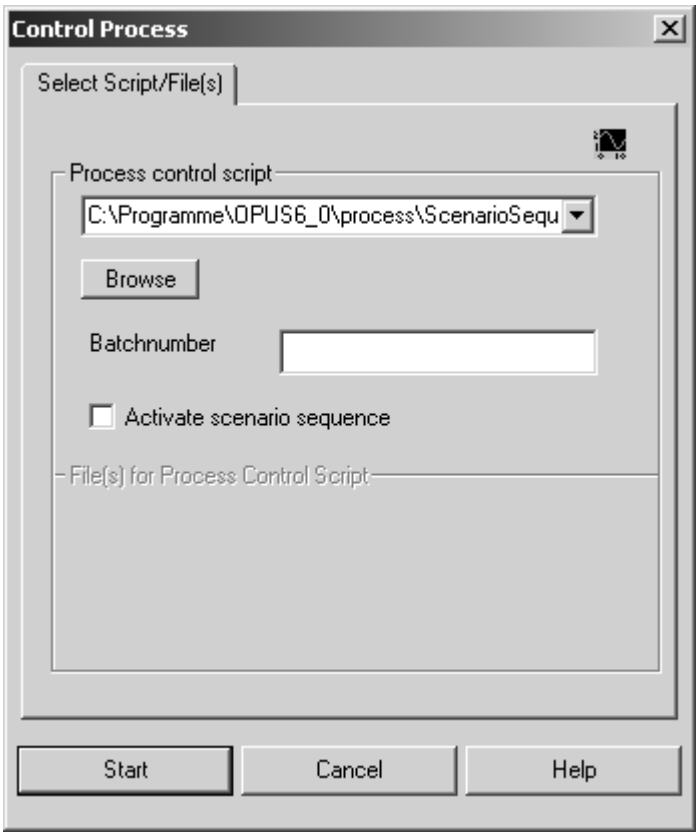


Figure 8: Process Control - Select Script/File(s) tab

The cyclic measurements are based on measurement scenarios which include:

- Measurement parameters
- Evaluation methods
- Graphical presentation

- Alarm signals
- Output interfaces
- Reactions to external triggers
- VBScripts

Define the *Process control script* by using the drop-down list or click on the *Browse* button and select the appropriate script from the dialog displayed.

It is also possible to enter a batch number before running a scenario. The batch number will be stored with each spectrum and added to the sample name. If you have activated the *Logfile* check box on the *Channel Setup* dialog (see figure 5), the batch number will also be stored in the log file.

Click on the *Start* button to load the scenario. A process control view (usually a trend chart) will be displayed. The cyclic measurements start automatically and the results are displayed. You can also start a reference or background measurement, if required.

If you want to start several scenarios in parallel, activate the *Activate scenario sequence* check box. In this case the *Process control script* selection box will be disabled. It is, however, possible to enter a batch number which will then be assigned to each script.

Click on the *Start* button to open the following dialog:

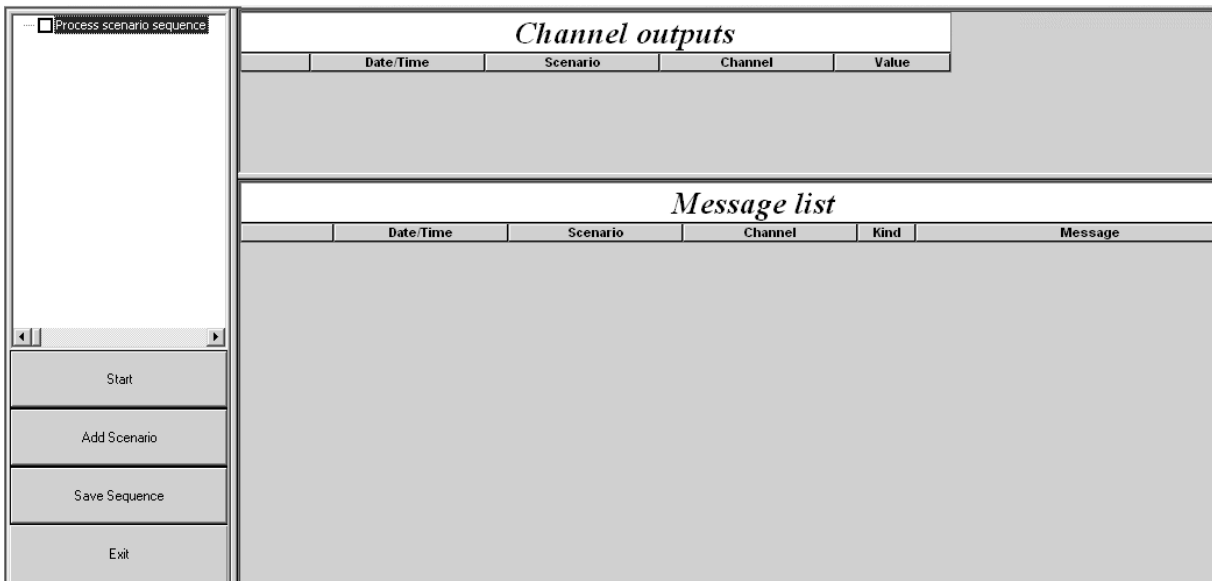


Figure 9: Scenario sequence dialog

When starting several scenarios the single sequences run one after the other and the results are displayed in the channel outputs list, i.e. the latest are on top. Additionally, the message list includes information on the process run of each scenario. The *Kind* column shows possible errors which can be of the following type:

- Error
- Information
- Warning

The errors included in the message list are also written into the error.log file (see chapter 5.2).

Select the respective scenarios by means of the *Add Scenario* button. The names of the scenarios are displayed in the browser window. Check the scenario you want to start the process run with. As soon as you check the Process scenario sequence level the *Start* button will change into *Stop*.

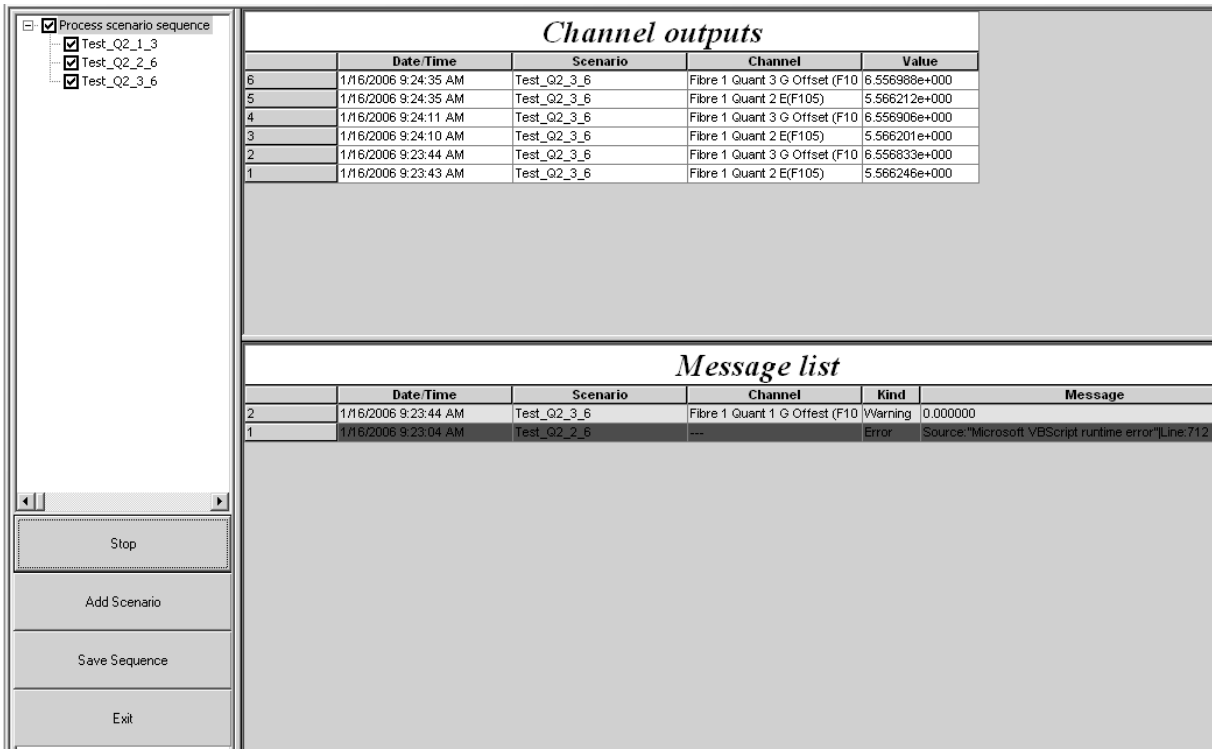


Figure 10: Scenario sequence with channel outputs and message list

5 Process Views

The different process views help you to monitor the process. All the measurement results can be graphically displayed by these views. The unique graphical interface is easy to use, even in case of untrained operators.

The graphical presentation of the measurement results permit a fast and clear overview of the results. Depending on the channel setup the following specific charts can be generated:

- Concentration/time plot
- Turnover/time plot
- Product output/time plot
- Changes in components/time

The process views are normal OPUS windows, i.e. they can be re-sized by using either the min./max. buttons on the title bar or by dragging the window edge. You can switch between the process window and normal spectrum window. Click on the respective window tab or use the OPUS *Window* menu and select the appropriate window from the list. The process views consist of two sections (see figure 13). On the left side some control elements indicate the measurement status, and the chart on the right shows the real-time data.

5.1 Control Elements

Sample measurements defined in the scenarios are initiated immediately after the scenario has been started (see chapter 4). A minimum and maximum limit can be set up in the scenario. If the current analysis value exceeds the limits defined, the process control system is informed about this circumstance by a signal. The alarm levels can also be read on the chart. If alarm values have been defined during the setup, the horizontal, red line on the chart indicates these values for the active channel. A yellow line indicates a warning. If, e.g., a QUANT value exceeds that limit, a special notification to the process control system can be configured.

The current status of the measurement cycle is indicated on the OPUS status bar below the OPUS spectrum window by a green field.

Figure 11: Process Control - status indicator

On the left side of the process view there are some control elements and buttons which will be described in the following.

Figure 12: Process Control - control elements

5.1.1 Seconds left before next cycle

This is a counter displaying the number of seconds before the next measurement will be performed. It counts down to 0 from the delay defined within the scenario.

5.1.2 Channel

This drop-down list indicates the number of the active channel. If the measurement cycle is in delay mode (i.e. the counter is counting down), the channel displayed is the one which has just been evaluated.

5.1.3 Measure Reference

If you click on the *Measure Reference* button, the background or reference measurements will be started for the channel defined in the *Channel* drop-down list. The background measurement may be different for each measuring position or probe. The parameters used for reference measurements are defined during the setup process and are stored in the scenario file. A reference measurement recorded in this way will be used as background for this channel during the next cyclic sample measurement.

At any time during the process run an appropriate background spectrum must be available for each measurement position (except for Raman measurements). This spectrum can be generated either before the measurement, or manually whenever the probe is in the right position, or from an external trigger of the process control system. Make sure that the probe/flow cell is clean (e.g. during the initial installation of the probe or flow cell) before running the reference measurement.

All reference measurements are stored in the scenario directory. The name of the directory is the same name as of the script and can be found in the PROCESS sub-directory in the path where OPUS has been installed. The files are named channel 1.0, i.e. the file name includes the channel number and the extension is incremented by each new reference recorded. If you want to use a previous reference spectrum for a certain channel, you have to rename this file manually to get the highest extension number. The spectrum file will automatically be loaded for the next measurement.

5.1.4 Change Scenario

Click on the *Change Scenario* button to select new scenario scripts from the dialog which opens. If you select a new scenario, the entire measurement context will change. The effects will be detected only if the current active run has been completed.

5.1.5 Stop

This button will abort the process control and close the chart. The active cycle will be completed before the scripts terminate.

5.1.6 Add Comment

The *Add Comment* button will be deactivated if the operator does not have the the right to change parameters. This option can be checked on the *Rights* tab of the *User Settings* command in the *Setup* menu. The comments added will be written into the error log file.

5.1.7 Pause

If you click on the *Pause* button, the internal measurement still continues. The display on the screen, however, will be interrupted and not any warnings or signals will be indicated.

> **Note:** The maintenance warnings are not entered manually, but the instrument status is permanently checked and automatically displayed.

5.1.8 Graph Type

Different graph types are available which will be described in the following. The *Trend* graph type is set by default. This kind of scroll mode allows the chart to be automatically scrolled when new data are measured. The other graph types (*Text*, *Bar*, *Meter* and *History*) acquire data and only display the current values for each channel. To switch between the different graph types, use the option buttons on the left.

5.2 Trend View

The real-time display depends on the particular channel, i.e each component measured or measurement position represents a data set or band in the trend chart.

For each band the scale can be adjusted, and each band has a separate axis.

The channel data shown indicate:

- Quantitative analysis
- OPC server data
- IDENT results
- Integrated bands
- Search results
- Conformity test result
- Script/macro result

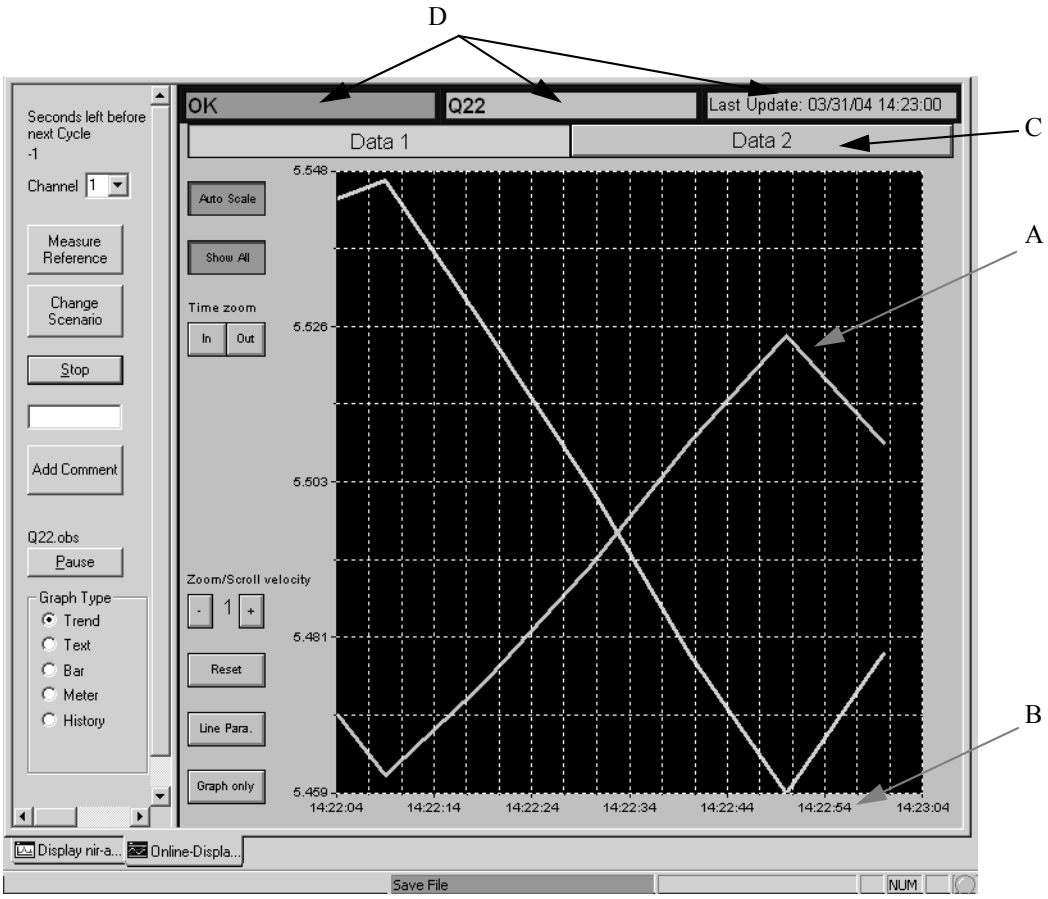


Figure 13: Process Control - Standard Trend View

The real-time results are displayed on the chart (A). In case of QUANT results the trend chart is a real-time chart of QUANT values achieved. The QUANT results defined for all channels measured are charted separately. The trend chart is continuously up-dated during the measurement cycle and shows the latest measurement results. You can unhide or hide the window at any time.

The chart pops up from left-to-right until the display is completely filled. The display automatically scrolls to the left to be able to display the latest values on the right side. Each channel has its own color. Yellow lines indicate that the warning limit defined for the currently selected channel is reached. Red lines indicate alarm limits.

The time axis (B in figure 13) is displayed on the lower part of the chart. At the beginning of a run the time axis is set to 0 and the default range is 60 seconds. If the process is slower than 60 seconds, the axis can be adjusted by the *Time Zoom In/Out* buttons.

The buttons on top of the chart (C in figure 13) represent the channels defined. Each button is labeled by the name of the component or measuring position as assigned during the setup. They all have a unique color that correlates to the respective band in the chart.

The chart header (D in figure 13) includes the status of the most recent measurements indicated by the left button. The following results are possible:

- **Green/OK:** measurements run successfully.
- **Yellow/WARNING:** the channel number and the value which caused the warning will be indicated and written into the log file.
- **Red/ALARM:** the channel number and the value which caused the alarm will be indicated and written into the log file.

If a measurement has completely failed, all errors will be listed in a so-called *error.log* file as exemplified in figure 14.

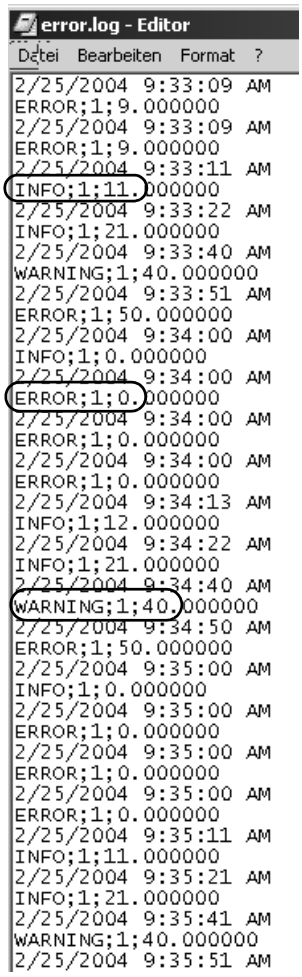


Figure 14: Process Control - error log file

The button in the middle (D in figure 13) shows the process control method. The last update (date and time) of this process control method is indicated on the right button (D in figure 13).

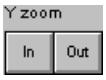
5.2.1 Active Channel

There is always one *Active* channel in a trend chart. If you click on one of the channel buttons (C in figure 13), this channel will be *Active* and represents the y-axis. As there can be several bands with completely different frequency ranges, the result may consist of several axes. To avoid this confusion the y-axis values displayed are the ones assigned to the active channel. If you want to absolutely scale a particular band, click on the respective channel button to activate this channel. The axis will automatically be adjusted.

If you select one active band, the other channels are automatically scaled, i.e. the scale is adjusted in so far as the absolute maximum for each channel will determine the whole y-range for the particular band.

5.2.2 Auto Scale/Show All

You can scale the y-axis (channel result value) of the active channel displayed by means of the *Auto Scale* button. A green *Auto Scale* button indicates that the scaling function is activated. To deactivate the scaling function click on the *Auto Scale* button. Additional scroll/scale buttons will be displayed. Click on the 

buttons to scroll the y-axis up and down, and on the 

buttons to zoom in and out the y-axis.

To show all channels click on the *Show All* button. A green *Show All* button indicates that this display function is activated. To deactivate this display function click on the *Show All* button, and the active channel only will be displayed on the chart.

5.2.3 Zoom/Scroll Velocity

It is possible to increase or decrease the velocity for the zooming and scrolling functions. Click on the 

button to increase the velocity, or on the 

button to decrease the velocity. The figure displayed between these two buttons indicates the active channel.

5.2.4 Reset

If the scaling factors for the individual channels have been modified, the *Reset* option will set them to default again, i.e. the y-axis is automatically scaled to their channel extremum.

5.2.5 Line Parameters

It is possible to change the parameters for the lines. If you click on the *Line*

Parameters button the following dialog pops up:

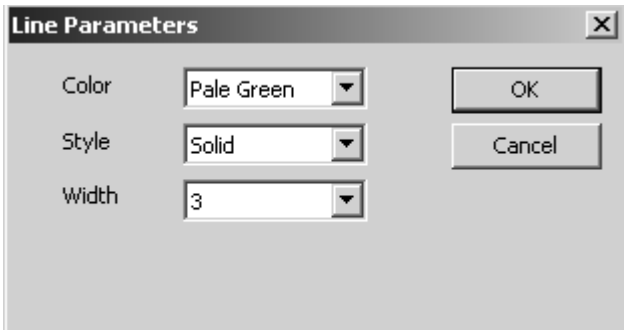


Figure 15: Process Control - Line Parameters options

Select one of the options available for color, style and width from the drop-down lists.

5.2.6 Graph Only

To display the graph only, click on the *Graph only* button. Double clicking on the graph will undo this view.

5.2.7 Assemble Traces

If you control a process, you primarily monitor the components, display them and adjust the process. These process data can be stored as an OPUS file for detailed off-line analysis.

Right click somewhere on the chart and select the *Assemble Traces* function from the menu that pops up. By means of this function the data acquired will be stored as traces into a 3-D file. This function requires the OPUS/3D software.

5.2.8 Printing

To print a chart use the *Quick Print* command from the *Print* menu, similar to printing normal spectrum windows. A default layout for the process view will be installed by OPUS. If you use a color printer, it is possible to have the chart printed in color.

You can also save the chart on the clipboard. Select the *Copy* command in the *Edit* menu. The particular chart is sent to the Windows clipboard puffer in the same form as it appears on the screen. The chart will then be directly pasted into the different Windows applications, e.g. all Microsoft Office programs.

5.3 Text View

During cyclic measurement the intermediate results can be displayed in the text view. In this view each row corresponds to one channel.

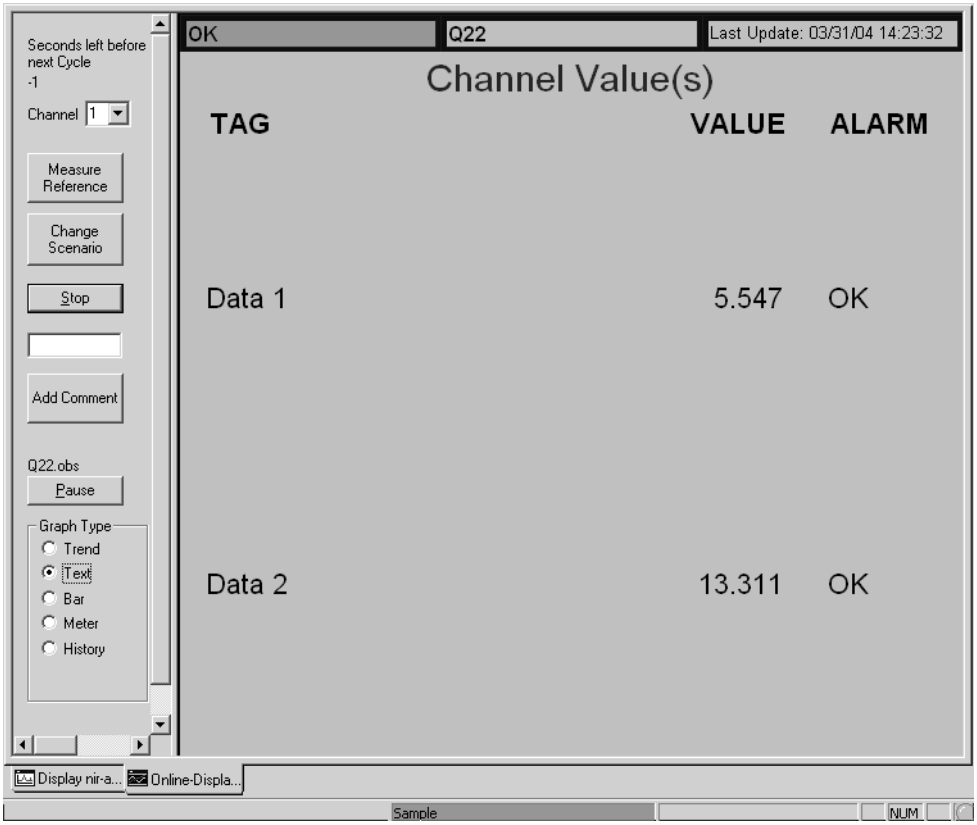


Figure 16: Process Control - Text View

The first column includes the names of the channels or components. These names correlate to the names of the channel buttons on the trend view. The second column includes the current value of the particular channel. This kind of view is very useful if the exact values are to be controlled.

The third column includes the alarm status. If you reach one of the limits defined in the setup, an alarm text pops up, e.g. *HIGH,* which refers to the particular channel. The alarm status is indicated by different colors:

- **Green:** process control is OK
- **Yellow:** general warning
- **Red:** fatal error

5.4 Bar View

You can also have data graphically displayed as bars, with the size of the bars indicating the numerical value for the particular channel. In this view each bar corresponds to one channel.

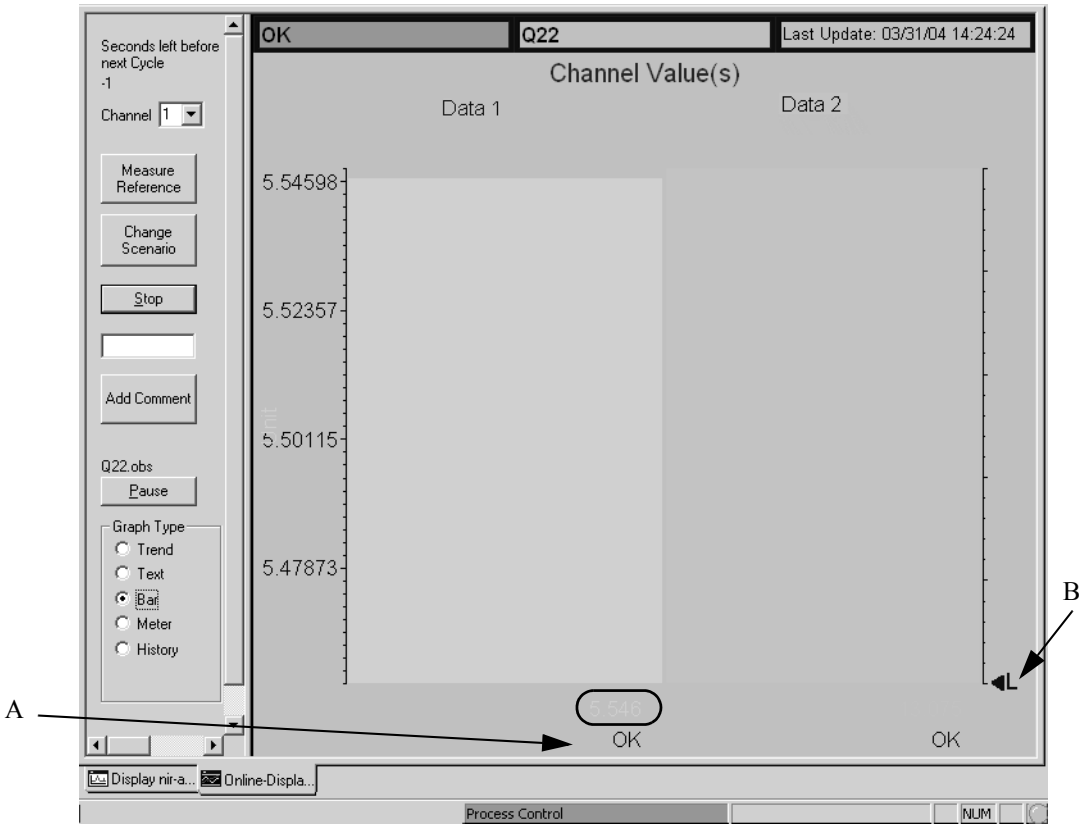


Figure 17: Process Control - Bar View

At the top the names of the channels or components are displayed. These names correlate to the channel buttons on the trend view, as well as to the order and colors of the data. At the bottom the analysis values achieved for each channel are displayed (see circle in figure 17).

Additional fields indicate the alarm status (A in figure 17). If you reach one of the limits defined in the setup, an alarm text pops up which refers to the particular channel. The alarm status is indicated by different colors:

- **Green:** process control is OK
- **Yellow:** general warning
- **Red:** fatal error

On the left side of the bar view is the axis which defines the scale. This scale always refers to the active channel. Small indicators (B in figure 17) correspond to low (L) and high (H) alarm values.

5.5 Meter View

The meter view is the most favorable if data are expected to move around a *target* value. Each range is on the same scale, and you can see whether the measurement values are within the red, yellow or green section.

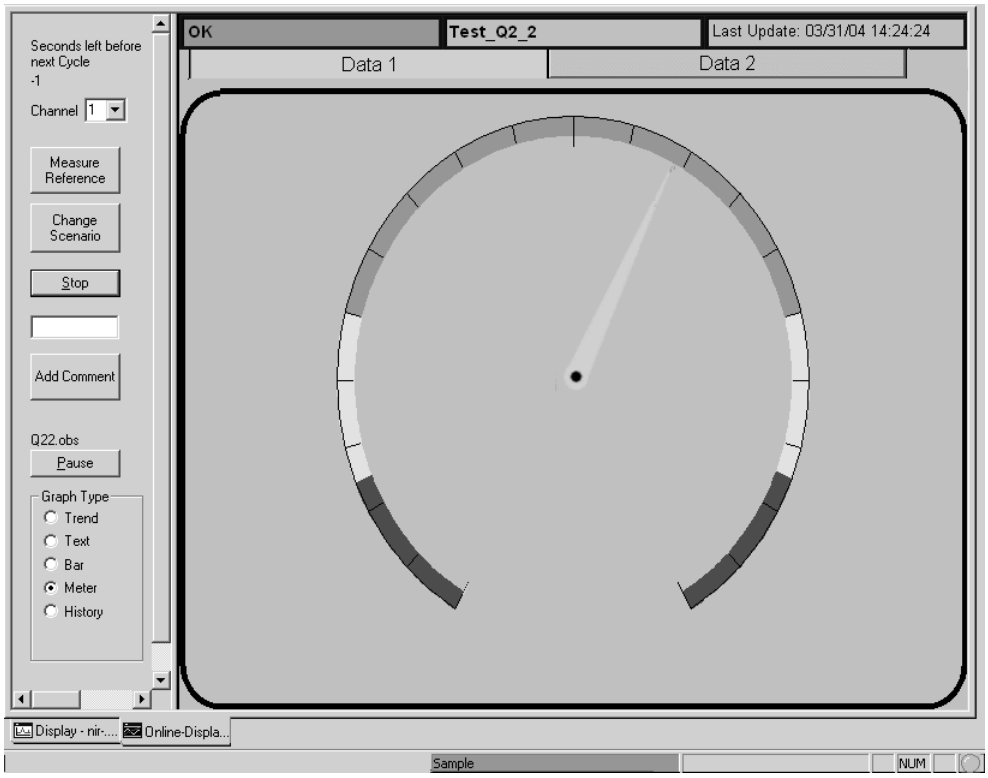


Figure 18: Process Control - Meter View

If you have not defined any alarm or warning limits in the process setup, the measurement values will always be in the green section. Otherwise, the alarm and warning indicators refer to the active channel.

5.6 History View

The history view is similar to the real-time trend view (see chapter 5.2). The difference is that the real-time trend view is updated automatically and always displays the most recently acquired data. The history view displays all data previously recorded (up to approx. 60,000 data records), but will not be automatically up-dated.

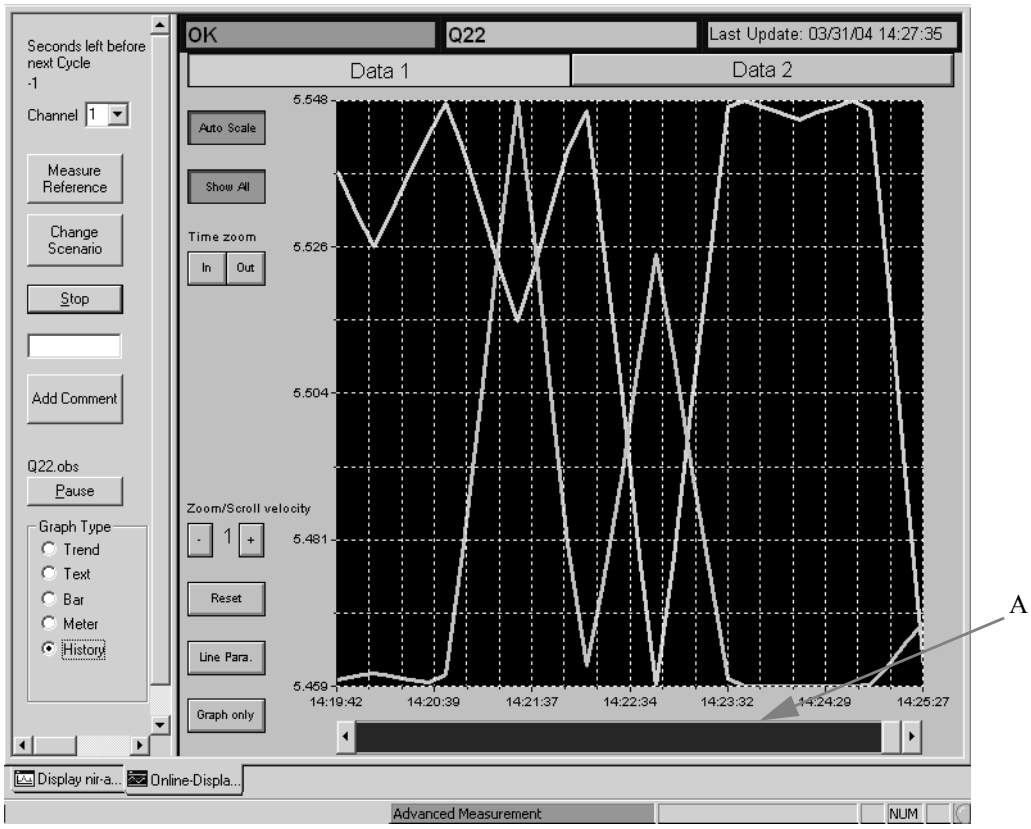


Figure 19: Process Control - History View

The history view allows to zoom into the previously acquired data and check values more precisely within a certain period of time. Select the area you want to zoom in, drag a rectangle around this area and click on the *Time Zoom In* button. Now, the chart displays the area zoomed. To undo the zooming double click on the chart.

The scroll bar (A in figure 19) below the chart corresponds to the complete measurement range. Use the arrow buttons to scroll back and forth.

5.7 Special Views

In case of specific applications a more sophisticated data presentation is helpful. OPUS PROCESS provides additional views which can be defined by the *Options* group field in the *Basic Process Setup* dialog (see figure 2).

It is possible to have the measured spectra displayed as 3-D stacked plots. Up to 16 band positions can be displayed in one chart. If you want to monitor more data items simultaneously, you can open several chart views. Each view shows up to 16 band positions of the current scenario. There can be channel views with 2 or 4 charts, with each chart including up to 16 different positions.

5.7.1 Multi View

All the view types previously described can be combined in one single window. It is possible to change the view type of each single chart individually. Click on the particular chart you want to change and select the view type from the *Graph Type* group field on the right. The different view types can be scaled individually and you can move the borders between the view types to change the screen section.

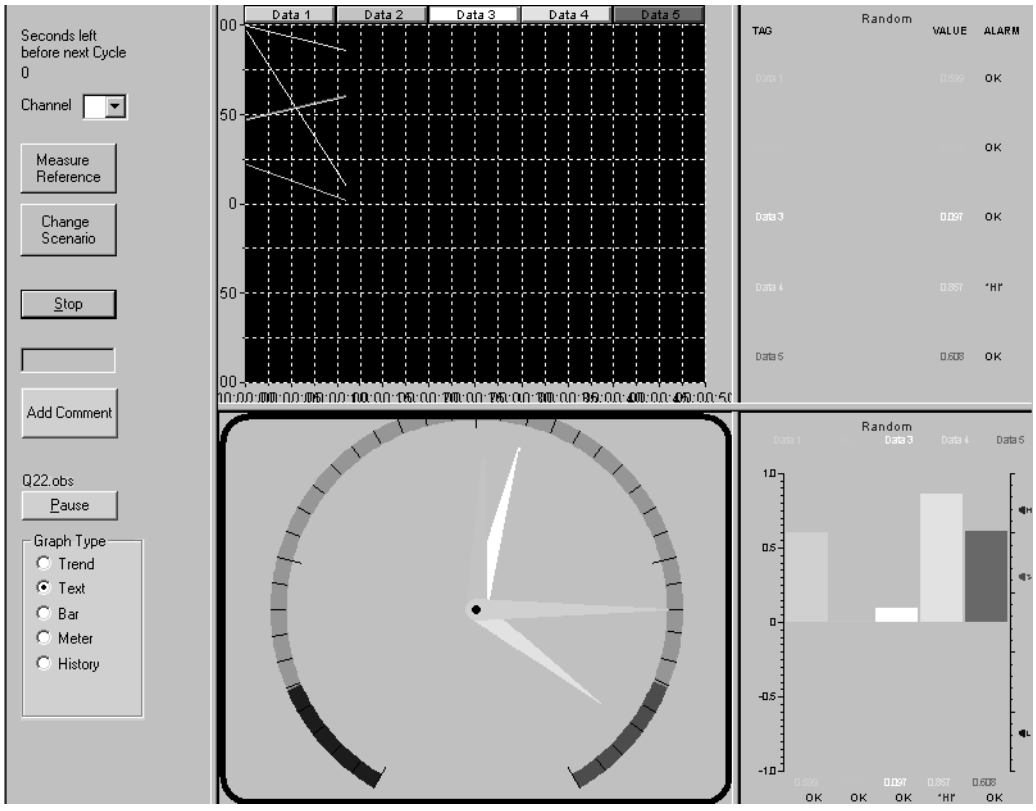


Figure 20: Process Control - Multi View

5.7.2 Form Control

You have the possibility to integrate graphical elements of a plant, e.g. boilers, pipes, probes into the process view.

It is, however, not possible to automatically define the integration of graphical elements by means of the process setup wizard. You need comprehensive programming experience.

Select an image presenting the plant or any other kind of graphical elements. After the setup you have to add these images manually to the process control script. Open this script by means of the VBScript editor. For each channel you need to have a button control element. This button control element has to have the same name as the channel. The control element corresponds to a specific channel, the bitmap assigned indicates the probe or measuring position. If all the settings are made, the form control view will be displayed.

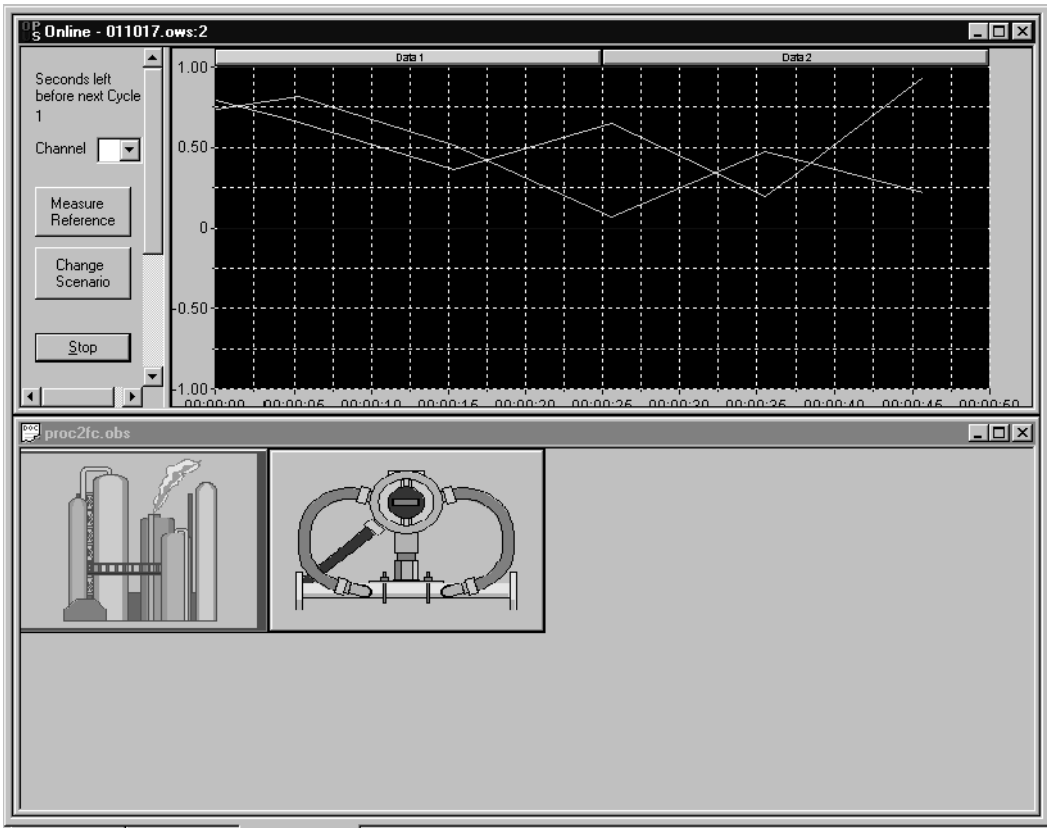


Figure 21: Process Control - Form Control View

The advantage of the form control view is to have plant facilities displayed. The assignment of images and bands is in both directions. If a band alarm level is reached, it will be indicated by the corresponding red flashing probe image.

If you click on a particular bitmap, the band assigned will be zoomed in the trend chart and displayed in full scale. All the other bands will be deactivated.

5.7.3 Waterfall

In many cases only the final evaluation results of measured spectra are interesting during an online monitoring. However, if you want to visually test all spectra, select the *Waterfall* option in the *Basic Process Setup* dialog (see figure 2) graphical output. In this case the spectra recently recorded will be shown in a 3-D stacked view.

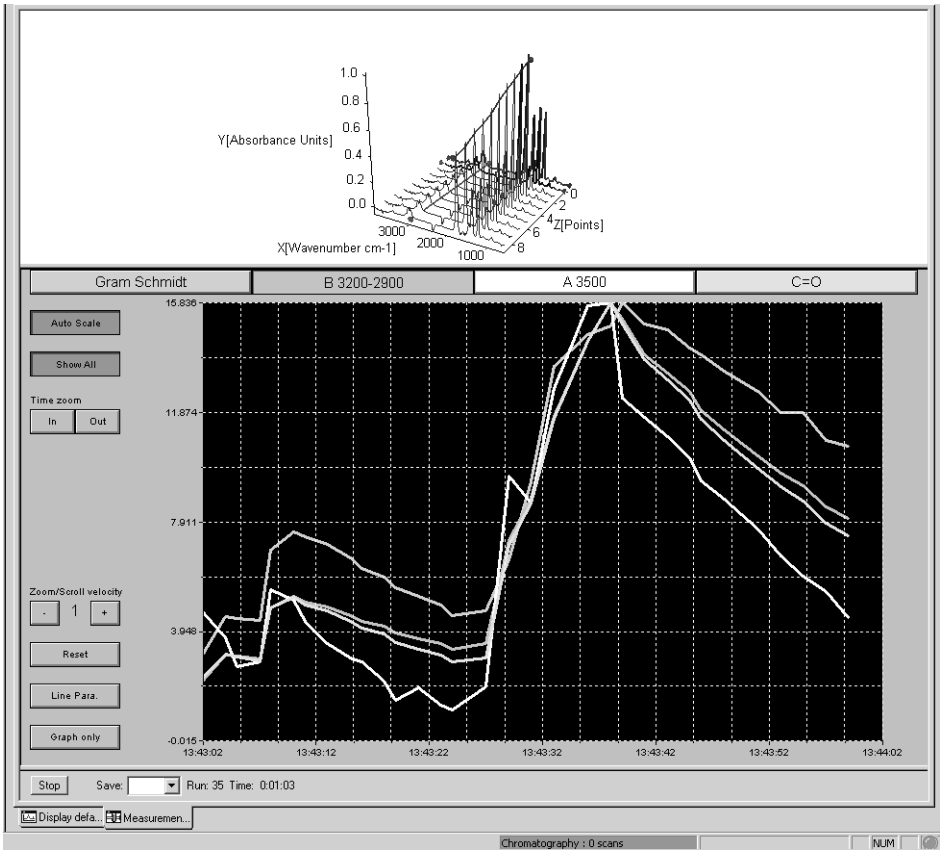


Figure 22: Process Control - Waterfall View

In the upper part a standard 3-D view is displayed. You can select all the view options, e.g. rotating, contour display, just as it is the case with a normal 3-D window. For further information on 3-D views refer to the OPUS 3D manual.

6 Setup Process Reference

This chapter describes the process setup function, including all possible dialogs and parameters. Note that only those dialogs will be displayed which are relevant for the channels and output parameters selected.

The *Back* button is used to open the settings made on previous pages. If all necessary information has been entered, click on the *Finish* button to generate the scenario script which will be saved on the hard disk. The new scenario will be immediately available for process control.

The process setup can be aborted at any time. If you click on the *Cancel* button, no scenario file will be saved.

6.1 Instrument Status

You do not have to manually set up the instrument status as output value. The instrument status is always automatically updated and available for a process control system.

The OPUS system diagnosis periodically checks the instrument status. It monitors the state of the source, laser, electronics and interferometer scanner. The results are indicated in the status bar, recorded in each spectrum, and the corresponding OPC (see appendix A) value is updated.

The OPUS Validation Program (OVP) allows an automated spectrometer validation by means of the PQ (Performance Qualification[1]) and OQ (Operational Qualification[2]) test. For further details refer to the OPUS Reference Manual.

A daily scheduled instrument test can be started by an external control system or the OPC time server.

Each diagnostic test component (e.g. source) can have the following status: OK, WARNING (i.e. maintenance required as life time has expired) or ERROR (see appendix B). All these test results are indicated by the spectrometer and read out as a special signal. The process control system can request even more detailed information, e.g. which component has caused the problem. For further details on the instrument test procedure refer to the OPUS Reference Manual.

1. For daily routine work
2. After installation and maintenance

6.2 Basic Process Setup

In the *Basic Process Setup* dialog you define the number of channels, path and file name of the resulting scenario stored and set display options.

The *Basic Process Setup* dialog consists of a scenario browser window (A in figure 23) and a dialog area (B) which correlate with each other. By default, if no scenario has yet been defined, three scenario levels are displayed in the scenario browser which can be run through by the *Next* button.

- Scenario*.obs
- Company
- Spectrometer

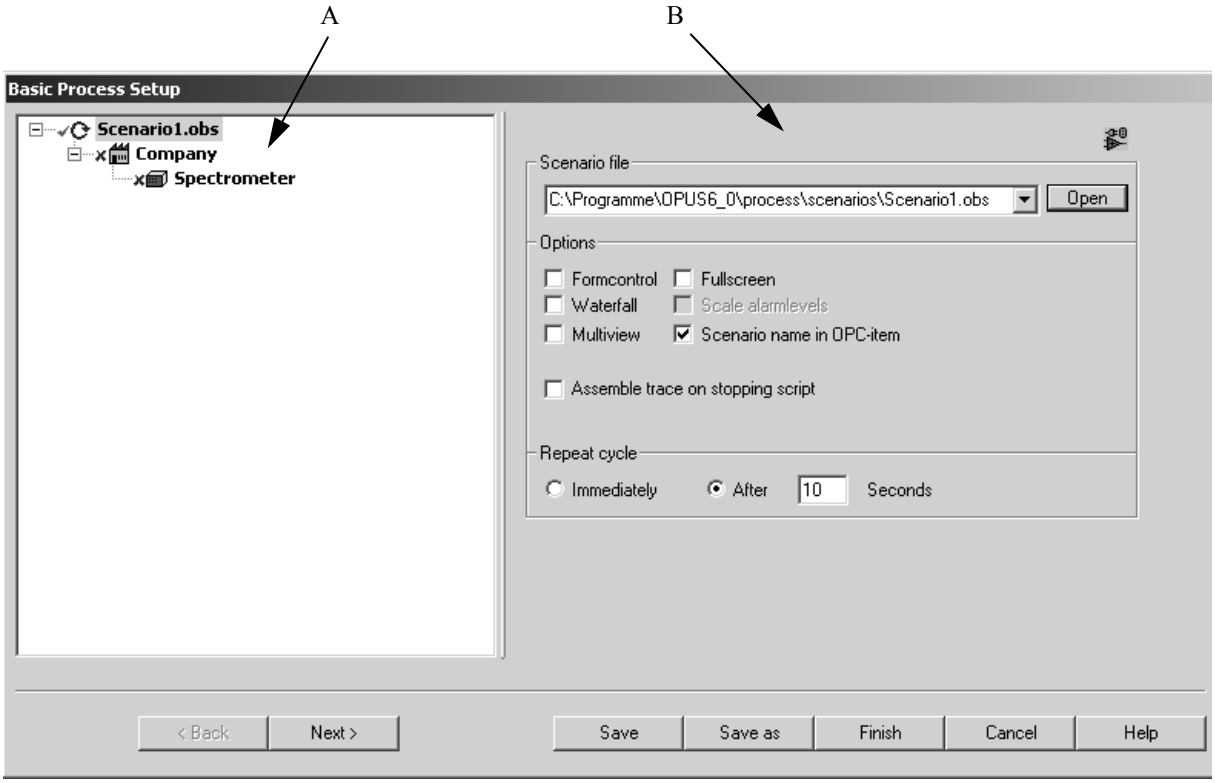


Figure 23: Basic Process Setup

To get access to the different scenario settings options right click on the particular scenario level and select the appropriate command from the pop-up menu.

Note: If you position the cursor on any scenario level a tool tip pops up in the form of a balloon. The tool tip explains how to get access to the different scenario setting options.

The red cross in front of the scenario level indicates that the values of this particular level are still invalid or incomplete. As soon as you run through the scenario levels by the *Next* button the red cross will turn into a green check mark. The following scenario level status can be indicated:

- **Red cross:** data inconsistent or incomplete; specific items have still to be defined
- **Green check mark:** data consistent and approved

  Note: Before you can execute a scenario you have to make sure that all scenario levels are approved by a green check mark and include at least 1 measuring point and 1 data channel. Otherwise, the scenario cannot be executed.
- **Orange exclamation mark:** correct values for data channel available which, however, may not make sense in this particular context. This can be the case if you e.g. copy previous data channels and allocate them to a different measuring point. In this case check the contents of the scenario level for its validity and make modifications, if required.

Scenario files always get the default name *Scenario*,* are stored as VBScripts and have the extension **.obs.* The file name is automatically incremented by the software. To change the file name, click into the *Scenario File* drop-down list (see figure 23), modify the name and store this scenario by clicking on the *Save* button. The drop-down list includes the scenarios recently used. Clicking on the *Open* button allows to load already existing scenarios.

When creating the scenario setup you can also copy particular components. Right click on the particular scenario component below the *Spectrometer* level and select the *Copy* command from the pop-up menu. All parameters and settings of the element selected will be read and used for the current setup.

By default, the *OPUS\Process\Scenarios* path is displayed. If you click on the *Save as* button, you can change the scenario file path from the dialog that pops up. In principle, the scenarios can be stored in any path, however, it is recommended to either use the OPUS directory or a well-defined sub-directory for all the scenarios.

Note: Do **not** use the <*OPUS Path*>*Process* path to store scenarios, as this path is reserved for log files.

Options

- **Form control**

If you activate the *Form Control* check box, an additional process view will be available. Apart from the usual *Trend* view the *Form Control* view enables a graphical depiction of the plant or the process (see figure 21).

Note: Graphical process presentations have to be set up manually.

- **Waterfall**

If you activate the *Waterfall* check box, an additional process view will be available. Apart from the usual *Trend* view the *Waterfall* view shows a 3-D display including the spectra of the last measurements (see figure 22).

- **Multiview**

If you activate the *MultiView* check box, an additional process view will be available. Apart from the usual *Trend* view the *Multiview* displays three additional views including the real-time data as text, bar and meter (see figure 20).

- **Full screen**

If you activate the *Full Screen* check box, an additional process view will be available in which all the normal OPUS menus and toolbars are deactivated. This is an easy way to remove all functions not required or not allowed during a process control run.

- **Scale alarm levels**

Not yet available.

- **Scenario name in OPC item**

If yo activate this check box, the names of the measurement channels are grouped below the respective scenario name on the OPC server. The scenario name is written above the default OPC items (see also chapter 2.14.2). This avoids possible problems caused by measurement channels which have the same name, as the channels are not displayed separately but always assigned to the respective scenario.

- **Assemble traces on stopping script**

If you activate this check box, traces are automatically assembled and saved when a script has been stopped.

Traces file path: *OPUS\PROCESS\Script name*
Traces file name: *assemble.x*; whereas *x = 0,...n*

Repeat Cycle

If you select the *Immediately* option button, a new measurement cycle will be started immediately as soon as the current measurement cycle has been finished.

If you select the *After* option button, a new measurement cycle will be delayed by *n* seconds as soon as the current measurement has been finished. Enter the number of seconds into the *Seconds* entry field to set the correct waiting time.

6.2.1 Company

Select the *Company* level either by the *Next* button or by clicking on the respective level in the scenario browser. The following dialog opens:

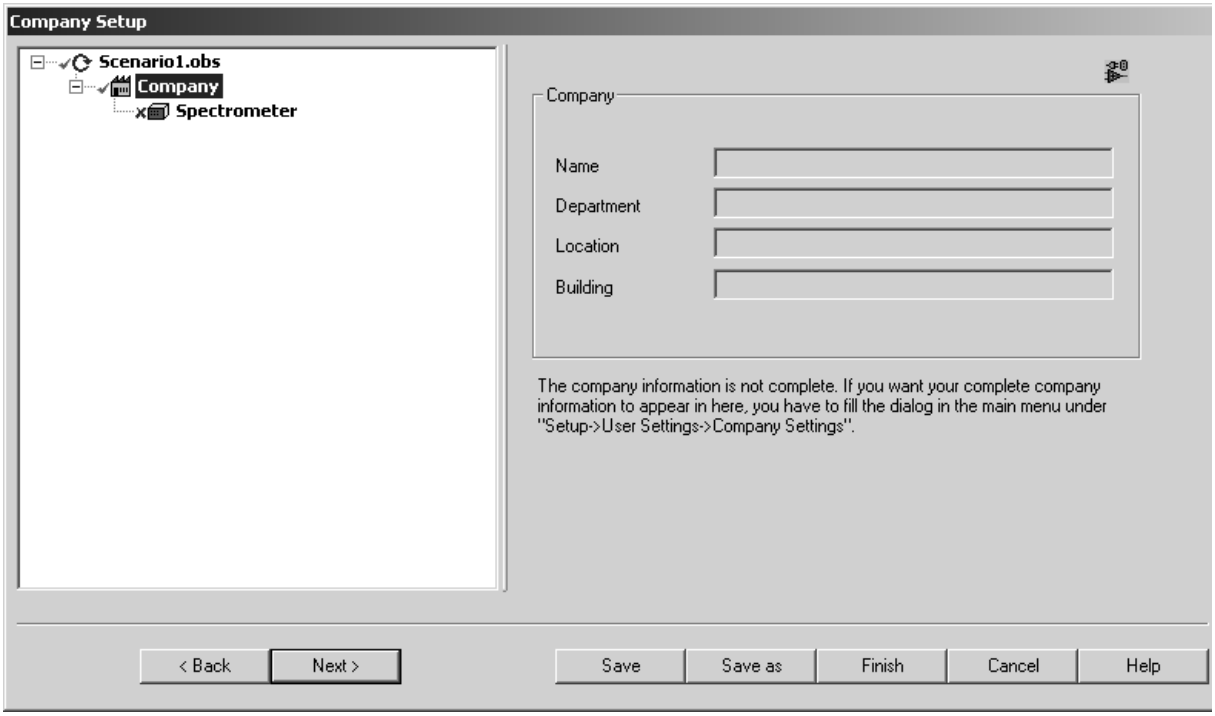


Figure 24: Company Setup

The company data in this dialog correlate with the entries made in the *User Settings* command from the *Setup* menu, i.e. the information given in the *User Settings* command will automatically be entered in the *Company Setup* dialog.

6.2.2 Spectrometer

Select the *Spectrometer* level either by the *Next* button or by clicking on the respective level in the scenario browser. The following dialog opens:

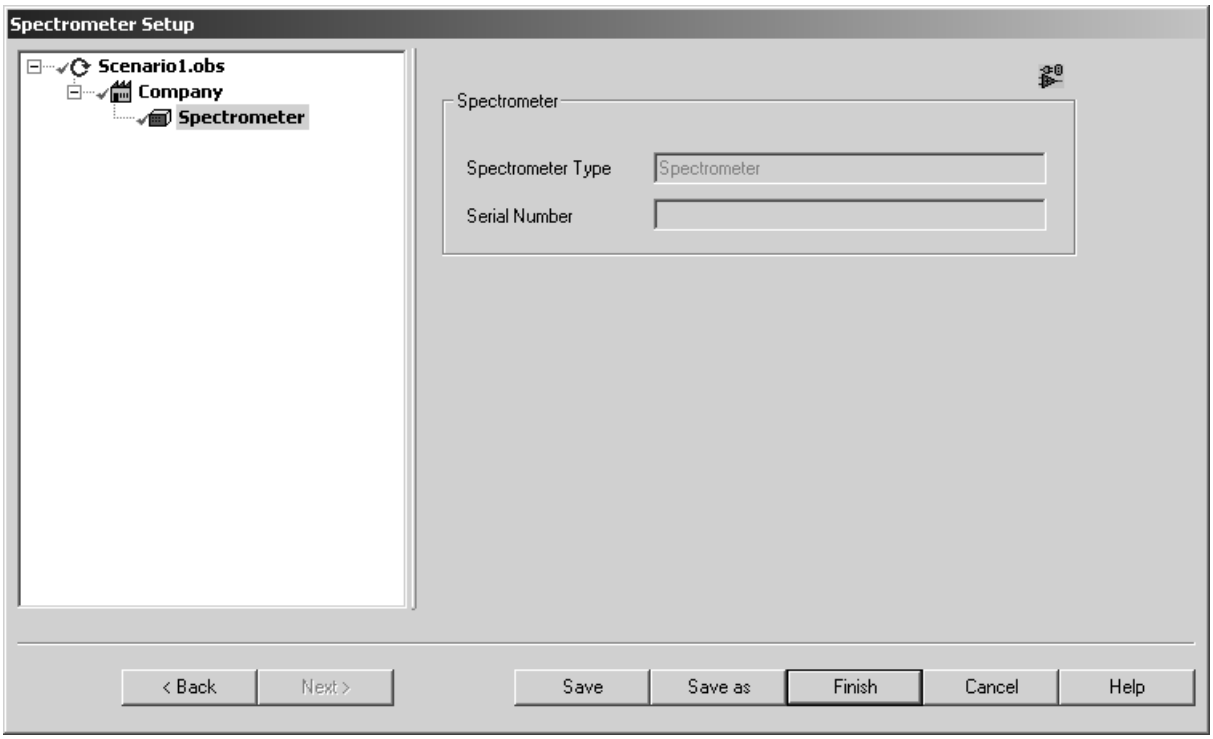


Figure 25: Spectrometer Setup

The entry fields are not editable in case of the latest spectrometer series e.g. MATRIX, i.e. the required data are automatically entered by the OPUS software. In case of former spectrometer series like VECTOR the entry fields can be filled in manually.

6.3 Measuring Point Setup

For each data channel to be measured you have to define a measuring point. Up to 128 measuring points can be defined. To create a measuring point select the *Spectrometer* level and open the corresponding pop-up menu by a right mouse click.

If you define several different measuring points, they will automatically be incremented by OPUS. If you copy a particular measuring point, all data channels, calculations etc. assigned to this measuring point will be copied as well.

Note: Make sure that all measuring points and data channels have a unique name when copying them. Otherwise, an error message will be displayed.

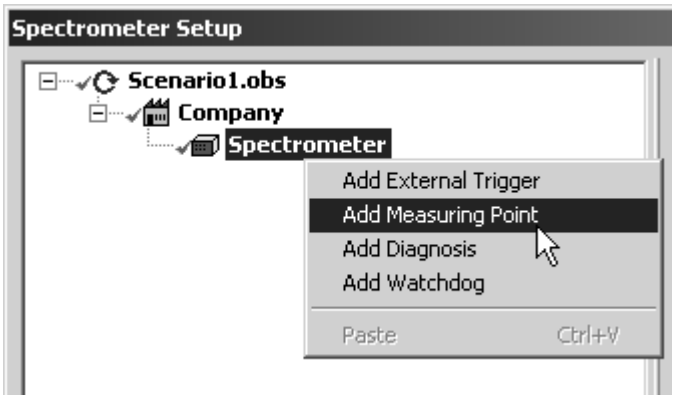


Figure 26: Pop-up menu on *Spectrometer* level

Click on the *Add Measuring Point* command. The *New Measuring Point* sub-level is displayed in the scenario browser.

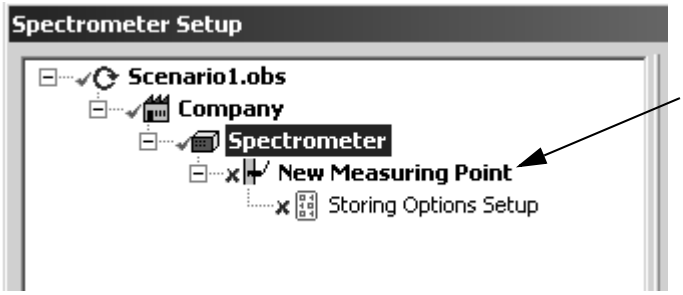


Figure 27: *New Measuring Point* sub-level in the browser

Clicking on the *New Measuring Point* sub-level opens the following dialog:

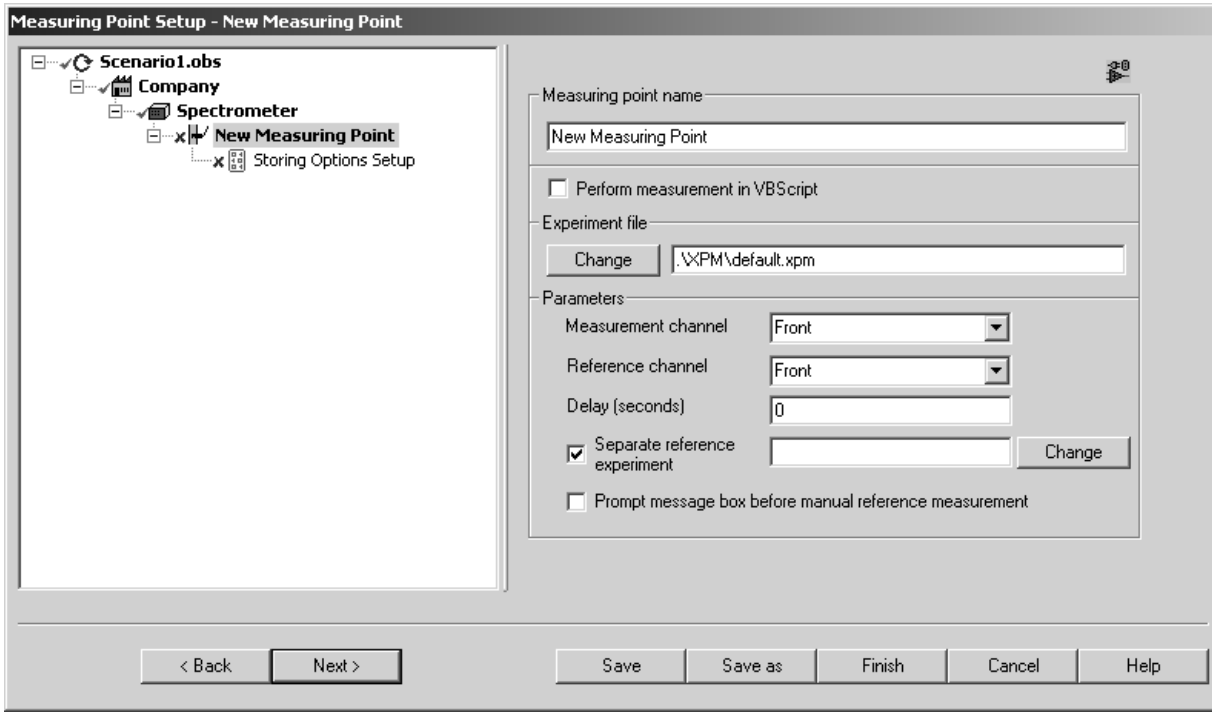


Figure 28: Measuring Point Setup - New Measuring Point

The name of the measuring point is pre-defined by OPUS. To change this name click into the *Measuring Point Name* entry field.

Activating the *Perform measurement in VB Script* check box performs measurements by using a Visual Basic Script. In this case you have to enter an appropriate file name as well as the correct parameters. The results of a script measurement must have the same format as for any other kind of measurement.

All parameters required for the cyclic measurements are stored in an measurement experiment file which has to be pre-defined in OPUS using the corresponding measurement function.

This, however, does not apply to the measurement channel nor to the delay before a measurement, which substantially simplifies the setup. Compared to the remaining manual in this case *Channel* means a physical measurement channel of the instrument and no logic data channel.

If you have to change between different resolutions, define two similar scenarios with two measurement experiment files which differ only in resolution. In the next dialog you can specify the storage mode regardless of the experiment file you use.

Enter the name of the measurement experiment file into the entry field or click on the *Change* button to select an appropriate file name from the dialog that opens. The measurement experiment file with the extension **.XPM* defines the measurement parameter for the current channel.

In general, you can store the files in any path, however, it is recommended to store the files in the OPUS PROCESS path. Make sure that an appropriate reference or background spectrum is available for each channel.

6.3.1 Parameters

- **Measurement Channel**

The *Measurement Channel* drop-down list includes all channels defined for the spectrometer used. Make sure that you select the correct channel for the measurement that will be evaluated afterwards.

- **Reference Channel**

The *Reference Channel* drop-down list includes all channels defined for the spectrometer used. Select the appropriate reference channel from the drop-down list.

This channel is used for background measurements and may be different from the one of the current measurements, e.g., if the reference spectra has been measured in a bypass.

- **Delay (Seconds)**

Add a delay between the end of the last measurement and the start of the new measurement for the particular channel. The delay can be entered in seconds.

- **Separate reference experiment**

If you activate this check box, an entry field will be displayed which can be used to manually enter the name of the reference experiment file. To select the appropriate reference experiment from a certain directory click on the *Change* button. The reference experiment will be used when performing reference (background) measurements.

- **Prompt message box before manual reference measurement**

Activate this check box if you want a message box to pop up after clicking on the *Measure Reference* button, see chapter 5.1.3, and thus initiating a manual reference measurement. Note that an activated check box will have no effect on reference measurements which have been initiated, e.g. by an external signal. In this case no message box will pop up.

6.3.2 Raman Measurements

OPUS PROCESS can also be used in connection with Raman measurements. In case of Raman measurements no reference spectrum is required. Therefore, the reference channel options in the *New Measuring Point* dialog will be disabled.

6.4 Storing Options Setup

OPUS PROCESS offers several storing options for the result file. The *Storing Options Setup* level is automatically displayed in the scenario browser if you define a measuring point or a data channel.

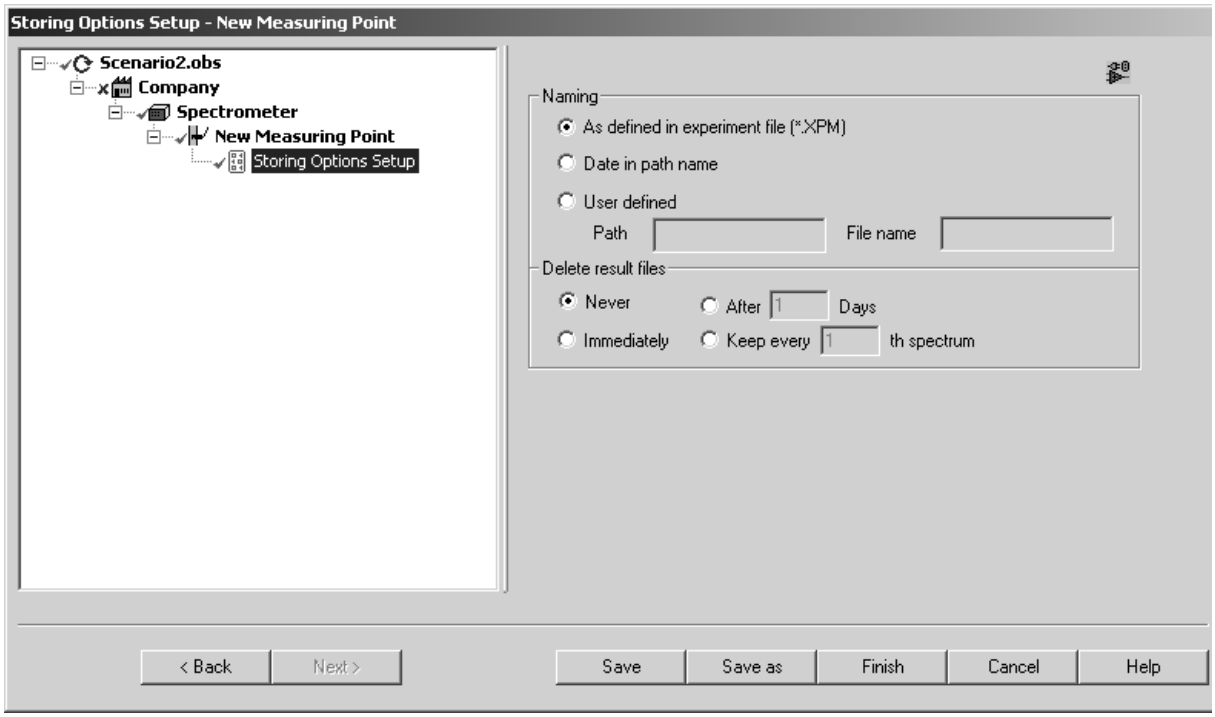


Figure 29: New Measuring Point

The *As defined in experiment file* option (see figure 29) uses the settings selected in the OPUS measurement experiment file. In this case the file name will automatically be incremented during measurement. It is recommended to store the data in a common directory or separate path which is defined by the current date, e.g. YYYYMMDDHHHH (year/month/day/hour).

Besides, there are several possibilities to define the storage path and automatically incorporate the sample name date or other measurement parameters.

If the amount of data from the current process run is very large, you can delete the spectra after the evaluation.

6.4.1 Naming

- **As defined in experiment file**

If you activate the *As defined in experiment file* option button, the name of the result files corresponds to the one defined for the measurement experiment file. In general, it will be a fixed name incremented either in the file name or the extension (according to the OPUS setup).

- **Date in path name**

The files measured are named according to the current date by using the following form: DD_MM_YY.0. The file extension will be incremented, and the current path and file name generated will be as follows:

<OPUS Program Path>\Process\<Scenario Name>\<DD_MM_YY>.0

- **User Defined**

Activate the *User Defined* option button if you want to specify an individual name and directory to store the spectra. Use the respective entry fields to configure the path and file name. The text may include fixed and/or variable parts.

Example: *<SNM>* if the sample name is to be used as file name or *<6SNM>* if the first 6 characters of the sample name are to be used as file name.

The date or certain measurement parameters are entered as special meta tags as defined by the measurement function (for details see the OPUS Reference Manual, chapter 7). Result files will not be overwritten, the file name or extension will be incremented instead.

6.4.2 Delete Result Files

The options available can be used to determine which spectral files have to be saved and when they have to be deleted.

- **Never**

If you activate the *Never* option button, all result spectra will be stored in the path defined. This may require huge amounts of disk space to store the data. To select *Never* may be useful during the early program phase if you acquire spectra for a QUANT calibration or IDENT library, or if you need the data for a subsequent analysis.

- **Immediately**

If you activate the *Immediately* option button, the recorded spectra will be deleted as soon as all components of the particular measurement have been evaluated. This would be the normal operation in a routine environment.

- **After x Days**

To define after how many days the result files will be deleted activate the *After* option button and enter the appropriate number of days into the entry field.

- **Keep every x th Spectrum**

If you activate the *Keep every...* option button, the result files are automatically deleted except for those files definitely entered, e.g. *5*, which means that every 5^{th} spectrum will be stored.

6.5 Data Channel Setup

Data channels are always assigned to a particular measuring point. For each channel to be measured you have to define what kind of data will be acquired and how you want to have the results presented. Each channel is uniquely identified by its specific number, i.e. if you define several different channels, they will automatically be incremented by OPUS.

You define the number of variables to be monitored. This is equivalent to the number of bands displayed in the real-time display. It may be the number of components or the number of probes/flow cells or a combination of both. For each evaluation of a measurement in a cycle you add one channel. This means that you have to define all the necessary measurement parameters for all channels.

To create a data channel select the *New Measuring Point* level and open the corresponding pop-up menu by a right mouse click.

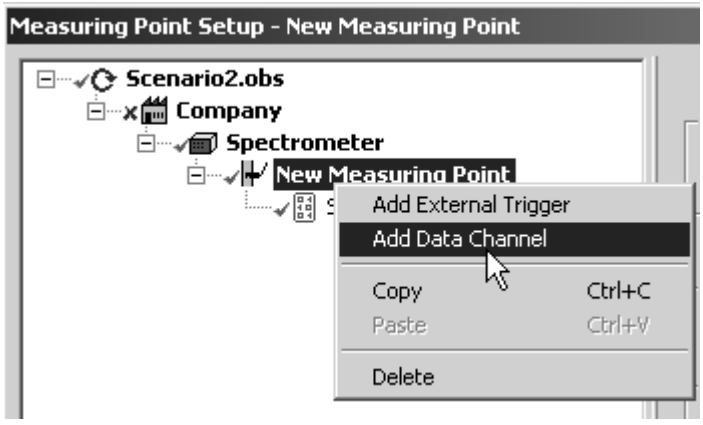


Figure 30: Pop-up menu on *New Measuring Point* level

Click on the *Add Data Channel* command. The *New Data Channel* sub-level is displayed in the scenario browser.

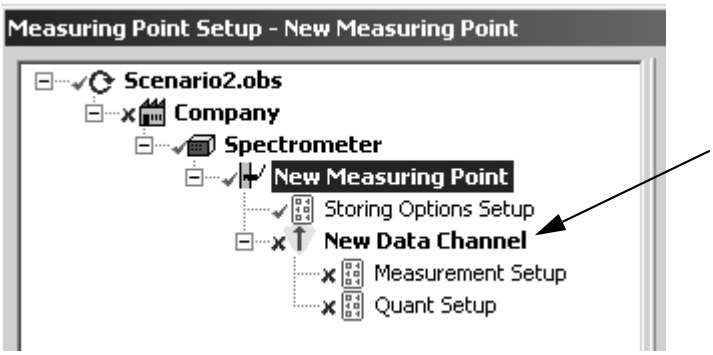


Figure 31: *New Data Channel* sub-level in the browser

Clicking on the *New Data Channel* level opens the following dialog:

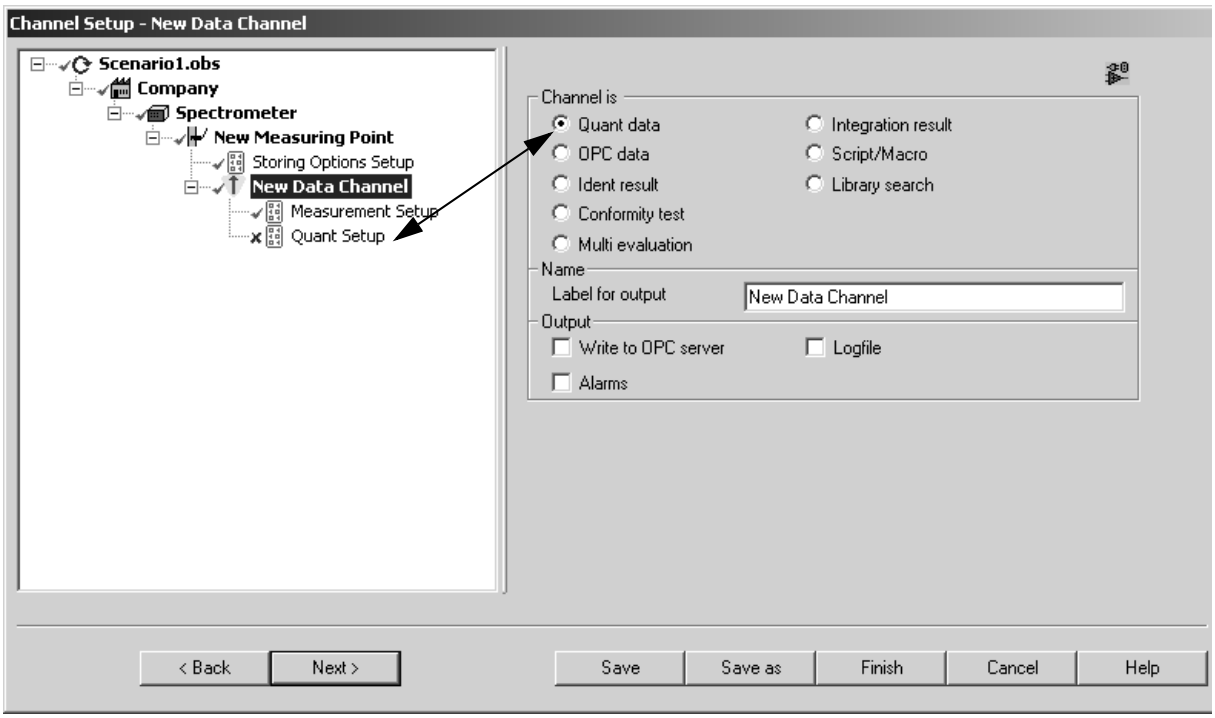


Figure 32: Process Setup - Channel Setup

A data channel can be:

- Measurement with evaluation
- Script or macro
- Data from other OPC servers

Depending on the channel type selected the corresponding sub-level will be displayed in the scenario browser (see arrows in figure 32). Click on this sub-level to be able to define the appropriate evaluation parameters.

In any case the data output will be performed by the OPUS OPC server. This is done automatically, i.e. you do not have to enter any configuration parameters.

The results can be

- written as log files or
- transferred to an OPC server.

Furthermore, alarm levels can be defined for each channel and a signal can be triggered as soon as these values are exceeded.

6.5.1 Channel type

- **QUANT Data**

The *QUANT Data* option button is activated by default. A quantitative analysis on the spectra measured will be performed by using the QUANT software package. Both QUANT 1 and QUANT 2 evaluations are possible. To define the measurement parameters and the method file click on the *Quant Setup* sub-level.

- **OPC Data**

To read and display data from a different OPC server activate the *OPC Data* option button. The content depends on the server type and may, e.g., originate from an external temperature control or pH-meter. To define the parameters click on the *OPC Setup* sub-level.

- **IDENT Result**

If you activate the *IDENT result* option button, a qualitative analysis will be performed on the spectra measured by using the IDENT software package. Select the method file after you have defined the measurement parameters. Activate the *IDENT result* option button even if you first perform an IDENT and subsequently a QUANT analysis. Later, you have to define whether the IDENT result has to be quantified as well. To define the measurement parameters and method file click on the *Identification Setup* sub-level.

- **Conformity Test**

To compare the spectra measured to a reference by using the conformity test you have to activate the *Conformity Test* option button. Click on the *Conformity Test Setup* sub-level to define the measurement parameters and conformity test method file.

- **Multi Evaluation**

If you activate the *Multi Evaluation* option button, NIR spectra will automatically be evaluated for qualitative or quantitative analysis. The *Multi Evaluation* function combines IDENT, QUANT and conformity test methods with the results being displayed in one single report. To define the measurement parameters and method file click on the *Multi Evaluation Setup* sub-level.

- **Integration Result**

To analyze certain pre-defined bands in the spectra measured by using integration activate the *Integration result* option button. Click on the *Integration Setup* sub-level to define the integration method file.

- **Script/Macro**

The *Script/Macro* option button enables user-defined analyses whose result will be calculated by a user-defined script or macro. Make sure that the script has been created before you start the process setup. To load the script click on the *Script/Macro Setup* sub-level.

- **Library Search**

If you activate the *Library Search* option button, the spectra measured will be compared to a reference library. To define the measurement parameters and library click on the *Search Setup* sub-level.

6.5.2 Name

- **Label for output**

The text entered into the *Label for output* entry field identifies the particular channel name. This channel name will be displayed as a label in the real-time views and be used as item name in the OPC server. By default, the *New Data Channel* label name is displayed. Click into the entry field to change this label name.

6.5.3 Output

- **Write to OPC Server**

Activate the *Write to OPC Server* check box if the channel values have to be sent to a different OPC server.

- **Alarms**

Activate the *Alarms* check box if you want to define alarm levels for the particular channel. You can enter high and low alarm limits as well as OPC items to be triggered as soon as the levels are reached.

> **Note:** Make sure that all OPC output channels are uniquely assigned to the measurement results. In case of I/O cards you have to use different data registers for each analysis values of a QUANT analysis.

- **Log File**

Activate the *Log File* check box if you want to store the analysis results of this channel into a text log file. Define the additional details to store the data in the dialog that opens.

6.6 Measurement Setup

The *Measurement Setup* sub-level is automatically displayed in the scenario browser if you define a new data channel. By default, the *As defined in measuring point* check box (figure 33) in the *Measurement Setup* dialog is activated. This allows to apply storing options of a particular measuring point for several different data channels. All the other options in the dialog are disabled.

If you deactivate the check box, the *Storing Options Setup* sub-level below the *New Data Channel* level appears. Clicking on this level opens the *Storing Options Setup* dialog and allows further individual storing settings. For details on this dialog refer to chapter 6.4.

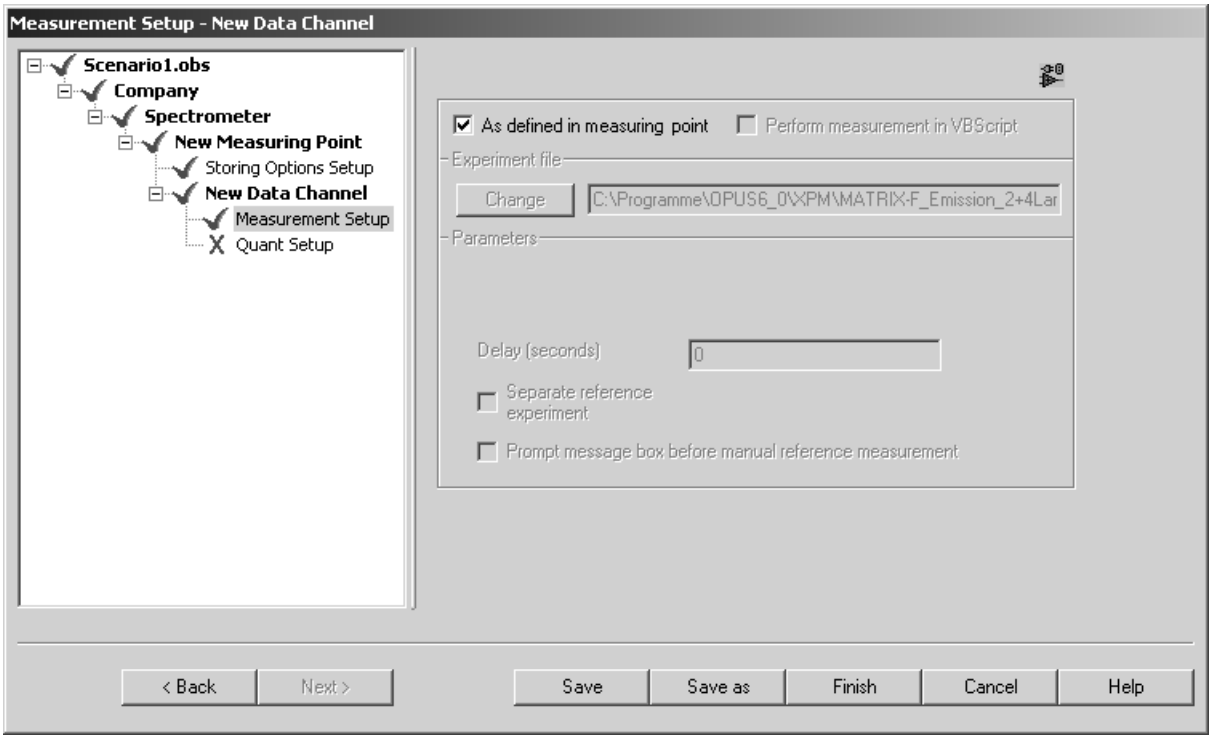


Figure 33: Measurement Setup

6.7 QUANT Setup

The QUANT (quantitative) analysis determines component concentration values or other continuous physical parameters of measured materials generated from their infrared spectra.

In case of a quantitative analysis the result is normally a floating-point number which is transferred to the process control system and trend-charted.

For each measuring position you can perform more than one QUANT evaluation. The number is mainly limited by the readability of the resulting trend charts. Multi-component QUANT 2 methods as well as QUANT 1 methods can be used for analysis purposes.

Clicking on the *QUANT Setup* sub-level in the scenario browser opens the following dialog:

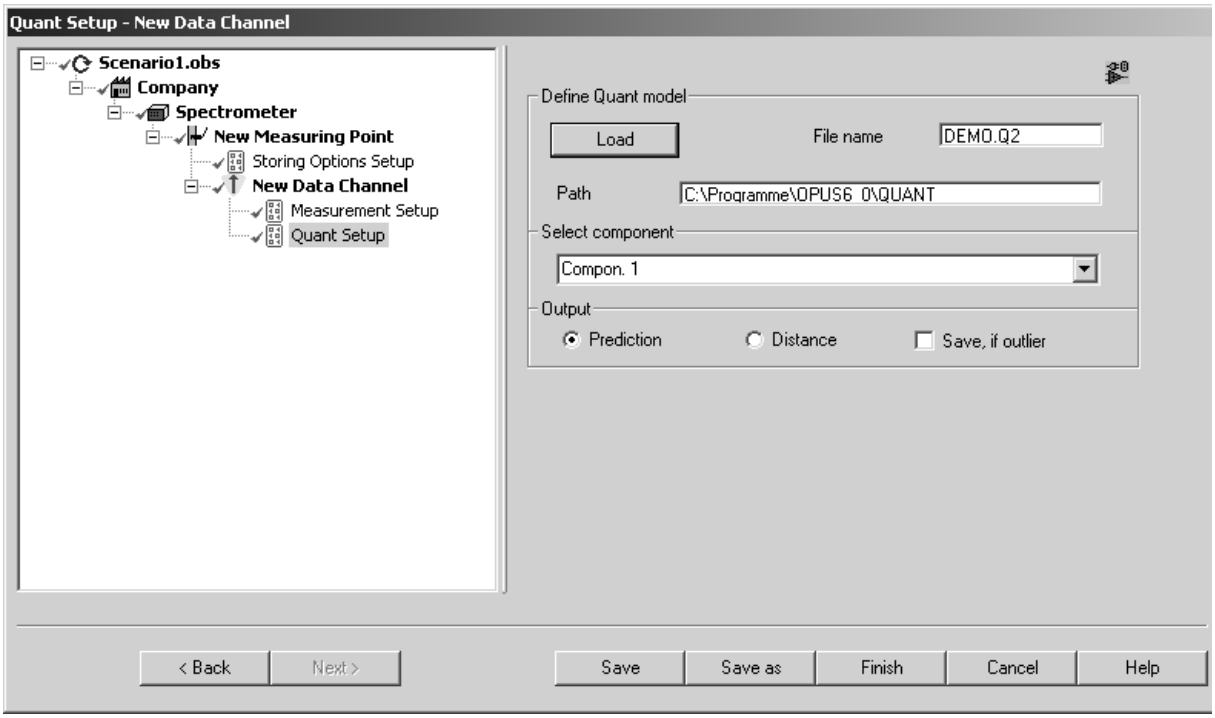


Figure 34: QUANT Setup

Enter the QUANT method file name into the *File name* entry field or click on the *Load* button to select the appropriate file from the dialog that opens. Depending on the method type selected the QUANT method file has the extension **.Q1* or **.Q2*.

You can load and use both QUANT 1 and QUANT 2 methods for quantitative analyses. They are used transparently, i.e. except for the file name you do not have to distinguish between them.

Define the path of the QUANT method. If you have selected the method file name by means of the *Load* button, the path is automatically entered into the *Path* entry field. In principle, the QUANT methods can be stored in any path, it is, however, recommended to either use the OPUS directory or a well-defined sub-directory of the process scenario path.

As soon as an existing QUANT method is loaded, the *Select component* drop-down list includes all the names of the components defined in the particular method file. Use the drop-down list to select the appropriate component.

6.7.1 Output

- **Prediction**

For quantitative analysis you mostly activate *Prediction* as output of the component value. Therefore, this option is set by default.

- **Distance**

Sometimes it is useful to monitor the Mahalanobis distance instead of (or in addition to) the actual prediction value.

- **Save, if outlier**

If the QUANT evaluation detects the spectrum to be analyzed as an outlier, you can store these spectra to perform a more detailed analysis. If you activate the *Save, if outlier* check box, these measurements will be saved in the scenario path by the name o*utlier.0*.

6.8 OPC Client Setup

OPC (OLE for Process Control) is an international standard used for process control systems to exchange data between different control systems. The *OPC Setup* is required if data from different servers are to be used by OPUS.

Various forms of data can be acquired by this mode, e.g. temperature, pH-value, which in general depends on the devices installed and on the form of data defined by the respective server.

Clicking on the *OPC Setup* sub-level in the scenario browser opens the following dialog:

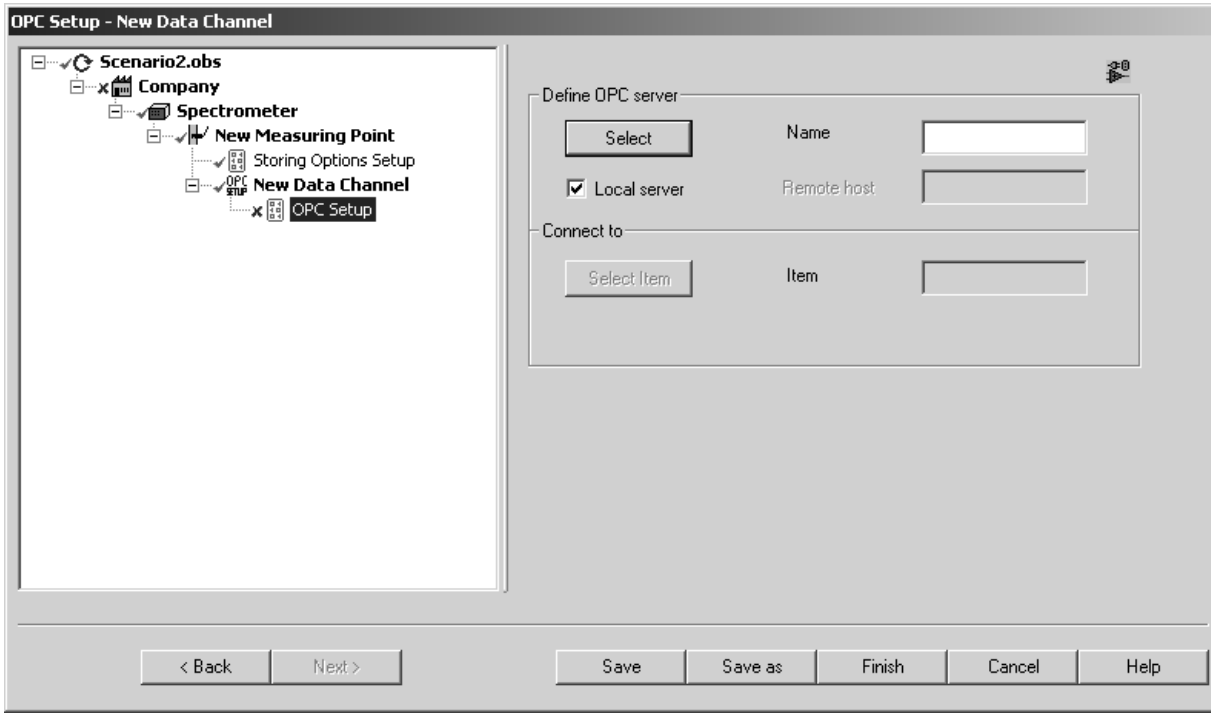


Figure 35: OPC Setup

The *Name* entry field identifies the OPC server. Each server registers itself in the system by a unique name. Click on the *Select* button to see which servers are available on your system.

Use the drop-down list from the dialog that pops up to select the appropriate OPC server. Note that OPC servers will not automatically be installed when installing OPUS, but have to be installed separately.

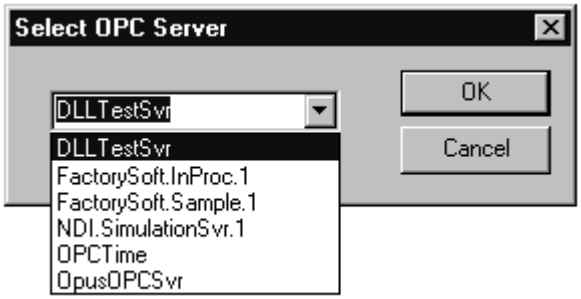


Figure 36: OPC servers available

The *Local Server* check box is activated by default. Deactivate the *Local server* check box if you want to retrieve data from a remote host. Make sure that you enter the host name of the server into the *Remote Host* entry field.

When connecting to an OPC server which is not installed on the local PC but accessible by the network, you have to enter the host name into the *Remote Host* entry field.

You enter the name to identify the item on the OPC server. Each server registers its item in the system by a unique name. If you click on the *Select Item* button, a dialog pops up including a drop-down list with the items available from the OPC server. Select one of the items which the OPC server exports.

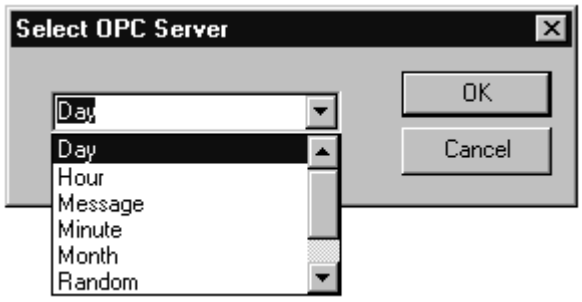


Figure 37: OPC server items

The combination of an OPC server name and an item uniquely identifies the data source.

6.9 IDENT Setup

The IDENT (qualitative) analysis compares a currently acquired spectrum of some new material to a library of spectra of known material in order to identify this new material. If the IDENT evaluation has to be used as channel, a previously created IDENT Method Library has to be available on hard disk.

If you select IDENT as channel type, each spectrum acquired is subjected to an IDENT analysis, using the specified library. The IDENT analysis compares the test spectrum with all reference spectra. The result of a comparison between spectrum *A* and *B* results in the spectral distance *D*, which is called *Hit Quality*. The better two spectra match, the smaller the spectral distance will be. For further details see the OPUS IDENT manual.

Clicking on the *Identification Setup* sub-level in the scenario browser opens the following dialog:

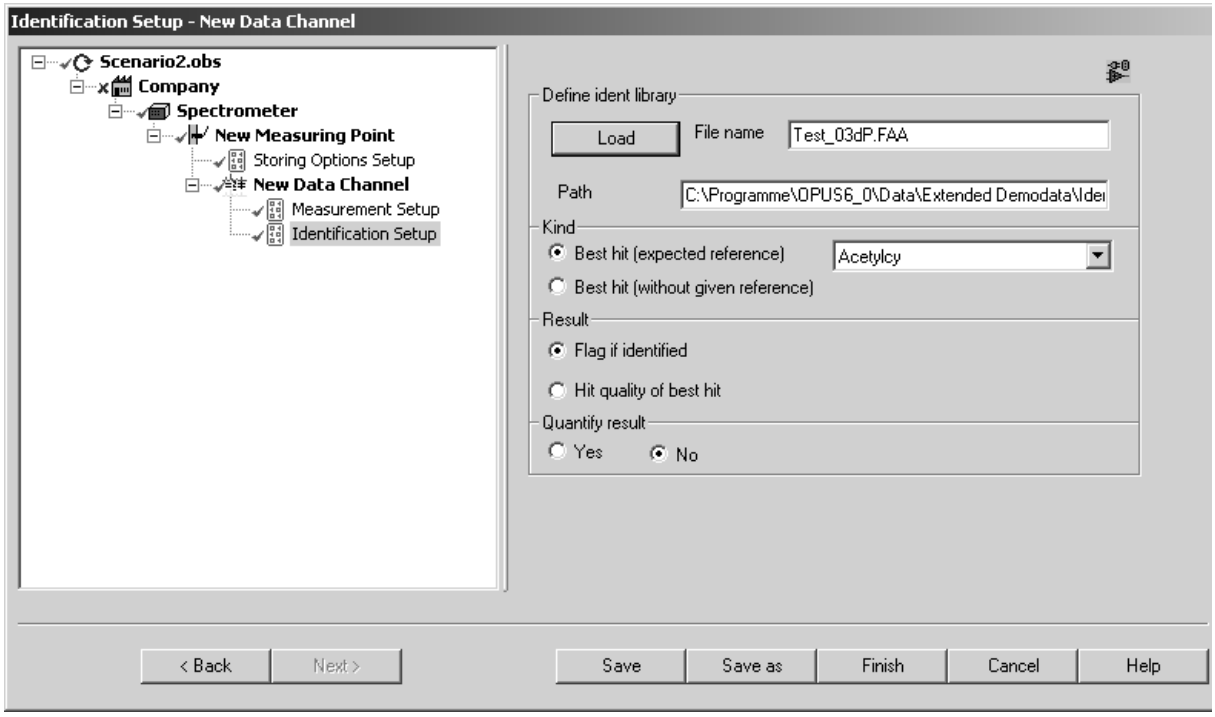


Figure 38: Identification Setup

Enter the IDENT method file name either manually into the *File name* entry field, or click on the *Load* button to select the method file from the respective directory. IDENT method files have the extension **.FAA*.

Define the path of the IDENT library. If you have selected the method file name by means of the *Load* button, the path is automatically entered into the *Path* entry field. In principle, the methods may be stored in any path, but it is recommended to either use the OPUS directory or a well-defined sub-directory of the process scenario path.

6.9.1 Kind

You can have several independent channels of IDENT results. If you select the *Best Hit (without given reference)* option button, the IDENT analysis result will not be compared to any reference.

If you select the *Best Hit (expected reference)* option button, the IDENT analysis result will be compared to an expected reference. Select the group name of the expected reference from the drop-down list.

The following output values are possible:

a) Best Hit (expected reference) and Quantify result *No:*
   1: Substance identified
   0: Substance not identified

b) Best Hit (expected reference) and Quantify result *Yes* or
   Best Hit (without given reference) and Quantify result *Yes*:
   evaluation result: if substance has been identified
   777.77: if substance has not been identified

A combined evaluation is also possible, i.e. the results of the IDENT analysis can be used to automatically select a specific QUANT analysis method. This quantification will define the final output value of the particular channel (see chapter 6.9.3).

6.9.2 Result

To mark the results which have been identified, check the *Flag if identified* option button. In this case *1* means *identified*, *0* means *not identified*. It is also possible to use the hit quality of the best hit as channel result. This is independent of the test result. The best hit is defined as the one with the smallest hit quality.

6.9.3 Quantify Result

As soon as a component has been identified by the IDENT library, it is possible to perform a quantitative analysis based on the search result. If you select the *Yes* option button, you have to supply QUANT methods for all the components that might be identified. These QUANT files need to have the same name as the search result, and have to be stored in the process scenario path.

How IDENT selects QUANT:

The program will automatically select a single QUANT method to be applied to spectra acquired on this channel, based on the result of the specified IDENT analysis. The result of the IDENT analysis serves as name for the QUANT method file.

This QUANT file name (with the extension *.Q2*) has to be available in the process scenario path. The QUANT method is selected and used to analyze the current spectrum. Only one QUANT analysis is performed in this way. Subsequently, it is important to coordinate the names of compounds identified by the selected IDENT method with the names of the QUANT files to be used to analyze these compounds. Therefore, the IDENT results also have to be unique in this case.

Example:

- The IDENT result is *MaterialA* (sample name).
- A *MaterialA.q2* file has to be available in the process scenario path.
- The *MaterialA.Q2* QUANT method is used to perform the QUANT analysis.

The *IDENT Selects QUANT* function can be very useful for automated QUANT analyses and different materials during different production runs. First, you need to have a successful IDENT library to distinguish one material from another, and second a QUANT method for each of these materials.

6.10 Conformity Test Setup

The conformity test can be used to check whether the spectrum recorded within the limits of a standard deviation is conform to the reference spectrum.

The result of this kind of evaluation is between 0 and 1. Make sure that the appropriate reference spectra are already included in the conformity test method.

Clicking on the *Conformity Test Setup* sub-level in the scenario browser opens the following dialog:

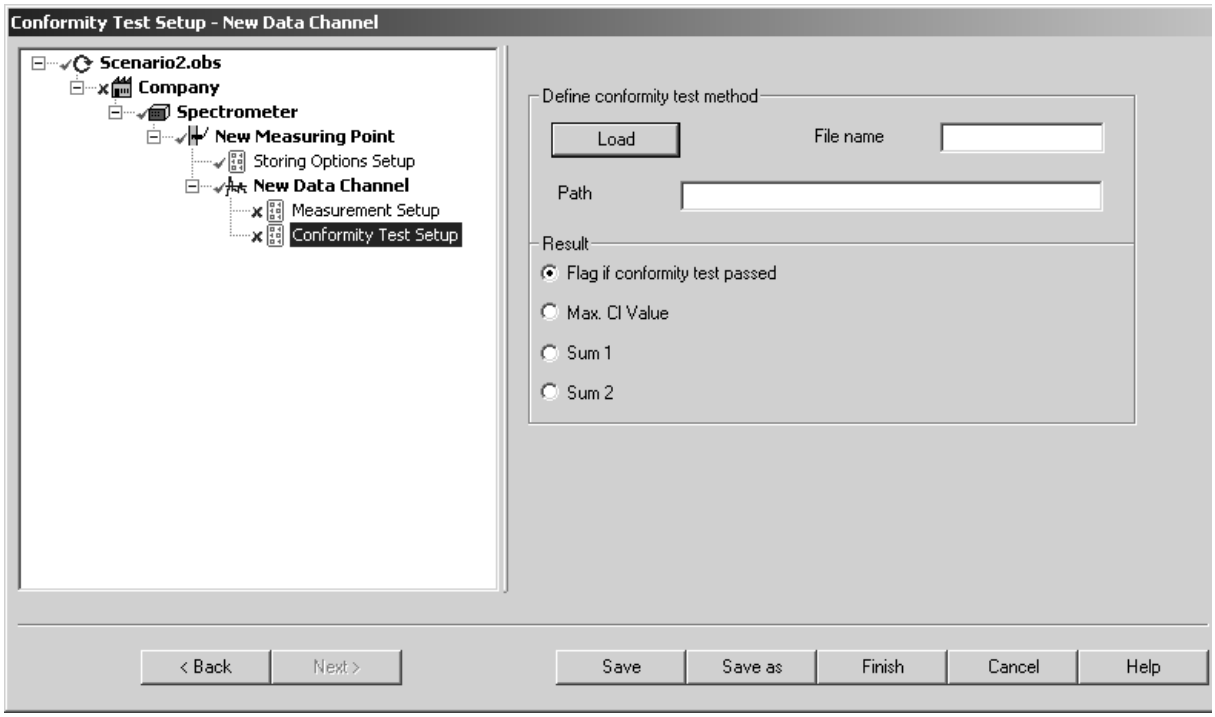


Figure 39: Conformity Test Setup

Enter the conformity test file name either manually into the *File name* entry field, or click on the *Load* button to select the conformity test file from the respective directory. Conformity test files have the extension **.CFT*.

Define the path of the conformity test method. If you have selected the conformity test method file name by means of the *Load* button, the path is automatically entered into the *Path* entry field. In principle, the conformity test method may be stored in any path but it is recommended to either use the OPUS directory or a well-defined sub-directory of the process scenario path.

6.10.1 Result

There are different possibilities for the channel result output:

- **Flag if conformity test passed**

If you activate this option button, the channel result will be identified, i.e. *1* means test has passed, *0* means test has not passed.

- **Max Cl value**

If you activate this option button, the maximum conformity index value will be displayed as channel result.

- **Sum 1**

If you activate this option button, the result will be displayed on the basis of CI > limit (/N total).

- **Sum 2**

If you activate this option button, the result will be displayed on the basis of CI > limit (/N over limit).

For detailed information on the conformity test, refer to the OPUS IDENT manual.

6.11 Multi Evaluation

In general, a multi evaluation is performed on the basis of an IDENT, QUANT and/or CONFORMITY TEST method. Make sure that all these methods used for multi evaluation are copied to the sub-directories of the multi evaluation root directory in OPUS. For further details on this subject, see the OPUS Reference Manual.

Clicking on the *Multi Evaluation Setup* sub-level in the scenario browser opens the following dialog:

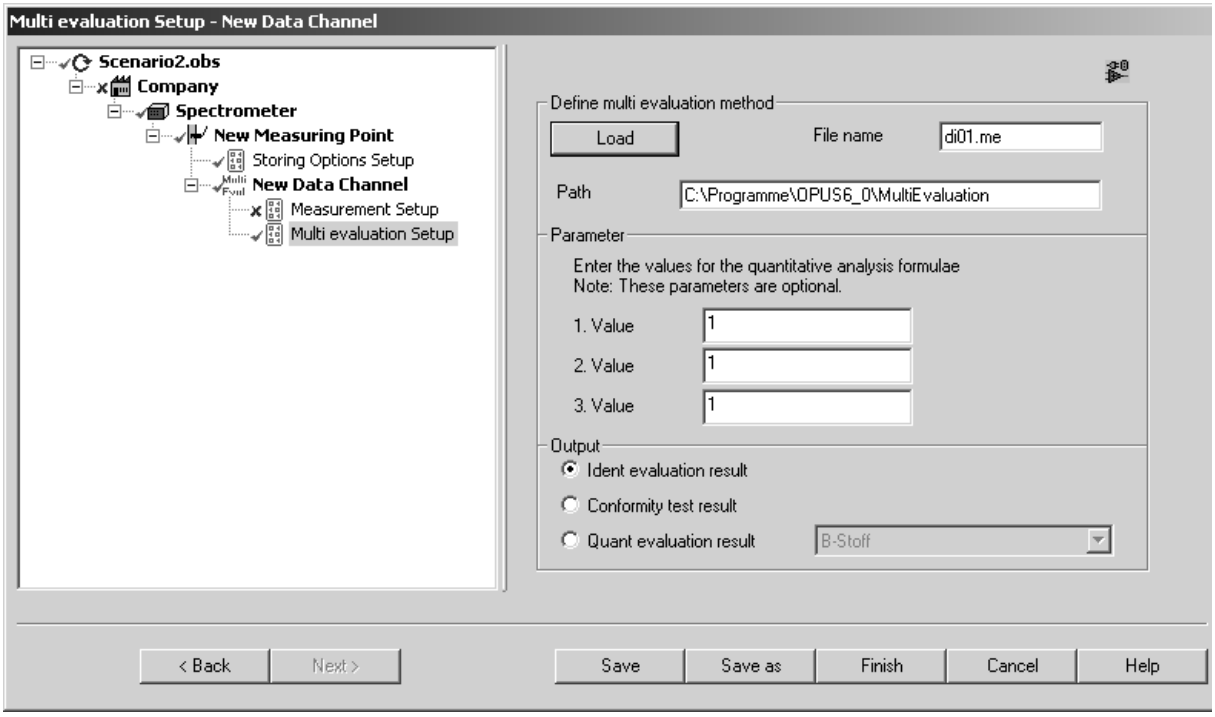


Figure 40: Multi Evaluation Setup

Enter the multi evaluation file name either manually into the *File name* entry field, or click on the *Load* button to select the multi evaluation file from the respective directory. Multi evaluation files have the extension **.ME.*

Define the path of the multi evaluation method. If you have selected the multi evaluation method file name by means of the *Load* button, the path is automatically entered into the *Path* entry field.

Enter the values (optional) of the QUANT analysis formulae which have been previously defined. For further details on this subject refer to the OPUS Reference Manual.

As the output channel always includes only one evaluation result, activate the respective option button to have the appropriate result displayed.

6.12 Integration Setup

An integration of a band area can serve as a simple quantitative analysis to determine component concentration values.

Each channel can be evaluated by using integration methods. Clicking on the *Integration Setup* sub-level in the scenario browser opens the following dialog:

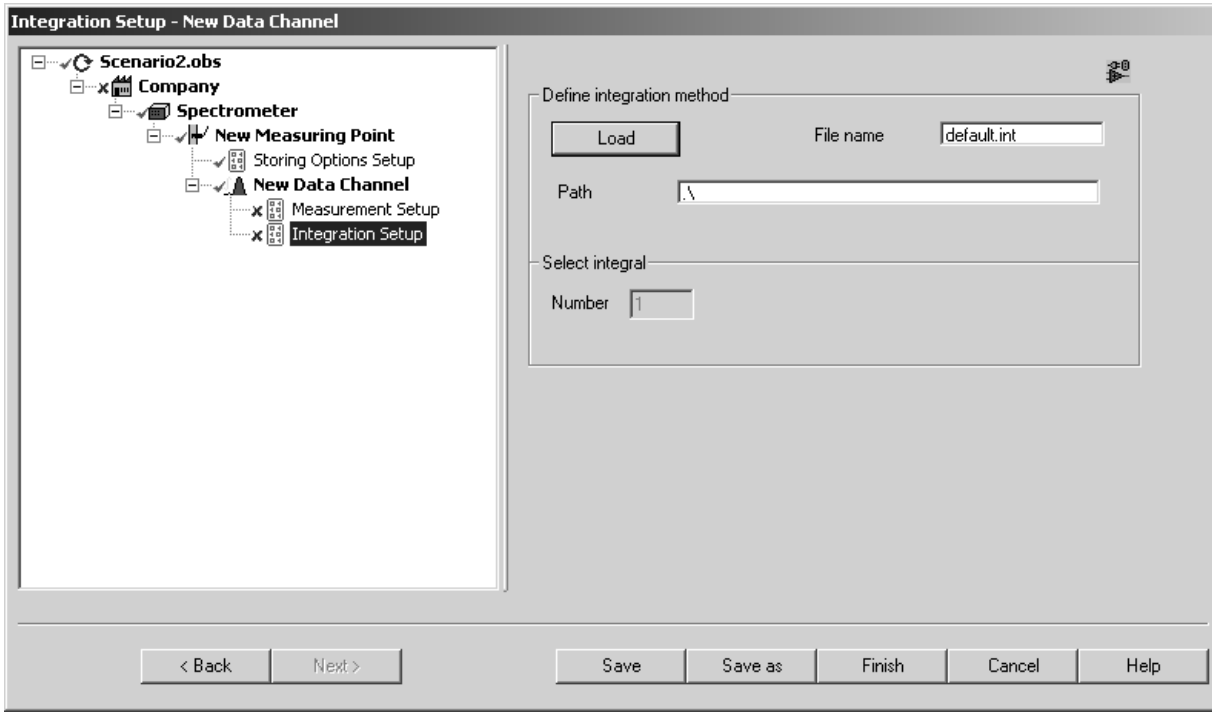


Figure 41: Integration Setup

Enter the integration method file name either manually into the *File name* entry field, or click on the *Load* button to select the method file from the respective directory. Integration method files have the extension **.int*.

Define the path of the integration method. If you have selected the method file name by means of the *Load* button, the path is automatically entered into the *Path* entry field. In principle, the methods may be stored in any path but it is recommended to either use the OPUS directory or a well-defined sub-directory of the process scenario path.

A method file can include more than one integral definition. Specify the number of the particular integral into the entry field.

6.13 Script/Macro Setup

Although many different channel types are available during the process setup, sometimes user-specific evaluations may be required.

If you use user-defined macros or scripts, a completely flexible programming language is added to OPUS PROCESS. If you specify user-defined components in the setup wizard, you can add these components by a script channel.

Clicking on the *Script/Macro Setup* sub-level in the scenario browser opens the following dialog:

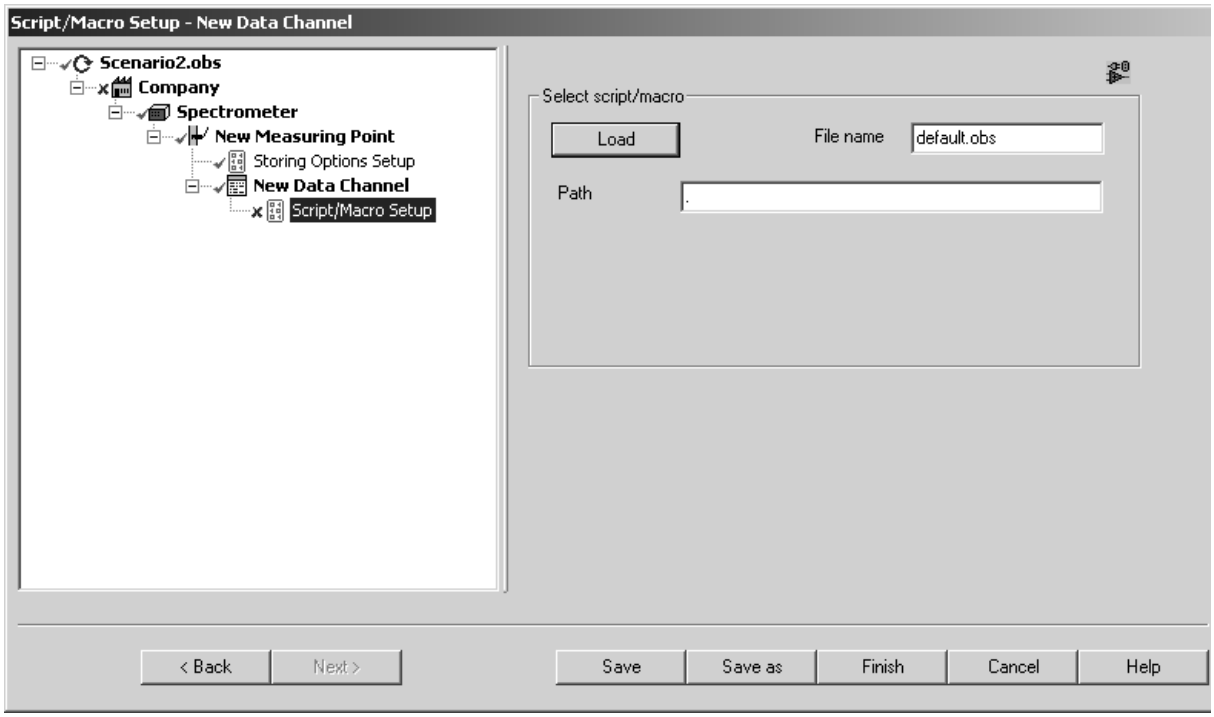


Figure 42: Script/Macro Setup

Use the OPUS script editor (for more information, refer to the OPUS Programming Manual) to generate the instructions for the calculations required. Within the script you can make measurements, send direct optic commands and perform an evaluation. The result that will become the channel data has to be returned using the *SetResult* function of the form.

A simple script, e.g., could contain the following code:

```
Randomize
Sub Form_OnOpusInform( ByVal strInfoText )
  Value = Rnd
  Form.SetResult Value
  Form.Close
End Sub
```

The calculations are made during the *OnOpusInform* event and the parameter transferred forms the number of the active channel.

Enter the script/macro file name either manually into the *File name* entry field, or click on the *Load* button to select the script/macro file from the respective directory. Script/macro files have the extension **.obs* for scripts or **.MTX* for macros.

You can load and use both macros and scripts for this channel type. They are used transparently, i.e. except for the file name you do not have to distinguish between them.

Define the script/macro path. If you have selected the script/macro file name by means of the *Load* button, the path is automatically entered into the *Path* entry field. In principle, the script/macro may be stored in any path but it is recommended to either use the OPUS directory or a well-defined sub-directory of the process scenario path.

6.14 Library Setup

An unknown substance can also be identified by a library search. The output value of the channel can either be the substance number in the library or the hit quality.

Clicking on the *Search Setup* sub-level in the scenario browser opens the following dialog:

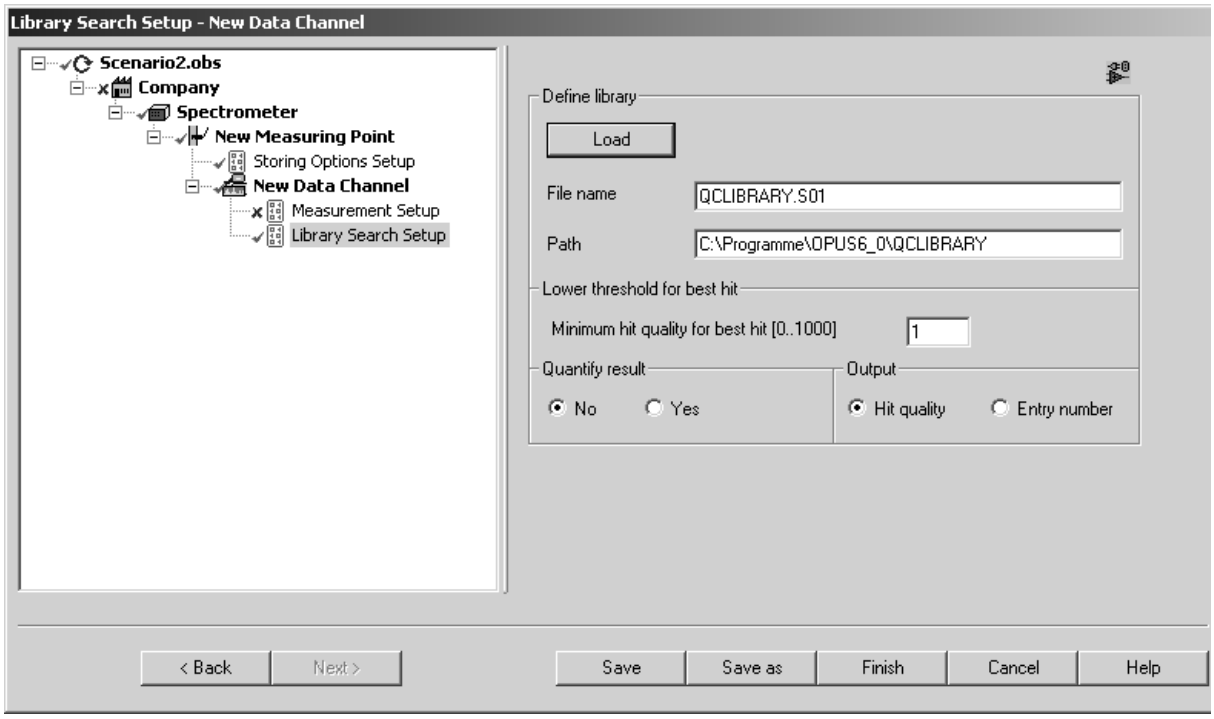


Figure 43: Search Setup

Enter the library method file name either manually into the *File name* entry field, or click on the *Load* button to select the library method file from the respective directory. Library method files have the extension **.s01*.

Define the library method path. If you have selected the library method file name by means of the *Load* button, the path is automatically entered into the *Path* entry field. In principle, the library may be stored in any path but it is recommended to either use the OPUS directory or a well-defined sub-directory of the process scenario path.

The result of a library search is a hit list. Enter the lower limit for the best hit, which can be defined between 0 and 1000 into the respective entry field.

6.14.1 Quantify Result

If you have identified a component by using the library search, it is possible to perform a quantitative analysis based on the search result. If you select the *Yes* option button you have to supply QUANT methods for all the components that might be identified. These QUANT files need to have the same name as the search result, and are loaded from the process scenario path. The *No* option button is activated by default.

6.14.2 Output

There are two possibilities to define the output value.

- **Hit Quality**

If you expect a certain hit quality to be reached, it can be used as an output value. This output value serves as some kind of semi-quantitative analysis to see how close the component comes to the optimal value.

- **Entry Number**

If you select the *Entry Number* option button, the output value corresponds to the entry number in the library. This enables the control system to determine, e.g., the type of reaction.

6.15 External Trigger Setup

A trigger is a certain kind of mechanism that initiates an action whenever an event occurs such as reaching a certain time or date or upon receiving some type of input. In general, a trigger causes a program routine to be executed.

All the scenario levels intended to use for external trigger will not be considered by the OPUS PROCESS software, i.e. an external trigger executed by an OPC server activates or deactivates the defined scenario level.

The external trigger option in OPUS PROCESS can be assigned to the following sub-levels:

- Measuring point
- Data channel
- Calculation

To set up an external trigger as a global scenario setting select the *Spectrometer* level in the browser window. If you want to set up an external trigger on one of the scenario sub-levels mentioned above, select the particular sub-level and open the corresponding pop-up menu by a right mouse click.

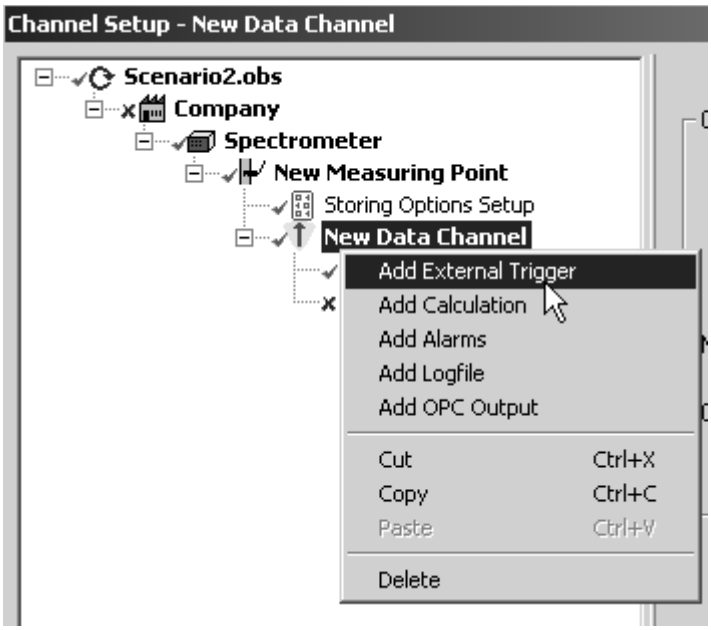


Figure 44: Pop-up menu on *New Data Channel* level

Click on the *Add External Trigger* command. The *External Trigger* sub-level is displayed in the scenario browser.

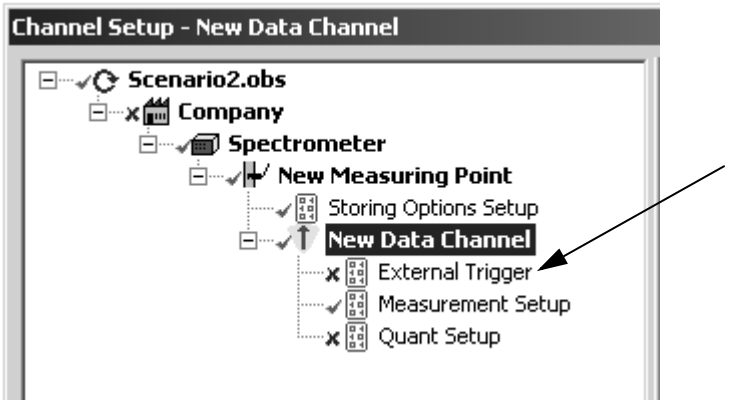


Figure 45: *External Trigger* sub-level in the browser

Clicking on the *External Trigger* sub-level opens the following dialog:

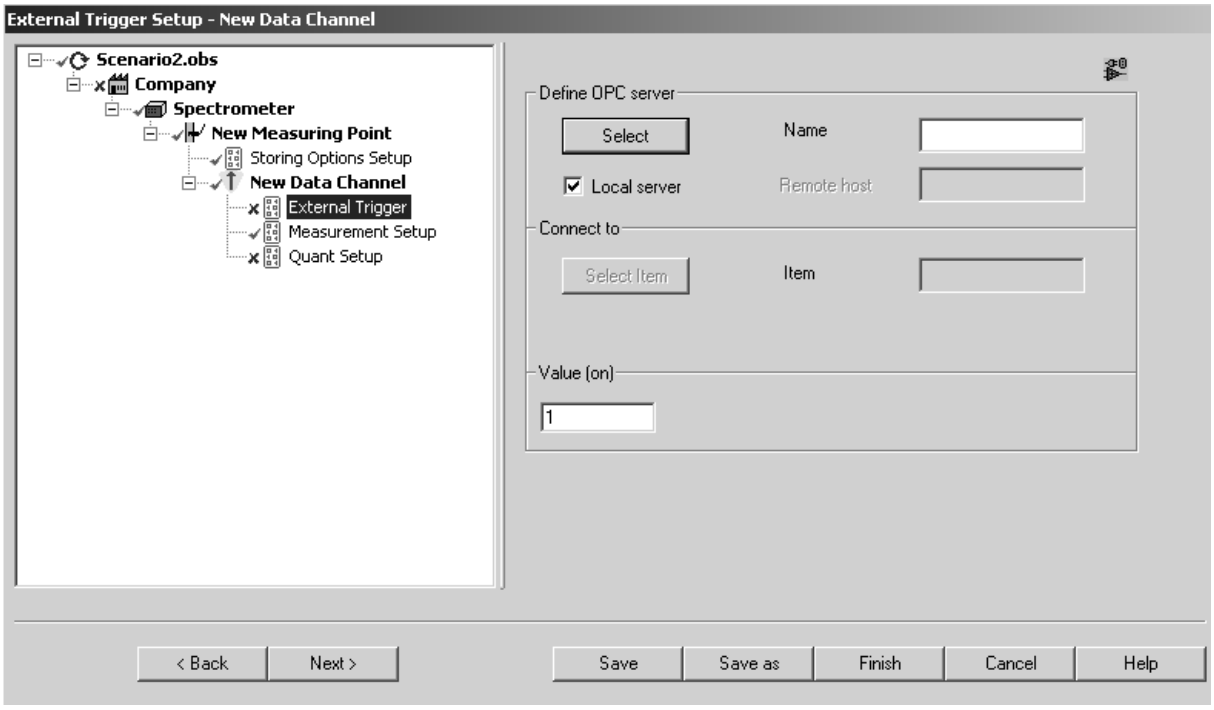


Figure 46: External Trigger Setup

Each OPC server registers itself on the system by a unique name. Click on the *Select* button to see which servers are available for the spectrometer used. The following dialog opens:

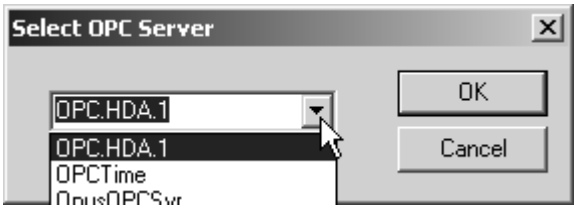


Figure 47: OPC servers available

Deactivate the *Local Server* check box if you want to access data from a remote host. This check box is activated by default. If you deactivate the check box, you have to enter the host name of the server into the *Remote Host* entry field.

If you want to set up a connection to an OPC server which is not installed on the local PC but somewhere on the network, you have to enter the network name of this host into the *Remote Host* field.

You enter the name to identify the item on the OPC server. Each server registers its items on the system by a unique name. If you click on the *Select Item* button, the data items available on the server will be displayed.

Enter an integer into the *Value* entry field to define the area to be triggered. By default, the integer 1 is specified.

6.16 Diagnosis Setup

Normally, OPC clients will be automatically informed whenever the status of the instrument changes. The diagnosis setup is a global scenario setting which transfers the instrument status to an OPC server defined.

To set up the diagnosis select the *Spectrometer* level and open the corresponding pop-up menu by a right mouse click.

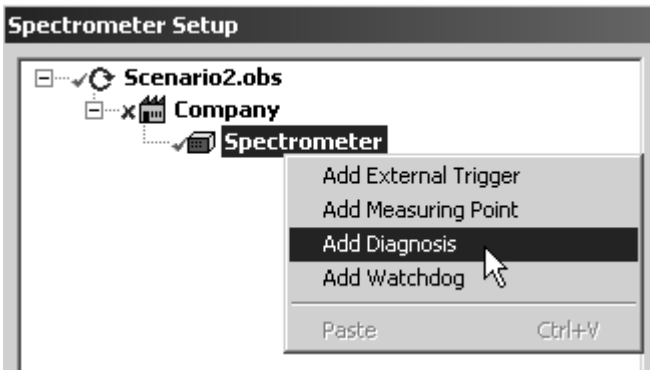


Figure 48: Pop-up menu on *Spectrometer* level

Click on the *Add Diagnosis* command. The *Diagnosis* sub-level is displayed in the scenario browser.

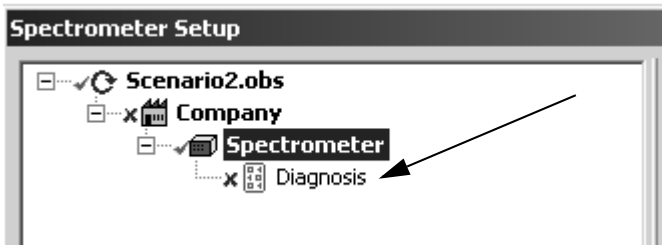


Figure 49: *Diagnosis* sub-level in the browser

Clicking on the *Diagnosis* sub-level opens the following dialog:

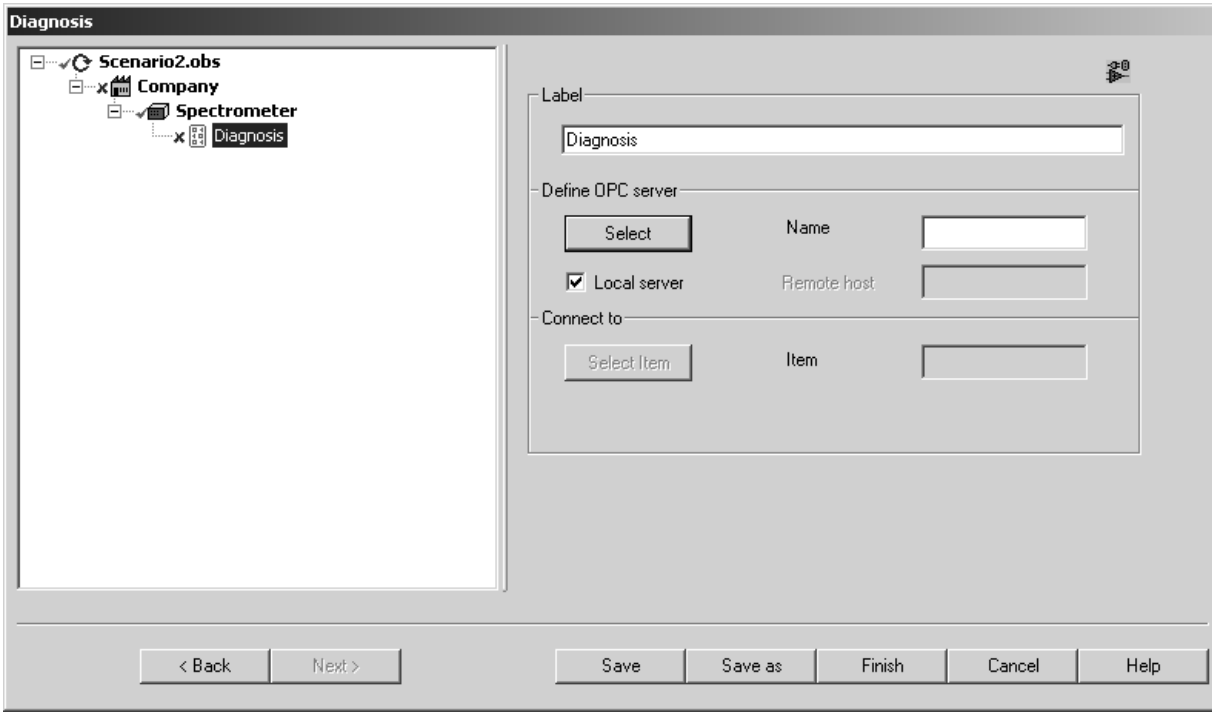


Figure 50: Diagnosis Setup

By default, the label is defined as *Diagnosis*. If you want to change the label, click into the entry field and specify a new name.

Each OPC server registers itself on the system by a unique name. Click on the *Select* button to see which servers are available for the spectrometer used. The following dialog opens:

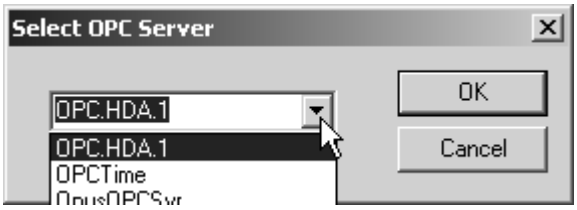


Figure 51: OPC servers available

Deactivate the *Local Server* check box if you want to access data from a remote host. This check box is activated by default. If you deactivate the check box, you have to enter the host name of the server into the *Remote Host* entry field.

If you want to set up a connection to an OPC server which is not installed on the local PC but somewhere on the network, you have to enter the network name of this host into the *Remote Host* field.

You enter the name to identify the item on the OPC server. Each server registers its items on the system by a unique name. If you click on the *Select Item* button, the data items available on the server will be displayed.

6.17 Watchdog Setup

In this context, a watchdog is a certain kind of control signal which lights up on a monitoring PC during the process run. A watchdog is useful if the entire system may respond e.g. in time delays due to problems in the process run. If you have defined a watchdog in OPUS PROCESS, a signal is sent to the monitoring PC within a specified interval indicating that OPUS PROCESS is still running.

To set up the watchdog select the *Spectrometer* level and open the corresponding pop-up menu by a right mouse click.

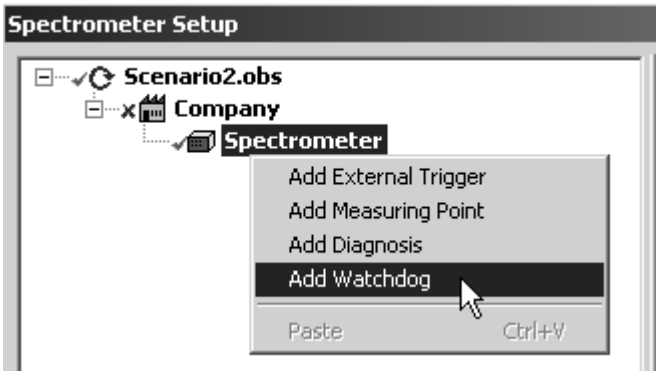


Figure 52: Pop-up menu on *Spectrometer* level

Click on the *Add Watchdog* command. The *Watchdog* sub-level is displayed in the scenario browser.

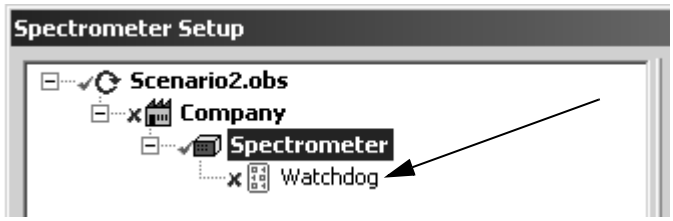


Figure 53: *Watchdog* sub-level in the browser

Clicking on the *Watchdog* sub-level opens the following dialog:

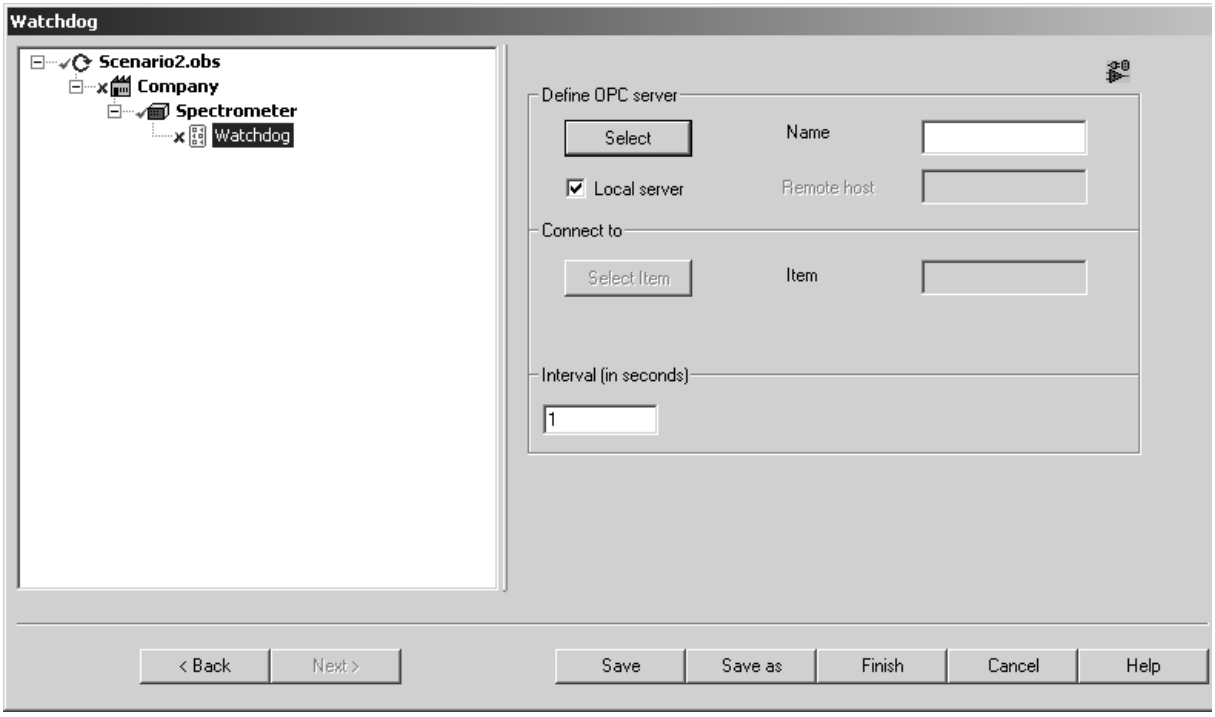


Figure 54: Watchdog Setup

Each OPC server registers itself on the system by a unique name. Click on the *Select* button to see which servers are available for the spectrometer used. The following dialog opens:

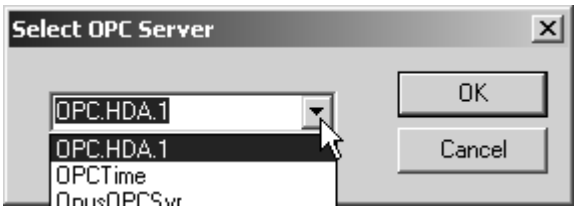


Figure 55: OPC servers available

Deactivate the *Local Server* check box if you want to access data from a remote host. This check box is activated by default. If you deactivate the check box, you have to enter the host name of the server into the *Remote Host* entry field.

If you want to set up a connection to an OPC server which is not installed on the local PC but somewhere on the network, you have to enter the network name of this host into the *Remote Host* field.

You enter the name to identify the item on the OPC server. Each server registers its items on the system by a unique name. If you click on the *Select Item* button, the data items available on the server will be displayed.

Define the interval within which the signal is to be sent to the monitoring PC. The interval is specified in seconds, with 1 being defined as default.

6.18 Calculation

This channel type uses the result of other channels as input value and performs a simple calculation, e.g. by averaging. To set up a calculation select the *New Data Channel* level and open the corresponding pop-up menu by a right mouse click.

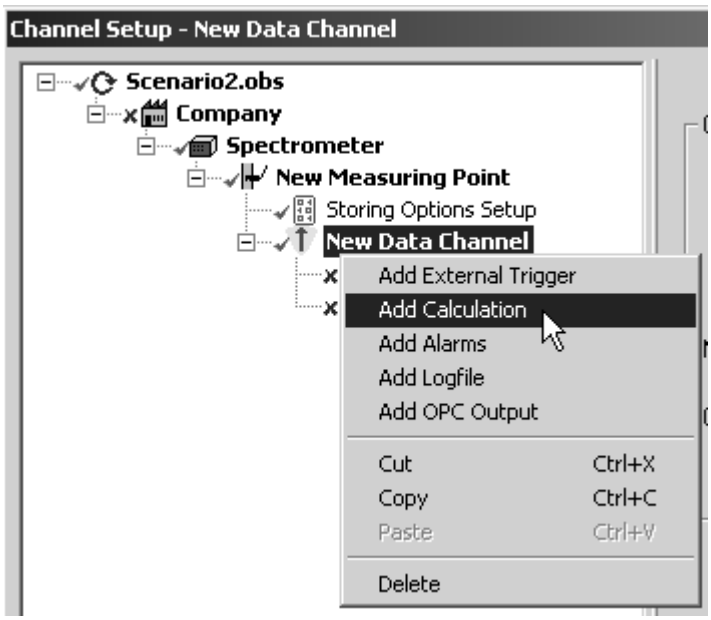


Figure 56: Pop-up menu on *New Data Channel* level

Click on the *Add Calculation* command. The *New Calculation* sub-level is displayed in the scenario browser.

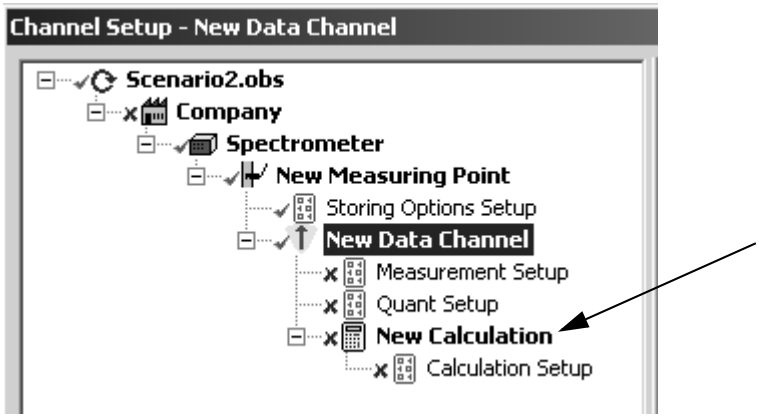


Figure 57: *New Calculation* sub-level in the browser

Clicking on the *New Calculation* level opens the following dialog:

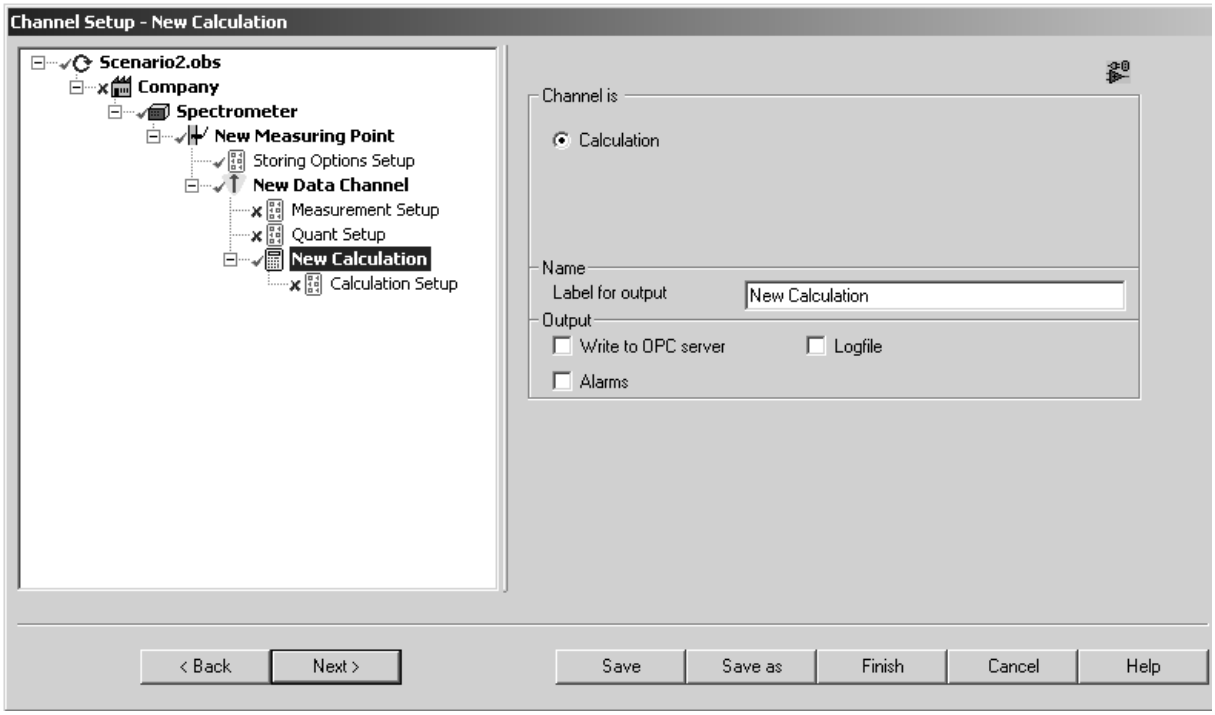


Figure 58: Channel Setup - New Calculation

Sometimes it is useful to define a set of calculation functions which can also be used for the data of any other channel. The variables which form the basis for the calculations can be, e.g., all components predicted by the QUANT model(s) such as *Prediction* and Mahalanobis distance. You can independently define the calculations on the basis of these variables and plot them versus time.

The *Calculation* option button is activated by default. It is also possible to define more than one calculation for a particular data channel. For details on the label and output options refer to chapter 6.5.2 and 6.5.3.

Clicking on the *Calculation Setup* sub-level opens the following dialog:

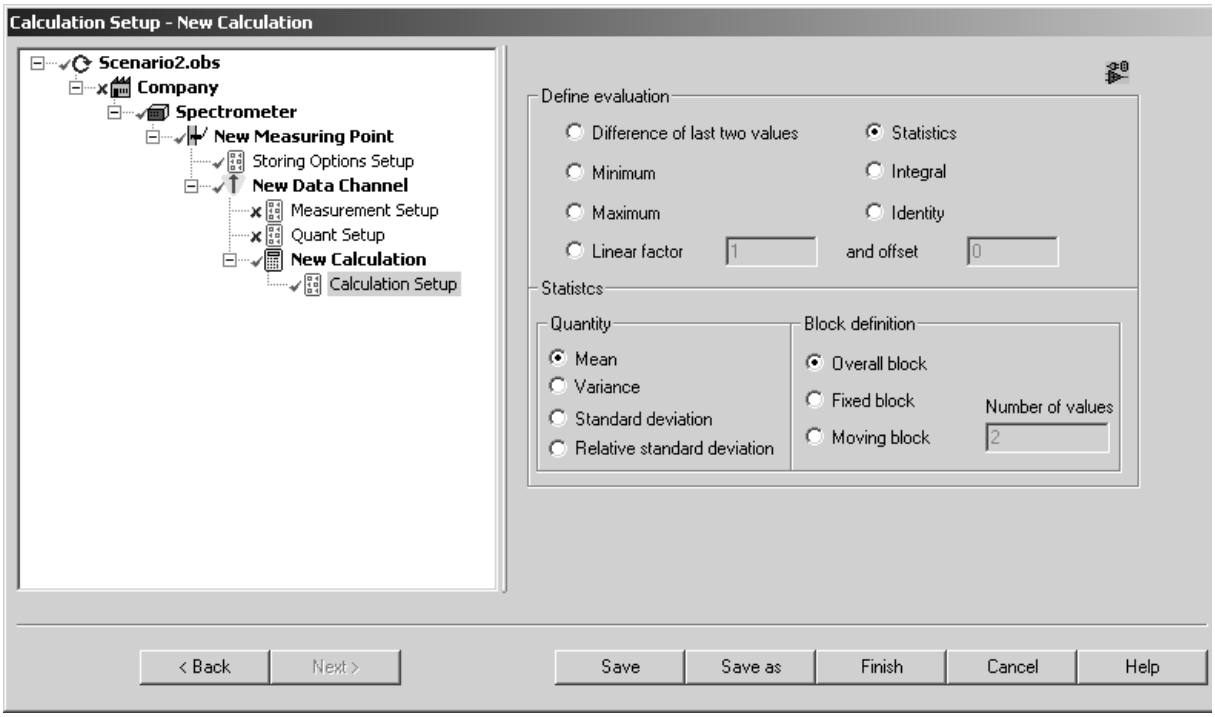


Figure 59: Calculation Setup

6.18.1 Define evaluation

- **Difference of last two values**

The output channel shows the difference between two successive values of the input channel. This difference has the same characteristics as a first derivative which has not been smoothed.

- **Minimum**

The output channel shows the absolute minimum values from the input channel up to the current measurement value.

- **Maximum**

The output channel shows the absolute maximum values from the input channel up to the current measurement value.

- **Linear Factor and Offset**

The result can be scaled linearly and corrected by an offset. Enter the appropriate linear and offset factor into the particular entry field.

- **Statistics**

The output channel calculates statistical terms. If you activate the *Statistics* option button, the statical evaluation options will be enabled.

- **Integral**

The output channel shows a running integral value of the input channel. All values from the beginning of the process control run will be added up.

- **Identity**

If you activate the *Identity* option button, the result of the reference channel will also be the result of the active channel.

6.18.2 Statistics

There are several evaluation functions available which provide statistical information on single spectra, file lists or 3D spectra files. Select one of them and define the block size of the spectrum or sample. The block size can be:

- Overall block: evaluation is performed on the basis of all values of the current run.
- Fixed block: evaluation is performed on the basis of a fixed-size value block. Enter the block size into the *Number of value* entry field.
- Moving block: evaluation is performed on the basis of the last *n* values defined in the entry field.

For further details on statistical evaluation in OPUS refer to the OPUS STATISTICS manual.

6.18.3 Reference Channel

The number specified defines the channel with the input data used for mathematical manipulations, and has to be smaller than the index of the current channel, as the data have to be available before any calculation will be performed.

6.19 OPUS writes Values to OPC Servers

No detailed description of the output interface has yet been given for the channels previously described. For each channel different check boxes for the output are available. This chapter will describe how to define the output. OPC servers allow access to all relevant communication interfaces.

Communication interfaces supported by busses can be

- Modbus
- Profibus DP
- Profibus FMS
- Industrial Ethernet

Communications via analog and digital values can be

- 4-20 mA interface card (ADLINK PC_6308A interface card)
- ADAM 5000
- Simatic S7

If you use one of these interfaces, it will be addressed by the appropriate OPC server. Define the right OPC server to select the output interface.

Frequently, this direct writing to servers enables to set up a connection to existing interfaces or process control systems that have not yet directly supported OPC. This also applies to the support of analog systems as it is very easy to develop OPC servers for existing hardware.

To set up the output select the *New Data Channel* level and open the corresponding pop-up menu by a right mouse click.

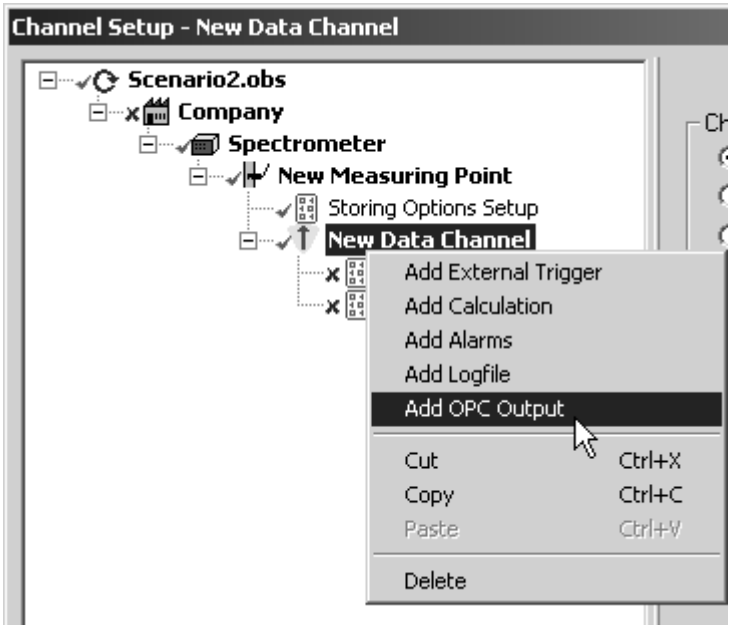


Figure 60: Pop-up menu on *New Data Channel* level

Click on the *Add OPC Output* command. The *New Calculation* sub-level is displayed in the scenario browser.

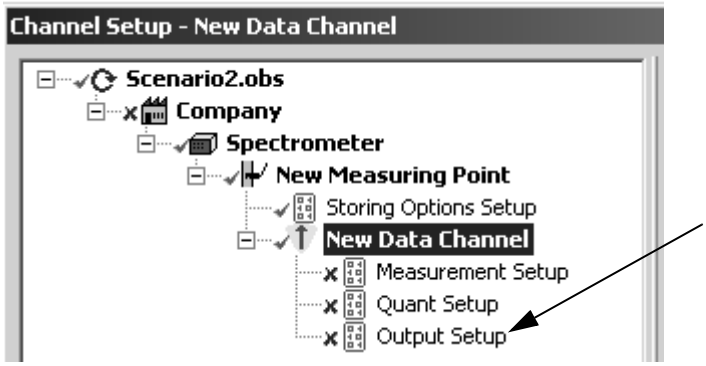


Figure 61: *Output Setup* sub-level in the browser

Clicking on the *Output Setup* sub-level opens the following dialog:

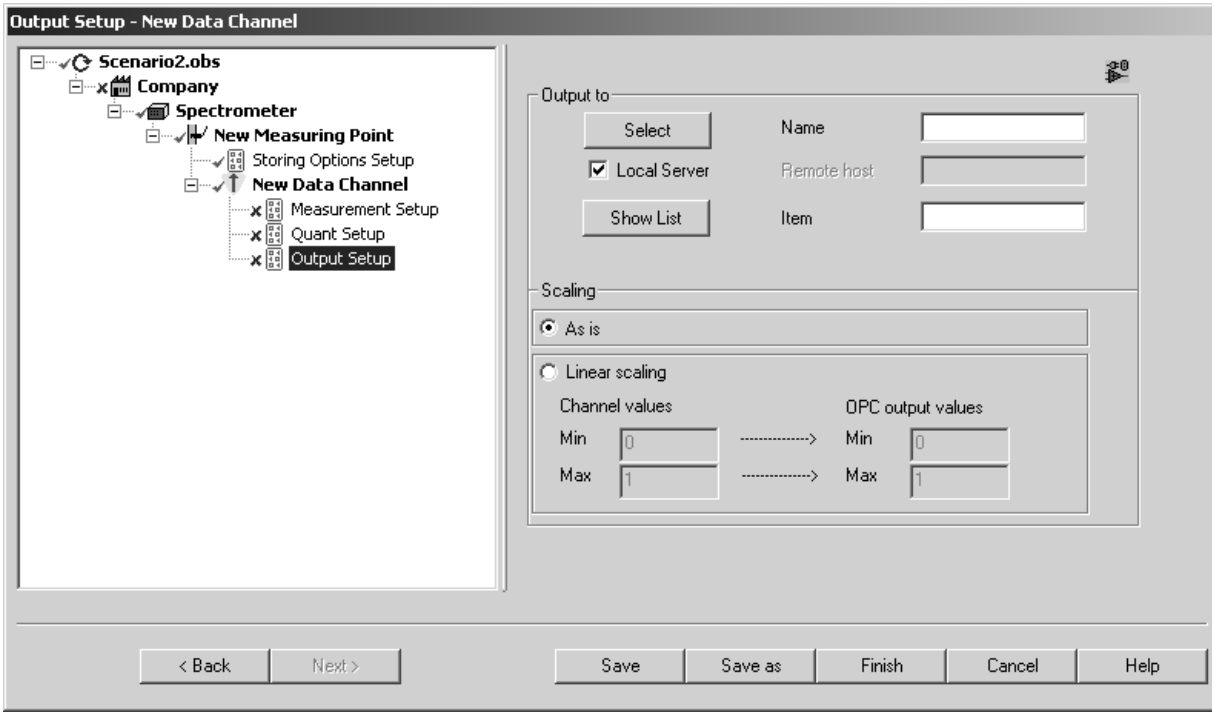


Figure 62: Output Setup

Each OPC server registers itself on the system by a unique name. Click on the *Select* button to see which servers are available for the spectrometer used. The following dialog opens:

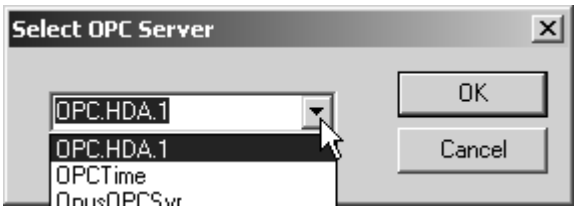


Figure 63: OPC servers available

Deactivate the *Local Server* check box if you want to access data from a remote host. This check box is activated by default. If you deactivate the check box, you have to enter the host name of the server into the *Remote Host* entry field.

If you want to set up a connection to an OPC server which is not installed on the local PC but somewhere on the network, you have to enter the network name of this host into the *Remote Host* field.

You enter the name to identify the item on the OPC server. Each server registers its item on the system by a unique name. If you click on the *Show List* button, the data items available on the server will be displayed.

The combination of an OPC server name and an item completely identifies the path for the output data.

6.19.1 Scaling

In case of communication via an A/D converter the relevant concentration ranges have to be scalable to ranges from 4 - 20mA. This is achieved by the following scaling options.

- **As is**

No scaling is performed at all, i.e. the result is transferred to the server regardless of the range you use. This may cause problems if the data exceed the maximum limits allowed.

- **Linear Scaling**

You can scale the channel and output values using a user-defined scale. Enter the minimum and maximum values for both the channel and the output.

6.20 Alarm Setup

OPUS PROCESS provides editable alarm limits for each channel, e.g. for a Mahalanobis distance of a quantitative analysis. These alarm limits can be set for each channel separately and are simply adjustable.

Alarm limits are used to identify outliers. The limits for these chemometric alarm levels for QUANT 2 evaluations can be easily defined. In case of QUANT the limits of the method stored are the default values for the alarm limits to detect outliers.

Apart from the graphical alarm indicators (alarm lines etc.), a variety of actions may become necessary when exceeding a limit. E.g., I/O signals can be triggered or specific data communication to the process control computer observed. All these possible reactions to one alarm can be caused by setting specific OPC values on different servers.

To set up alarm limits select the *New Data Channel* level and open the corresponding pop-up menu by a right mouse click.

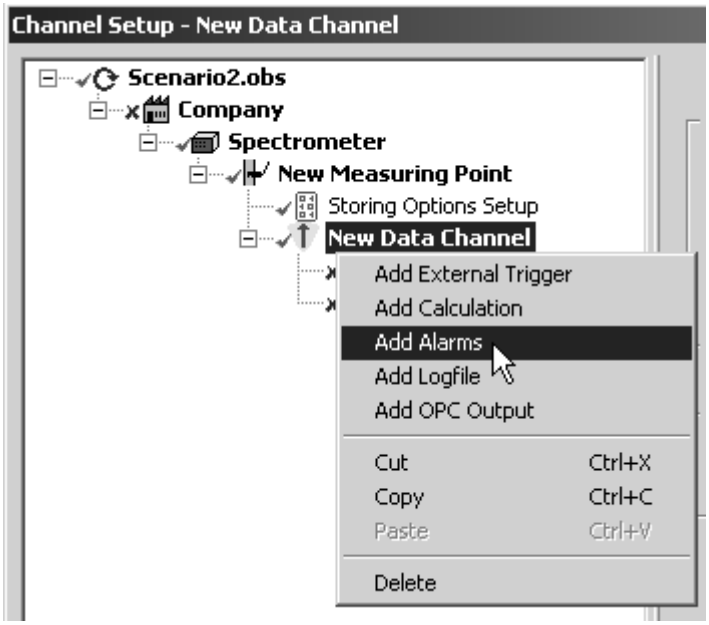


Figure 64: Pop-up menu on *New Data Channel* level

Click on the *Add Alarms* command. The *Alarm* sub-level is displayed in the scenario browser.

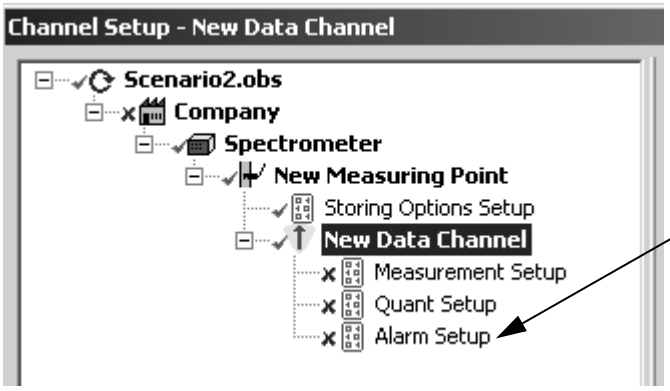


Figure 65: *Alarm Setup* sub-level in the browser

Clicking on the *Alarm Setup* sub-level opens the following dialog:

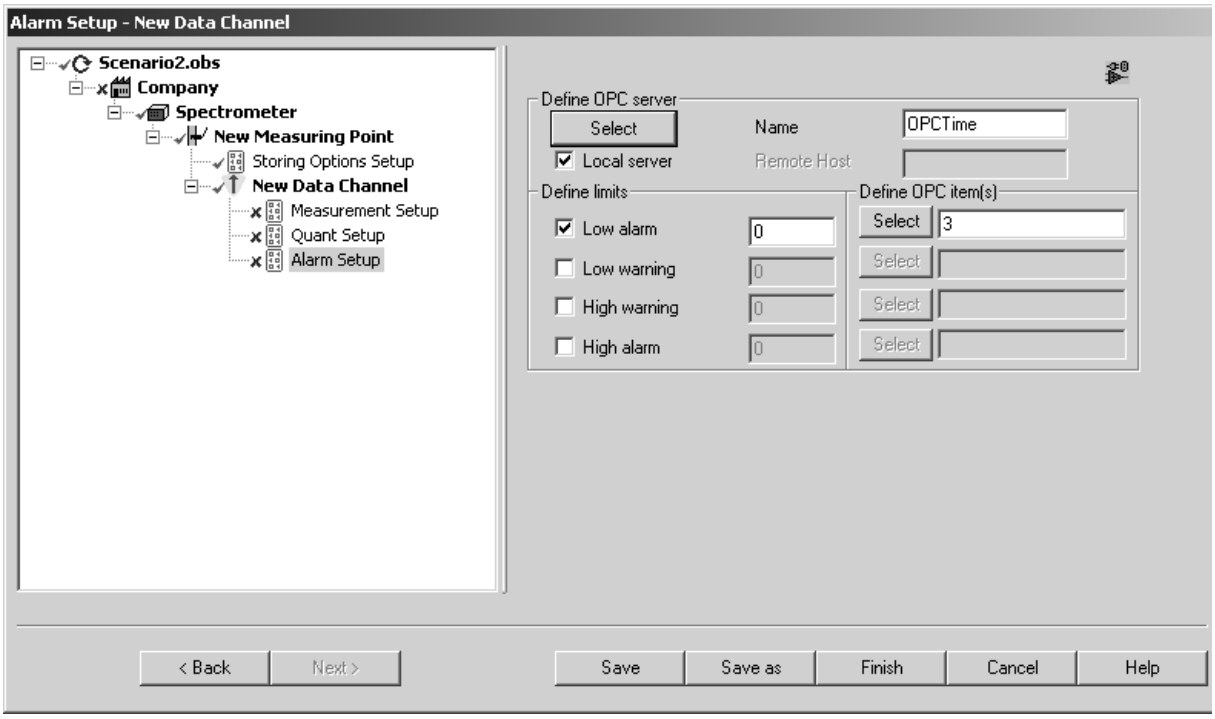


Figure 66: Alarm Setup

Each OPC server registers itself on the system by a unique name. If no OPC server has been defined, the alarms will not be transferred but indicated only. Click on the *Select* button to see which servers are available for the spectrometer used. The following dialog opens:

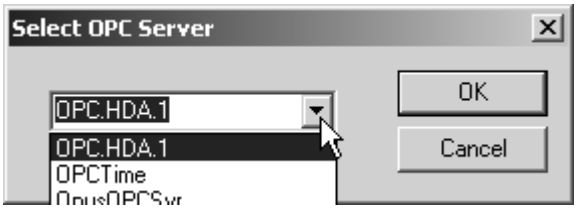


Figure 67: OPC servers available

Deactivate the *Local Server* check box if you want to access data from a remote host. This check box is activated by default. If you deactivate the check box, you have to enter the host name of the server into the *Remote Host* entry field.

If you want to set up a connection to an OPC server which is not installed on the local PC but somewhere on the network, you have to enter the network name of this host into the *Remote Host* field.

Define the upper and lower warning/alarm limits for the channel and enter the OPC items either manually into the entry field or select them by clicking on the *Select* button.

6.21 Log File Setup

The result of each channel can either be presented graphically, exported to an OPC server or reported into a log file. At the beginning of a new run it is possible to automatically delete old reports.

For each measurement a single text line separated by comma is stored in the log file. This line can easily be imported into a spreadsheet. If you want to log several channels into one single file, use the same file name for all channels.

To set up a log file select the *New Data Channel* level and open the corresponding pop-up menu by a right mouse click.

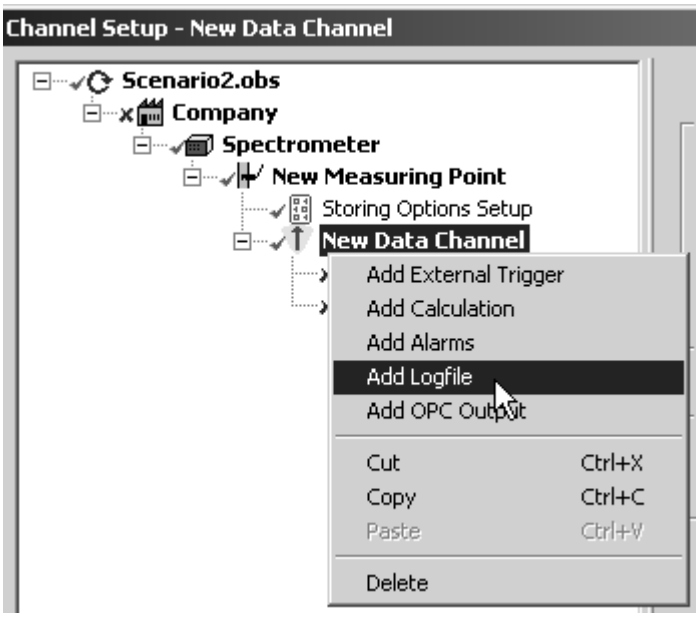


Figure 68: Pop-up menu on *New Data Channel* level

Click on the *Add Logfile* command. The *Logfile Setup* sub-level is displayed in the scenario browser.

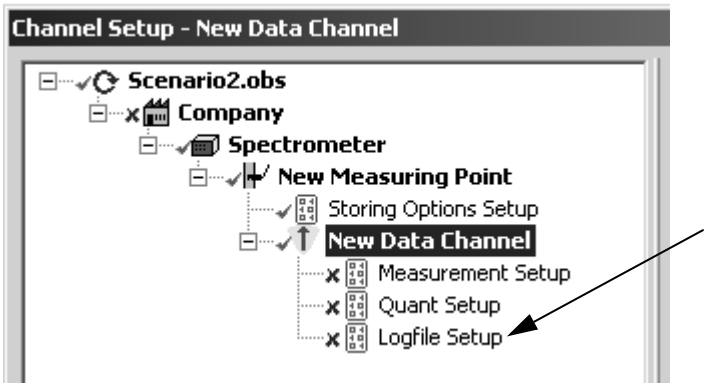


Figure 69: *Logfile Setup* sub-level in the browser

Clicking on the *Logfile Setup* sub-level opens the following dialog:

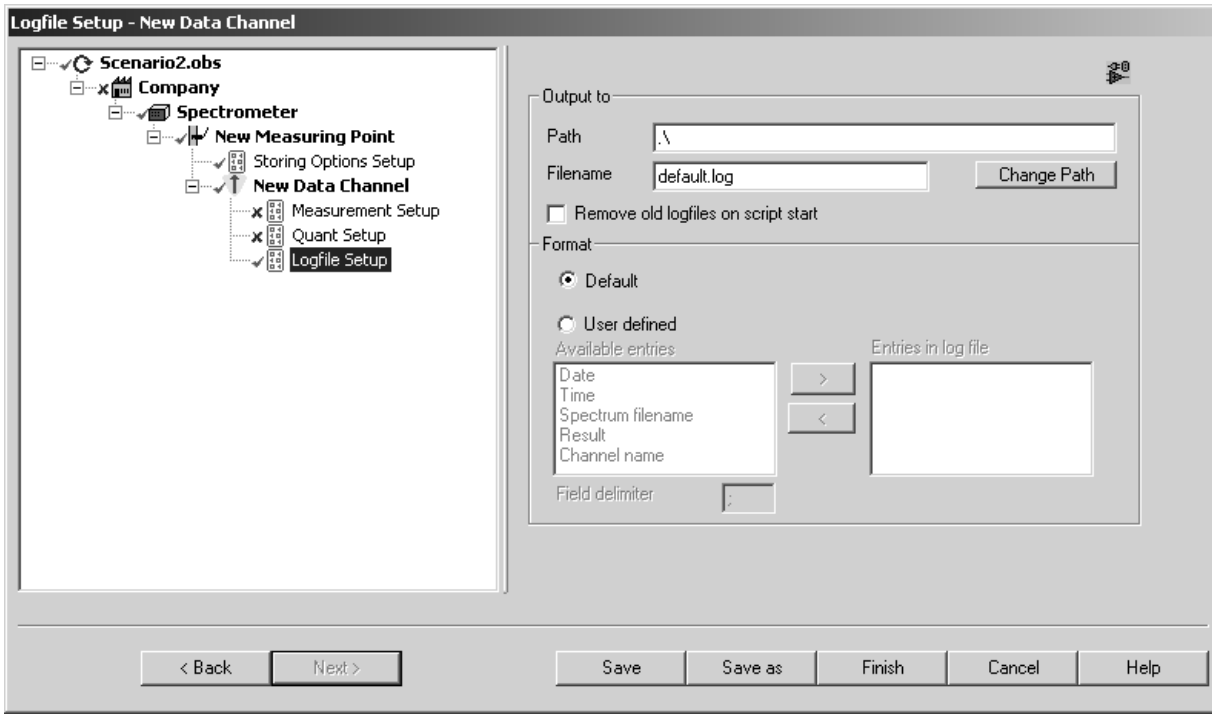


Figure 70: Log File Setup

Define the file name of the log file to be stored. The file is stored in text format which can be easily imported into other applications. Log files have the extension **.log*.

Define the path of the log file. You can also change the path by clicking on the *Change Path* button. In principle, the log file may be stored in any path but it is recommended to either use the OPUS directory or a well-defined sub-directory of the process scenario path.

If you activate the *Remove old log files on script start* check box, all the previous log files will be deleted as soon as you start the script.

6.21.1 Format

- **Default**

If you activate the *Default* option button, the date and time, the name of the measured file and the channel data will be logged.

- **User Defined**

It is possible to define a user-defined output format for the log file. If you activate the *User defined* option button, the selection field with the available entries will be activated. Select the respective entries and move them by the >

button to the *Entries in log file* selection field. To undo the selection use the  button. All entries will automatically be separated by the *Field delimiter* which is a semicolon.

6.22 External Control

This chapter describes how external events trigger special tasks in OPUS PROCESS. These external events will be triggered if one OPC value on the server changes. Possible reactions to these events can be:

- Measuring new reference
- Using a different scenario
- Calling VBScripts

OPUS PROCESS can be operated by external programs, or by an input of commands by standardized OPC interfaces. To facilitate the setup all important measurement and evaluation parameters are pre-defined in the measurement scenarios.

Almost all changes caused by an external signal can be met by using a new scenario. If you want to modify the measurement parameters during a cycle, a new measurement scenario must be defined. Instrument or method parameters cannot be changed by a direct control system command. Different measurement scenarios can be used to adjust the method and cycle times. Thus, more detailed measurements in shorter time intervals can be performed if a reaction reaches the final stage.

The *Run Macro* command in the *Macro* menu increases the flexibility of possible reactions and can optionally be used for additional OPUS control options. The command allows to selectively collect calibration spectra, i.e. to record individual spectra in a separate directory. The calibration spectra are used afterwards to extend the existing QUANT and IDENT methods.

A new reference measurement can be directly effected by OPUS PROCESS or by an external control system, for each measurement channel individually - even during an active cycle. The control system needs to indicate the number of the channel to define the corresponding reference for each channel. The spectra for background measurements are automatically archived.

To add an external control select the *Company* level and open the corresponding pop-up menu by a right mouse click.

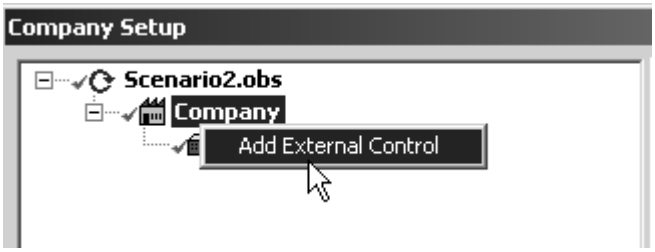


Figure 71: Pop-up menu on *Company* level

Click on the *Add External Control* command. The *External Control* sub-level is displayed in the scenario browser. If more than one external control is defined, the number is automatically incremented by OPUS.

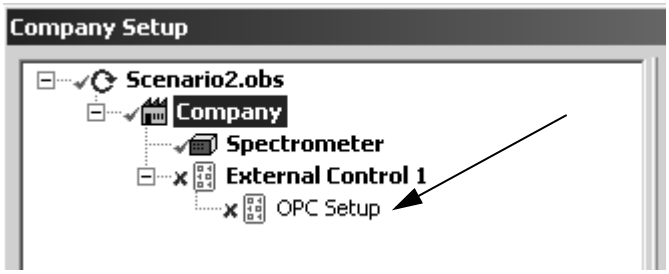


Figure 72: *External Control* sub-level in the browser

Clicking on the *External Control* sub-level opens the following dialog:

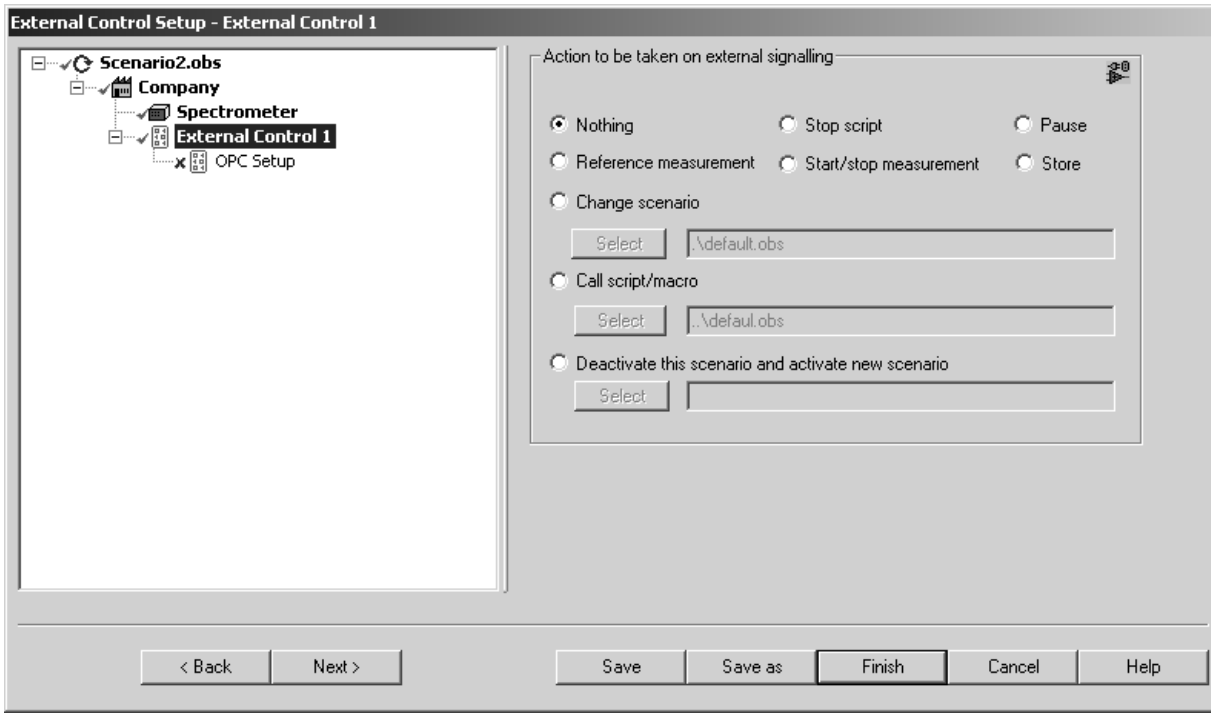


Figure 73: External Control Setup

6.22.1 Action to be taken on external signalling

These are the signals of a process system which are generated by a certain control system. For each signal you can specify a certain type of reaction. The process control system indicates whether you have to acquire a new background spectrum or to use a completely new scenario.

- **Nothing**

If you activate this option button, trigger signals will be registered without ensuing any actions.

- **Stop Script**

If you activate this option button, the script will be stopped.

- **Pause**

If you activate this option button, no more data will be added to the real-time display. The first external signal activates the *Pause* function, the next will start the process run again.

- **Reference Measurement**

If you activate this option button, the acquisition of a background measurement will be started. The channel parameters have to be already defined in the setup. The control system needs to indicate the number of the channel only, to define which reference has to be acquired.

- **Start/Stop Measurement**

If you activate this option button, an external signal is directly sent to the measurement which will immediately be stopped. The spectrum, however, will be evaluated.

- **Store**

If you activate this option button, a spectrum will always be stored. E.g., if you want to measure calibration spectra at a certain period of time, the measurement will be stopped not until the *Store* option button is deactivated.

- **Change Scenario**

If you activate this option button, the process scenario will be terminated after the current process cycle has been finished. The file name and path define a new scenario script which will then be started. Either type in the scenario manually or use the *Select* button and select the scenario from the dialog that opens. In principle, the scenarios may be stored in any path but it is recommended to use the OPUS directory.

- **Call Script/Macro**

The file name and path define a script that will be started. This script/macro can perform an instrument test and send direct commands to the optical bench, or transfer data required to the control system. For further evaluation the script receives a parameter which includes the value of the OPC item that has triggered the event.

Either type in the script/macro manually or use the *Select* button and select the script/macro from the dialog that opens. In principle, the scripts/macro may be stored in any path but it is recommended to use the OPUS directory.

- **Deactivate scenario and activate new one**

If you activate this option button, the current process scenario will be deactivated. The new scenario can be selected by using the *Select* button. In principle, the scenarios may be stored in any path but it is recommended to use the OPUS directory.

6.22.2 Defining external OPC server

When defining an external control in a process scenario you also have to define the external OPC server. Click on the *OPC Setup* level which is automatically displayed below the *External Control* level (see figure 73) to open the following dialog:

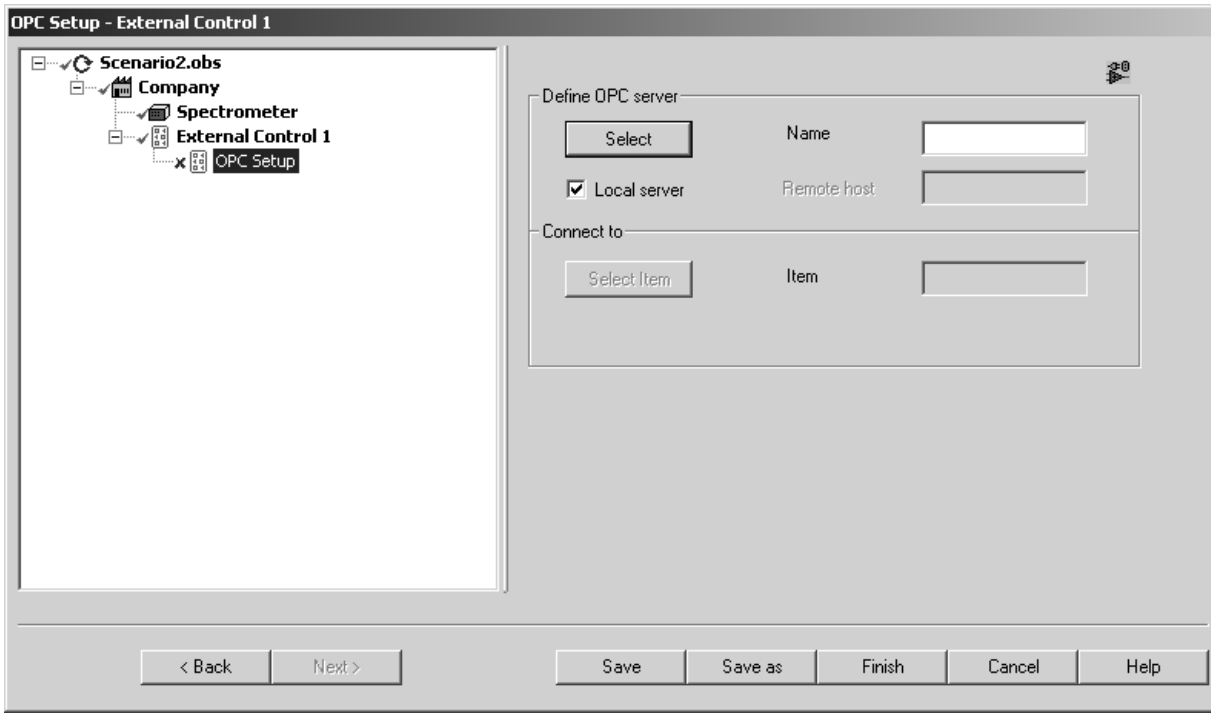


Figure 74: External OPC Setup

Each OPC server registers itself on the system by a unique name. Click on the *Select* button to see which servers are available for the spectrometer used. The following dialog opens:

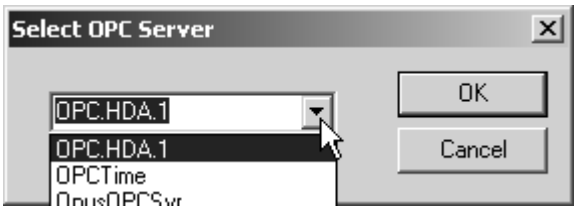


Figure 75: OPC servers available

Deactivate the *Local Server* check box if you want to access data from a remote host. This check box is activated by default. If you deactivate the check box, you have to enter the host name of the server into the *Remote Host* entry field.

If you want to set up a connection to an OPC server which is not installed on the local PC but somewhere on the network, you have to enter the network name of this host into the *Remote Host* field.

You enter the name to identify the item on the OPC server. Each server registers its items on the system by a unique name. If you click on the *Select Item* button, the data items available on the server will be displayed.

7 Converting Old Scenarios

For reasons of compatibility OPUS PROCESS allows to convert the setup of previous process control environments. Existing ADIO data can be converted to OPUS PROCESS by means of a kind of wizard.

It is, however, not possible to convert all ADIO setup features one-to-one into OPUS PROCESS for two reasons:

1) There are many customer-specific adapted ADIO versions in which some system components are not stored in the parameter files, but hardwired in the program code.
2) The ADIO definition of the measuring points is slightly different from the *channel* term in OPUS PROCESS.

7.1 ADIO

To convert ADIO data select the *Convert Process* command from the OPUS *Measure* menu. The following dialog opens:

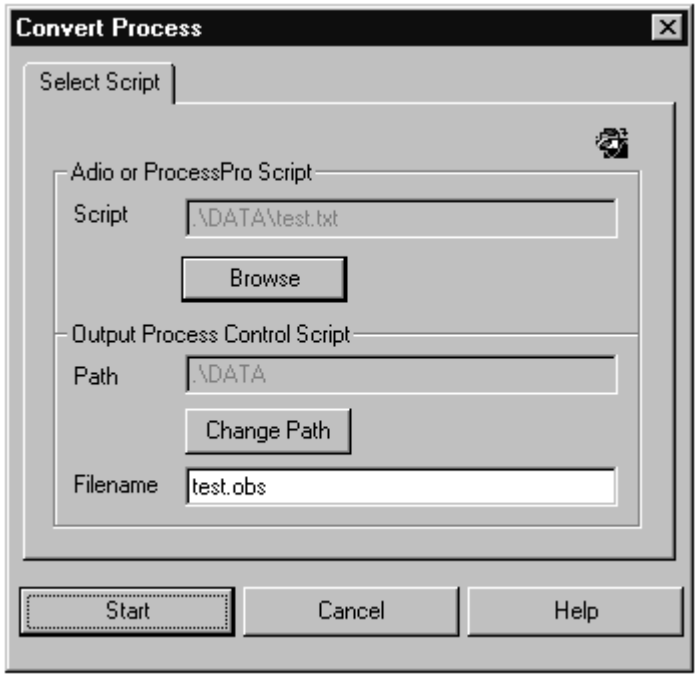


Figure 76: Convert Process - Select Script tab

Click on the *Browse* button to locate the ADIO configuration file you want to convert.

Enter a file name for the output file, i.e. the new scenario. To change the script path click on the *Change Path* button.

If you click on the *Start* button, and a new scenario will be generated. The process run is similar to the initial ADIO setup.

7.2 PROCESS PRO

You can also convert configuration files of the PROCESS PRO system. Select the appropriate input file, and the conversion routine automatically detects the file format and performs the right conversion.

8 Connecting to Other Systems

All configuration steps previously described do not include a detailed explanation of any particular interface. The reason is that a very simple setup has been used which allows access to all currently important communication interfaces. Today, almost every I/O hardware works with an OPC server which can be addressed by OPUS via a single interface. This enables the use of communication bus interfaces, e.g. Modbus or Profibus.

For analog and digital communications you should use a 4-20mA interface card (ADLINK PC_6308A), or connect to an ADAM 5000 or Simatic S7.

The next chapter describes the setup of the most commonly used interface types.

8.1 Modbus

OPUS PROCESS can communicate with a control system by means of an Applicom PCI1000 Modbus interface card.

8.1.1 Hardware and OPC Server Installation

For further information on how to install the hardware and software, refer to the appropriate Applicom documentation. The card is connected to the control system by a RS-485-interface.

8.2 Profibus

Graduated, matching industrial communication systems such as the Ethernet-based PROFInet, the fieldbus PROFIBUS and other systems, e.g. the AS-Interface sensor/actuator bus have the necessary qualifications for transparent networking in all areas and levels of the automation process.

Distributed peripherals, such as I/O modules, measuring transducers, drive units, valves and operator terminals communicate with the automation systems via an efficient, real-time communication system. The transmission of the process data is performed cyclically, while alarms, parameters and diagnostic data have to be transmitted acyclically, if required. PROFIBUS meets these requirements and offers a transparent solution for manufacturing as well as for process automation.

Appendix A

OLE for Process Control

OPC Basics

OPC is an industry standard created by different leading automation and hardware software suppliers. The organization which manages this standard is the OPC Foundation. The Foundation has over 150 members based throughout the world, including nearly all famous major providers of control systems, instrumentation and process control systems.

Figure 77: OPC logo

The objective of the OPC Foundation is to develop an open, flexible, plug-and-play standard that allows a greater choice of hardware and software suppliers. Customers can choose the appropriate instrument from the most suitable supplier to meet their unique requirements by a standardized software.

The name of this standard is OPC. The letters O-P-C derive from OLE (Object Linking and Embedding) for Process Control. According to the OPC Foundation this standard will bring the same benefits to industrial hardware and software that standard printer drivers brought to word-processing.

Today, each automation system installed requires a significant amount of time and money to ensure that the system can share information with other systems and devices. OPC will save the customer time and money by reducing the system integration problems caused by the lack of open standards that exist between automation devices and software manufacturing.

- **Software standard for automation**

  The standard creates a common interface for communication between various devices controlling technological processes. The objective is to prevent given monitoring or control software from being dependant on the hardware manufacturer. OPC is based on the OLE/COM/DCOM technology of Microsoft, Inc.

  Many client applications developed collect data from data sources and make that data available using independently developed drivers

for the given software package. This may cause the following problems: each application must include a separate driver for a particular hardware device (figure 77).

Problems between drivers of various manufacturers can be put down to the fact that various hardware features are not supported by all driver developers. The change of hardware features may result in functionality failures of some drivers.

Two different software packages cannot address the same device simultaneously as each one of them works with an independent driver. This may cause severe hardware access problems.

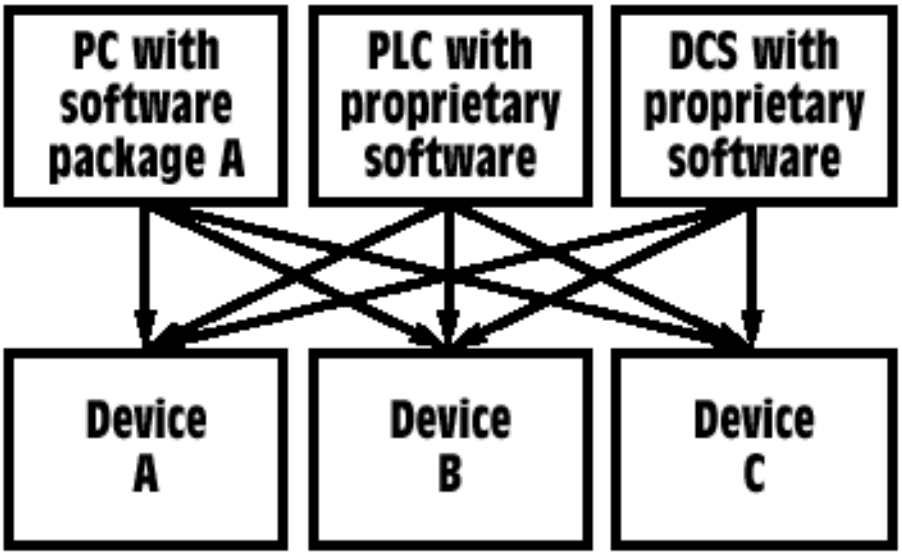


Figure 78: Scheme of an I/O driver problem

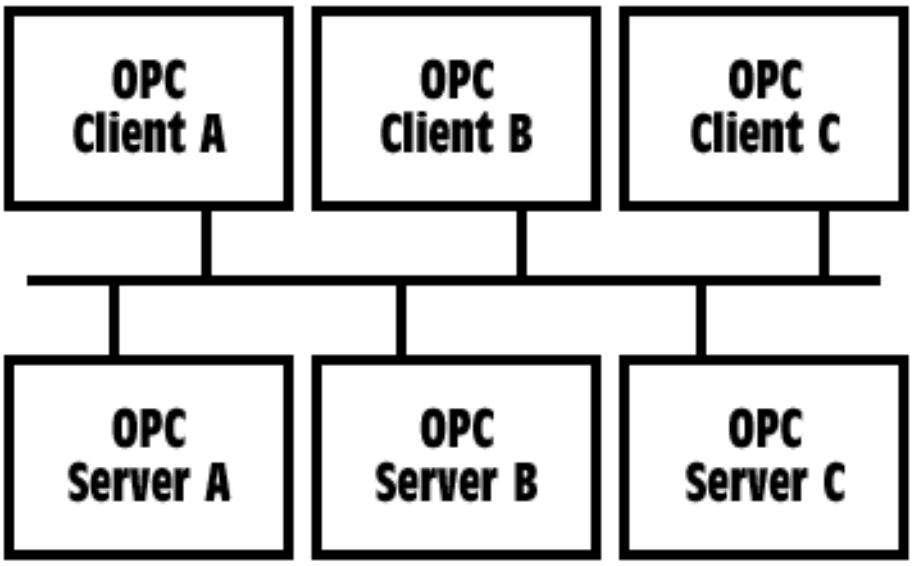


Figure 79: ...and its OPC solution

OPC draws a line between hardware and software developers. It collects data from data sources and transfers the data to any client application, independent of any hardware manufacturer. This feature allows manufacturers to develop a performance-optimized server to communicate with the data source.

- **COM/OLE is a Microsoft technology for data exchange between applications**

  Based on Microsoft OLE (now ActiveX), COM (component object model) and DCOM (distributed component object model) technologies, OPC consists of a standard set of interfaces, properties and methods for the use in process-control and manufacturing-automation applications. The ActiveX/COM technologies define how individual software components can interact with and share data.

  The concept of the standard is plug-and-play. If you use a standard method to automatically configure computer hardware (and software interfaces), a device can easily be connected to another and immediately operates without the need of lengthy installation or complex configuration procedures. Instead of learning how to use 100 or more commercial toolkits, users will have to deal with only one set of tools, as all OPC drivers work on the same principle.

  These devices are used as OPC servers, permanently providing data to OPC client applications. Application developers can write codes in any appropriate language.

- **OPC is based on COM**

  COM (Component Object Model) provides standard interfaces and inter-component communications.

  When using COM, an application may use features of any other application object or operating system, or allow software component upgrades without affecting the operation of the overall solution.

  OLE (Object Linking and Embedding) is used to provide the integration of different applications, enabling a high degree of application compatibility even among different types of information. OLE is based on COM and enables the development of re-usable, plug-and-play objects that are interoperable between multiple applications.

  The Distributed Component Object Model extends COM to networks (remote objects). It is a new, highly optimized protocol in which remote components appear to be local.

- **OPC activities aim at a uniform software interface**

  The OPC principle is that any client system - either located in the control room or in an executive office - has to deal with only one interface to get data from any device. The OPC client application can be connected to any supplier OPC server without any differences to be expected regarding the servers' feedback.

- **OPC future**

  In the meantime the OPC standard has been very well established due to the large organization of suppliers. OPC servers are now an integral part of hardware deliveries provided by the majority of manufacturers who are specialized in automation technology and control systems. Similarly, an ever increasing number of manufacturers of visualization systems provide an option for data collection using OPC servers in their OPC clients. Thus, the OPC technology is gradually becoming a worldwide communication standard in industrial information systems.

Advantages

A standard that provides real plug-and-play software technology for process control and factory automation, enabling each system, device and driver to be freely connected with each other is the basis of an open and easy communication between systems and devices. Therefore, the OPC design allows client applications to have consistently access to plant floor data.

Due to the increased acceptance within the industrial environment, the hardware manufacturers only have to use one set of software components for all their customer applications. And software developers will not have to rewrite drivers because of feature changes or extensions made in a new hardware release.

Customers have the freedom of choice between different manufacturers of various components and devices. They also can decide where to integrate the monitoring and control of technologies, either on the plant floor or throughout the entire company.

- **Independence of hardware and software suppliers**

  Bigger choice, better access to process data and easy plug-and-play operation are the main benefits of OPC technology.

  Customers used to be limited in their choice of client applications supporting the communication to their installation devices.

  With OPC, customers are no longer bound to a single supplier. If a plant has installed a legacy system, end-users do not inevitably depend on this system supplier. Using OPC ensures that any future process control system can read data generated by Bruker spectrometers.

  OPC technology enables to select optimum process control or visualization software, without depending on any supplier.

- **Plug and play data exchange**

  Another advantage is the time reduction realized by lower system integration costs. OPC avoids the need of costly customer software integration. OPC provides plug-and-play software and hardware components from a variety of automation software, device and system suppliers.

By the ease of integrating plug-and-play (connectivity) the PC technology develops, beyond hardware I/O, to ever more complex control and business systems. DCS, SCADA, HMI, plant scheduling, maintenance and others.

In general, a communication can easily be realized. Any kind of data are displayed as simple tags which can be grouped.

- **Multi-client access**

  OPC facilitates data distribution, e.g. you can use the same data for HMI and the process control system and store them in one database. Thus, everybody can have access to process-related data and the widespread use of OPC results in substantial information sharing across multiple applications at the same time.

- **Network capability**

  One major advantage of OPC is that distributed, client/server networking is made transparent to the OPC application. By DCOM the underlying network communication protocol is made transparent to the OPC client/server. DCOM may send OPC messages using a variety of transports such as UDP, TCP/IP and IPX with the same OPC applications.

  DCOM also handles retries and time-outs between an OPC client and a remote OPC server and tries to re-establish communications. This supports multi-user systems via intranet or internet. Remote data access, e.g. from different monitoring terminals is also possible.

OPC Background

The OPC standard data exchange is based on the generally accepted and well-established client/server architecture. Thus, multi-client systems of various manufacturers can be connected to a single server. Similarly, the standard also allows to connect servers of various manufacturers to a single client.

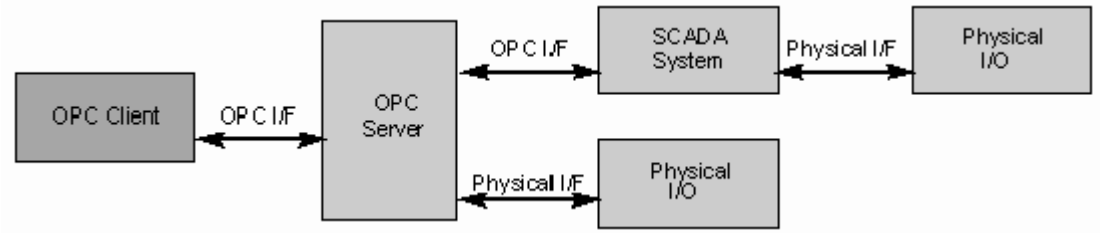


Figure 80: OPC client - OPC server architecture in an industrial information system

One OPC server operates as driver for each hardware feature. Data are read and prepared for visual interpretation, control purposes or data storage by one or more OPC clients.

The process management is also performed by an OPC client. Additional functionality implemented as OPC client may be SCADA HMI software (Supervisory Control And Data Acquisition; Human Machine Interface).

These systems are connected to OPC servers via a computer network (LAN).

They exchange data that are, if required, further transferred from/to sub-systems using OPC servers.

- **OPC Interface**

  The OPC specifications include OPC Data Access providing real-time data access as well as OPC Alarm & Events providing information on specified events and alarms to OPC clients.

  Figure 81 shows several programming language possibilities to develop a client application - C/C++, Visual Basic, Delphi, etc. Each OPC specification has 2 different approaches. To implement OPC using C/C++, use custom interface and to implement OPC in a Visual Basic application, use automation interface. Generally, but not unconditionally, OPC servers are written in C/C++.

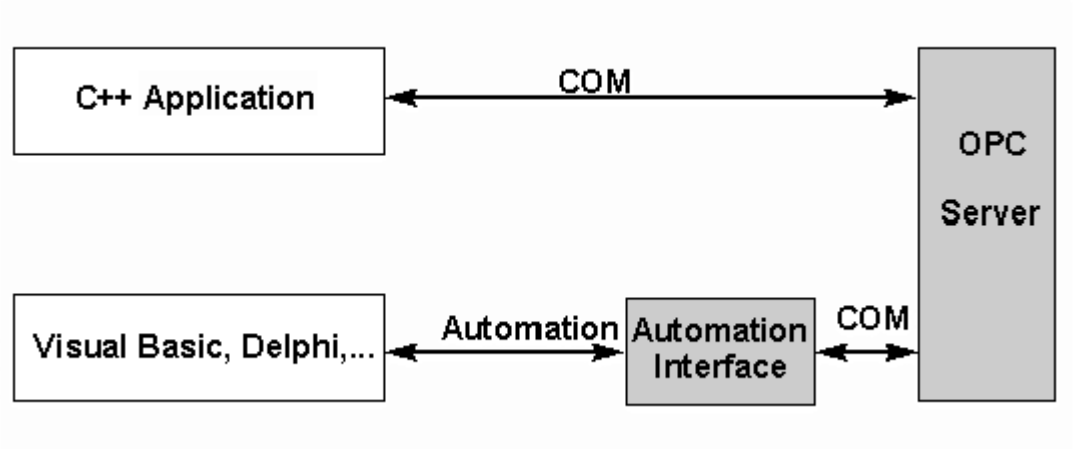


Figure 81: OPC scheme to use the automation interface wrapper connection link

One of the essential components of OPC communication is the COM layer and its network version DCOM. DCOM is a standard component included in the Windows NT 4.0, Windows 98, Windows 2000 and Windows XP operating systems. Windows 95 allows an additional installation of DCOM. All these systems allow OPC data transmission both on a single PC and a LAN basis. The OPC standard is also implemented to Linux applications.

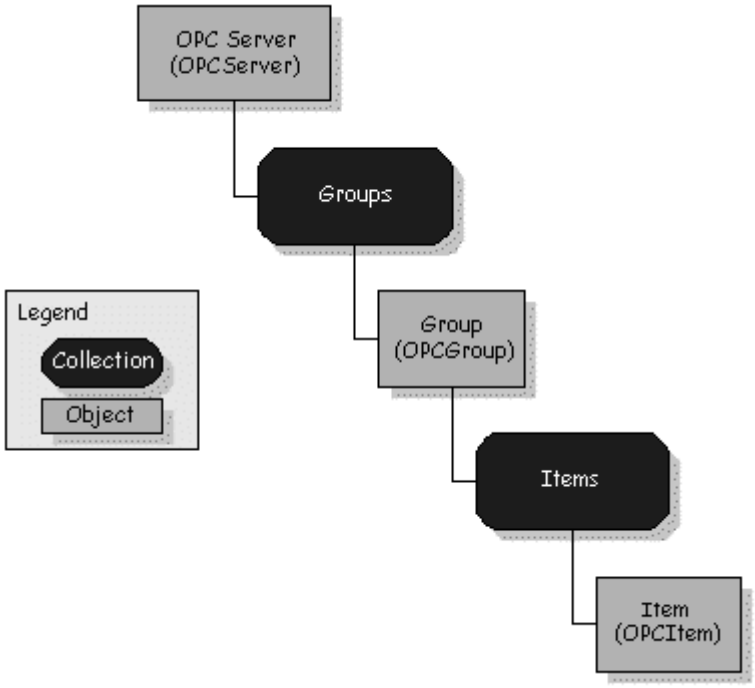


Figure 82: OPC object hierarchy chart

The object-orientated hierarchy chart of an OPC server is shown in Figure 82. The server sends items to the outside world which can be organized in groups.

- **OPC Server**

  Before connecting the OPC server to a process it first has to be connected to a PC or LAN. If you connect an OPC server to an OPC client, the COM technology allows the searching of the OPC list of servers installed on the respective computer. This enables a fast and simple connection to an OPC server. The searching is also called OPC server browsing.

  In the second step the process data from the OPC server configuration are connected to the OPC client configuration. OPUS PROCESS supports data browsing. These data can easily be connected to the OPC client after the OPC server address-space has been searched.

OPC in OPUS

How can this more general introduction be related to OPUS? By the use of the process package, OPUS becomes both an OPC server and an OPC client.

- **OPUS as server**

  The server is an integral part of the measuring device in the OPC context. OPUS PROCESS collects spectral data, evaluates them and indicates the result as an OPC process data. These process data are available to all clients involved in the system.

  Some data are always displayed while the availability of other depends on the setup of the process control scenario. The instrument

status is one piece of information that is always displayed, whether a process control scenario is running or not. So, the process control system can always test if the spectrometer is ready or if it is in warning or error condition. This status is indicated by the green or red light in the OPUS status bar. For more information on this diagnostics output, refer to OPUS Reference Manual.

The complete programming interface is another item always displayed. It is not routinely used in normal process control, but it offers the full C/S functionality for the experienced programmer.

The *normal* items a process control system will read are automatically created by OPUS PROCESS for all channels defined in the running scenario. If a channel is defined as QUANT result of a given component, you do not need to care about any OPC setup - the item is always there.

- **OPUS as client**

  OPUS PROCESS can also act as an OPC client for several reasons:

  OPUS PROCESS can query data from other OPC servers. In this case OPUS *is* the process control system and will get the data from other devices e.g., temperature controllers. The data are shown in OPUS and can be stored and processed as normal OPUS files.

  The OPC client side can detect changes in data items of other servers. This mechanism is used for external triggering, i.e. by writing a value into one of its items another OPC server will trigger OPUS PROCESS to collect a new background etc.

  OPUS PROCESS can write into items of other OPC servers, e.g. in environments with multiple OPC servers. This feature is also useful in case of process control systems that are not yet based on OPC, e.g. in case of existing Modbus or Profibus systems. To realize the connection to these systems an interface board (hardware) is needed. Today, all modern suppliers deliver these devices with corresponding OPC servers.

Appendix B

Paths

The basic path for each process control scenario is:

<OPUS Program Path>\Process\<Script Name>.obs

In this path reference files are stored. For each channel a background measurement will be stored, i.e. a measurement without a sample in the sample compartment. The ratio between the sample and background measurement results in the reference measurement. When performing reference measurements, make sure that optimal conditions are given as these reference measurements are the basis for all subsequent measurements.

The appropriate reference file is always loaded prior to each sample measurement. If a new reference measurement is stored, the file name or extension of the old reference file will be incremented. Reference measurements are stored by the following names:

Channel<Number>.0

Although it is not absolutely necessary we recommend to store all the files belonging to a particular scenario in a single directory and sub-directories. Make sure that the following features are stored:

- Data
  All the spectra measured and data saved by automatic naming.
- IDENT
  Suggested location to store IDENT or search libraries as well as conformity test methods or multi evaluation methods.
- Scripts
  VBScripts or macros called by external triggers.
- Log
  Log file storage location.
- QUANT
  Suggested location to store QUANT method files. If you are using QUANT after IDENT, the QUANT files will have to be located in this sub-directory.
- Reference
  Location where the reference spectra are automatically stored.
- XPM
  Suggested location to store experiment files associated with each measurement.

OPC Time Server

This is an OPUS accessory program. It will be installed during the normal OPUS installation, but you have to run it once to register it as OPC server. If you have registered the program, it comes up whenever you open an OPUS OPC server selection box (figure 36) or any other application which allows to browse through the installed servers.

This server has been mainly used

- as test server and
- to trigger time-repeating events.

If you try to read values from other OPC servers, you have to access the example server. You can read out random values or count the seconds. The server can also display a message that can be written by a client. The message can be used to test the extended data export capabilities or to see how it is assigned to an alarm level. A server message box indicates that the error has been communicated.

The other application area of this server is to trigger periodical actions, regardless of the current measurement cycle running. If you want a certain test to be performed daily, you have to assign the date item of the server to an external control. If these data change, i.e. every new day, an event will be triggered and, e.g., a script or macro running the desired instrument test will be started.

The server includes the following items

Year
The year of the current date.

Month
The month of the current date.

Day
The day of the current date.

Hour
The hour of the current time.

Minute
The minute of the current time.

Second
The second of the current time.

Random
Random number (to be up-dated every second).

Message
This item can be written and will generate a message box indicating the written value.

Limitations

Apart from the computer memory there is no basic limit on the number of channels that can be used. You can freely define the number of measuring points or QUANT components. However, one single view will only display up to 16 channels. If you define not more than 64 channels, two or four views in one window will be used automatically. If you really need more channels, you have to split the process into two or more scenarios that can be executed in parallel.

GMP Considerations

If you work in a validated environment, refer to the 21CFR Part 11 compliance of OPUS (see OPUS Reference Manual). The 21CFR Part 11[1] regulation describes in detail how to use signatures to release QUANT or IDENT methods, and explains the audit trail stored in the measured files.

Error Messages

There are several kinds of problems that might occur during a process control run. Spectrometer problems have to be automatically diagnosed by OPUS. The errors can be reported to a process control system in the status item of the OPUS OPC server.

1. Regulation issued by the United States Food and Drug Administration, Federal Register 62, n. 54 (1997), for Electronic Records and Electronic Signatures

There are several kinds of error:

- **Green:** OPUS status = 0

  The process run is **OK**.
- **Yellow:** OPUS status = 1

  Indicates a **Warning**, but the measurement process can continue without any problems.
- **Red:** OPUS status = 2

  Indicates an **Alarm**. Usually in case of hardware problems. Depending on the type and location of the error, measurement data may neither completely nor partly be generated.
- **Yellow + Red**: OPUS status = 3

  Indicates a **Warning and** an **Alarm**. No measurement data can be generated.

In case of instrument maintenance requests the same status, warning or alarm items are used. An instrument maintenance request may occur if the lifetime of a component, e.g. the source, has just expired. The error messages will not interrupt the measurement cycle, although it might not be sensible to perform a measurement.

If the process runtime system is not able to perform a measurement or detect any other kind of problem, this error will be recorded in the log file. In this case it is tried to restart the measurement at the beginning of the next cycle. This may cause further errors, however, OPUS PROCESS tries to continue in spite of temporary error conditions. Regardless of the cause for this runtime error a special bit indicating this error will be set in the instrument status and is therefore available for the process control system.

There might be a few cases when OPUS PROCESS is unable to recover an error and calls Dr. Watson. In this case send or e-mail the *drwtsn32.log* file together with the log files of your scenario to the Bruker Technical Support for troubleshooting.

Try to provide as much information as possible, e.g. what sequence of events took place prior to this error.

Safety Instructions

A technical instrument like a spectrometer can occasionally break down. Several tests are performed inside the spectrometer and with OPUS, to frequently check the source, the laser etc. If the lifetime of one of these components nearly expires, this will be indicated by an instrument warning status. However, these error and warning indicators do not automatically guarantee that the spectrometer and OPUS are functioning correctly.

Furthermore, it is not possible to use OPUS PROCESS to test whether the output signal is of correct amperage. The user has to ensure that there is no cable damage or noise affecting the output signal.

When working with OPUS PROCESS make sure that the entire process control systems works properly, especially after breakdowns.

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