

PROCHEM

User manual



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Table of contents

1. PRESENTATION	5
1.1 Basic functionalities	5
1.2 Sampling management	5
1.3 Recovery of additional data	5
1.4 Analytical calculations	6
1.5 User interface	6
1.6 Alarms	6
1.7 Backup and filing	6
1.8 Data transmission	7
1.9 Compatibilities	7
2. PROCHEM CONFIGURATION	8
2.1 The Instrument menu	9
2.2 The Sampling menu	12
2.2.1 Configuration	13
a) Selection by electrovalves	14
b) Selection by series multi-position valves	15
2.2.2 Vici valve serial control	15
2.2.3 Stream	17
2.2.4 Auxiliary commands	18
2.2.5 Alarm input	19
2.3 The Module menu	20
2.3.1 Remote module	20
2.3.2 TES module configuration	21
2.3.3 Analog inputs	25
2.4 The Alarms menu	26
2.4.1 Property	26
2.4.2 Options	27
2.5 The Settings menu	28
2.5.1 Options	28
2.5.2 Calculated value	29
2.5.3 Report\Company	29
2.5.4 Report\Certificate	30
2.6 The Maintenance menu	31

3. USING PROCHEM	32
3.1 Sequence management	32
3.1.1 Sequence table	32
3.1.2 Auxiliary commands	34
3.1.3 Scheduler	35
3.1.4 Control	36
3.1.5 Assignment	36
3.2 Analysis launch	37
3.3 Analysis printing	39
3.4 Selection of displayed results	39
3.5 Alarms	40
3.5.1 Alarms acknowledgment	40
3.5.2 Definitions	40
3.5.3 Options	41
3.6 Parameters	42
3.6.1 Export file	42
3.6.2 Trends	44
3.6.3 Average	46
3.6.4 4-20 mA analog outputs	47
3.6.5 User program	48
3.7 Display	48
3.8 Coupling between two sessions	49
3.9 About ...	50
3.10 RGA calculations	51
3.10.1 Component names and values	51
3.10.2 Calculation selection	51
3.11 Excel calculations	52
4. USING THE MODBUS MODULE	53
4.1 Software installation	54
4.2 Software configuration	54
4.2.1 Configuring the communication parameters	54
4.2.2 Modbus addresses	55
4.2.3 Options	59
4.3 Process menu	59
4.3.1 Connect sub-menu	59
4.3.2 Exit sub-menu	59
4.4 View menu	60

4.4.1 Display select sub-menu	60
4.4.2 Selection of displayed values	60
4.5 About menu	61
4.6 Features	62
5. APPENDIX I : MANAGING DIRECTORIES WITH OPENLAB AND PROCHEM	63
6. APPENDIX II : MANAGING USERS' NAME WITH OPENLAB	64
7. APPENDIX III : COUPLING WITH MSD CHEMSTATION AND MASS HUNTER	66
7.1 Software installation	66
7.2 Use with Mass Hunter	66
7.2.1 Analyses launch	66
7.2.2 Transfer of results	68
8. APPENDIX IV : USING PROCHEM WITH A MARKES THERMAL DESORBER	72
8.1 Prochem configuration	72
8.1.1 Instrument menu	72
8.1.2 Sampling/Configuration menu	73
8.1.3 Auxiliary commands menu	74
8.2 Using Prochem	75
8.2.1 Event table	75
8.2.2 Analysis sequences	76
8.2.3 Launching analyses	76
9. APPENDIX V : DESCRIPTION OF THE PROCHEM DATABASE	77
9.1 Definition of tables (information and common)	77
9.2 Definition of the tables for each sample line (stream)	78

1. Presentation

Prochem is a workstation supervision software of Agilent Openlab Chemstation, MSD Chemstation and Mass Hunter, which allows you to increase the functionality of your analyzer in order to use it in "online" mode.

Prochem is used to control analysis sequences, either in continuous or in delayed mode and to allow complete control of a sampling system with different devices. It can receive some analog signals to insert them into the analysis results.

Prochem also simplifies the operator interface and the visibility of results by minimizing the actions required by the user thanks to programming of integrated calculations, integration of external sensors...

By favoring the integration of Agilent Technologies laboratory chromatographs in an industrial environment, Prochem enables to combine process operation requirements and analytical performance.

1.1 Basic functionalities

- Possibility to control up to 16 sample streams via multi-position valve or electro valve.
- Programming of analyses sequences allowing to define, for each analysis, the selected stream, the analysis method, the number of injections and the sequence of events (auxiliary commands).
- Possibility to program the sequences to launch a certain number of analyses, a sequence, continuous analyses or a sequence at a given time (example: Sequence 1 at 2 p.m., Sequence 2 at 4.30 p.m. or verification scheduled every week at a fixed time).
- Possibility to change sequence following an alarm of components, to launch a specific software in order to signal the information.

1.2 Sampling management

- Intelligent stream change management: Prochem anticipates the following selection during the current analysis to optimize the analysis time. It can also select a purging stream after injection.
- Possibility to control pumps or auxiliary gas ejectors with a programmable pumping time thanks to an event table.
- Possibility of atmospheric pressure or isolation of the sample.
- Possibility of waiting for an external action on a logic input (hardware ready waiting, injection waiting...)

1.3 Recovery of additional data

Prochem allows you to retrieve signals from different sensors or additional analyzers such as pressure, temperature, flow rate or values from an external analyzer (NO_x, H₂O, etc.), by reading analog inputs, of Keller or Bronkhorst flow sensors or by Modbus. It is possible to set alarms on these signals and thus to prohibit or not the start of analyses. It is also possible to send these values via Modbus.

At the time of injection, Prochem can retrieve the values of these sensors or analyzers and integrate them into the analysis results ; they can then be used in post-analytical calculations. These values can be viewed in reprocessing mode.

1.4 Analytical calculations

Prochem recovers the values calculated by the integration method:

- Retention time
- Peak area
- Raw concentration
- Peak height
- Any additional result (temperature, pressure)

to perform programmed calculations.

Calculation results can be included in the final report for printing.

Possibility of specific calculations: NGA/RGA according to ISO 6976:1995 or GPA 2261 and GPL according to ISO 8973/ISO 7941/ISO 6578 or customized calculations.

1.5 User interface

Prochem allows you to visualize :

- All results in the form of a table.
- All results in the form of trends: up to 8 graphs of any value over time by stream of analysis.
- Calculation of hourly or daily average or over a programmable range (0-9999 h).
- When used with OpenLab ChemStation, it is possible to have two sessions on the same computer. These two sessions can be coupled to synchronize the injections on the two chromatographs. In this case, the results can be grouped together in a single results file.

1.6 Alarms

Prochem allows you to:

- Program 16 concentration alarms on all peaks. Examples:
 - o Pre-alarm at 10 %, then Alarm 2 at 15 %, etc.
 - o Alarm on the sum of known peaks or the sum of unknown peaks
 - o Alarm on the calculations performed
 - o Alarm on any other read value

These alarms display the results in red color on the screen.

As an option, Prochem can associate these alarms with relays.

- Change the analysis sequence (method or sampling stream) if an alarm is present. It is also possible to launch a post-program to send a message by email or SMS for example.

1.7 Backup and filing

Creation of archive files by stream as and when analyses are performed. Date and time of injection in hourly format and different results (Excel® compatible).

When used with Mass Hunter Data Analysis, it is possible to export the results in PDF format. In all cases, the generated PDF files can be transferred to remote servers.

1.8 Data transmission

As an option, Prochem can communicate all results in ASCII file, 4-20 mA, Modbus, Profibus, Profinet.

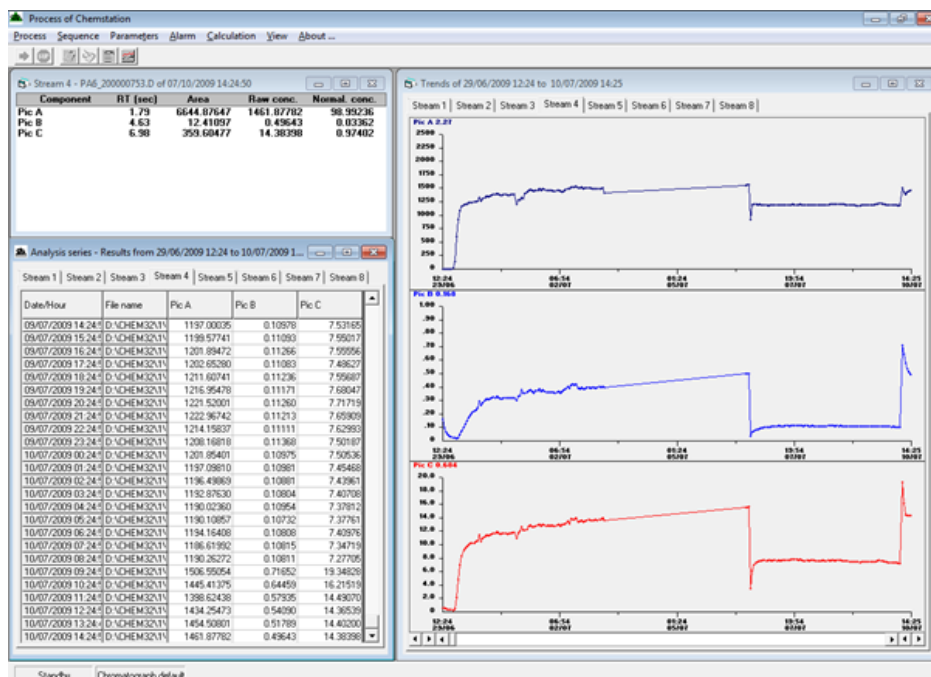
1.9 Compatibilities

Prochem is compatible with the following software versions:

- Chemstation GC B.04.03 and previous versions
- Openlab CDS Chemstation C01.10 and previous versions
- Chemstation MSD E.02 and previous versions
- Mass Hunter for GC/MS with Data Analysis, version B.07.06/Build 7.06.0.0.2704 and previous versions

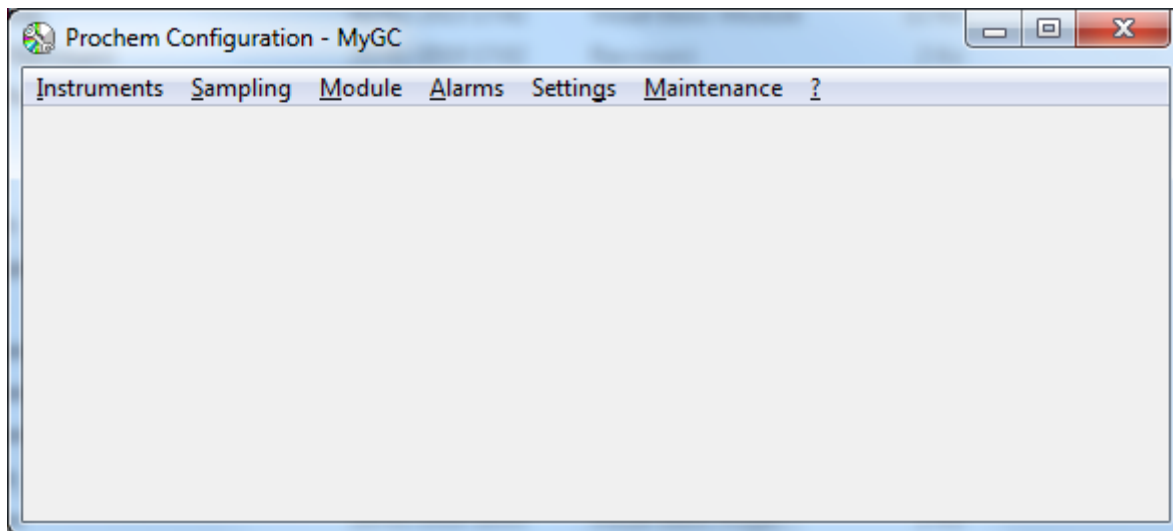
Prochem is compatible with the following instruments:

- GC Agilent 5890, 6890, 6850, 7820, 7890, 8860 and 8890
- MSD Agilent 5973, 5975, 5977
- Interface 35900^E
- Hplc 1260

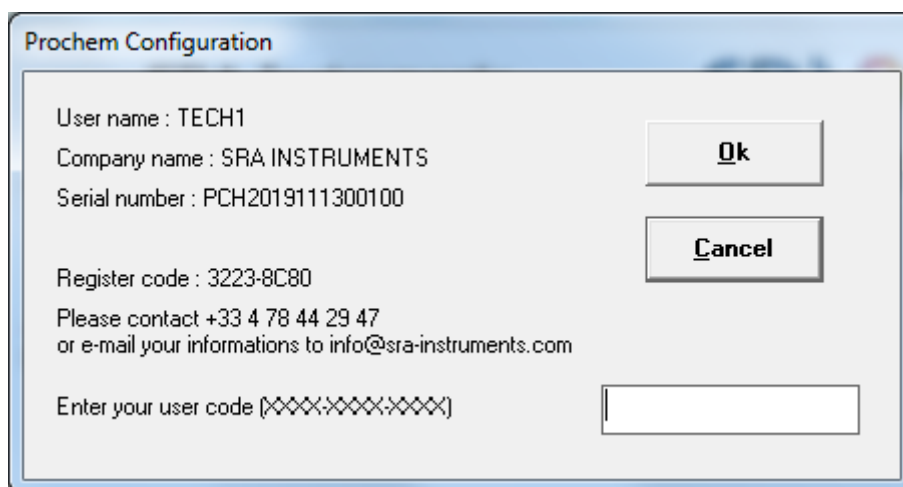


2. Prochem configuration

The Prochem Setup software in the PROCHEM installation directory allows you to define all parameters. It can be called by the Start / Programs / SRA Instruments / Prochem Setup command.



If the option "Using Prochem without a protection key" is activated, the following window appears in order to enter a user code.



Contact SRA Instruments and give the information that is displayed in this window. In return, we will provide you with a user code to enter in the field without omitting the dashes separating the different elements constituting this code.

Warning: In case of hard disk failure or replacement, you will need to contact SRA Instruments for a new code.

2.1 The Instrument menu

From version 3.0.0, Prochem can control one or two chromatographs with OpenLab ChemStation. With MSD Chemstation or Mass Hunter, if you have installed several instruments on the same computer, you must make a choice.

The "**Instrument\Chromatograph n°1**" sub-menu allows you to choose one of the analyzers that will be controlled by Prochem.

'Repeater of GC Ready' : This option allows you to transmit the state of the analyzer (ready/not ready) to another instrument by activating (or not) the relay defined according to the state of the analyzer.

'Remote start' options : These options allow an external system (PLC, supervisor or other) to transmit an analysis start command to Prochem either via a logical input (define the module and its logical input), or by a DDE command (External Command, 'Start' command)).

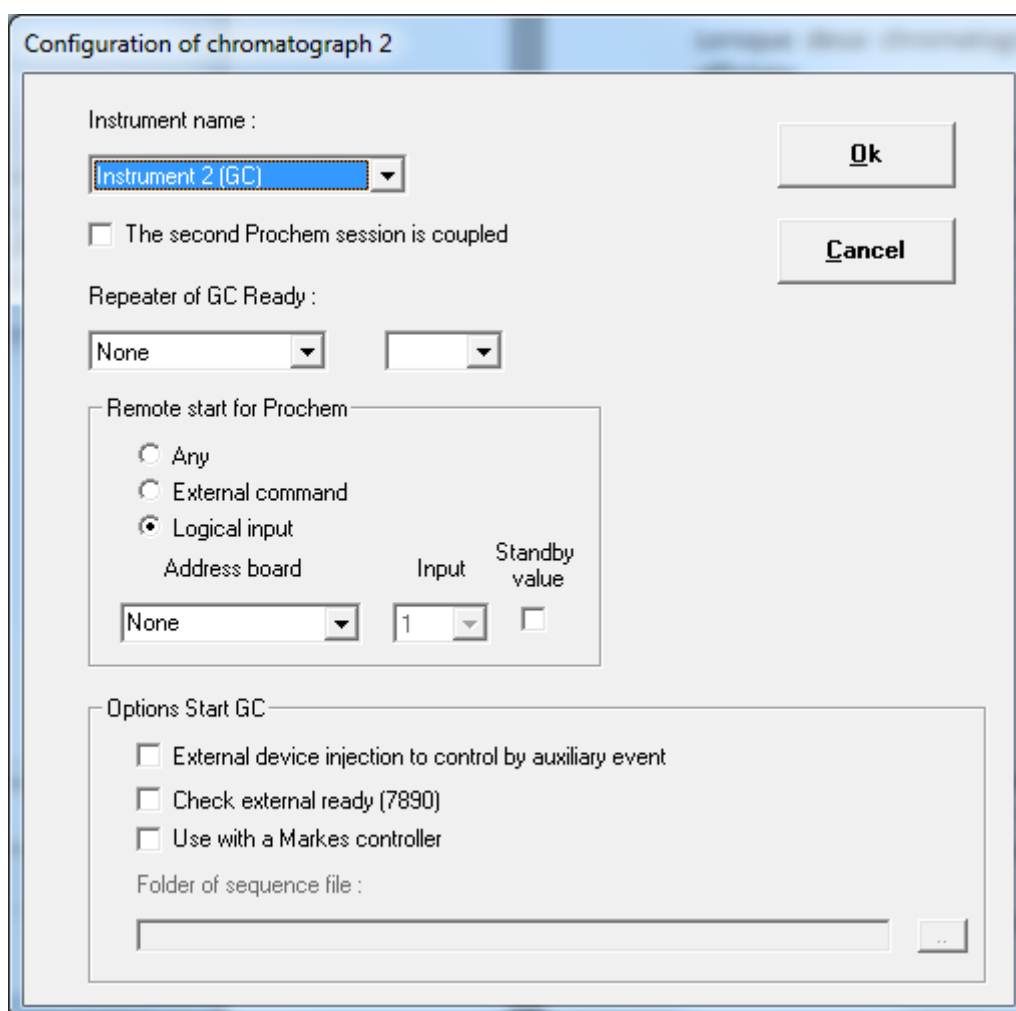
'External device injection' option : This option allows Prochem to manage the analysis launch differently according to particular cases. If Prochem is used with Chemstation (or Openlab Chemstation) on an instrument equipped with an automatic injector or controlled by an external program, Prochem will have to start the injection cycle and wait for the start that will be sent by the passer. In this case you must check

this box. However, if the instrument uses a sampling valve (GSV), the system works by itself, this option is not necessary, and the box should not be checked.

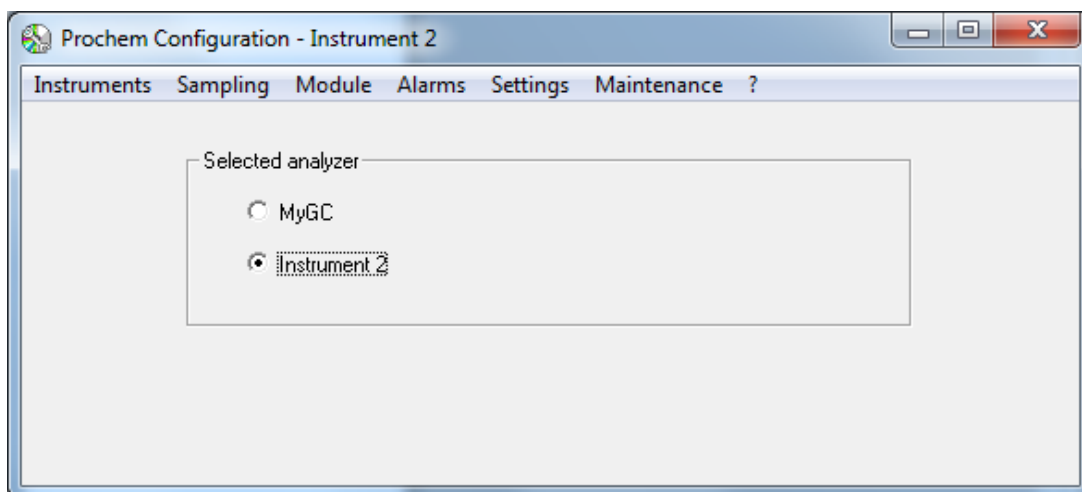
'Check external ready' option : This option is enabled if the chromatograph used is a GC7890. It makes it possible to wait until an element external to the chromatograph is ready to launch the analyses.

'Use with a Markes controller' option: This option is to be activated when an On-line thermal desorber of the Markes brand is coupled to the chromatograph. In this case, Prochem retrieves the stream number injected by the sample multiplexer and stored in the 'sequence.csv' file generated at each new sequence. It is then necessary to fill in the storage directory of these files. It is also important to check the option 'Automatically export sequence report file' in the Settings menu of the Markes software, tab 'Sequence options'.

The **"Instrument \Chromatograph n°2"** sub-menu allows you to choose the other analyzer that can be controlled by Prochem and, possibly coupled.



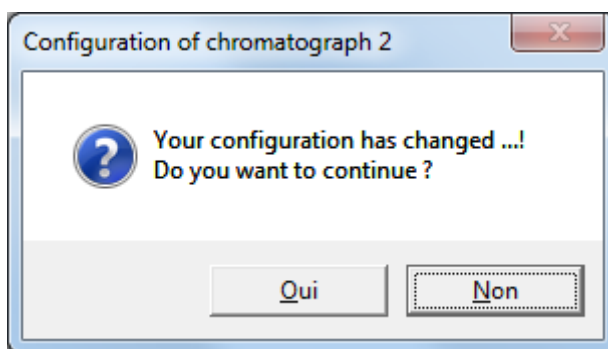
When two chromatographs are configured, a selection on the main window is displayed.



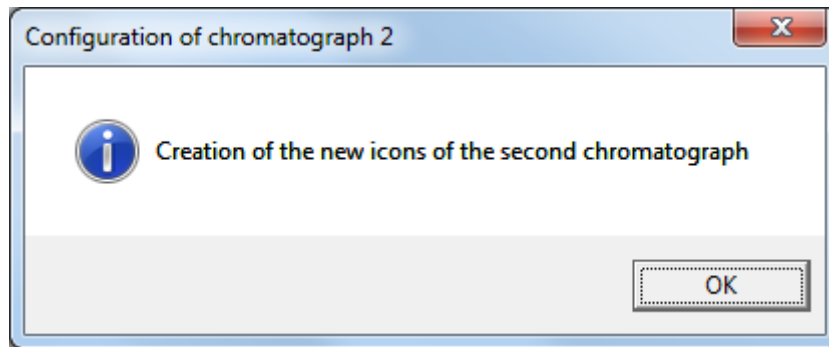
This selection allows you to choose the instrument to be configured. These two configurations are dissociated : if they use serial ports to communicate to different modules, they must have their own serial port.

If the option '**The second session is coupled**' is selected, the two sessions are coupled and the analyses can be started at the same time. The results are retrieved at the master session (chromatograph n°1) when both analyses are completed.

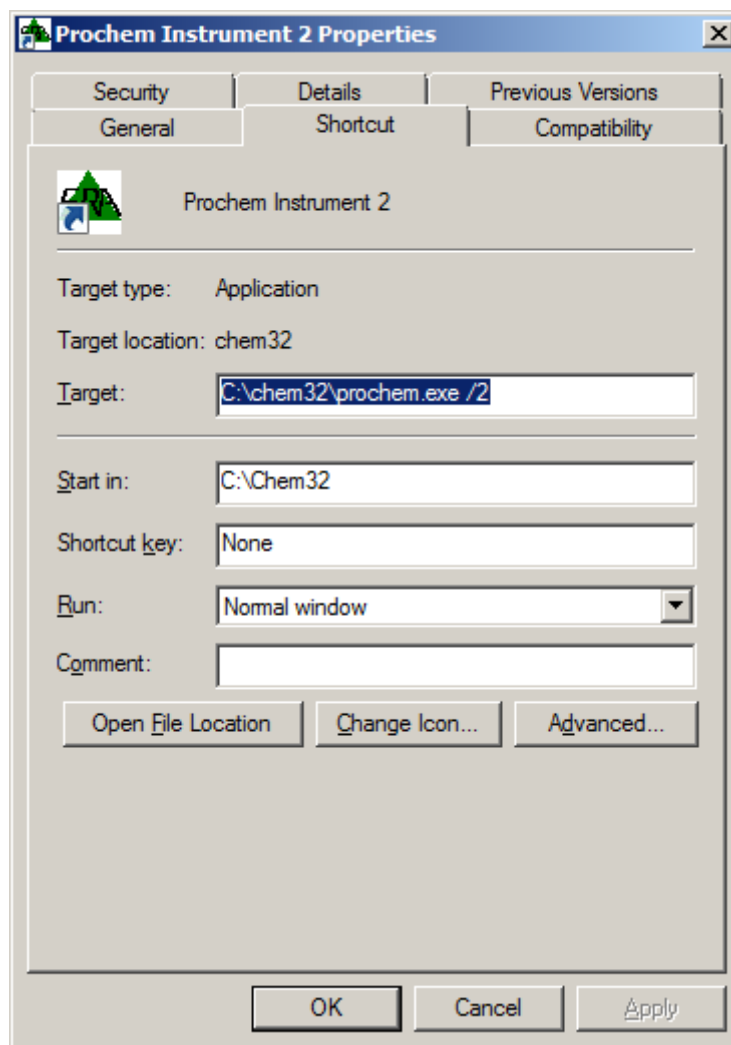
After entering the name of chromatograph n°2 and confirming, the program asks you to confirm the new configuration.



If you validate, a shortcut on the 'Windows' desktop is created to launch this second session.



If you accidentally delete this shortcut, simply create a shortcut on the Prochem executable and add the term '/2' to the property of this shortcut preceded by a space.



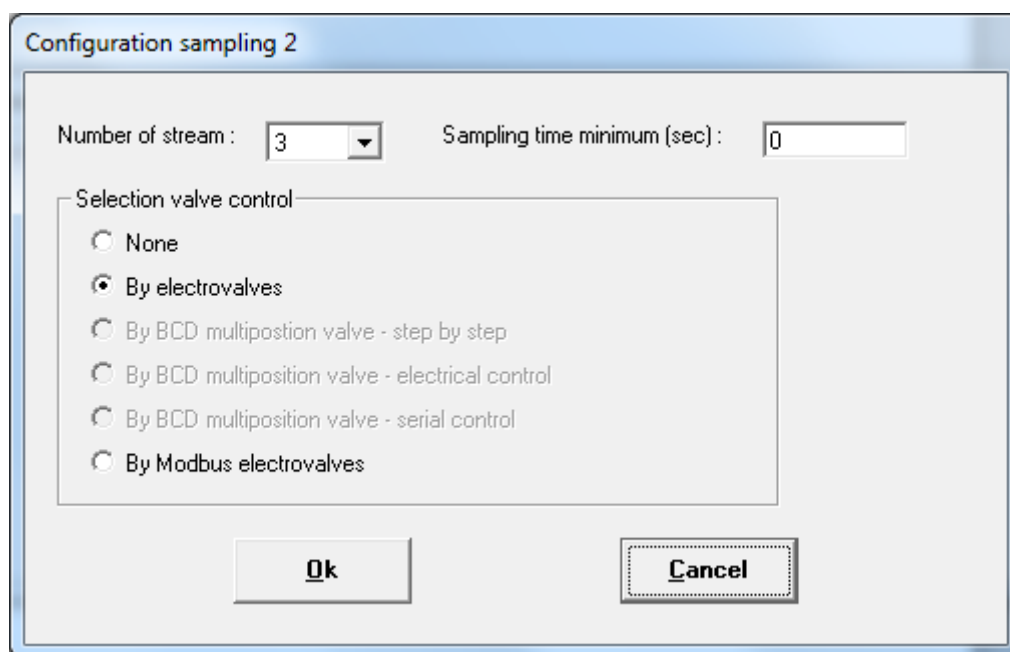
2.2 The Sampling menu

Before performing the configuration, check that you have selected the correct instrument.

2.2.1 Configuration

Be careful, the selection of samples is an option of the Prochem software therefore the following description is valid only in the case where this option is present in the protection key.

Note: Each instrument has its own configuration ; if the two sessions are coupled, you must configure the control system on the first instrument but it is important to enter the same number of streams and names, on the second instrument.



Prochem can control up to 16 sample streams:

- either by electro valves
- either by multi-position valves. These can be managed either by reading in BCD and advancing step by step, by reading and positioning in BCD or by Valco type valve controlled by serial link.
- or by sending an order by Modbus.

When using the BCD, your computer must be equipped with a logical I/O card.

The '**By Modbus electrovalves**' option is available only if the Modbus option is activated and the corresponding application is launched. In this case, the address corresponding to the stream number must be entered manually in the file Prochem.ini with a text editor type Notepad in the section 'Chromato x' where x corresponds to the analyzer assignment number in the Agilent workstation and under the variable 'Stream address y' where y corresponds to the stream number.

Example for the case where addresses are defined as bit:

[Chromato 1]

Stream address 1 =51	Stream address 5 =55
Stream address 2 =52	Stream address 6 =56
Stream address 3 =53	Stream address 7 =57
Stream address 4 =54	Stream address 8 =58

Example for the case where there is only one common address as an integer:

[Chromato 1]

Stream address 1 =51	Stream address 5 =51
Stream address 2 =51	Stream address 6 =51
Stream address 3 =51	Stream address 7 =51
Stream address 4 =51	Stream address 8 =51

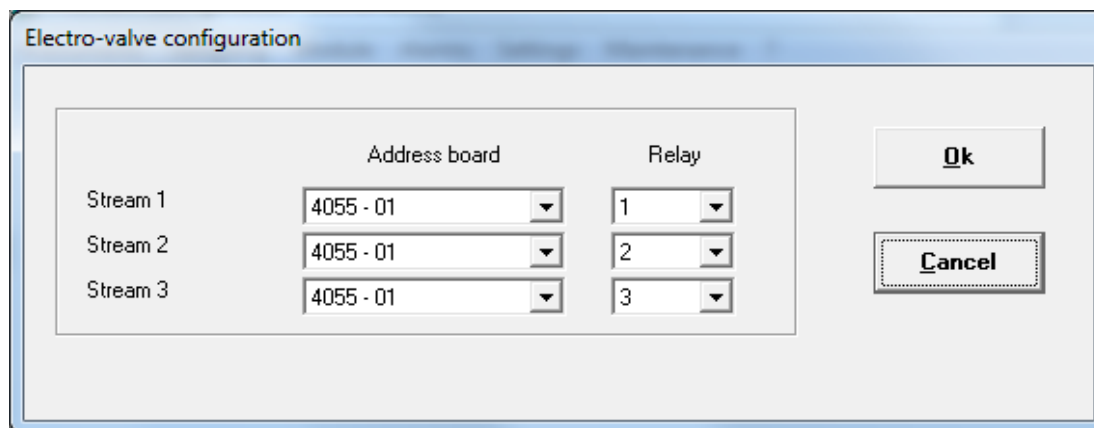
The '**Sampling time minimum**' field allows you to enter a default sweep time for each stream. This time is used when a sample line switch occurs just before injection. This ensures minimum sample sweeping prior to injection.

Select the interface type used for sample stream control and click on the "Ok" button.

Depending on the option selected, a new window will appear.

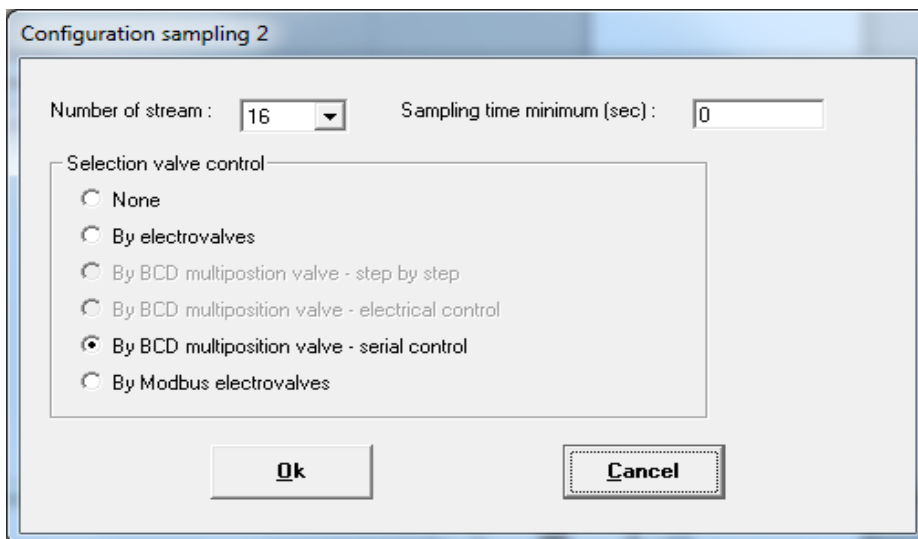
a) Selection by electrovalves

In the case of selection by electro valves, the following window is displayed:

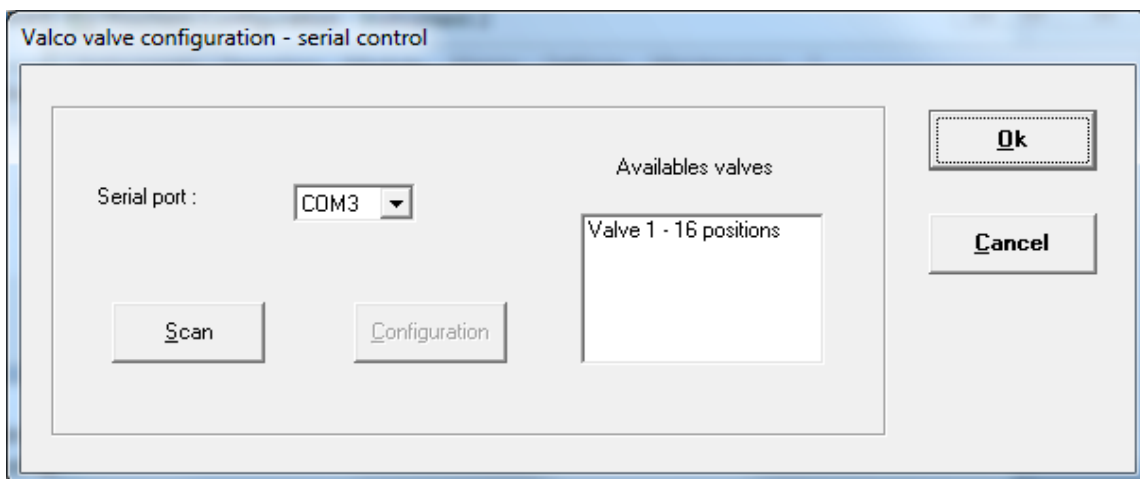


Select the board or control module and the relay number corresponding to the electro valve.

b) Selection by series multi-position valves



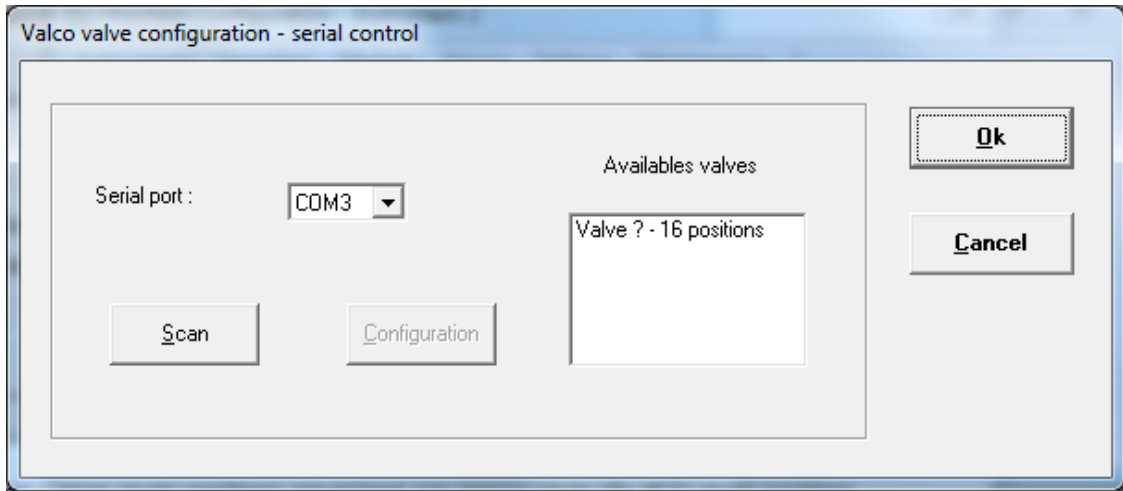
When selecting an electric multi-position valve via serial link (By BCD multiposition valve - serial control), the following window is displayed:



See the following paragraph for more information.

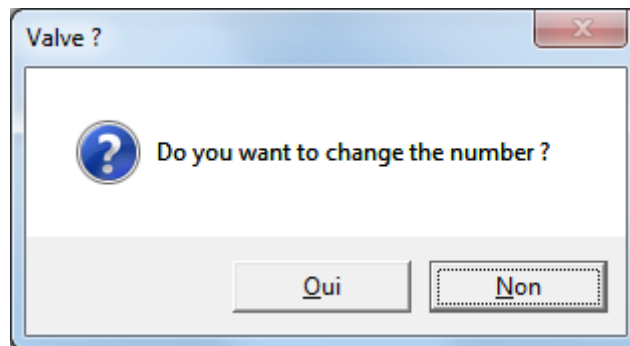
2.2.2 Vici valve serial control

The "Sampling\Vici valve serial control" sub-menu allows to configure the multi-position valves and the switching valves used by Prochem.

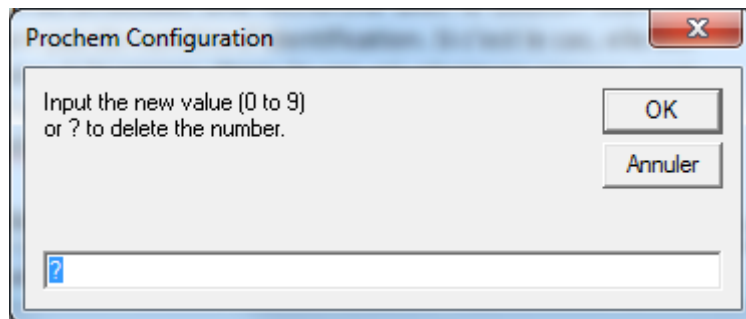


Select the serial port for communication and search with the Scan button. The search is first performed on valves that do not have an identification number. If this is the case, it is stopped to allow a number to be assigned to the valve. In case several valves are connected and without identification, it is necessary to carry out this search valve by valve. The detected valves are then displayed in the 'Available valves' list.

It is possible to change the identifier by selecting the valve in the list and using the 'Configuration' button. The following message is displayed:

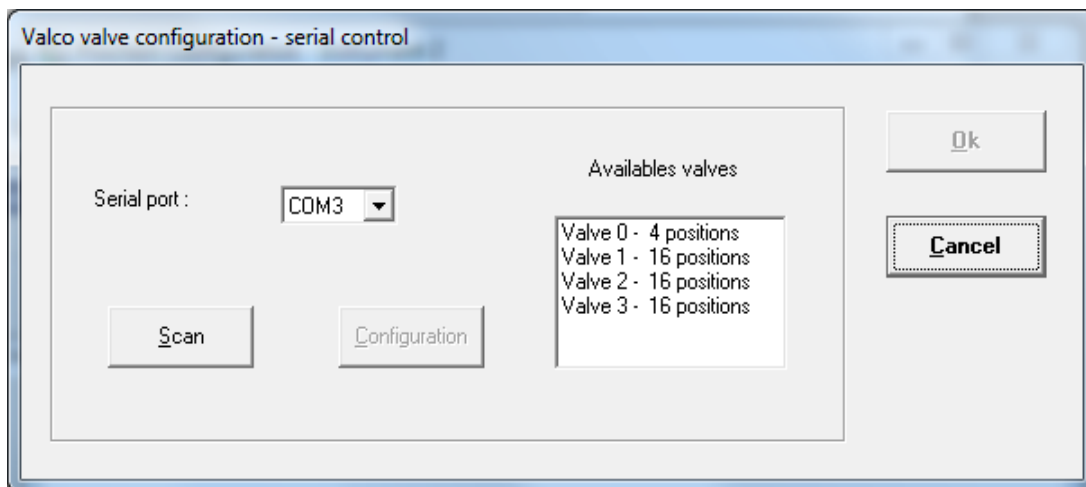


Confirm with Yes, a new window allows you to enter the number. You have the choice between 0 and 9 or ? if you want to delete the ID.



After validating with Ok, the software performs a new search.

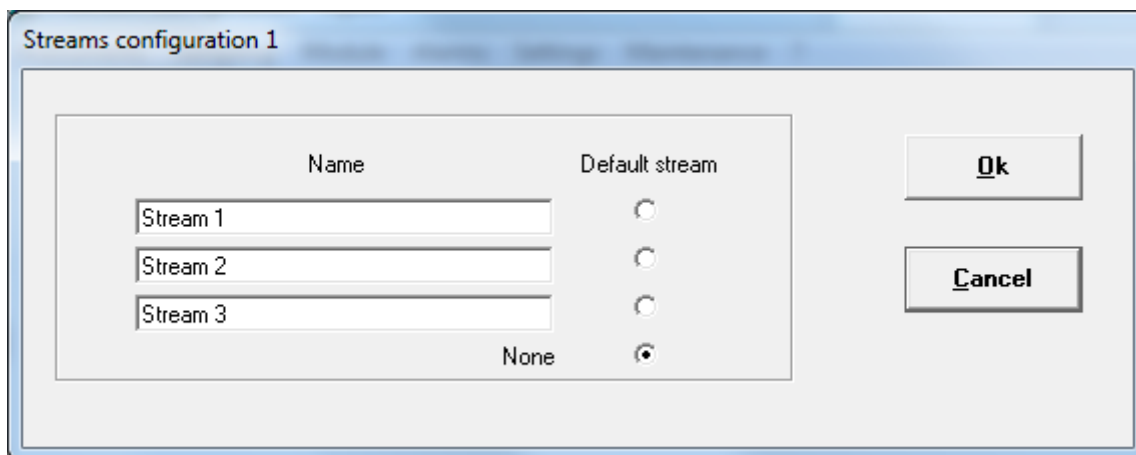
Note that there may be several multi-position valves and one of them may be used to select the others. In this case, this valve must have the identifier 0.



2.2.3 Stream

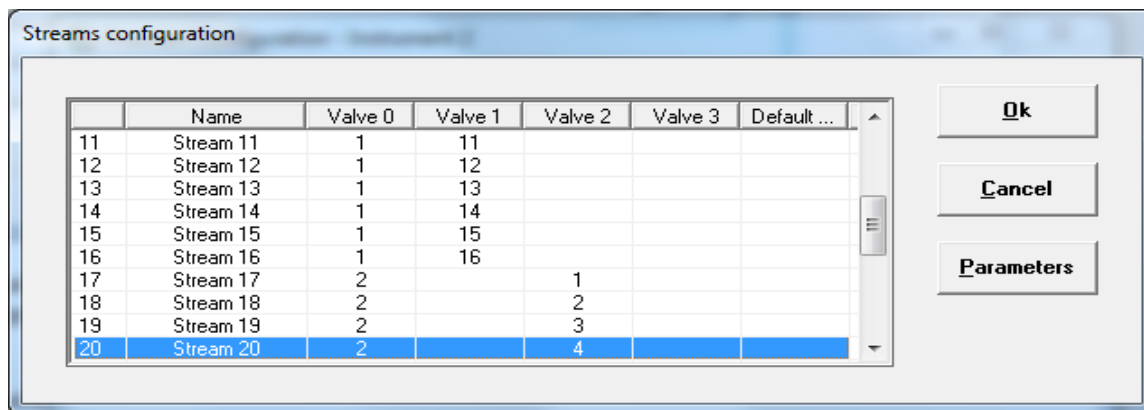
Once you have configured the sample stream selection interface, you can name the different streams via the "**Sampling\Stream**" sub-menu.

If you have opted for selection via electro valves, the following window appears:

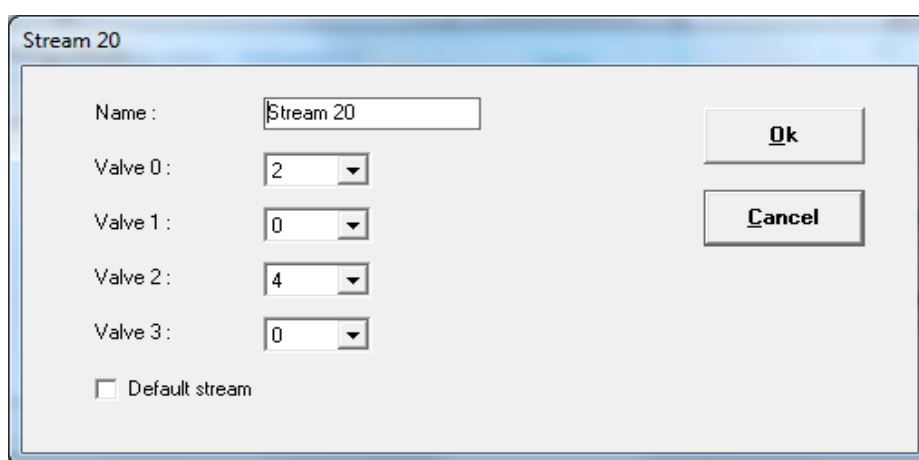


Enter the stream names and press Ok. The 'Default stream' option allows you to define if one of the streams is used as purge steam or default stream. If none of the streams is used, select the 'None' choice.

If you have opted for multi-way valve selection, the following window will appear:



The 'Parameters' button allows you to configure the parameters of each stream.



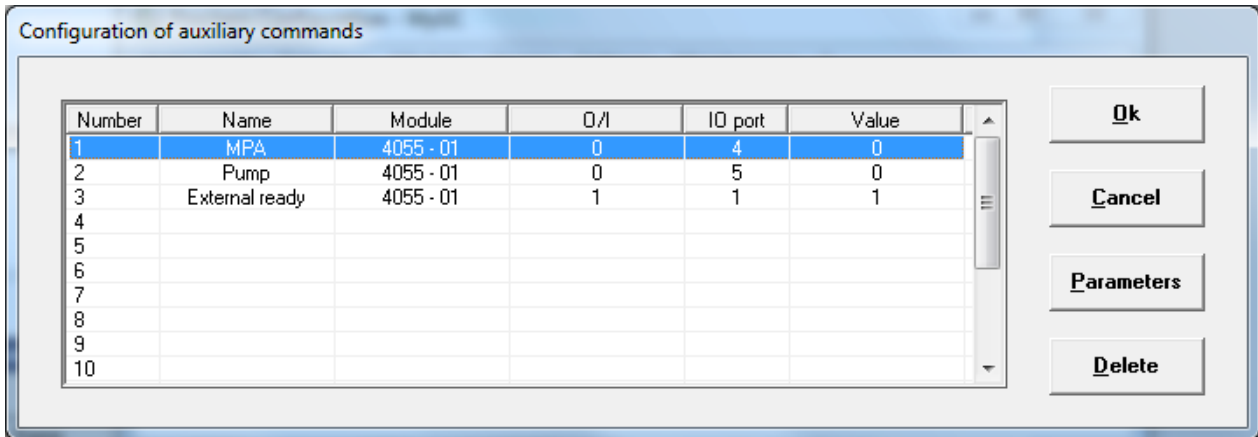
Enter the name and check the 'Default stream' option if this is the default stream. If the selection requires switching several multi-position valves, specify the positions of each valve.

2.2.4 Auxiliary commands

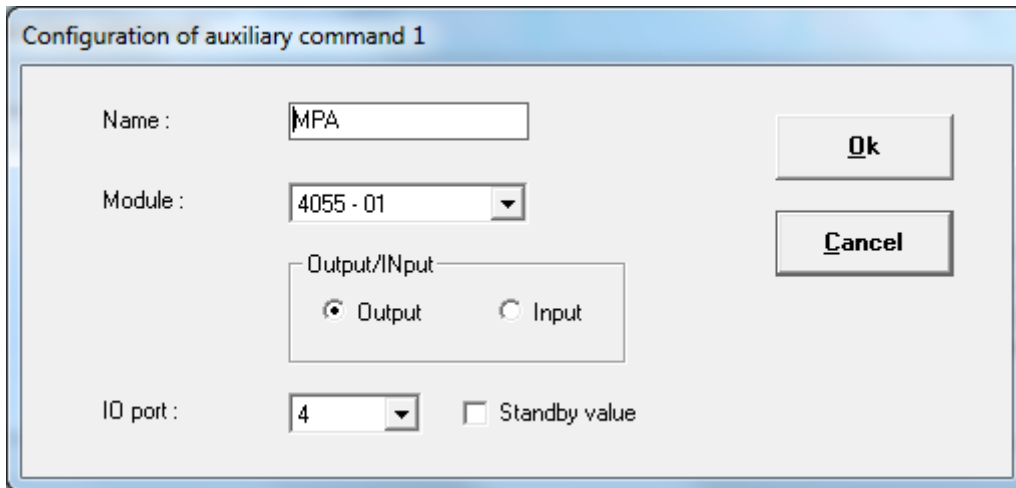
Prochem allows to control various commands before and after injection, such as suction pump, isolation valve or atmospheric pressure setting valve. Similarly, if the chromatograph is not equipped with an injection valve, Prochem can manage the start of the analysis.

In some configurations, Prochem allows to wait for an external action to continue the cycle.

For this, go to the "**Sampling\Auxiliary commands**" sub-menu ; the following window is displayed:



The parameters of these commands are accessible via the 'Parameters' button. Then simply select the control device, relay number or logic input number.



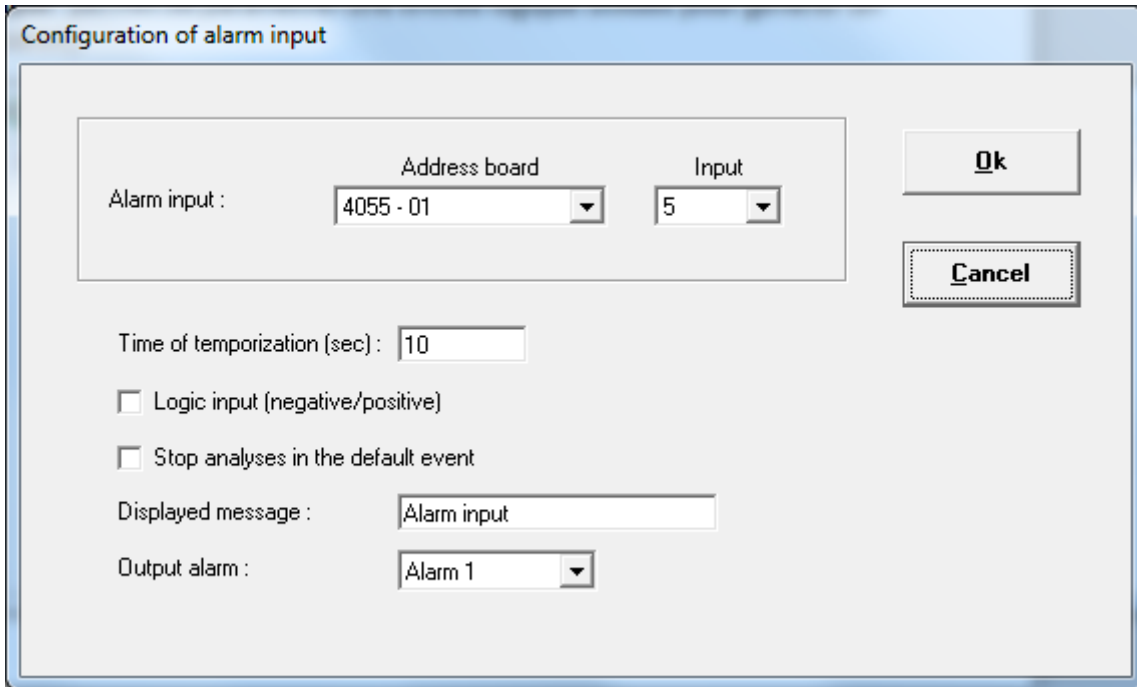
If the 'Output' option is selected, the configuration is for a logical output. If the 'Input' option is selected, it concerns a logical input.

The value 'Standby value' corresponds either to the idle state for a relay or to the value when the input is inactive.

2.2.5 Alarm input

The "**Sampling\Alarm input**" sub-menu makes it possible to set a logic input used to generate a fault (pressure or flow defect).

The following window allows you to define the different parameters of this alarm.



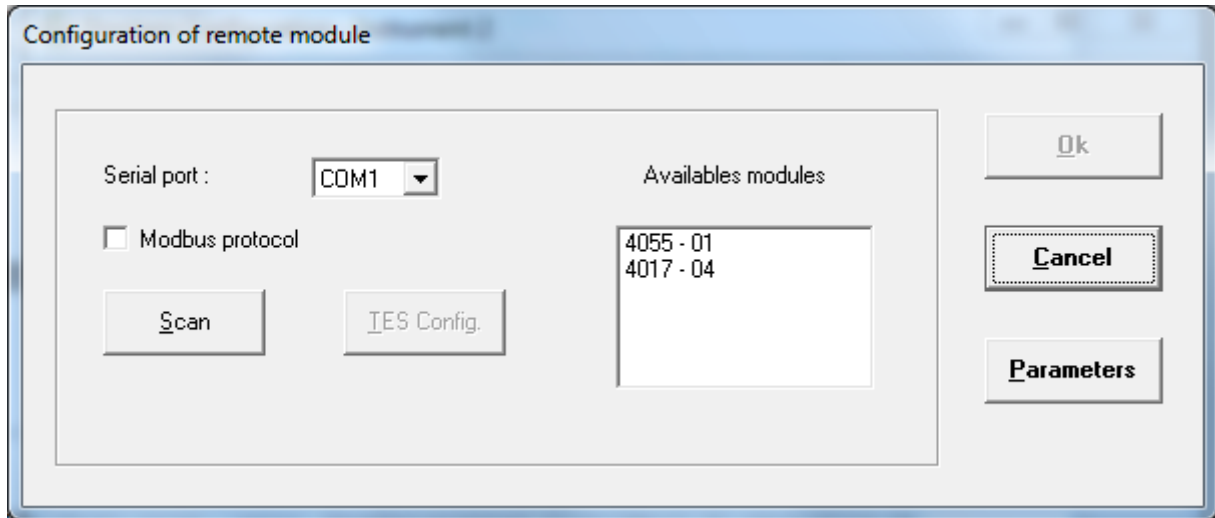
- Select the board or module and then the input used.
- The 'Time of temporization' timer is used to filter state changes to avoid untimely alarms.
- The checkbox 'Logic input' allows you to define the type of input (positive or negative) at idle.
- The checkbox "Stop analyses in the default event" allows you to stop the cycle in case of a fault.
- The message 'Displayed message' will be displayed in the Status bar in case of a fault.
- The 'Output alarm' field is used to define the alarm relay that will be activated in the event of a fault.

2.3 The Module menu

2.3.1 Remote module

Prochem uses either relay cards installed in the computer or remote modules such as Adam or TES. If the relay cards are directly detected by the software, it is necessary to search for the modules used.

The "**Module\Remote module**" sub-menu allows you to configure the serial port used to communicate with these modules.



Once you have selected the serial port you can search for the modules connected to the computer.

The 'Parameters' button is used to configure the communication parameters.

In the case of Adam modules, the protocol is 9600 baud, 8 data bits, no parity and 1 stop bit. The configuration of the Adam modules is done directly from the supplier's software.

If communication is in Modbus, check the option 'Modbus protocol'.

In the TES module frame, you must check the 'Modbus protocol' option and configure the communication parameters with the 'Parameters' button. Note, if the communication is in RS232, the parameters are 9600 baud, 8 data bits, even parity and 1 stop bit. These modules are configured using the Test button and only in RS232 (see chapter 2.3.2).

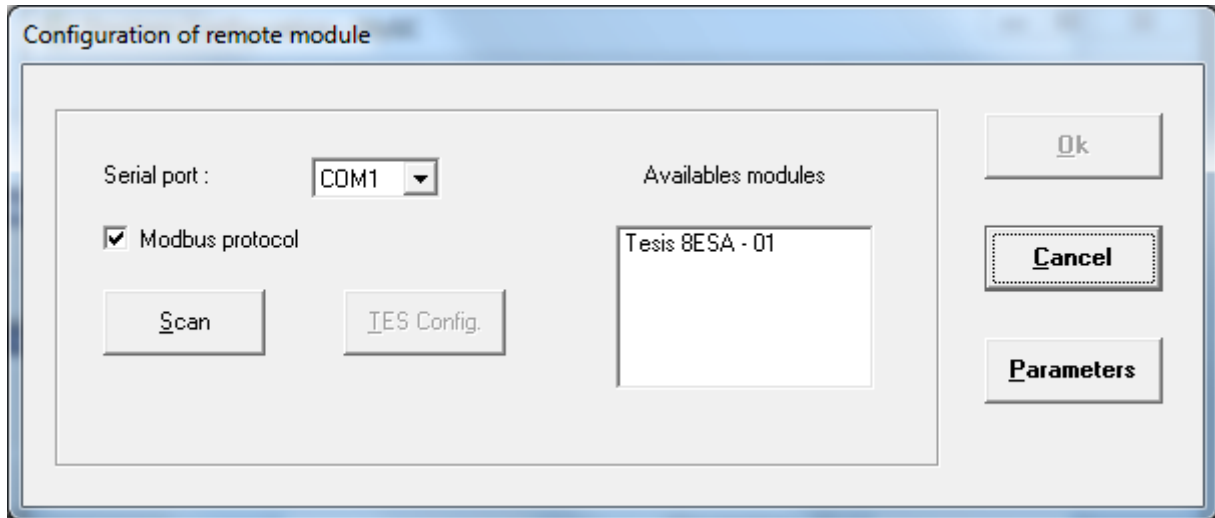
If you have connected Adam 4024 modules or a TES to the computer, you can transmit the results via 4- 20 mA analog signals. The values are selected directly from the Prochem software.

2.3.2 TES module configuration

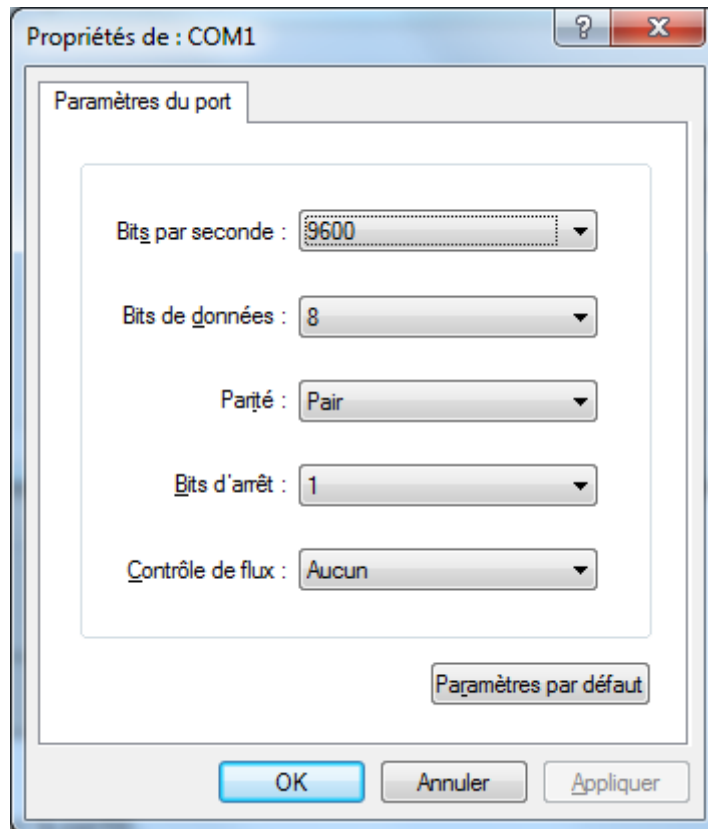
To configure the TES module, use the RS232 serial port.

From the Prochem setup software, select the "**Module\Remote module**" sub-menu.

The following window is displayed :

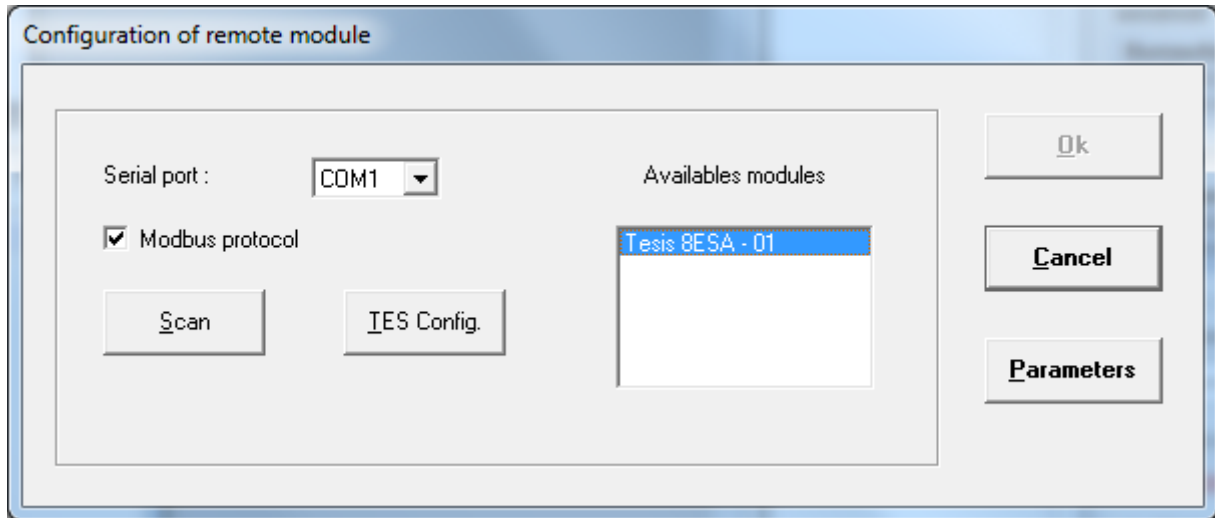


Check the 'Modbus protocol' box and verify the RS232 port parameters.

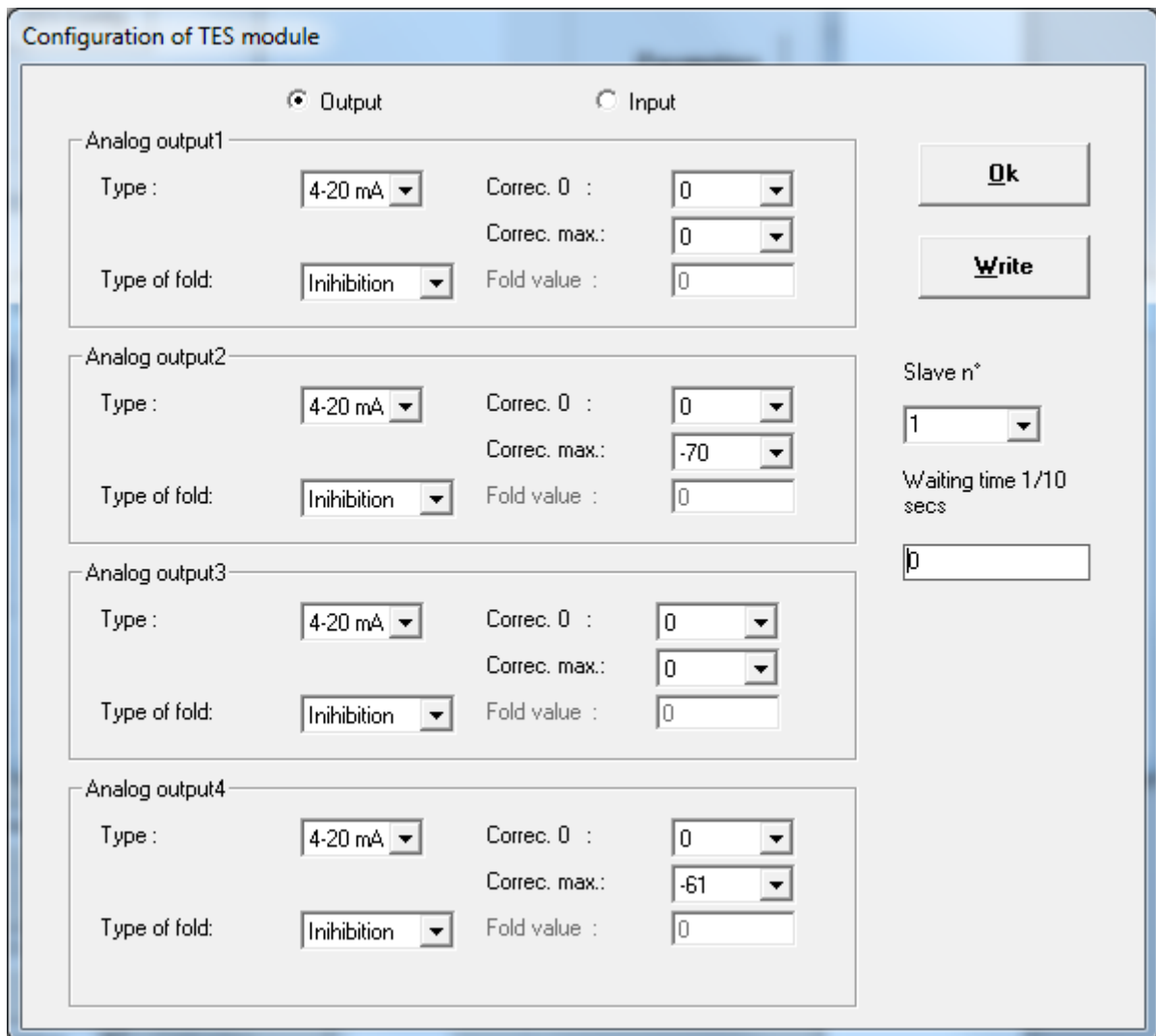


Warning: Select 'Even' for the parity.

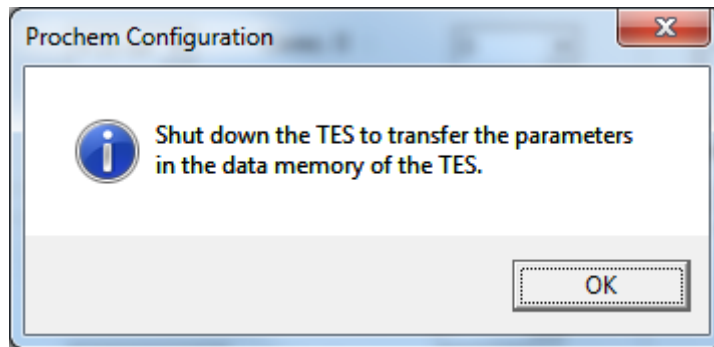
Then click on the 'Scan' button.



To configure the TES module, select it from the list and click on the 'TES Config.' Button

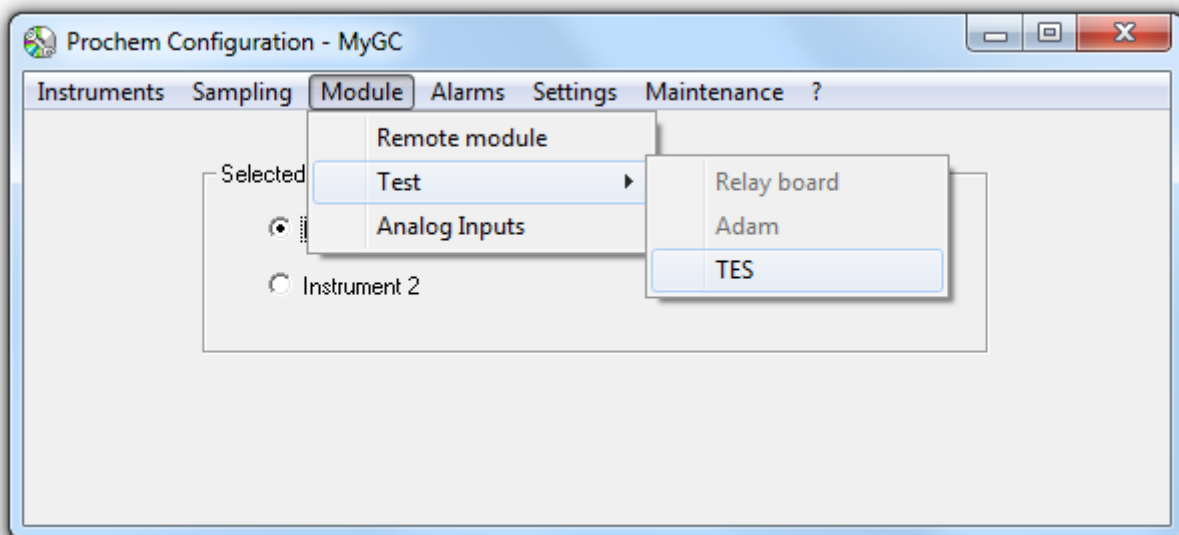


Change the various parameters (Analog output type, slave number, analog input type). The waiting time is only used with a RS485 serial link. It allows in the event of loss of dialogue (system blocking or loss of power of the computer) to activate or deactivate the relays and the Watchdog output of the TES.

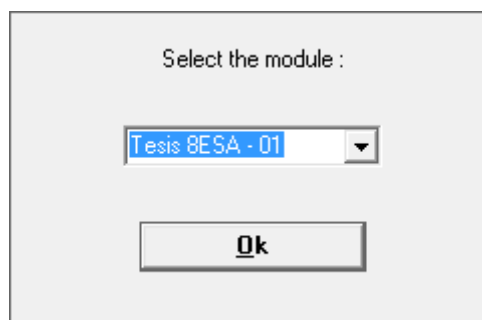


When all modules are configured, perform an on/off on the modules so that the changes are taken into account. If you are using a RS485 serial port, connect the TES to the correct port and scan again.

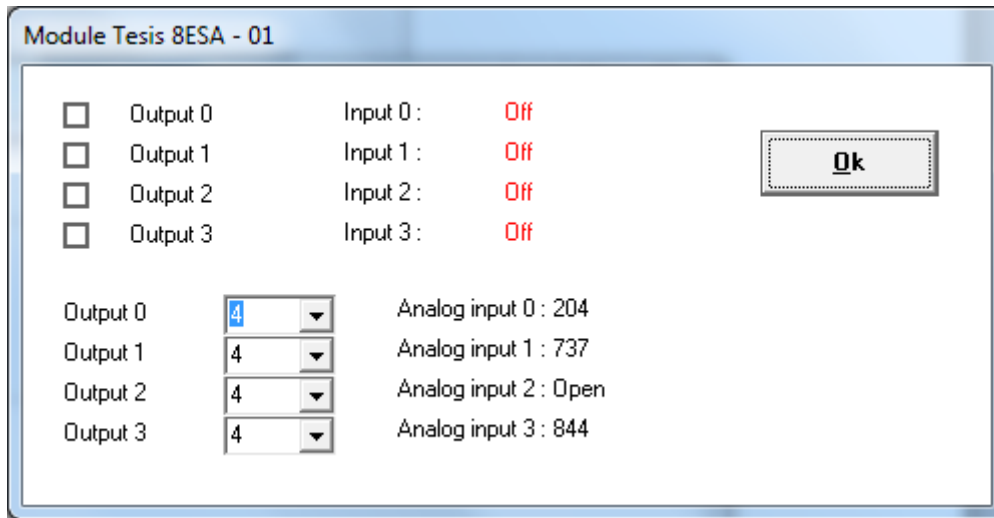
To test the TES module, select the "**Module\Test\TES**" sub-menu.



Select the TES module you want to test.



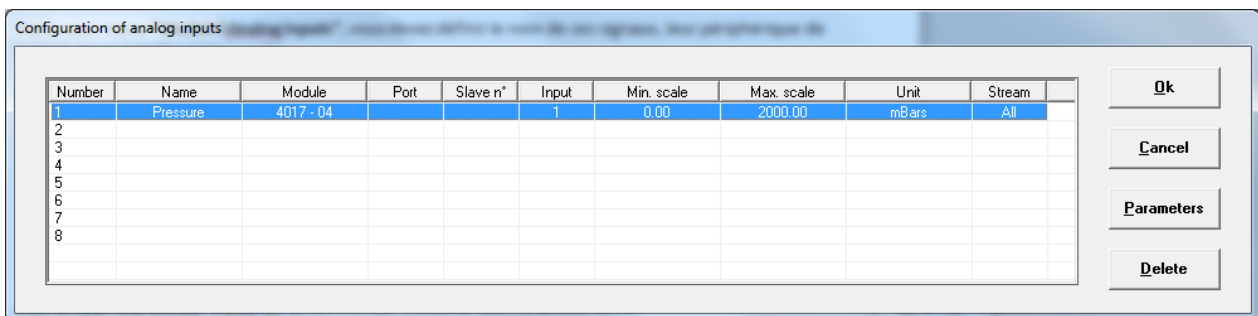
The following window is displayed:



2.3.3 Analog inputs

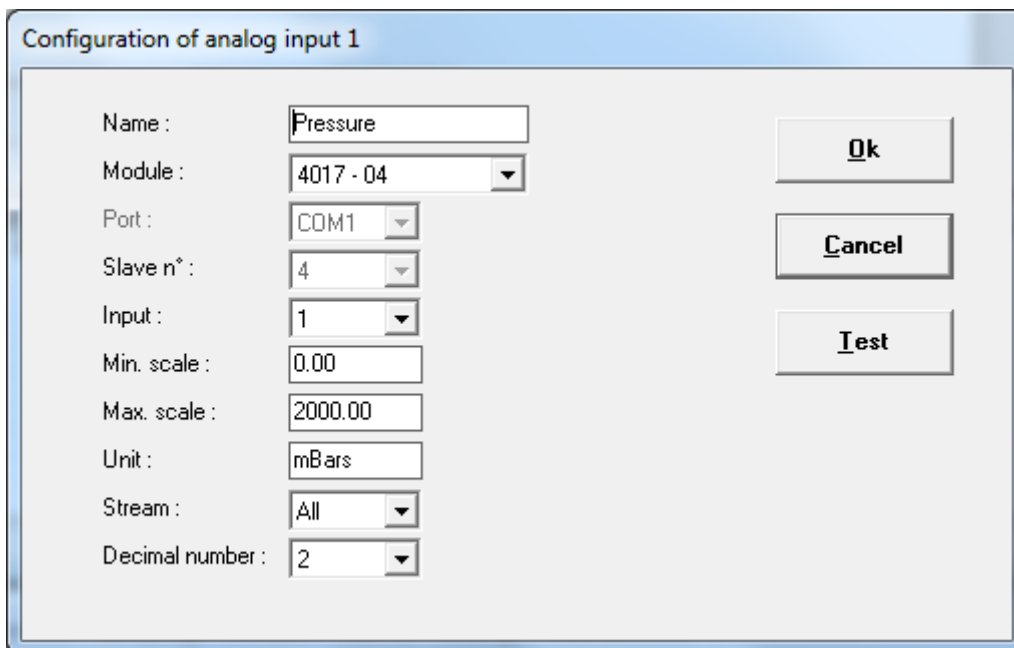
As explained previously, Prochem allows the acquisition of analog signals in order to integrate the value to analysis results.

Via the "**Module\Analog inputs**" sub-menu, you must define the name of these signals, their reading device, their scales and their unit.



To delete an entry, simply delete the name entered in the 'Name' field.

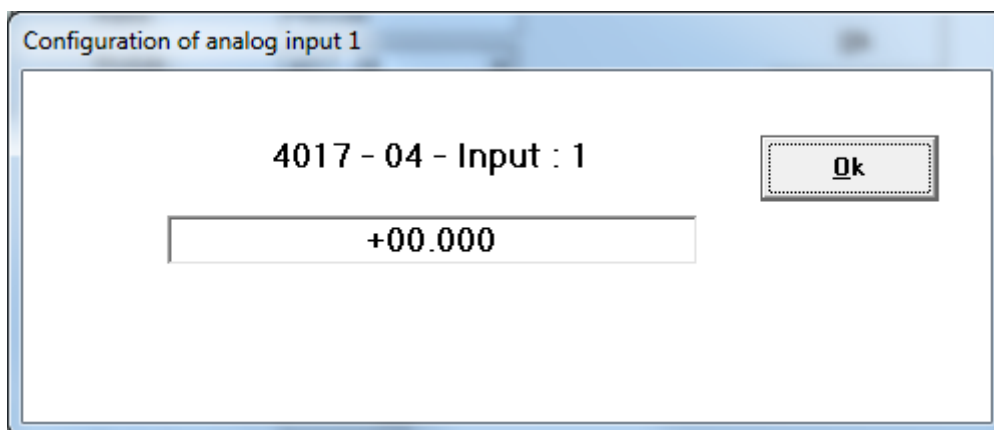
Select a line and click on the 'Parameters' button to define, modify the analog signal parameters.



The choice of modules can depend on the defined configuration: Adam module equipped with analog inputs or not, TES module. For sensors monitored with West 8010 modules, select the Modbus module and the address of the value read in the N° Input list.

For Bronkhorst modules, it is necessary to install the software from this supplier for dialogue with these sensors.

By clicking on the 'Test' button, the following window appears:



2.4 The Alarms menu

2.4.1 Property

In the "Alarms\Property" sub-menu, alarms can be set on the different values related to the detected components. Similarly, a general alarm (Alarm 0) can be generated in the case of a fault on the whole chromatograph-stream selection-stopped cycle-application.

	Address board	Relay
General alarm	4055 - 01	1
Alarm 1	None	1
Alarm 2	None	1
Alarm 3	None	1
Alarm 4	None	1
Alarm 5	None	1
Alarm 6	None	1
Alarm 7	None	1
Alarm 8	None	1
Alarm 9	None	1
Alarm 10	None	1
Alarm 11	None	1
Alarm 12	None	1
Alarm 13	None	1
Alarm 14	None	1
Alarm 15	None	1

You must assign a control device and a relay to each alarm.

2.4.2 Options

In the "Alarms\Options" sub-menu, the following window appears:

Display general alarm
 Positive logic for alarms
 Stop analyses if analog input alarm

Time before alarm if analyzes not carried out (mn):

Time before inhibition of alarms (secs):

It is not necessary to display the general alarm, uncheck the **'Display general alarm'** option.

'Positive logic for alarms' option : this option must be checked if the relay contact is to be opened on alarm.

'Stop analyses if analog input alarm' option: this option is useful if there are configured analog inputs. If the value of the analog input exceeds a programmed threshold, it is then possible to stop the analysis cycle, for example if the temperature of an oven is below a setpoint.

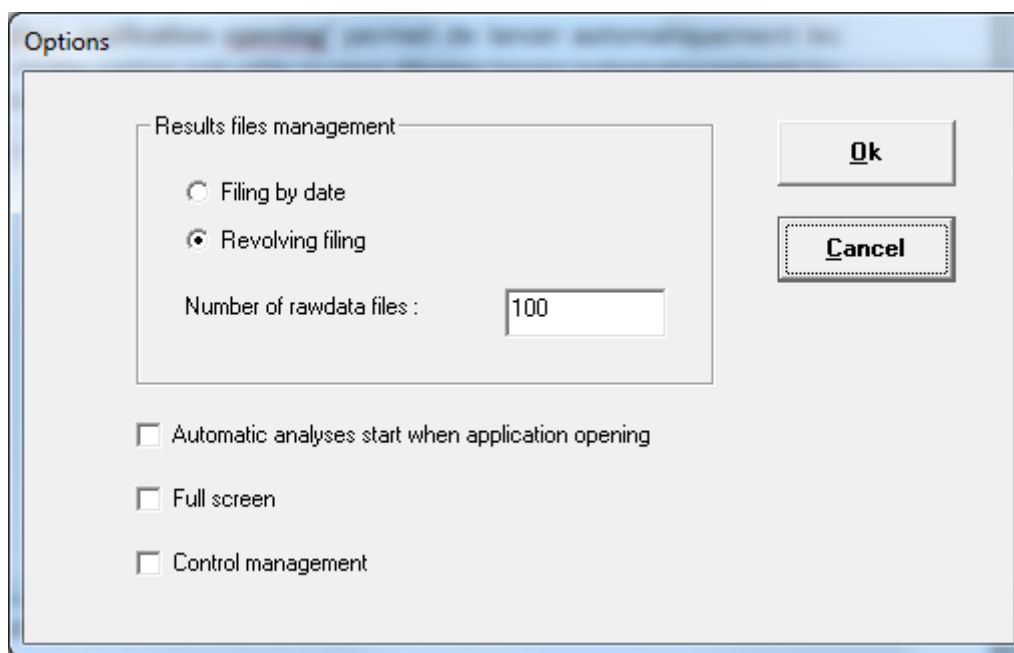
'Time before alarm if analyzes not carried out' : If no analysis has been performed after this time, Prochem generates an alarm. This option is used to generate an alarm if the chromatograph has a fault and it is unable to obtain its ready state.

'Time before inhibition of alarms' : If after this time the alarms have not been acknowledged, Prochem inhibits these alarms. This option is interesting if no action is to be taken in the event of an alarm.

2.5 The Settings menu

2.5.1 Options

Via the "Settings\Options" sub-menu, you can select the following different options :



The **'Results files management'** option allows you to define the name of the analysis files and the storage directory. It will be date dependent with the option 'Filing by date'. With the 'revolving filing' option, the directory is always the same but after a certain number, the counter is reset to 1.

The **'Automatic analyses start when application opening'** option allows to start automatically the analyses when Prochem is launched. This option is useful if you wish to automatically start the analyses after a power failure.

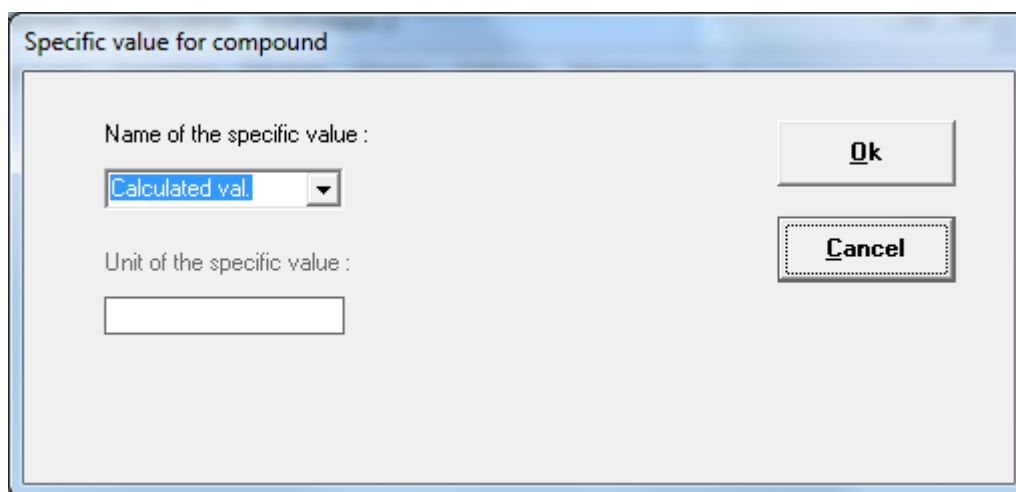
The '**Full screen**' option is no longer used.

The '**Control management**' option: By default, Prochem allows programming sequences at fixed times every day. By checking the 'Control management' option, this programming is modified, and it is possible to program a sequence at a fixed time, but the programming can be located after a certain number of hours (every day, every week, every month) to carry out a check for example.

2.5.2 Calculated value

The "**Settings\Calculated value**" sub-menu is used when there is a specific calculation performed in the Chemstation results processing macro.

For example, it can allow the calculation of a quantity in relation to a read flow. In this case, Prochem must take this calculation into account and display it in the results window.

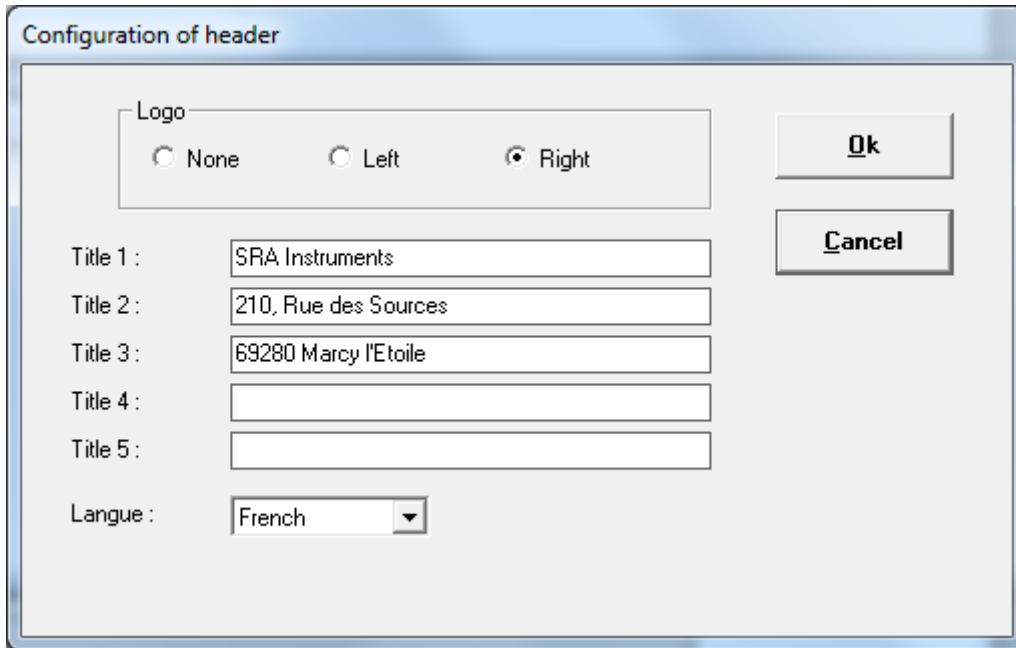


If no calculation is performed, it is then possible to display the height of the peak.

2.5.3 Report\Company

In some cases, it is necessary for the company name to appear when an analysis report is printed. It is then necessary to fill in the company's information.

This can be done via the "**Settings\Report\Company**" sub-menu ; the following window is displayed:

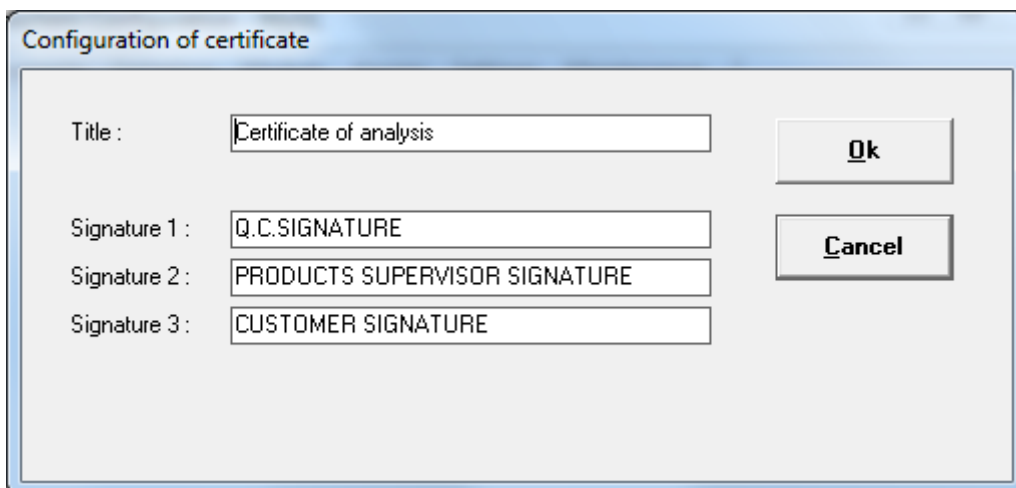


It is possible to add a logo to the print. The file must be in image format, must be in the same directory as Prochem and must be called 'logo.bmp'

Note, this menu is protected by password 0478442947

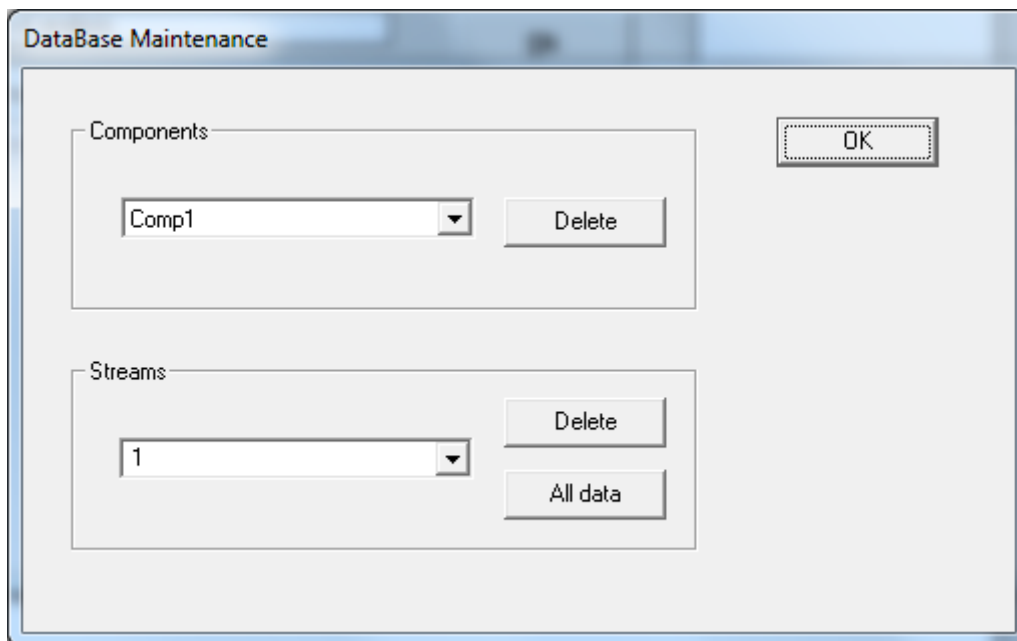
2.5.4 Report\Certificate

In some cases, it is necessary that the report be printed in certificate form. This sub-menu allows you to fill in the different fields of the certificate. Note that this menu is only visible if the 'Calculations' option is activated on the protection key.



2.6 The Maintenance menu

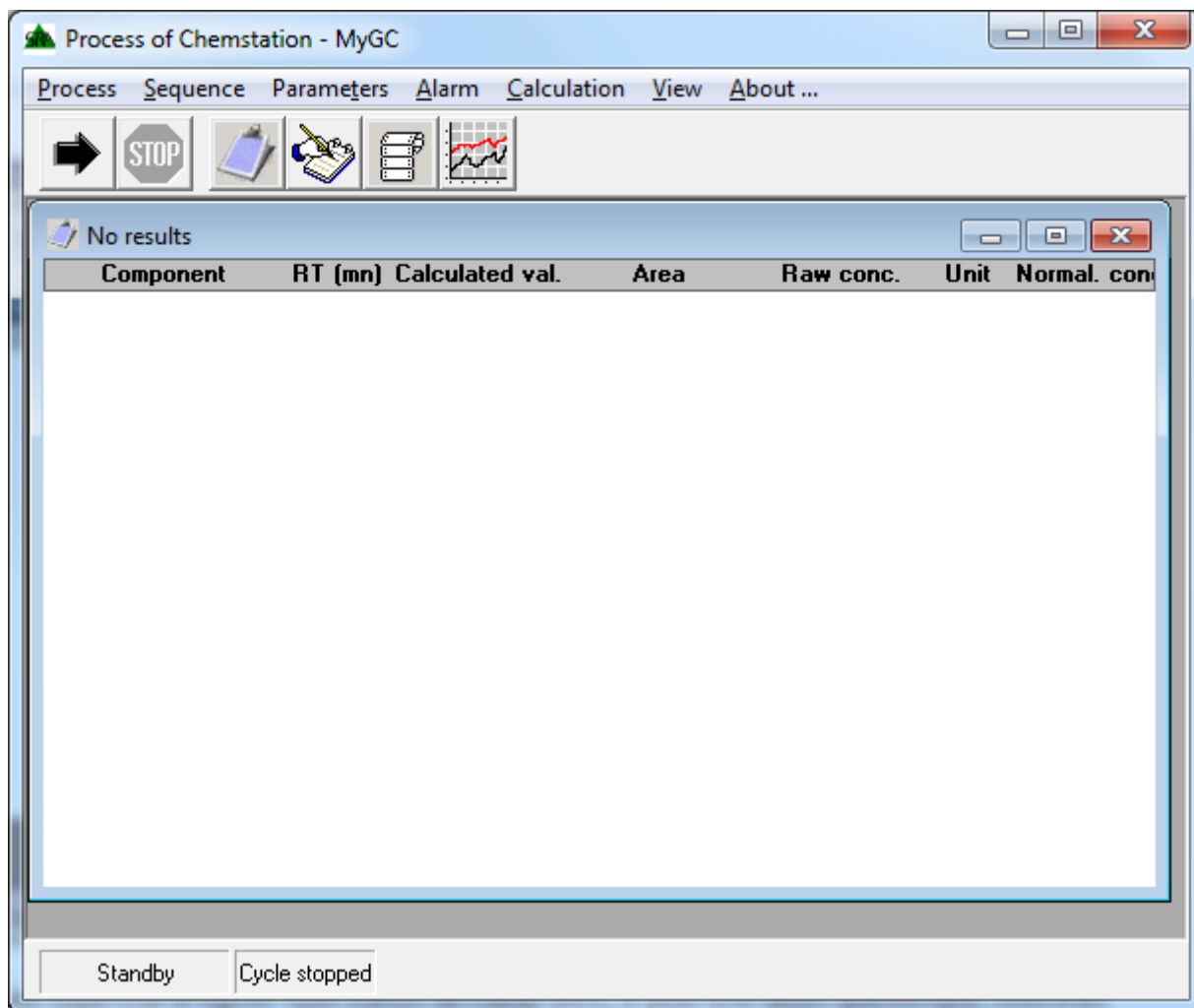
The "**Maintenance**" menu allows you to perform certain actions on the Prochem database (see chapter 8 - description of the database).



For each analysis, Prochem retrieves the results from the workstation and if a new component is created, it adds this new component to the database. But if a component is removed from the table, the component name is not removed from the database and is always displayed. So, you can delete it with this menu.

Also, in some cases, you may not want to keep some results for analysis streams, so it is possible to delete them at this level.

3. Using Prochem



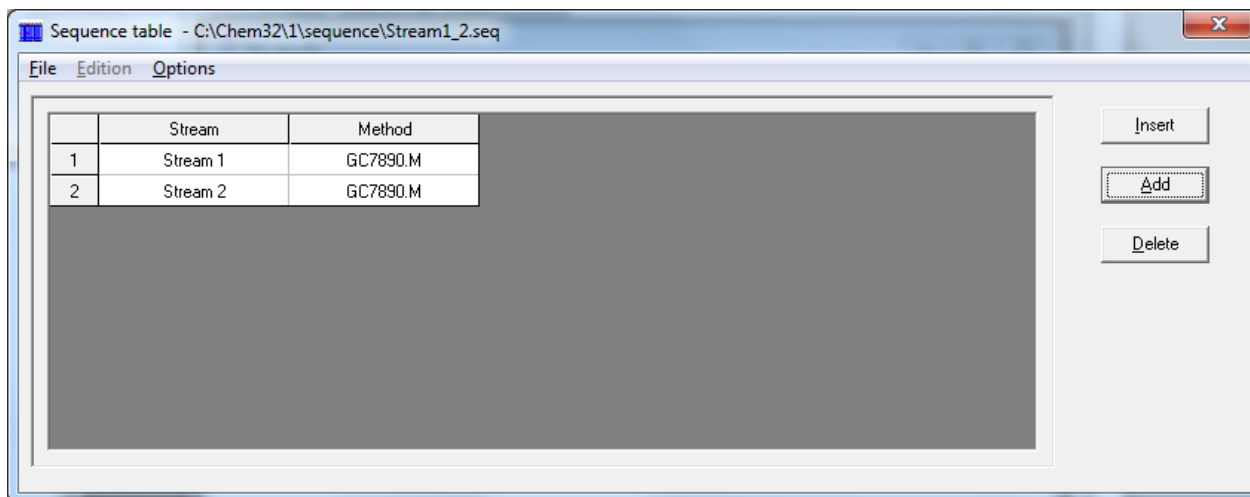
NOTE: This software supervises the workstation type software so if for any reason you have to close this application, it is better to close the Prochem software as well.

3.1 Sequence management

3.1.1 Sequence table

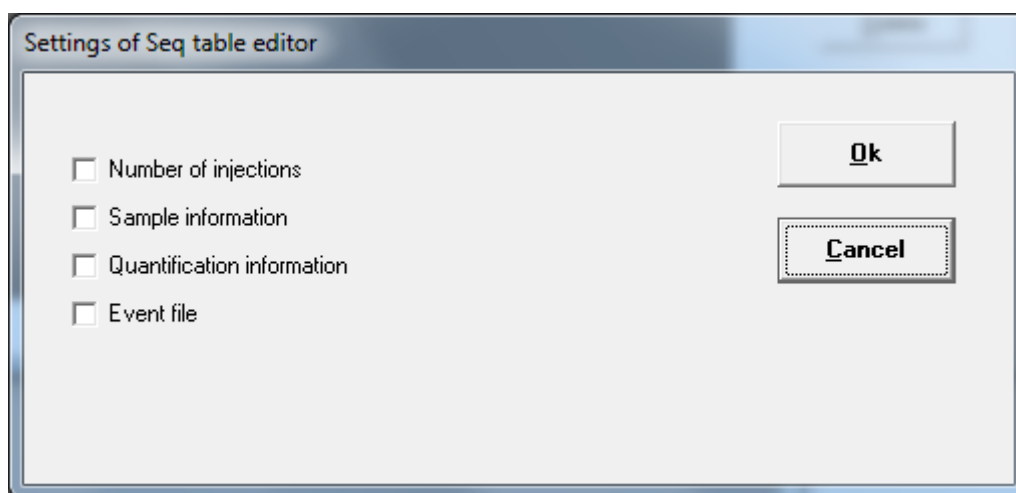
Prochem allows you to create and manage analyses by sequences. These sequences are edited directly at the software level via the "**Sequence\Sequence table**" sub-menu.

The management of these sequences then depends on how the analyses are launched (see paragraph 3.1.3).



If the 'Stream Selector' option is not active, the 'Stream' parameter is replaced by the location of the 'Location' vial to be analyzed.

The Options menu allows you to add additional columns to the editing of the sequence.



The 'Sample information' option allows to display the columns 'Sample Type' and 'Cal level' in the sequence table. It is then possible to define standard analysis types, blank, verification or calibration. In the latter choice, it is necessary to enter the calibration level in the 'Cal level' column.

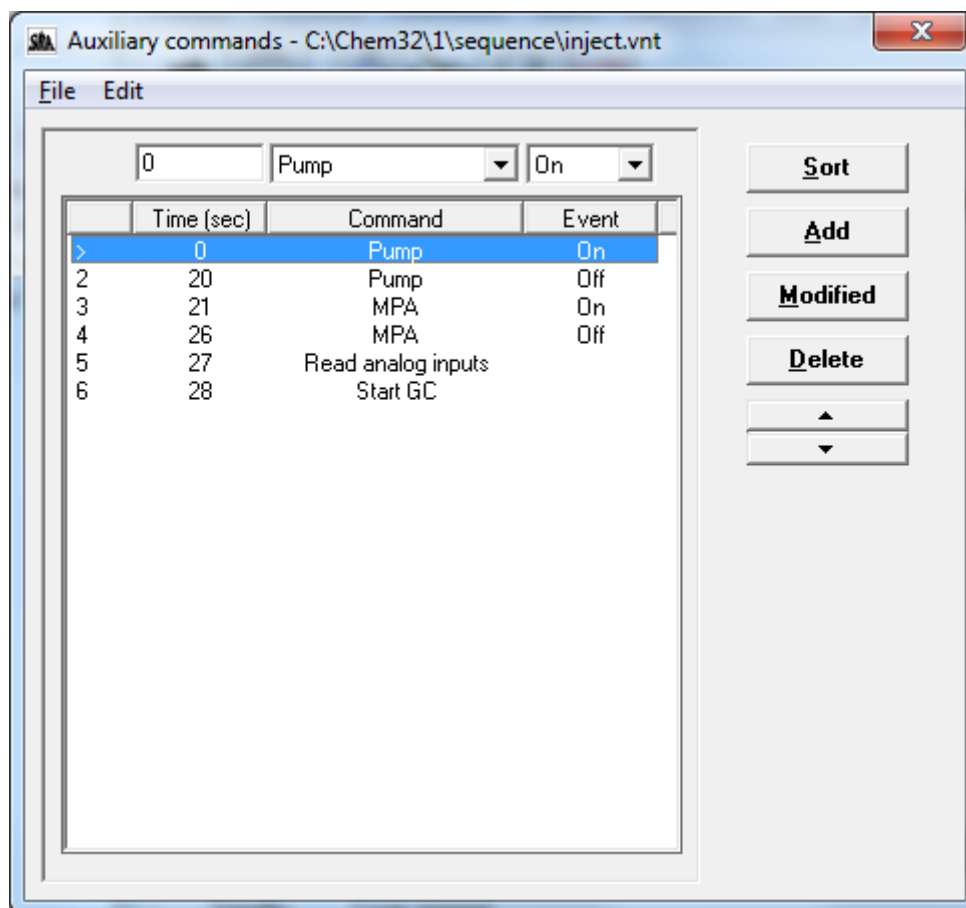
If the 'Quantification information' option is checked, the following columns are displayed :

- Sample amount
- Istd amount
- Multiplier
- Dilution

If the 'Event file' option is checked, it is possible to define an event table for each analysis. But in this case, it is no longer possible to select an event table when starting the analyses.

3.1.2 Auxiliary commands

Prochem can be used to control various commands before and after injection, such as selecting an analysis stream, switching a suction pump, isolation valve or atmospheric pressure setting valve. These commands are programmed into an event table that can be edited via the "**Sequence\Auxiliary commands**" sub-menu.



Depending on the configuration, you can choose between several commands :

- **'Read analog inputs'** : this command saves the value of the analog inputs at one time.
- **'Select the current stream'** : generally, to be used before injection. It allows to select the stream to analyze and to wait a certain time before the injection. If this time is not programmed, it can be replaced by the time entered in the 'Sampling time minimum' field of Prochem Configuration.
- **'Select the next stream'** : this time is generally filled after the injection and allows to switch to the analysis stream which will be carried out afterwards.
- **'Select the default stream'** : this time is usually filled after injection and allows to switch to the default stream in order to save the sample to analyze.
- **'Select the stream'** : this event allows you to switch to a particular analysis stream.

The **'Start GC'** command is a very particular function according to the configuration defined with Prochem Configuration and depending on the controlled workstation; it indicates when Prochem must prepare the analysis.

In the case of OpenLab ChemStation, several cases can be encountered depending on the configuration:

- If the ChemStation parameter 'Injection Source' is configured in 'Manual' and the 'External device injection' option of Prochem is not active, this command is not necessary and Prochem prepares the analysis directly.
- If the ChemStation parameter 'Injection Source' is configured in 'GC Valve' mode and there is no event to be handled or the 'External device injection' option of Prochem is activated (example: case where the start is given by a software executed as PreRun Command in the ChemStation method or a dry contact for the MSD ChemStation), the command is not necessary and Prochem prepares the analysis directly.
- In other cases, it must be programmed into the event table. If it is not present, it is added at the end of the event table.

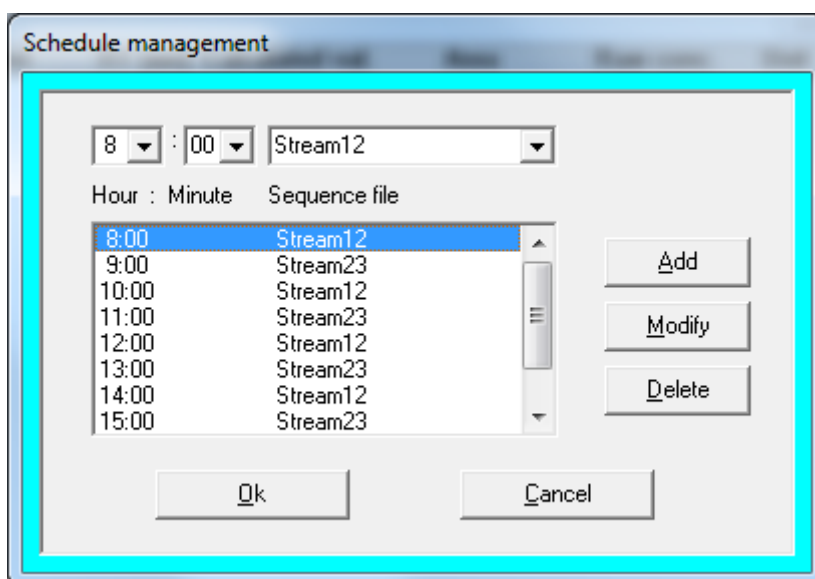
In the case of Mass Hunter, it is not necessarily required because Prochem automatically starts the preparation of the analyses so that Mass Hunter (chromatograph) switches from the 'Idle' state to the 'Prerun' state.

Depending on the injection system, switching to the 'PreRun' state starts its injection cycle. But in some cases, Prochem must activate an auxiliary command before injection and deactivate this command after injection. Then the 'Start GC' command is necessary to indicate to Prochem that it must wait for the end of the injection to take into account the injection time and not take it into account in relation to the times of the commands to be carried out after the injection. For method configuration, see chapter 6.2.1.

From version 3.0.0, it is possible to insert an action to be validated by a logical input in the cycle of the event table (example : waiting for a ready state or for external start). As long as the action has not been validated, the cycle of the event table is on hold. After validation, it resumes its cycle where it was. If actions have to be carried out afterwards, it is not necessary to take time into account.

3.1.3 Scheduler

If the 'Control management' option of Prochem Setup is not activated, it is possible to program the start of sequences at fixed times every day.

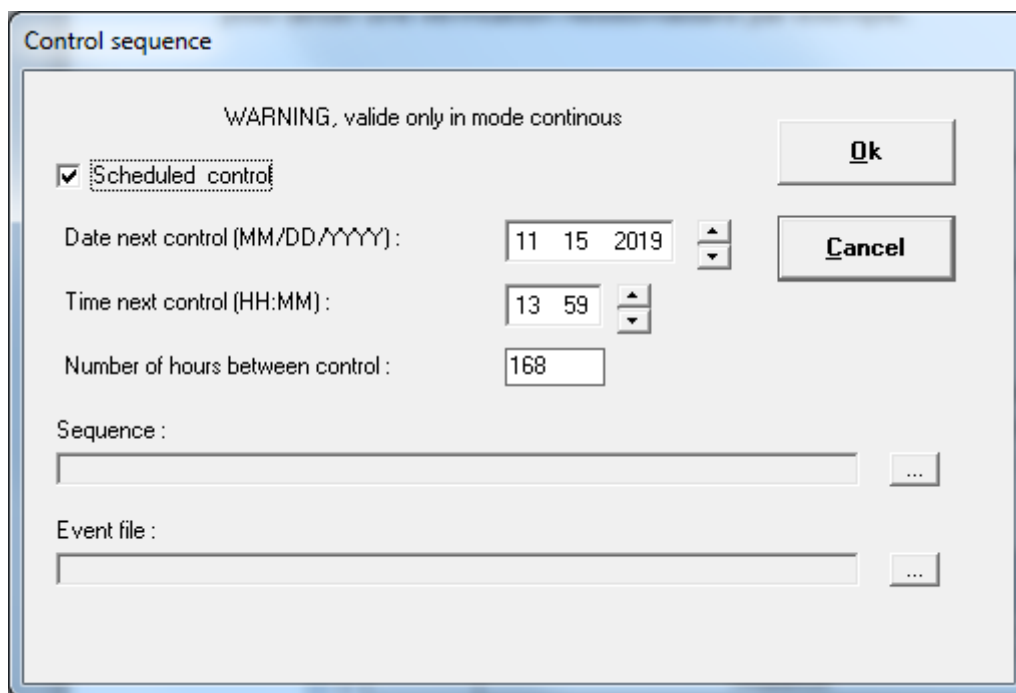


Enter the list of times and sequences used. Note that the sequence file must be in the Sequence directory of the instrument directory.

Of course, this table is only active if the analyses are started with the 'Schedule' option.

3.1.4 Control

If the 'Control management' option of Prochem Setup is activated, it is possible to program the start of a sequence at a fixed time and repeat it every x hours. This option can be useful to run a weekly check for example.

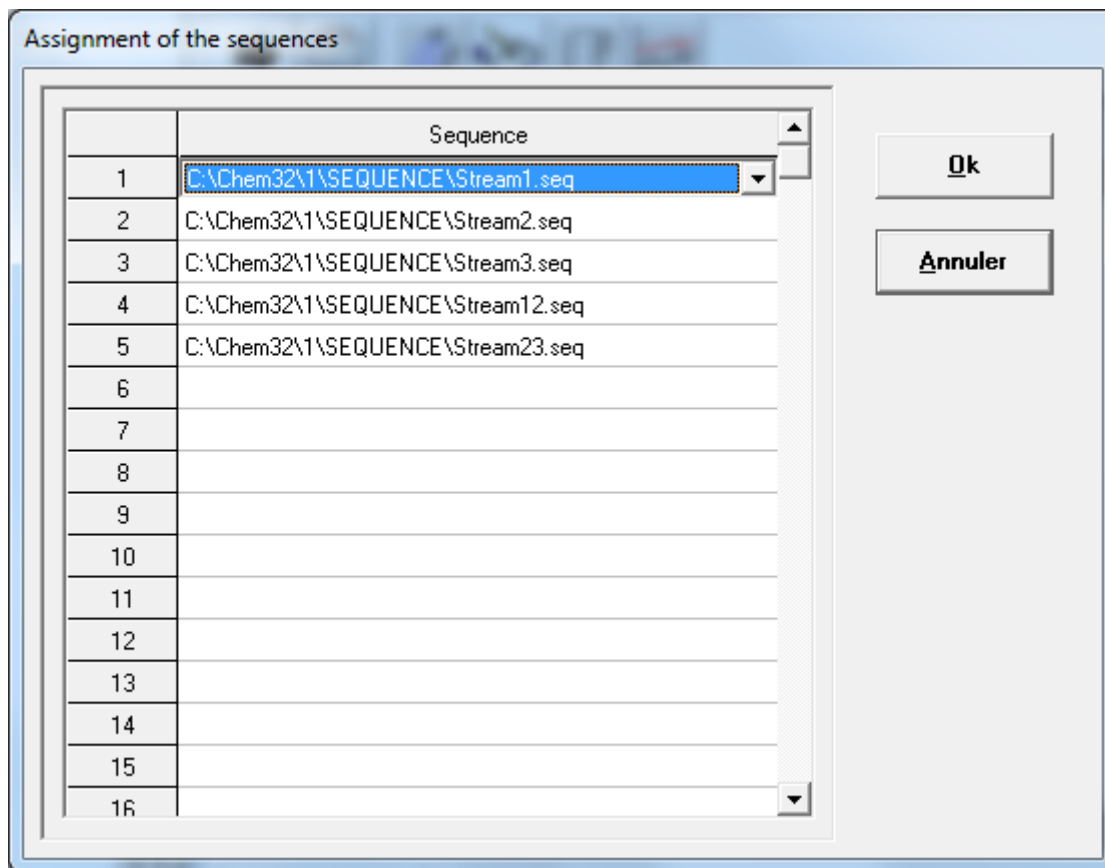


Enter the time and date of the next sequence start, the sequence to be performed and the event table to be used.

Note: the sequence will only be started if the analyses are performed in continuous mode.

3.1.5 Assignment

If the 'Modbus' option is activated, it is possible to run analyses from an external supervisor either in analysis mode or in sequence mode. For sequence mode, it is necessary to enter a number corresponding to the chosen sequence. These numbers are assigned with the "**Sequence\Assignment**" sub-menu.



The sequence file must be stored in the Sequence directory of the instrument directory.

3.2 Analysis launch

The analyses are launched by the "**Process\Start**" menu or by the "Arrow" icon.

The analysis storage directory is composed of a 'path' parameter and a 'Subdirectory' sub-parameter. The 'path' parameter is configured in the ChemStation .

The analysis name consists of the 'Data file name' parameter and the 'Counter' parameter. It will be incremented with each analysis.

You can select the working mode:

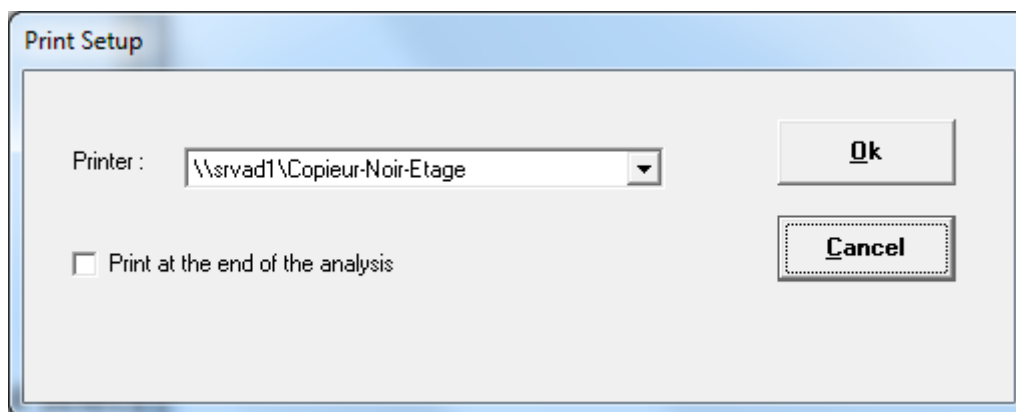
- **'Analysis'**: Prochem will perform the number of analyses programmed in the 'Number of programmed analyses' field. If you select 'Continuous', it will continuously chain the analyses. You must choose the method used and select the stream to scan. The 'Options' button allows you to program a time between each injection.
- **'Sequence'**: You must select the sequence used. You can program a number of sequences to be performed or work continuously. The 'Options' button allows you to program a time between each sequence.
- **'Schedule'**: With this option selected, the analyses are performed according to the programming defined in the **"Sequence\Scheduler"** menu. Note that the 'Options' button allows you to modify this programming.

The 'Apply' button is used to validate the choices made (method and event table) in the case of an analysis launch by Modbus.

3.3 Analysis printing

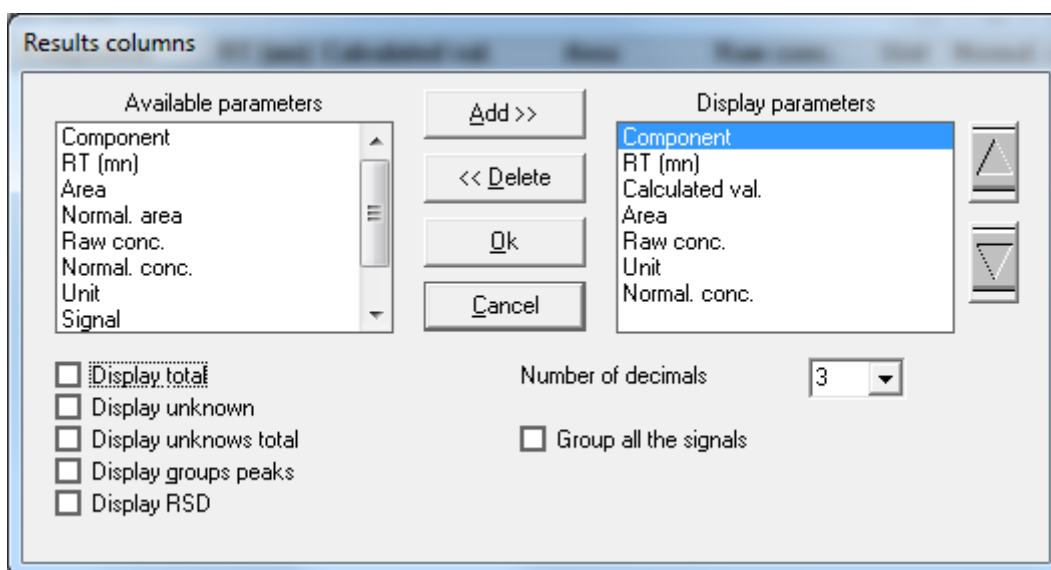
The "Process\Print\Analysis" sub-menu is used to print the results displayed in the "Results" window.

The "Process\Print\Setup" sub-menu allows you to configure the printer to use. You can also request to print these results at each end of analysis.



3.4 Selection of displayed results

The "Parameters\Display columns" sub-menu allows you to select the results displayed in the "Results" window.



Select the parameter from the 'Available parameters' list and click on the 'Add' button to add it to the 'Display parameters' list.

The 'Normal. area' parameter corresponds to the normalization of surfaces. This calculation is performed on all the detectors of the chromatograph if the option 'group all the signals' is active.

The 'Signal' parameter corresponds to the detector number used to analyze the component.

The '**Normal. conc.**' parameter corresponds to the normalization of concentrations. This calculation is performed on all the detectors of the chromatograph if the option 'group all the signals' is active.

The '**Calculated val.**' parameter corresponds to the display of a value calculated in relation to the concentration. In the case of a Prochem RGA version, it will be the mass concentration, but this value can also correspond to a concentration value corrected with respect to a flow, a pressure, a temperature or a calculation defined by a specially developed macro (see paragraph 2.5.2 Calculated value). This parameter can be replaced by the height.

The '**Number of decimals**' is used to define the number of significant digits when displaying concentrations in the "Results" window and in the "Analysis series" window.

Similarly, the display options: '**Display total**', '**Display unknown**', '**Display unknowns total**' and '**Display groups peaks**' are used for both windows.

Only the '**Display RSD**' option is used to display the sum of the squares of the deviations (Relative Standard Deviation) in the "Analysis series" window.

The results can be displayed completely for an analysis ("**View\Results**" menu) or as a series of analyses ("**View\Analysis series**" menu). In this case, the displayed value is selected by right-clicking on the table in the "Analysis series" window.

If you double left-click on the line of an analysis, you can view all the results of that analysis in the "Results" window.

3.5 Alarms

3.5.1 Alarms acknowledgment

Alarms are acknowledged via the "**Alarm\Acquit**" sub-menu, whether for an alarm linked to the chromatograph, to the sample selector or if it is linked to a fault exceeding thresholds.

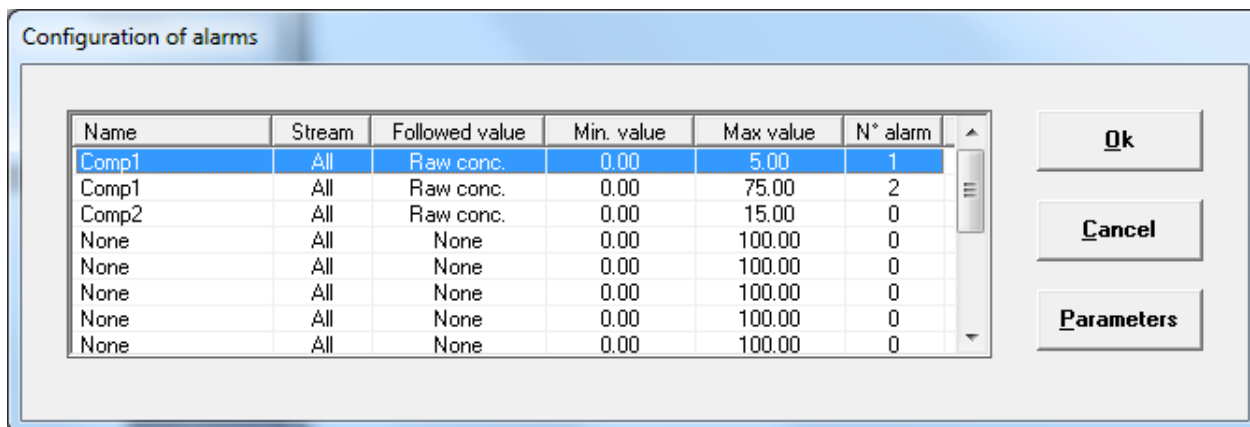
You can also click on the "Alarm" icon.

If the threshold is exceeded, the fault is acknowledged when new results are processed.

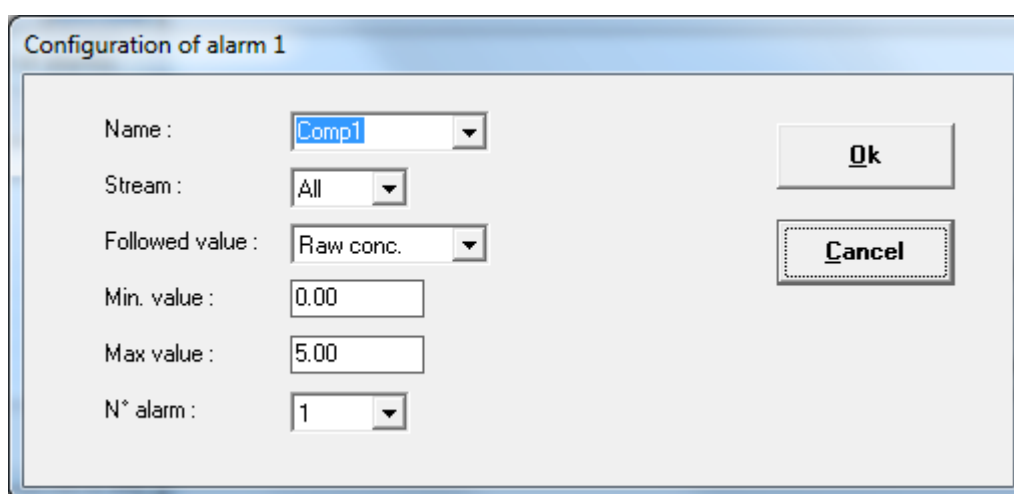
3.5.2 Definitions

Prochem allows the programming of 16 threshold alarms related to the concentration of constituents. In case of an alarm, the values corresponding to this component are displayed in red. These alarms can be associated with relays according to the alarm number, knowing that alarm 0 corresponds to the general alarm.

You can set the alarms via the "**Alarm\Parameters**" sub-menu.



If you click on the 'Parameters' button, you get the following display :

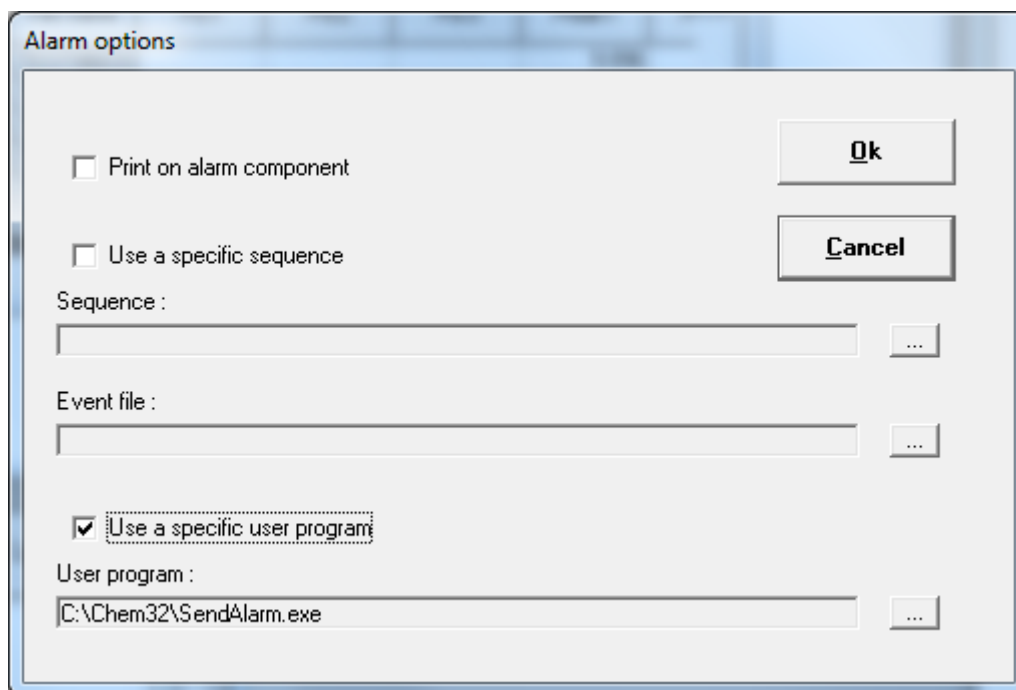


The alarm number is used to assign a relay to this alarm (see chapter 3.4).

3.5.3 Options

In case of a component alarm, it is possible to modify the sequence management or launch a specific program, via the "**Alarm\Options**" sub-menu.

Fill in the different fields in the window below to perform the appropriate action.

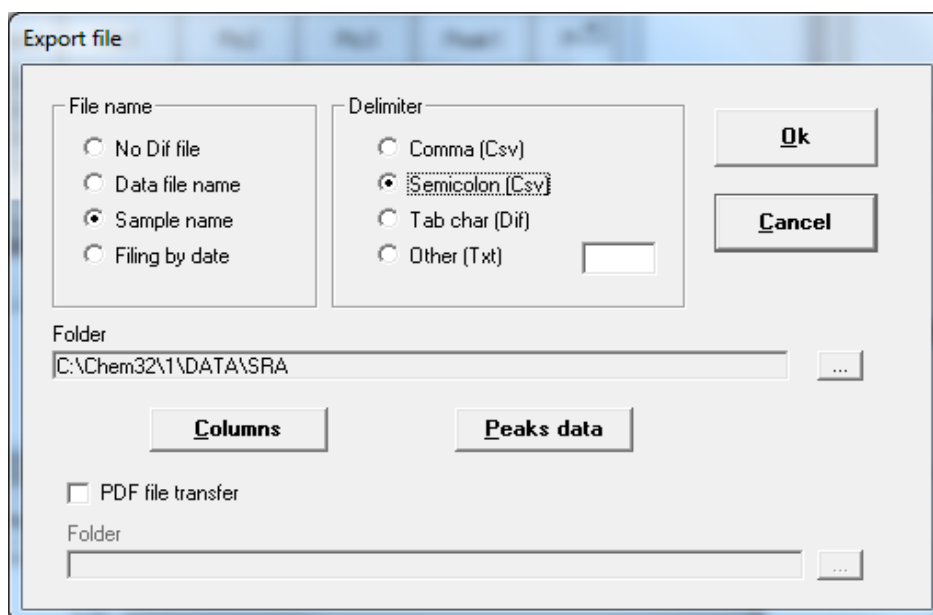


3.6 Parameters

3.6.1 Export file

Prochem allows to store the results of the analyses, in historical form, in a file directly exploitable by spreadsheets (Excel for example). These files are also viewable by a text editor because each field is in ASCII separated by a special character. Prochem creates a file for each sample stream.

To configure the editing of these files, select the "Parameters\Export file" sub-menu. The window below appears :

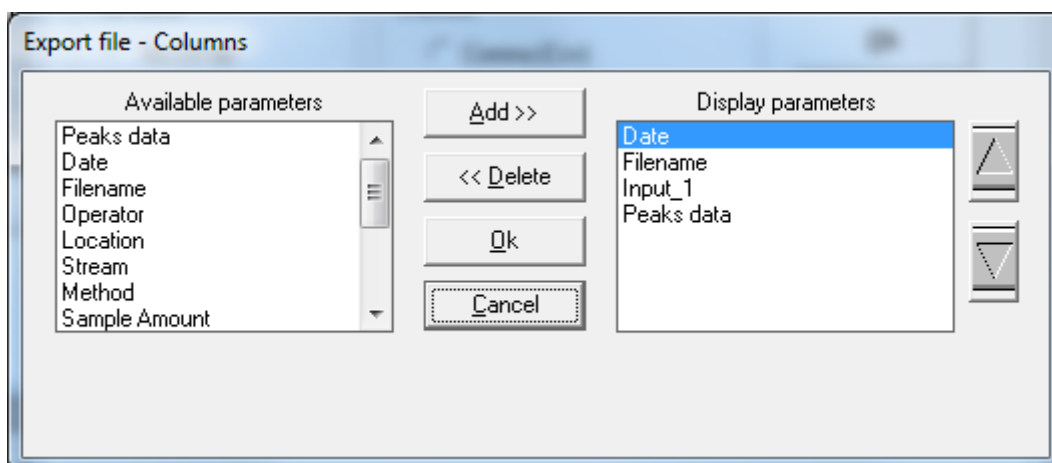


Select how the file will be named, the desired file type.

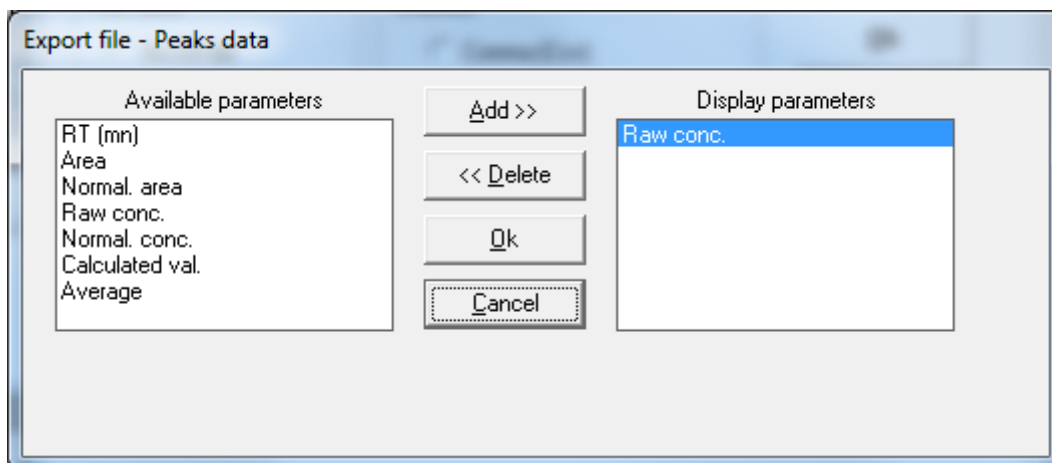
The name of the file is obtained either by retrieving the name of the analysis ('Data file name'), by the name of the sample ('Sample name') or from the date of the analysis if the option 'Filing by date' is checked.

You can also define the directory for these files. If it is not defined, Prochem stores the file in the analysis directory.

The 'Columns' button gives access to the different information of the analysis.

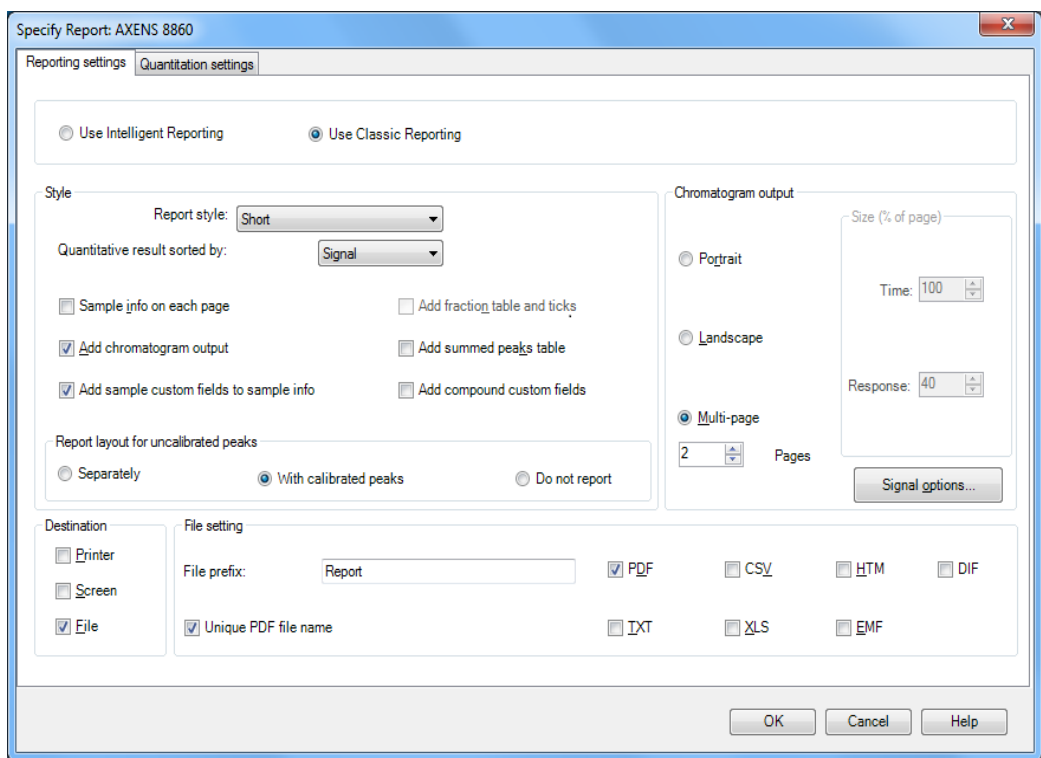


The 'Peaks data' button gives access to all component results.



PDF file transfer option

With OpenLab Chemstation, it is possible to create PDF files in the analysis directory but it is not possible to transfer them to a network disk. Prochem allows this possibility thanks to the option '**PDF file transfer**'. Select the directory on the network and Prochem will store the generated files in the same place. If the network is not available at the time of creation, it stores them on the computer until the network is restored and then copies the stored files. This option requires that PDF file generation is configured correctly on the Chemstation.

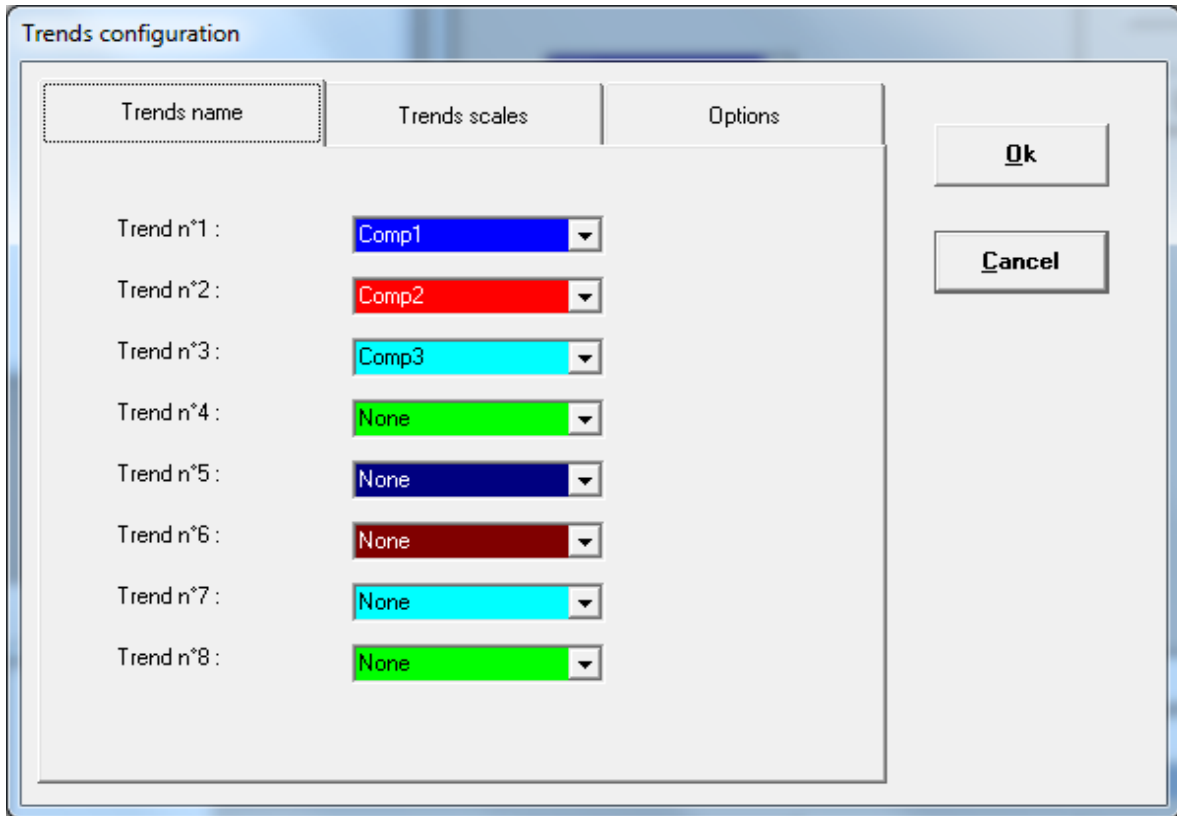


With Mass Hunter, it is not possible to generate PDF files. Prochem then uses the 'PDF Creator' application to generate its own PDF reports. This application is available on Prochem's installation USB key.

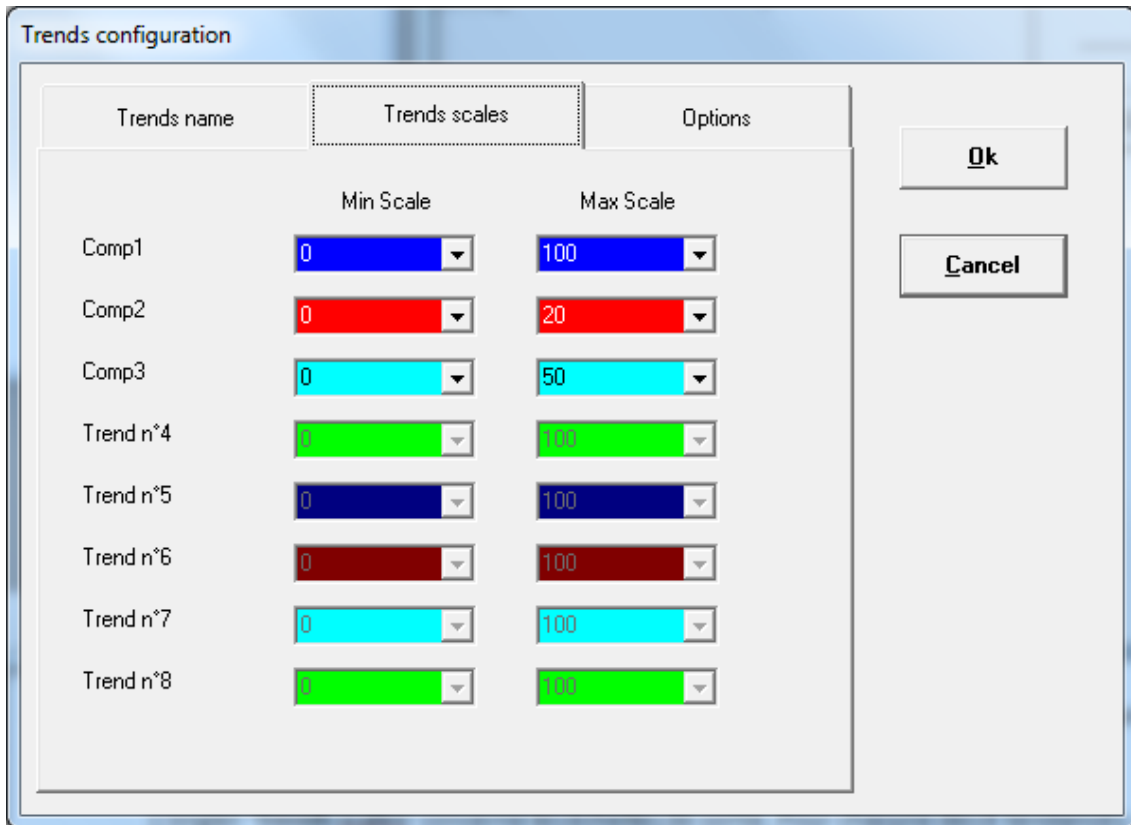
3.6.2 Trends

Prochem displays the evolution of concentrations or calculated values over a period of time.

The "**Parameters\Trends\Property**" sub-menu allows access to a sheet used for programming these trends:



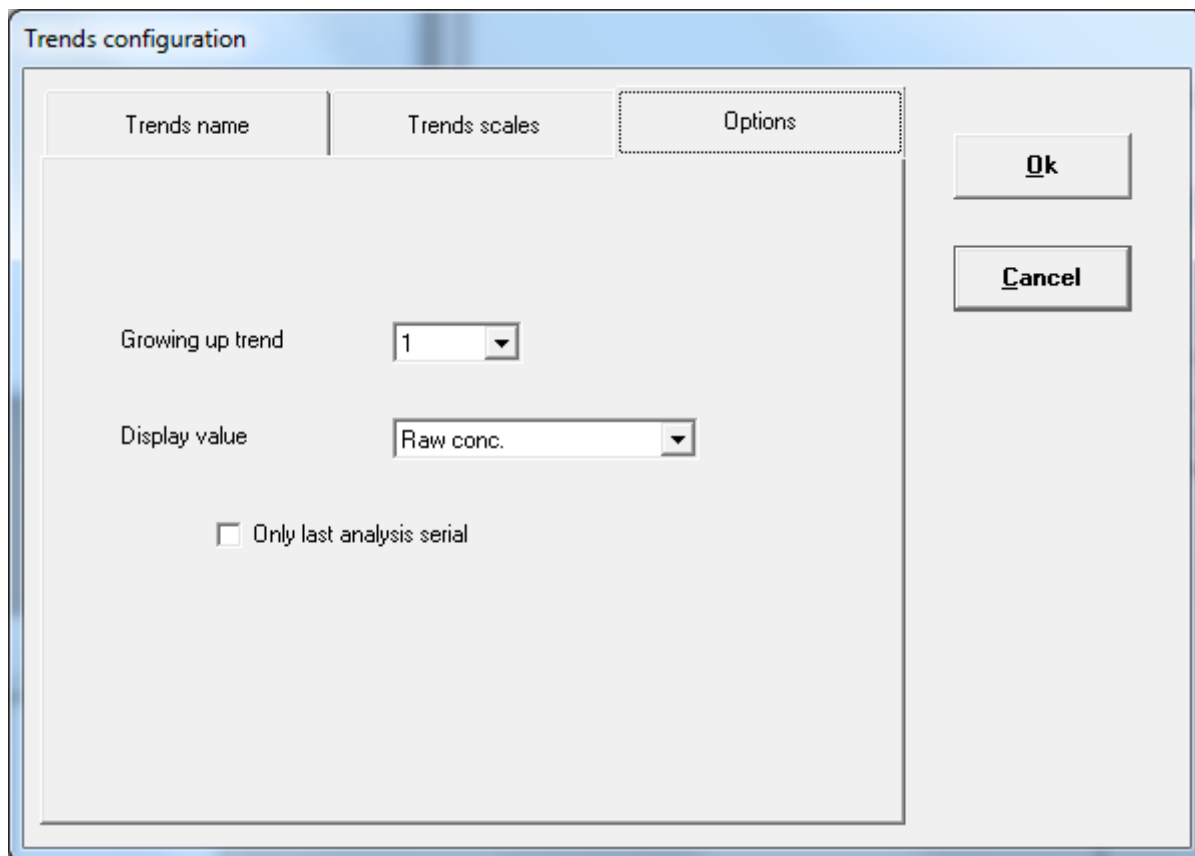
The 'Trends name' tab allows you to define the 8 values followed independently of each other.



The '**Trends scales**' tab concerns output scales. For each of the 8 trends, you must indicate a minimum value and a maximum value to be taken into account during the graphical representation.

By default, these values are 0 and 100 respectively. **It is preferable to change the maximum value first.**

Usable values can be in the range suggested by Prochem, which allows great flexibility without risk of error, or can be written directly.

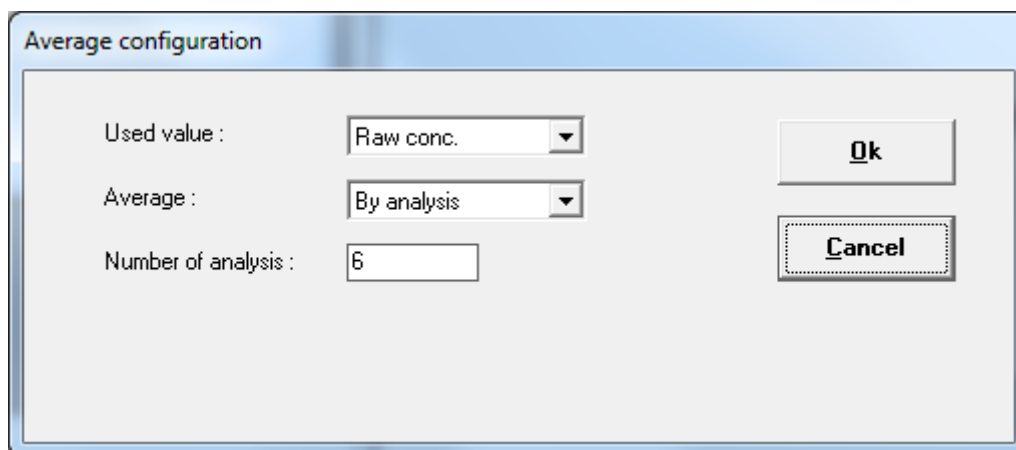


In the '**Options**' tab, you can define a time range in order to visualize the evolution of the values or display the totality of trends. You can also set the displayed value.

3.6.3 Average

Prochem allows to calculate hourly average values or over a number of analyses.

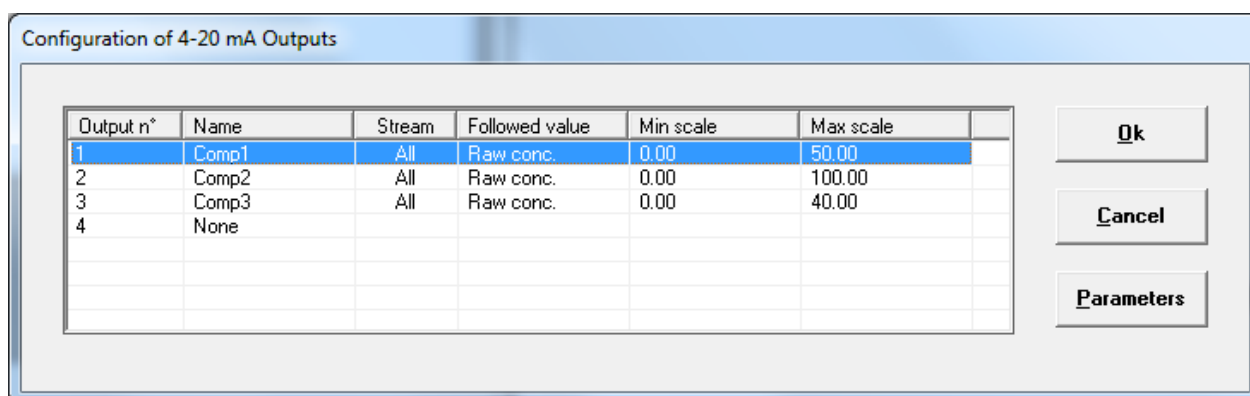
Select the "**Parameters\Average**" sub-menu; the window below appears:



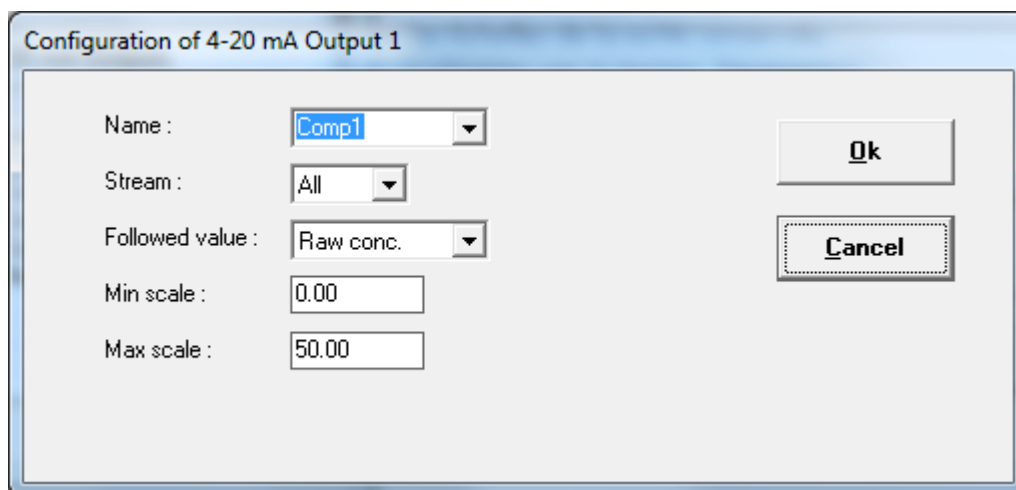
You must select the followed value, the type of average and either the time range or the number of analyses.

3.6.4 4-20 mA analog outputs

This menu is accessible only if your configuration is equipped with 4-20 mA analog outputs.

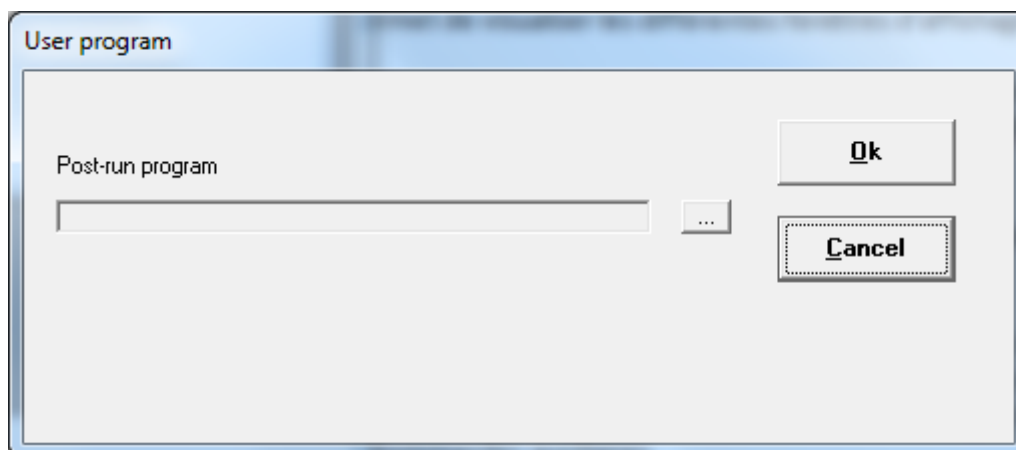


You can then define the name of the component, the number of the sample stream if the value is specific to one stream, the value followed, and the scales of the output concerned. All these parameters can be modified by the 'Parameters' button.



3.6.5 User program

This window allows you to select a program that will be launched when the analysis results have been transmitted to Prochem.



3.7 Display

The **"View"** menu allows you to view the different result display windows.

Once you have defined a specific display order, it can be saved via the **"Save windows positions"** sub-menu. So, if you click on the **"View\Customized"** sub-menu, the displayed windows will automatically reframe.

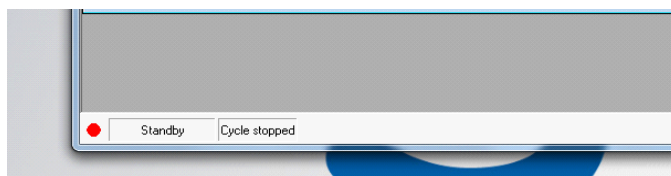
The **"Last analyse"** sub-menu allows you to view the latest results processed in the workstation. In the case of OpenLab, these results may come from reprocessing.

The **"Prochem Status"** window displays a window showing the selected stream, the status of the auxiliary commands, the value of the analog inputs and the status of Prochem (time, next event). When the system is out of analysis, it is possible to change stream manually or to enable/disable auxiliary commands.

From the "Analysis series" window, if you right-click in the result columns, you can select the value to display, the number of decimals and the statistics display. If you right-click in the line header, you can copy the selected lines and transfer them to another application (Notepad, Word, Excel etc...). If you double left-click, you can view all the results of the analysis in the "Results" window.

3.8 Coupling between two sessions

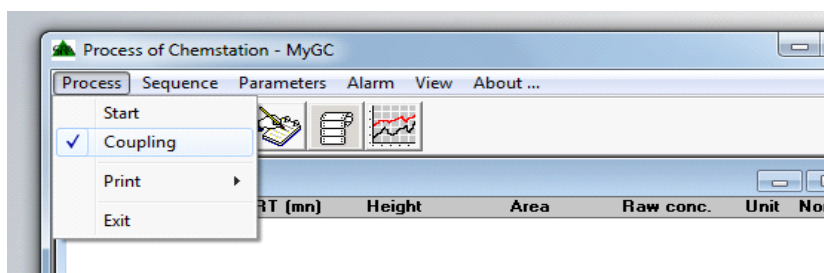
Since version 3.0.0, it is possible to couple two sessions of Prochem present on the same computer. In this configuration, an indicator appears on the left of the status bar at the bottom of the screen.



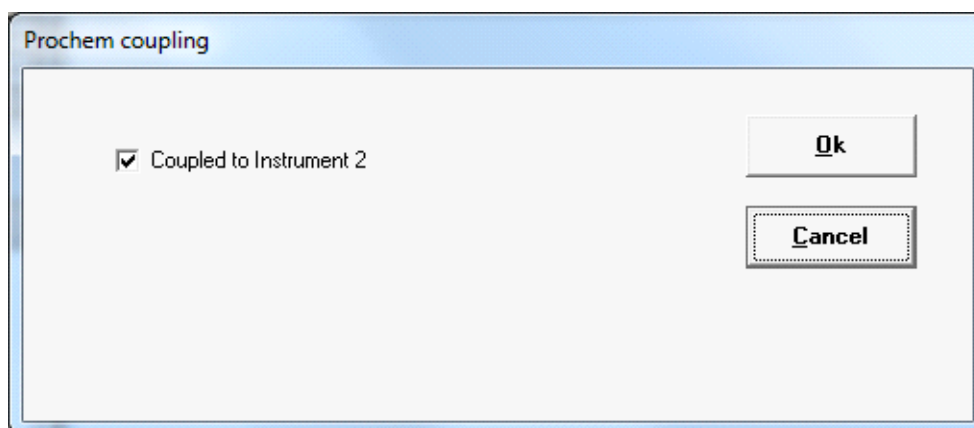
Depending on the state, it can be in different colors:

- Red: there is no dialogue between the two sessions.
- Black: the coupling is deactivated.
- Blue: this is the master session.
- Green: this is the slave session.

When both sessions are coupled, it is possible to temporarily stop the coupling with the "Coupling" menu.



By unchecking the box, the two instruments can then be launched separately.



When the two instruments are coupled, the analyses must be started normally from the master instrument. If the analyses are started in 'Analysis' mode, you must make sure that the method of the slave instrument is loaded correctly.

It is possible to change the directory and the name of the analysis files; to do this, open the Start window of the slave instrument, fill in the fields and validate with the 'Apply' button.

If you start the analyses in 'Sequence' mode, you must create the same sequences at the slave session level and assign them the same numbers with the 'Sequence\Assignment' menu. They do not need to have the same name.

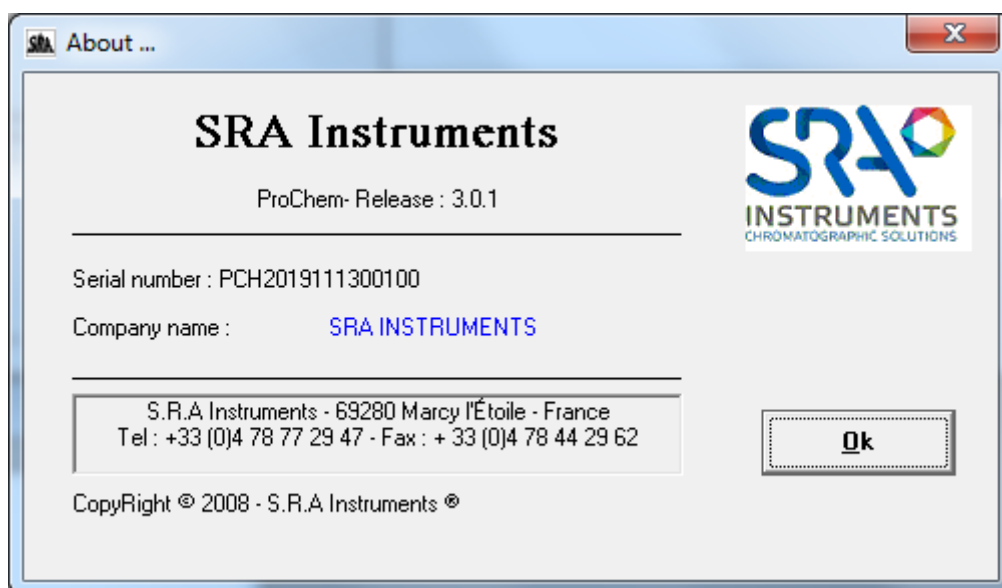
Concerning the event table, all commands must be managed by the master session.

It is not necessary for the analysis time to be the same, the master session waits until the slave session has completed its analysis to process all the results: print, alarm, 4-20 mA outputs and results file. If alarms on the components need to be programmed at the slave session level, they must be configured at this level for display but also at the master level for relay management.

For Modbus, each session has its own address table.

3.9 About ...

This menu displays the version of Prochem.



3.10 RGA calculations

These menus are accessible only if the "Calculations" option is activated.

3.10.1 Component names and values

The "**Name, molar and calorific values**" menu allows the definition of component names and their coefficients used during calculations.

	Components	Formula	Molar mass
			g/mol
1	Helium	He	4.003
2	Hydrogen	H2	2.016
3	Oxygen	O2	31.999
4	Nitrogen	N2	28.014
5	Methane	CH4	16.043
6	Carbon monoxyde	CO	28.010
7	Carbon dioxyde	CO2	44.010
8	Ethylene	C2H4	28.054
9	Ethane	C2H6	30.070
10	Propylene	C3H6	42.081
11	Propane	C3H8	44.097

Display the second calculation

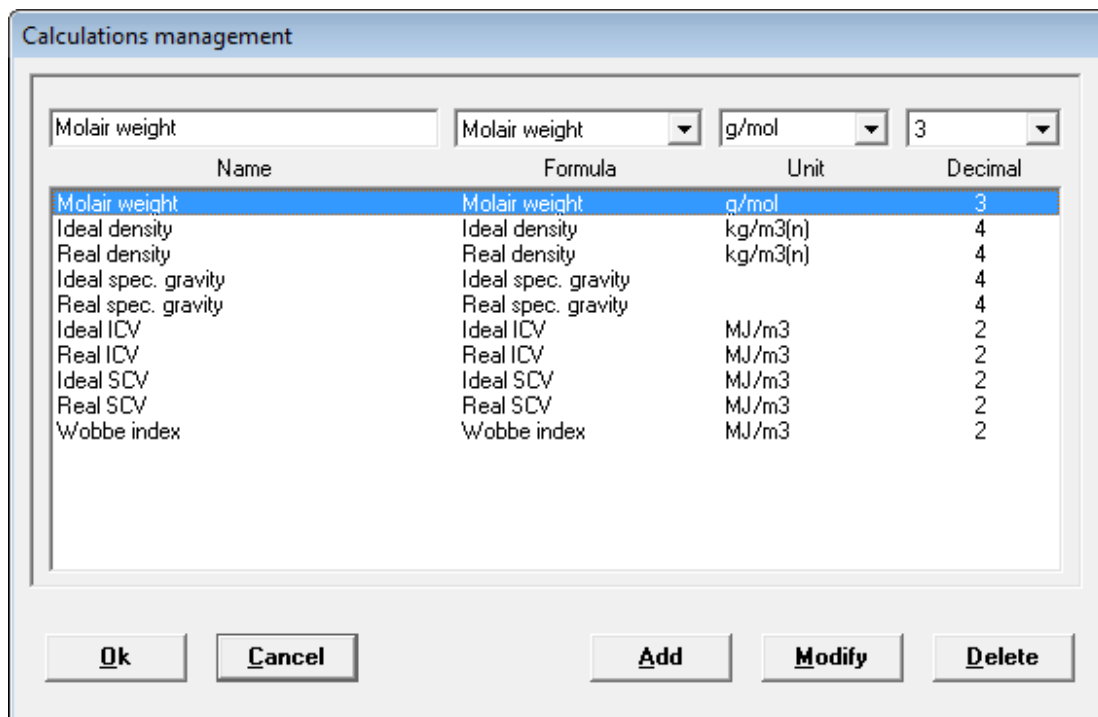
The spelling of the name of the constituents must be identical to the capital letters with respect to the Chemstation peak table. The constituent formula is used to calculate the carbon.

The "Compounds" menu allows you to enter the name of the component, its chemical formula and molar mass. The "Calorifics values 1" menu is used to define the values for the calculations in the first column and the "Calorifics values 2" menu for the calculations in the second column. The default values are from ISO/DIS 6976:1995. The "Conditions" menu is used to fill in the calculation conditions and is only used as comments.

To display the second calculation column, the option "Display the second calculation" must be checked.

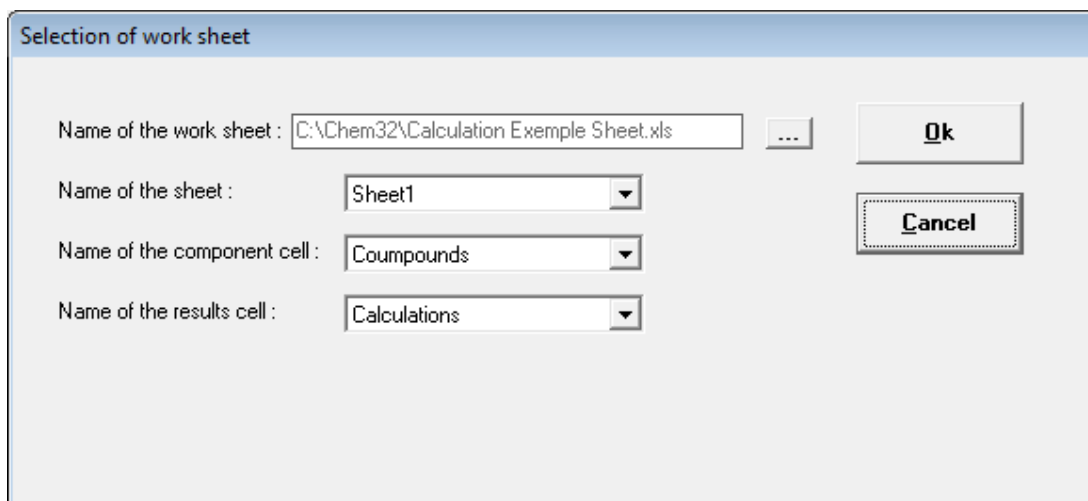
3.10.2 Calculation selection

The "Calculation select" menu is used to define the desired calculations. The formula for these calculations complies with ISO/DIS 6976:1995 and the experimental standard X 20-522 and are not accessible. However, the name of the calculation can be changed.



3.11 Excel calculations

The "Excel Calculations" menu is accessible only if the "Excel" option is activated.



The Excel sheet must follow a specific format.

Select the cell name from column A of the sheet corresponding to the component name.
 Select the name of the cell in column A of the sheet corresponding to the name of the calculations.

For each analysis, Prochem will store in the second column, the raw concentration corresponding to the component name of the first column. If calculations are performed in the sheet, it will retrieve these calculations in the following lines to the cell "results cell".

A sample sheet is delivered by default. Contact us for more information.

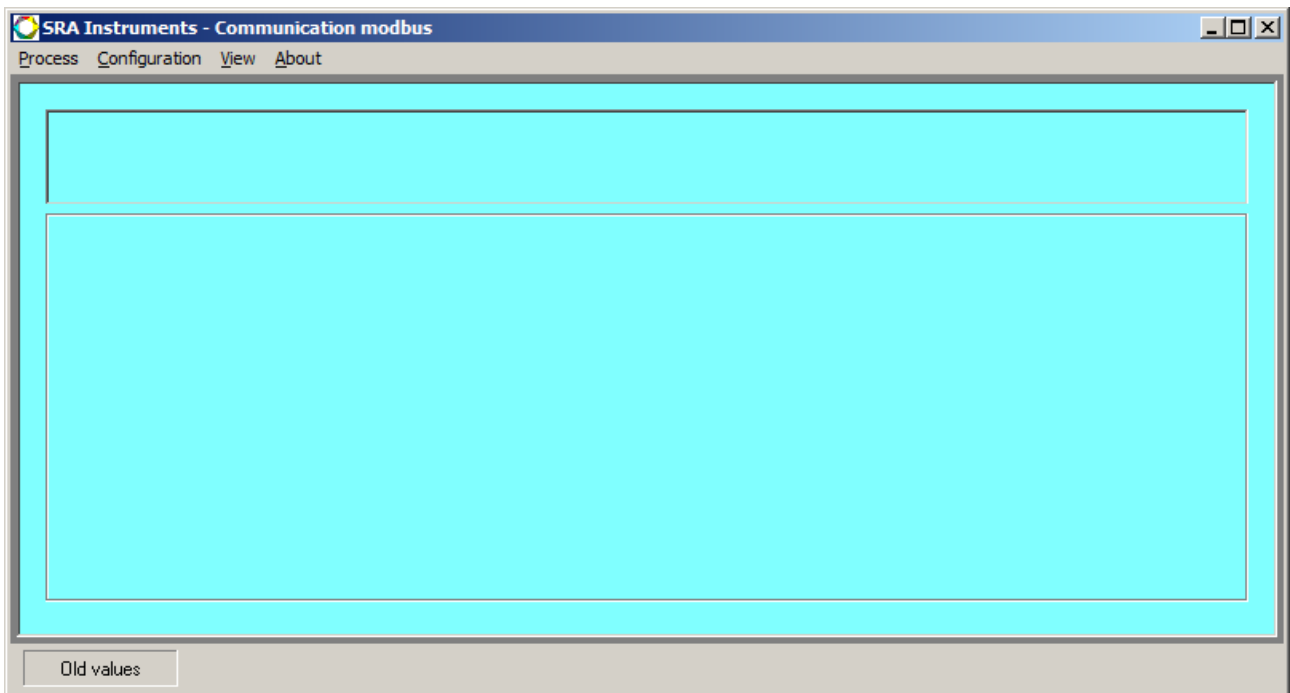
4. Using the Modbus module

The specific SendToBus software, allows data exchange between Prochem and another remote computer or a centralized control via the industrial network of type Modbus (Lan or serial), Profibus or Profinet.

Thus, the results of an analysis can be fully transmitted: date, time, stream, type of measurement, concentrations, calculation results.

The data is stored in an address table and the communication consists in exchanging this information (16 bit integer, 32 bit integer or real) between the master equipment and one or more slave equipment(s). The master asks a question or asks for the value of one or more addresses, and in response, the slave returns the stored value to these addresses.

Just define an exchange table according to the variables you want to read and assign the desired address and format. These parameters are not fixed and can be modified at will.



The presence of this software is visible in the Windows taskbar under the SRA icon. You can display the main window by right clicking on this icon and selecting 'Maximized'.



4.1 Software installation

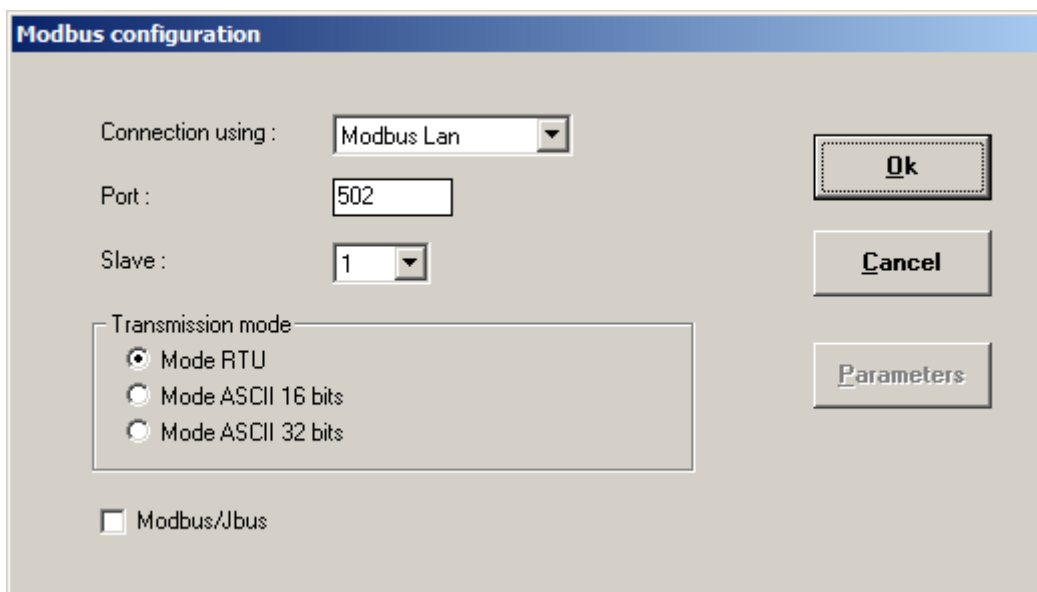
This module is installed when Prochem is installed if the Modbus box is checked.

4.2 Software configuration

4.2.1 Configuring the communication parameters

Select the "**Configuration\Communication**" sub-menu. The following page appears.

Note that this menu is accessible only if the link is disconnected, i.e. if the message 'Disconnected' appears in the status bar. To log out, go to the "Process\Disconnect" menu.



In this window:

- Choose the bus type, that is to say the communication protocol to interact with the remote system.
 - If you choose Modbus to serial port, select the serial port used. In this case, the "Parameters" button is used to view and modify the transmission parameters (speed, number of bits, parity, number of stop bits, control type).
 - If you choose Modbus to TCP/IP, keep the 502 value for the port number.
- Indicate a slave number for Prochem.
- Select a transmission mode. The 32-bit ASCII mode corresponds to the Daniel ASCII mode.
- Choose to use a Modbus/Jbus transmission protocol.

By default, keep the transmission mode in RTU mode and the Modbus/Jbus option unchecked.

Validate with the Ok button.

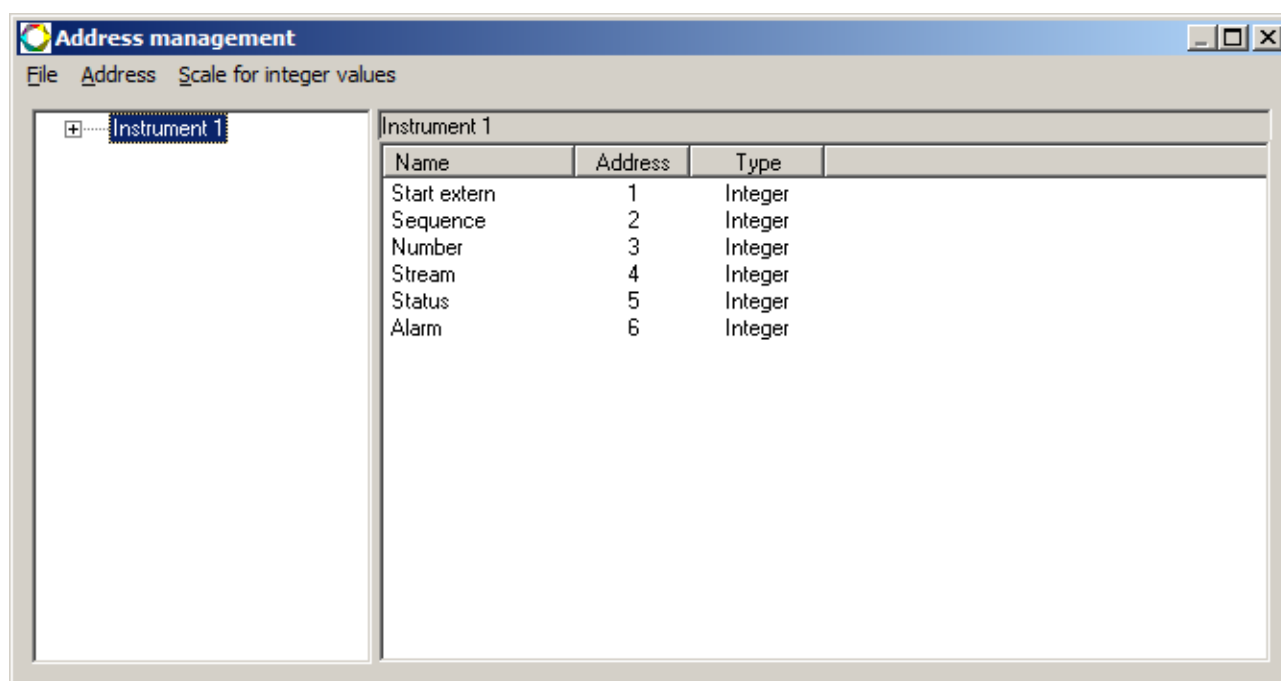
4.2.2 Modbus addresses

The available data are separated into three types:

- Data concerning the analyzer.
- Data concerning the analysis.
- Data concerning the results.

Each transferred data is assigned an address, a value type and, for results, a coefficient when transmitted as an integer.

This setting is done by selecting the "Configuration\Modbus Address" sub-menu.

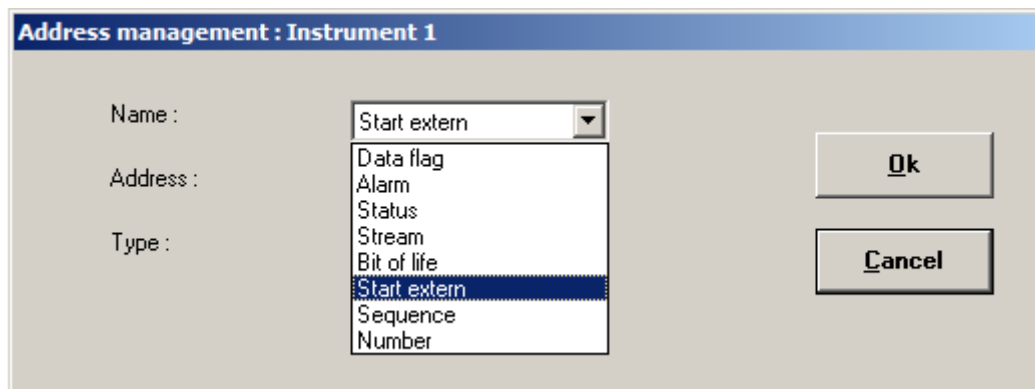


This screen displays two areas:

- The area on the left allowing the selection and display of all variables specific to a type. (Click on the + to expand the chromatograph tree).
- The area on the right allows you to edit the desired values for each type either via the "Address" menu or by right-clicking within this area.

No test is performed on the address entry, you must be careful not to use the same address twice, as this address is imposed by the central control system anyway.

Data concerning the analyzer:

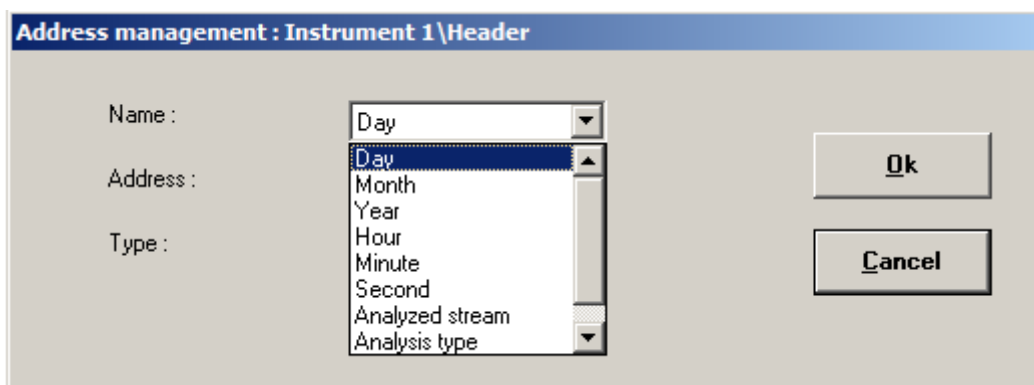


- **Data flag:** SendToBus uses this variable and passes it to 1 to indicate that the results of the analysis are available. It is up to the remote computer to reset it to 0 when it has read these values.
- **Alarm:** This value indicates faults with the analyzer or alarms coming from the results. It can take several values; these values are obtained according to a combination of bits.
 - Bit 0: chromatograph default
 - Bit 1 : cycle stopped
 - Bit 2 : results not recovered at the end of the analysis
 - Bit 3 : default with stream selector
 - Bit 4 : default with Chemstation that did not open
 - Bit 5 : alarm input default
 - Bit 6 : calibration default
 - Bit 7 : with Modbus, the results are not refreshed
 - Bit 8 : concentration alarm
- **Status:** This variable is used to monitor the status of the analysis cycle. The value 0 indicates that the whole is out of analysis, the value 1 that it is waiting for injection and the value 2 that the analysis is in progress.
- **Stream:** In the case of a multi stream application, this value allows the number of the selected stream to be changed.
- **Bit of life:** This variable is used to monitor transmission. Its value is updated every second.
- **Start extern:** this variable is used to launch analyses.
 - 0 : stop of the current cycle
 - 1 : single analysis mode, any value for Sequence ; if Number at value = 0, continuous analysis ; if it is different from 0, it is the number of analyses
 - 2 : analysis sequence mode, Sequence = number of the desired sequence ; if Number at value = 0, continuous mode ; if it is different from 0, it is the number of times that the sequence is repeated.
 - 3 : stop requested at the end of the cycle
- **Sequence:** number of the sequence

- **Number:** 0 = continuous mode; other = number of cycles

Data concerning the analysis:

- **Values concerning the date of the analysis**, i.e. year, month, day, hour, minutes and seconds.
- **Analyzed stream:** indicates the sample stream of the last analysis.
- **Analysis type:** (reserved for future applications)
- **Compounds alarm:** the value of this variable is decomposed into 16 bits. If an alarm is triggered, the bit corresponding to this alarm will be active. *Example: If the value is 5, this means that alarm 1 is activated, alarm 2 is not activated and alarm 3 is activated.*



Data concerning the results:

In this section you can select the names of the peaks, peak groups and any calculations that will be transmitted.

You must enter the name of the value in the "Name" field. This field is a free input field, so it is necessary that the word entered corresponds to a name of components or groups used in Prochem, the application not taking into account capital letters.

You must also enter the address, the type of value (floating or integer), the analysis stream (signal) and the value returned. In the case of a floating value, you must specify the number of decimal places to be transmitted and in the case of an integer value, you must also enter the coefficient of decimal places, i.e. if you want to return values with 2 decimal places, you must select the value 100. Thus, when the software will deposit the value in the address, it will be multiplied by 100 and the remote computer will have to carry out the opposite operation.

In the choice of the value to transmit, you have the possibility to select an "other value". This choice is possible only if you perform additional calculations on the peaks.

Address management : Instrument 1 \Compounds

Name :

Address :

Type :

Decimals number :

Signal :

Value :

Ok

Cancel

Options

This menu is accessible from the address configuration window. They concern the format of the values transmitted.

Options

Scale for the integers values

Swap 32 bits integer bytes

Swap Floating point bytes

Ok

Cancel

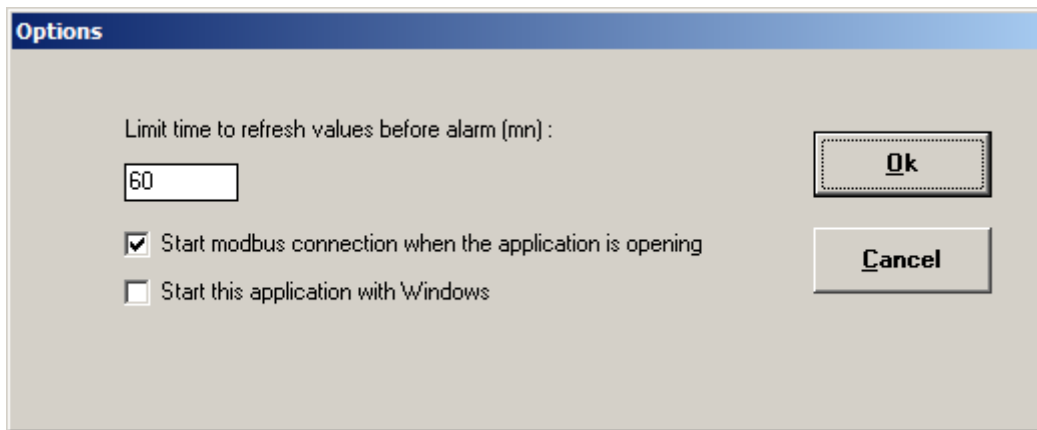
The value '**Scale for integer values**' is used when you have chosen to report values in the integer format. If the value obtained in the results and multiplied by the determined coefficient is greater than this value, then the software sets this value to full scale.

If the values are sent as a 32-bit integer data type, they use two addresses. As a general rule, the word of high weight is the first and the word of low weight is the second. But it may be that this rule is reversed and therefore, in this case, it is necessary to check the option '**Bytes inversion for 32-bit integers**' (Big Endian or Little Endian order).

If the values are sent as real or floating data type, they use two addresses. As a general rule, the word of high weight is the first and the word of low weight is the second. But it may be that this rule is reversed and therefore, in this case, it is necessary to check the option '**Bytes inversion for reals**' (Big Endian or Little Endian order).

4.2.3 Options

This menu is accessible from the main window. They concern the use of the software.



This window allows you to select different options available in this software.

- **Limit time to refresh values before alarm.** This value is used to generate an alarm if the values are not refreshed after the time programmed in this field.
- **Start Modbus connection when the application is opening.** When you launch the SendToBus application, the software automatically connects to the Modbus network.
- **Start this application with Windows.** When you turn on the computer, the application is loaded directly into memory. These last two options allow the system to be reconnected when the power supply fails.

Note:

If you choose to automatically launch the software, SendToBus is automatically launched when Windows is initialized, and the main window is hidden. To access this window, right-click above the application icon in the taskbar and select the Enlarge menu. If communication changes are made to the configuration, you must restart SendToBus or Windows.

4.3 Process menu

4.3.1 Connect sub-menu

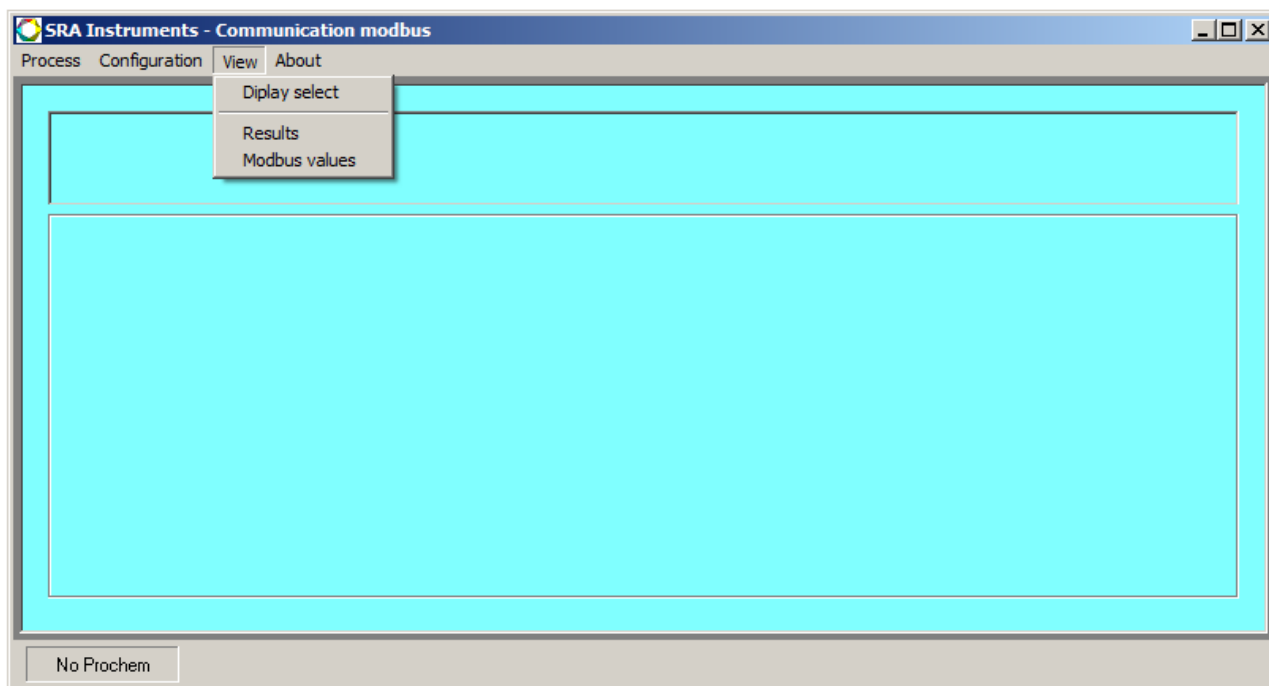
This sub-menu is used to connect the application to the Modbus network to ensure dialogue with the remote computer. This menu is replaced by the Disconnect menu when the connection is active.

The software indicates the status of the connection in the status bar if it is inactive. Otherwise, you have a red spot that appears in the lower right corner of the window at each dialog.

4.3.2 Exit sub-menu

This sub-menu closes the application.

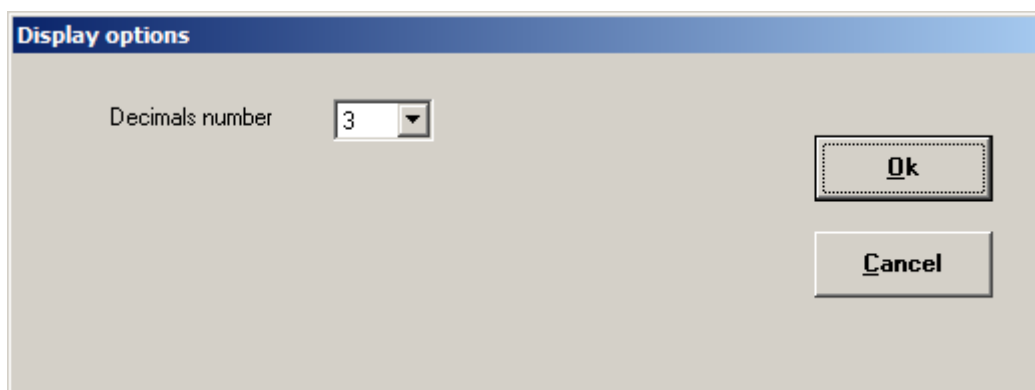
4.4 View menu



If you have configured two instruments in Prochem, it is not possible to view all the results obtained on the same screen. You must select the instrument whose results you want to view.

4.4.1 Display select sub-menu

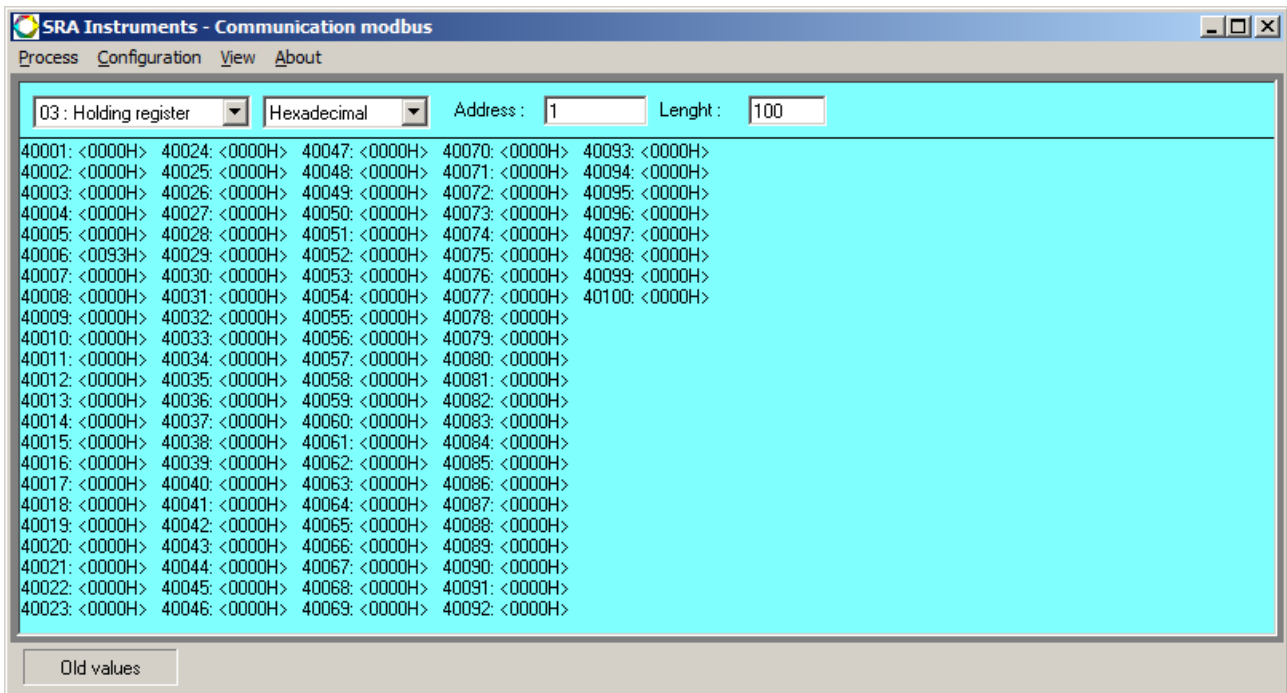
This sub-menu allows you to define the number of decimal places for the values displayed in the "Results" window.



4.4.2 Selection of displayed values

The "**View\Results**" sub-menu displays the values of the last analysis performed.

The "View\Modbus Values" sub-menu provides access to:



- Select from the list the table to be displayed (01:0000 - bit read/write, 02:10000 - bit read only, **03:40000 - word read/write**, 04:30000 - word read only)
- Select from the list the type of values you want to view (hexadecimal, decimal, floating).
- Enter the value of the first address to be displayed
- Enter the number of addresses

4.5 About menu



This menu allows to display the software version.

4.6 Features

- Connection :
 - o Protocol:
 - Standard serial Modbus : RS 232, RS 422, RS 485 (depends on computer port)
 - Modbus Lan
 - Profibus
 - Profinet
 - o Parameters for serial link : 75 to 115200 baud, parity: none, even and odd, 1 or 2 stop bits.
 - o Slave : 1 to 255
 - o Mode : RTU, 16-bit ASCII, 32-bit ASCII (Daniel)
 - o Turnaround time : 300 ms (depending on screen length)
 - o Cyclic interrogation in 100 ms steps

- Data :
 - o Address range: 1 to 8192 words of 2 bytes
 - o Type : 16-bit or 32-bit integer words or 32-bit real

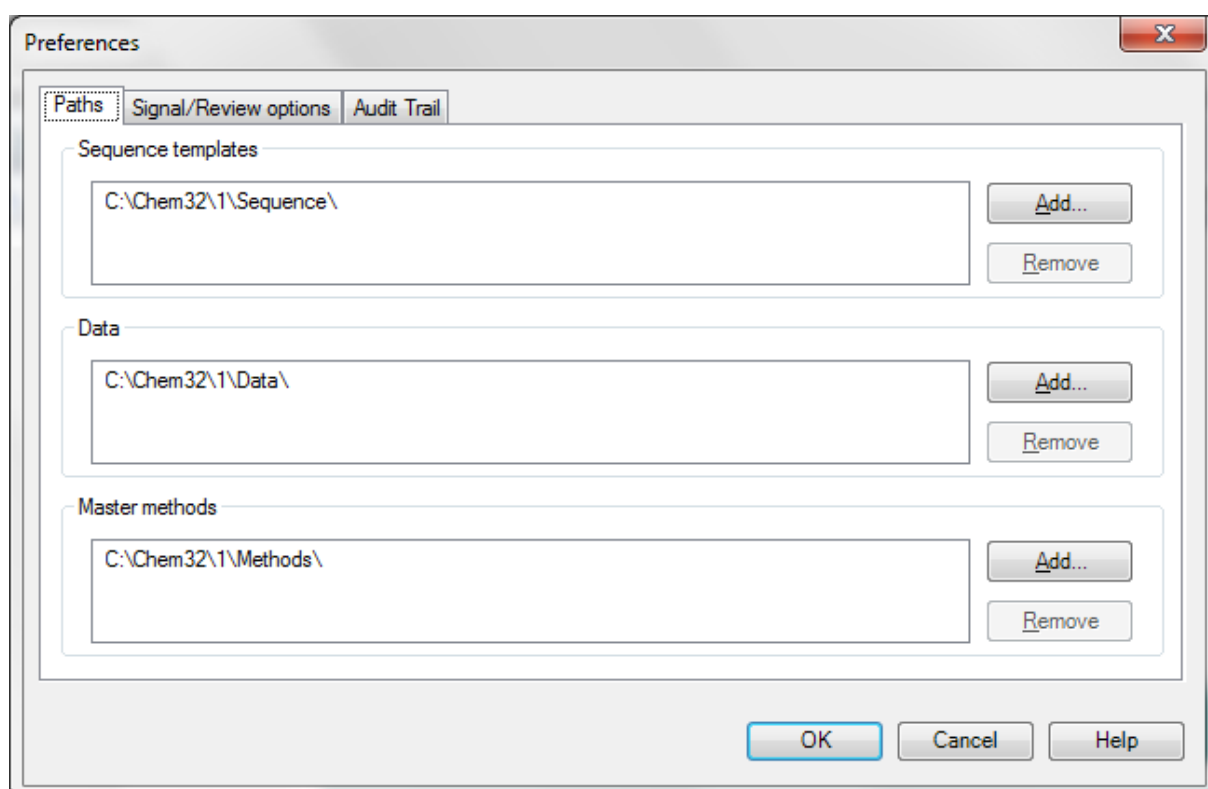
- Query :
 - o 3 Reading n words
 - o 6 Writing one word
 - o 16 Writing n words

5. Appendix I : Managing directories with OpenLab and Prochem

With the OpenLab ChemStation version, directory management has changed and now it is no longer possible to create directories for saving files when running analyses as before. These directories must be known to ChemStation.

First, it is necessary to create the backup directory with Windows Explorer. Then, it is necessary to identify at the OpenLab level, this directory as data backup directory.

From the main screen, click on the **View** menu, then **Preferences**. The following window opens:



Click on the **Add** button in the Data frame and select the desired new directory.

When this choice has been made, this directory will then be visible in Prochem in the Start window.

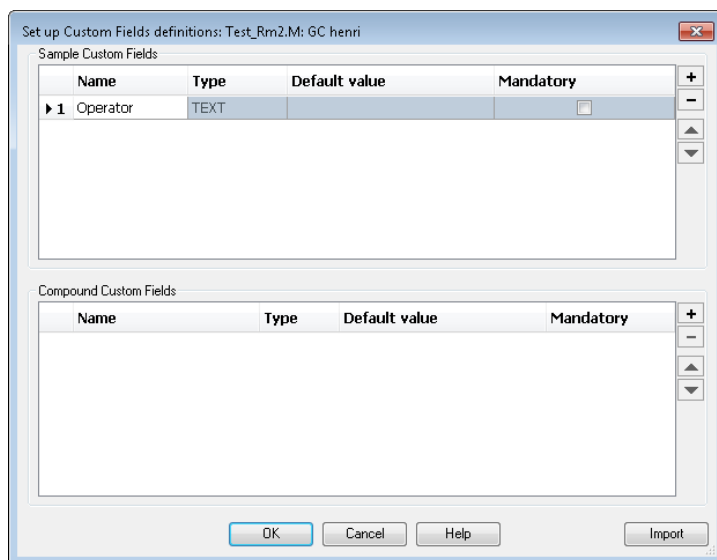
Then, you can enter the SubDirectory name, this directory will be created as a subdirectory of the main Path data directory, selected in the list.

6. Appendix II : Managing users' name with Openlab

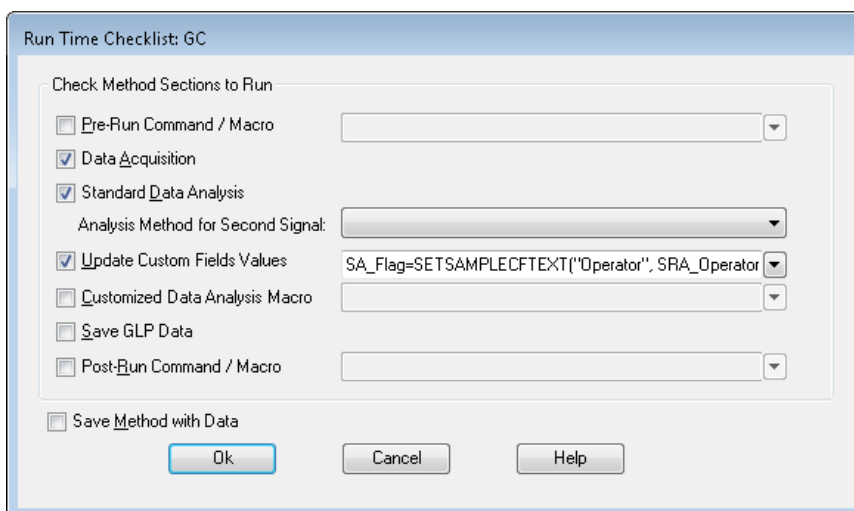
Since OpenLab version C.01.08, it is no longer possible to change the operator name. The application always uses the name 'System'.

In some cases, the user wants to be able to identify the person who performed the analyses. In Prochem, there is a specific field in the 'Start' window. To be able to transmit this name to the final results, it is necessary to configure OpenLab correctly.

On the '**Method and Run Control**' screen, click on the '**Method\Custom fields setup**' menu. The following window is displayed:



In the '**Sample Custom Fields**' box, click on the **+** button: a new line is added to the list. Enter **Operator** in the **Name** field, select '**Text**' in the '**Type**' cell, confirm with Ok. Then click on the '**Method \Run Time Checklist**' menu, the following window appears:



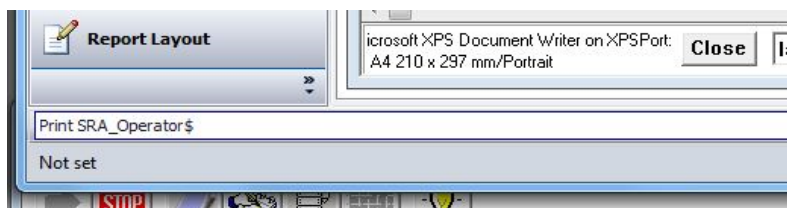
Check the box **"Update Custom Fields Values"** and, in the next field, enter the command while respecting the uppercase characters:

SA_Flag=SETSAMPLECFTEXT("Operator", SRA_Operator\$)

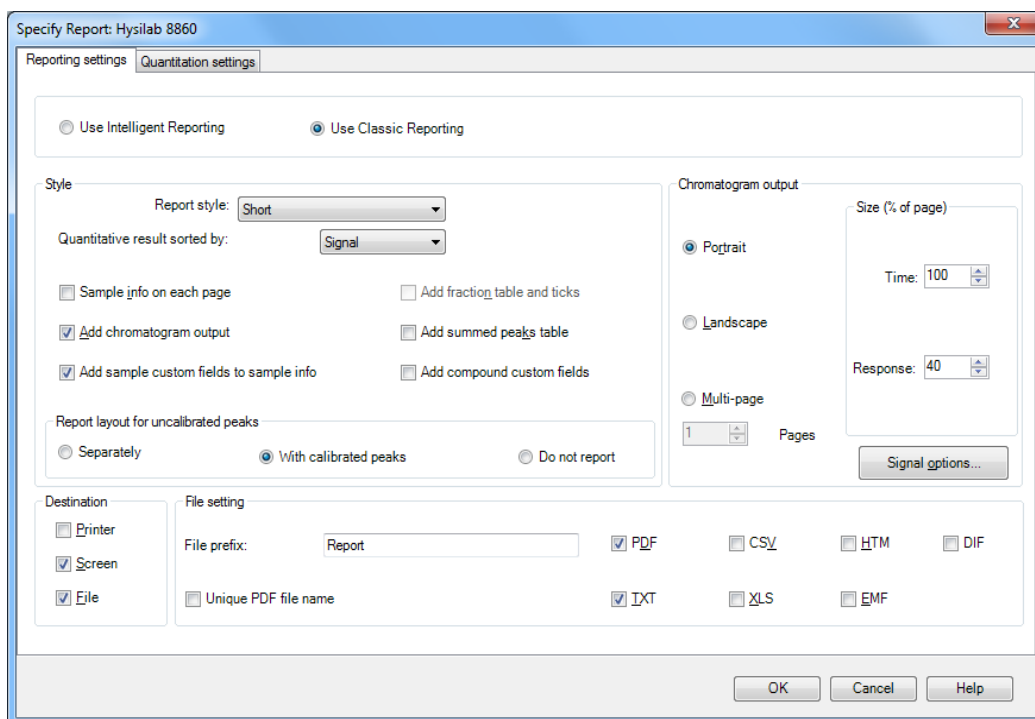
where **"Operator"** is the same name as **"Sample Custom Field"**.

SRA_Operator\$ is the name of the operator transmitted by Prochem. To check if this name is correct, type **"Print SRA_Operator\$"** in the command line.

The name should normally be displayed as below.. This allows you to check if the SRA Instruments macros are correctly installed.



To display the operator's name in the report, select the **'Data Analysis'** screen and click on the **'Report\Specify report'** menu. The following window appears:



Check the box **'Add sample custom fields to sample info'** and confirm with Ok.

! The modifications must be done for each method.

7. Appendix III : Coupling with MSD ChemStation and Mass Hunter

7.1 Software installation

For the installation to be successful, Mass Hunter must be installed and configured first. Then, the user must install Prochem on the same computer.

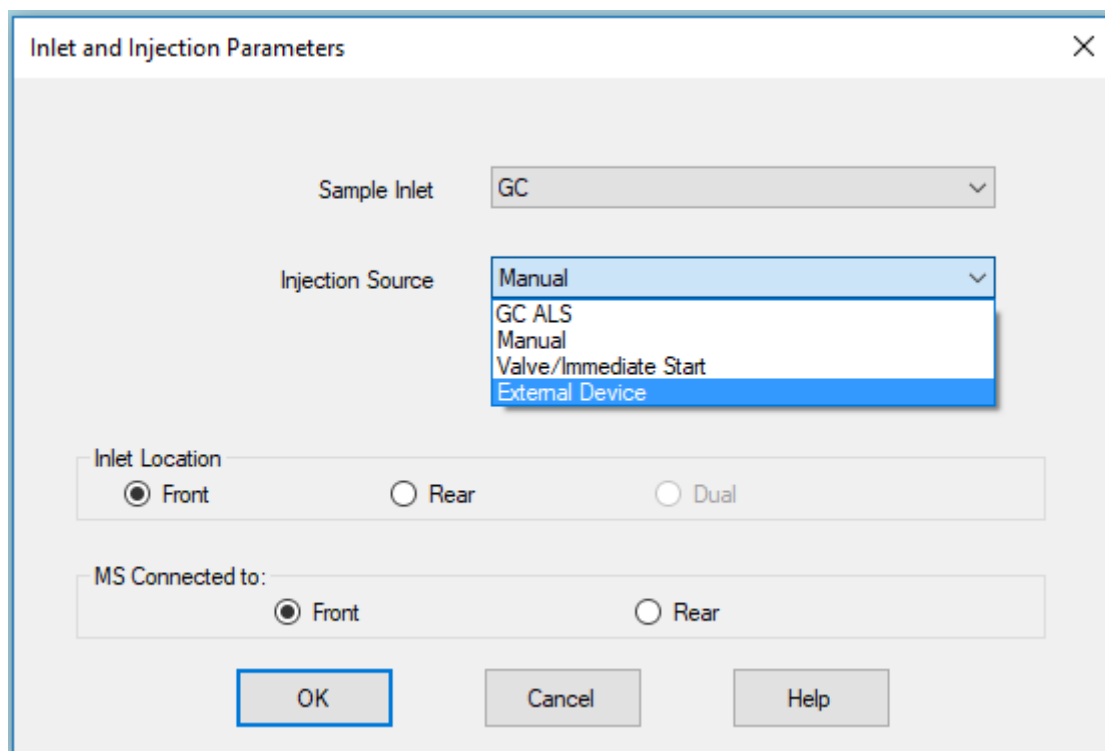
The Prochem installation installs different macros at the Mass Hunter level and the intermediate software CpPHunter.exe (SRA program). After this installation, it is necessary to restart Mass Hunter so that it takes into account the modifications brought by the installation of Prochem.

7.2 Use with Mass Hunter

7.2.1 Analyses launch

Prochem launches the analyses. When it is out of analysis, Mass Hunter's state is 'Idle'. When the chromatograph is 'Ready', Prochem asks Mass Hunter to go into 'PreRun' analysis preparation mode and the analysis is then started either by the action of a valve, or by a dry contact controlled by Prochem or by an injection system (purge & trap or desorber).

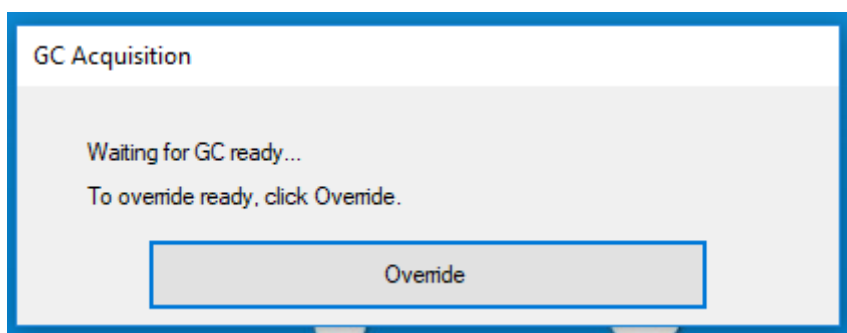
When editing the GC method, it is important to choose the correct injection mode 'Source injection'.



In the case of a valve, select the 'Valve/Immediate Start' mode.

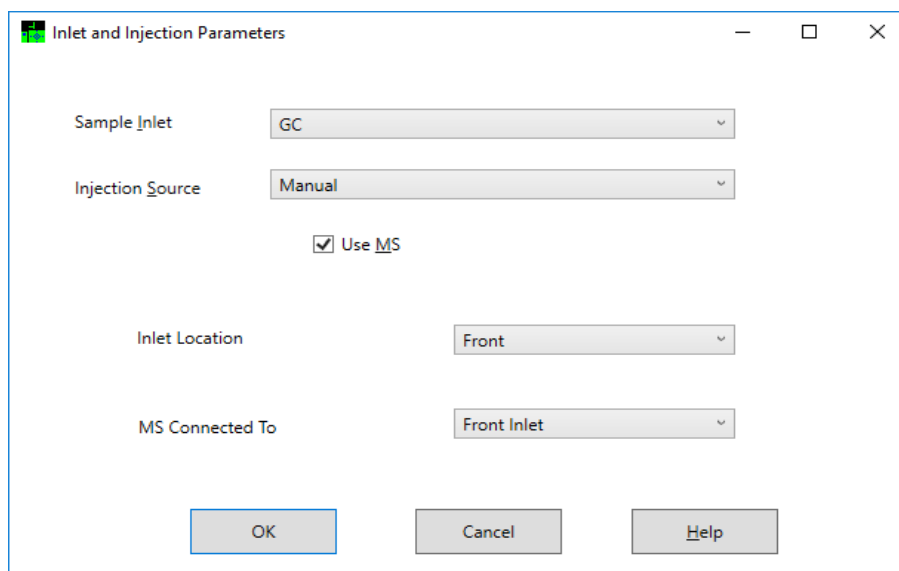
In the other cases, it is preferable to privilege the 'External Device' mode instead of the 'Manual' one, especially in the case of a system of injection type 'purge & trap' or 'desorber' which waits that Mass Hunter is in 'PreRun' mode to launch their cycle of injection.

If the method uses a temperature ramp, it is possible that after loading the method, the GC will switch several times from Ready to Not Ready state. When Prochem prepares Mass Hunter to perform the analysis (Idle to PreRun), the following message may appear:



If the 'Start' contact closes at this time, the cycle is started at GC level but not at mass spectrometer level. This signal is therefore not acquired.

The solution to avoid this phenomenon is to use the Prochem event table, program a "Start GC" command and configure the injection source in "Manual" mode. When preparing the analysis, Mass Hunter can easily switch from Ready to Not Ready state and display the 'Override' window. Prochem will wait until the 'Start' window is displayed to confirm the start and execute the analysis on both channels.



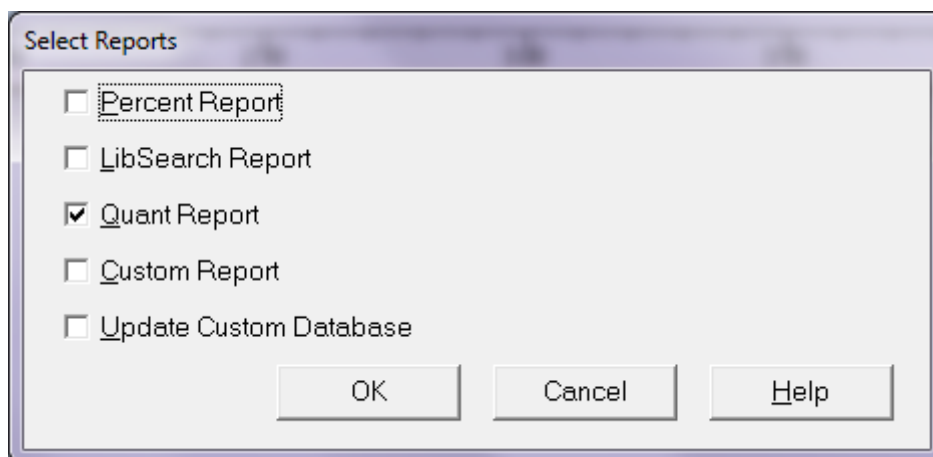
This can also be a solution to start the analyses without auxiliary command (dry contact via Adam).

7.2.2 Transfer of results

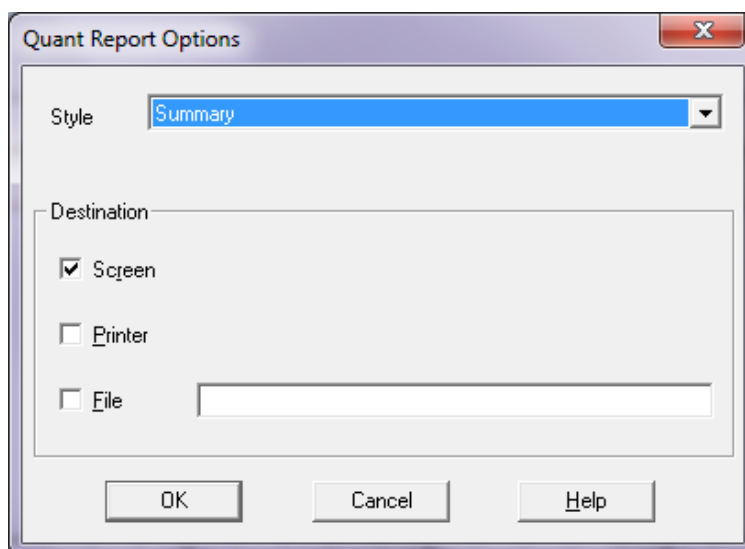
Prochem retrieves Mass Hunter results **only if the analyses are processed with Data Analysis**.

To obtain this transfer, it is necessary to correctly set the Mass Hunter method in order to generate the results. This setting is made from the Data Analysis application.

Select the menu **'Method'** then **'Edit Method'**. The following window appears:

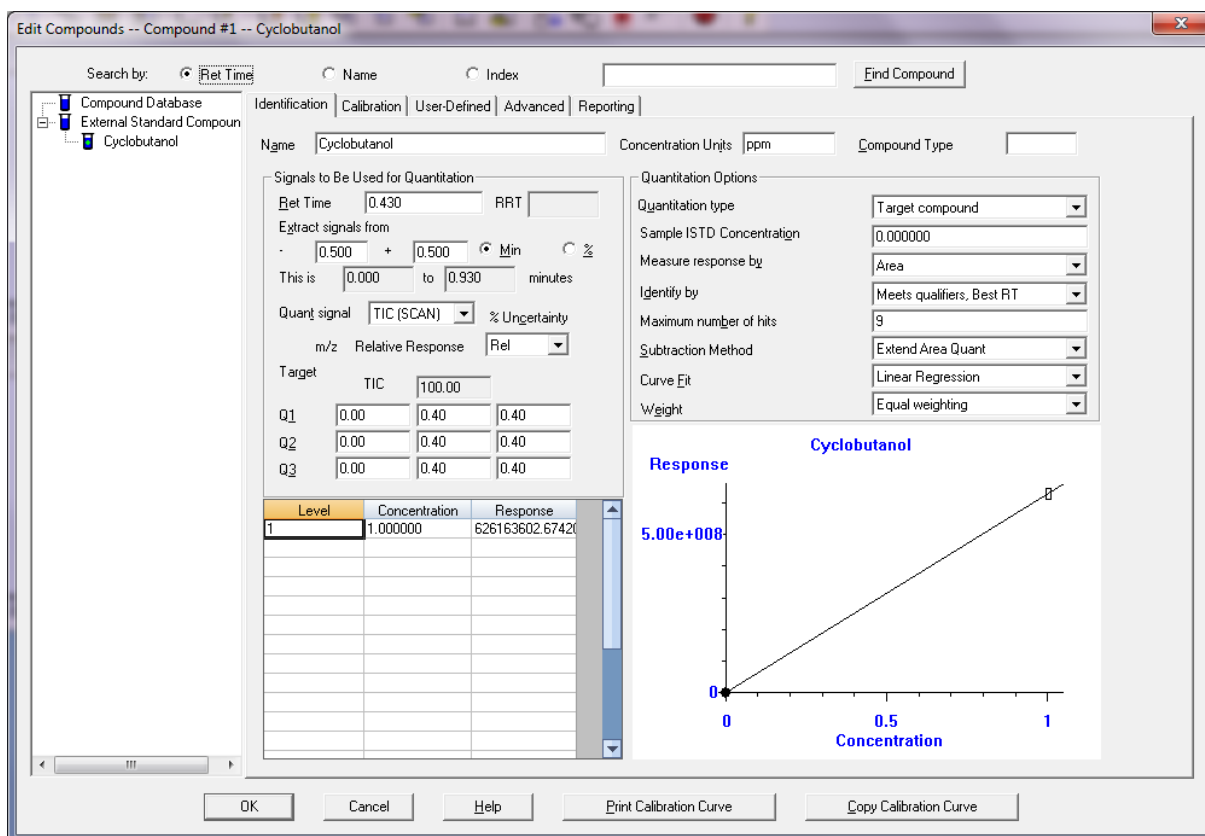


Check the box 'Quant Report' and confirm with Ok, the following window appears.



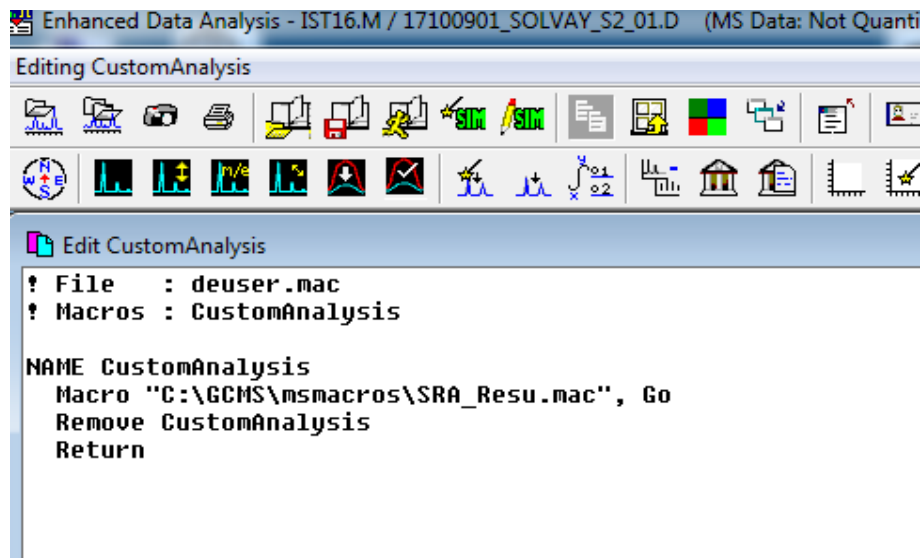
It is not necessary to check one of the boxes, validate with Ok.

Then, it is necessary to create a table with at least one component. Select the menu **'Calibrate'** then **'Edit Compounds'**.

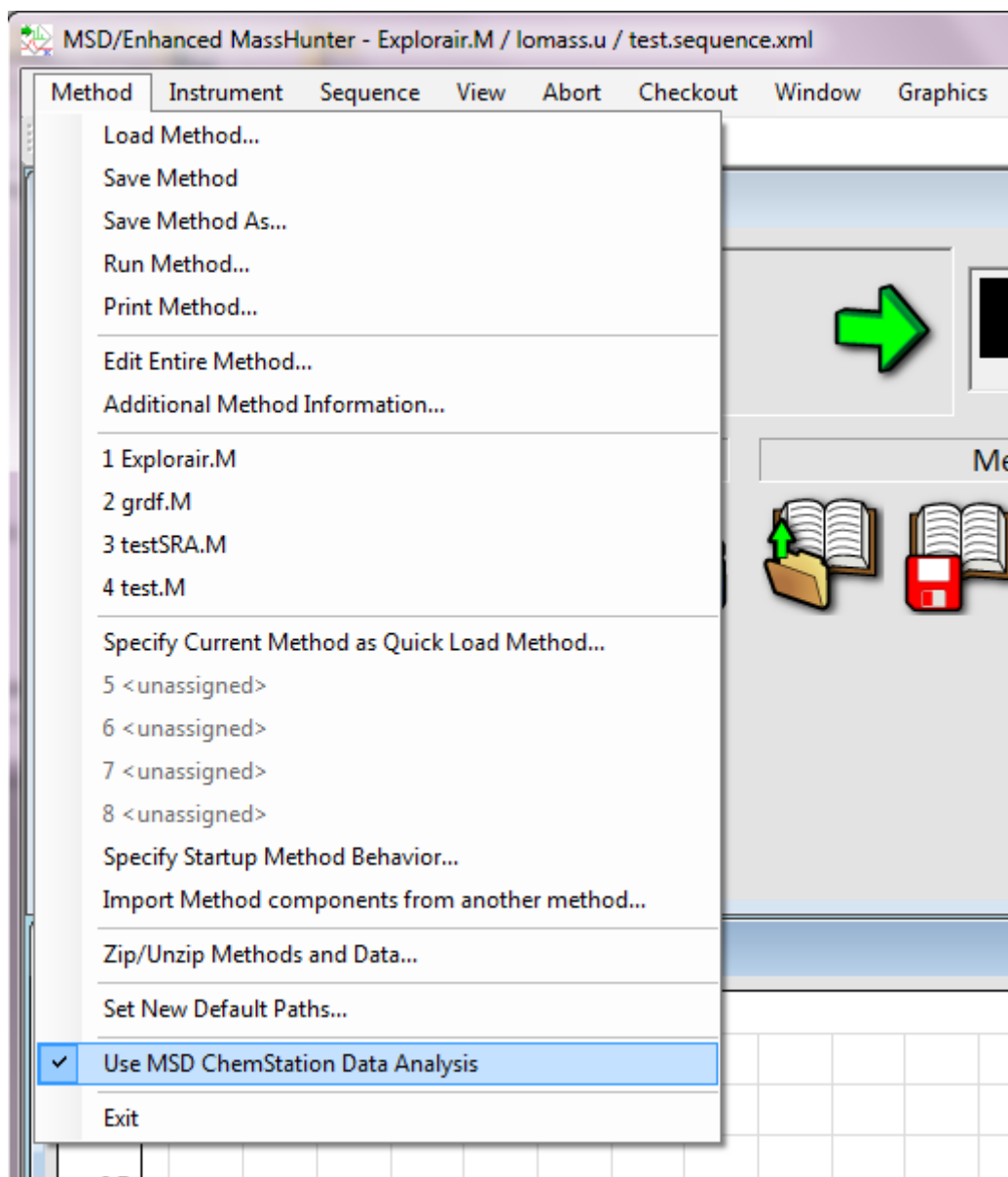


Create a component by entering its various integration and quantification parameters, validate with Ok, and save the method to finish.

To finalize this setting at the Data Analysis level, it is necessary to modify the "CustomAnalysis" part of the method so that the macro that generates the results file is launched at the end of processing. This action is performed using the 'Result transfer' menu and 'Add Custom macro in method'. The result of this action can be viewed using the 'Method' menu and 'Edit CustomAnalysis'.



Finally, to complete the Mass Hunter settings, it is necessary to ask the GC-MS Acquisition application to use Data Analysis during processing. This action is enabled when the '**Method\Use MSD ChemStation Data Analysis**' menu is checked.



When these actions are performed, the 'SRA_Results.Txt' file must be created for each analysis in Mass Hunter's 'Executable' directory (C:\GCMS).

8. Appendix IV : Using Prochem with a Markes Thermal Desorber

Prochem can be used with a Unity-xr thermal desorber from Markes.

In the standard configuration, the user prepares the sequence to be injected via the Markes Instrument Control software. The desorber launches the analyses as soon as the chromatograph is ready via its start command.

For a configuration with Prochem it is necessary to use a relay which will intercept the ready state of the chromatograph and prevent the desorber from starting the analyses.

Similarly, the system can be equipped with a CIA Advantage Markes sampler which allows the injection of several channels into the desorber. In this case, Prochem must retrieve the number of the injected channel.

8.1 Prochem configuration

The configuration of Prochem is carried out at three levels.

8.1.1 Instrument menu

Configuration of chromatograph 1

Instrument name :
 TD-GC (GC) [v] [Ok]

Repeater of GC Ready :
 None [v] [v] [Cancel]

Remote start for Prochem

Any
 External command
 Logical input

Address board Input Standby value

None [v] 1 [v]

Options Start GC

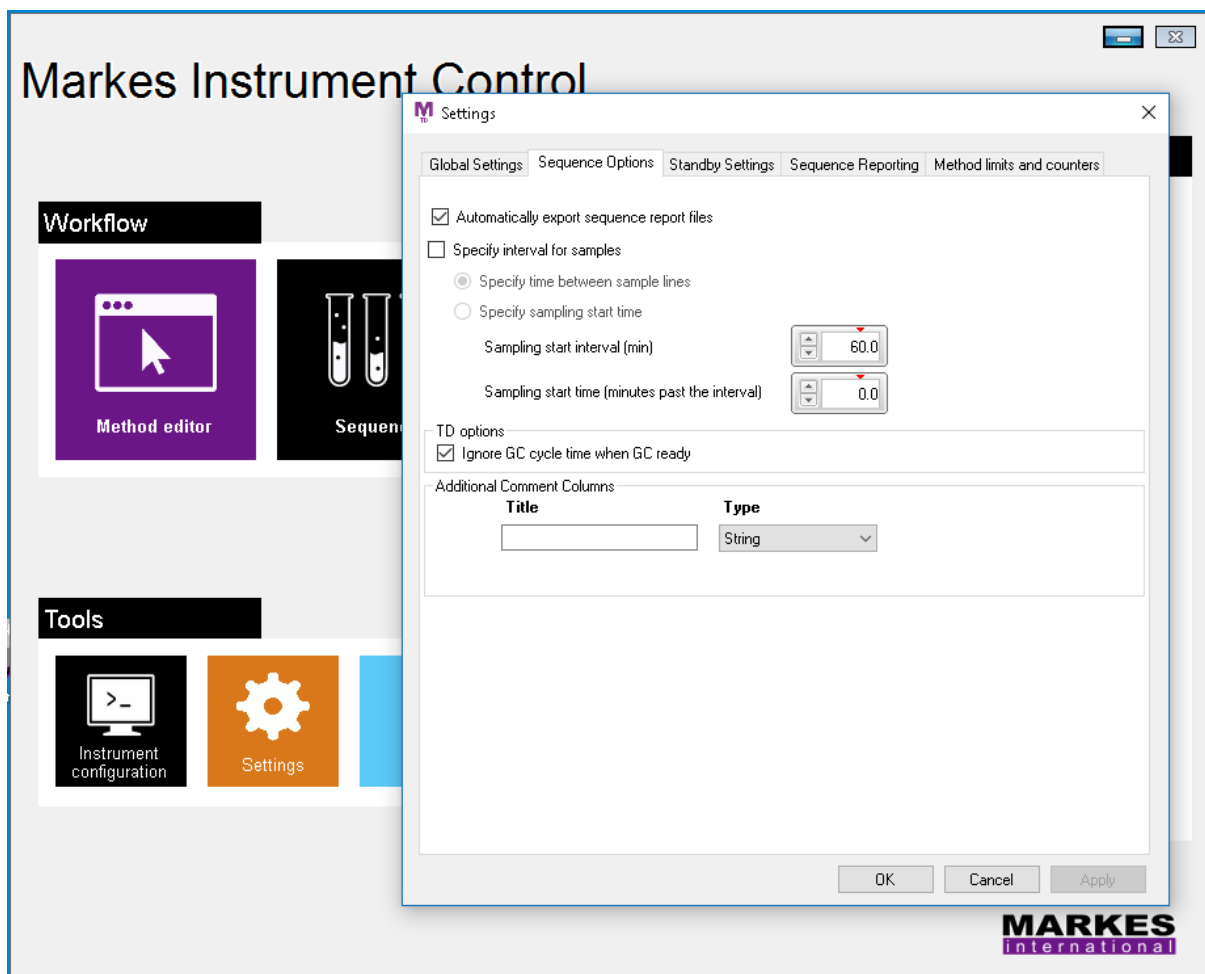
External device injection to control by auxiliary event
 Check external ready (7890)
 Use with a Markes controller

Folder of sequence file :
 C:\ProgramData\Markes International\TD\Sequences [..]

The 'External device ...' checkbox is used to indicate to Prochem that there is an external command to start the analyses, i.e. the start of the desorber.

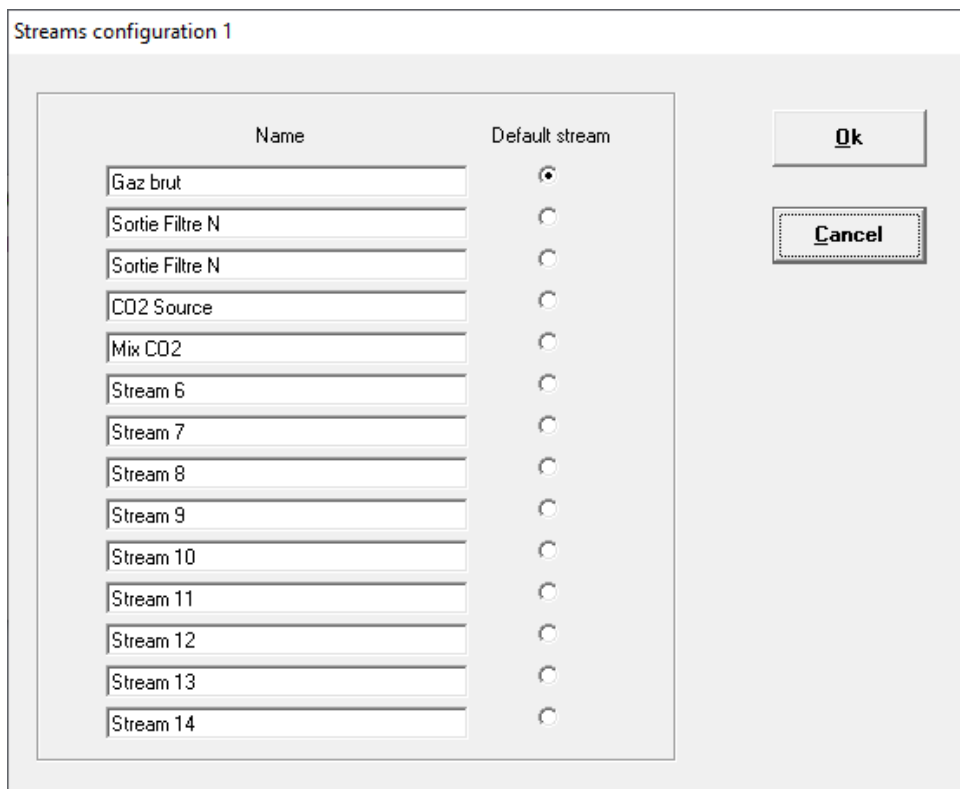
The 'Use with a Markes controller' checkbox adds an optional 'Read Markes channel' command to the event table to read the number of the channel injected. It is also necessary to fill in the directory where the file to be read is stored to know this information.

In the Markes software, the user must check that the 'Automatically export sequence report files' option in the Settings menu of Tools is enabled.

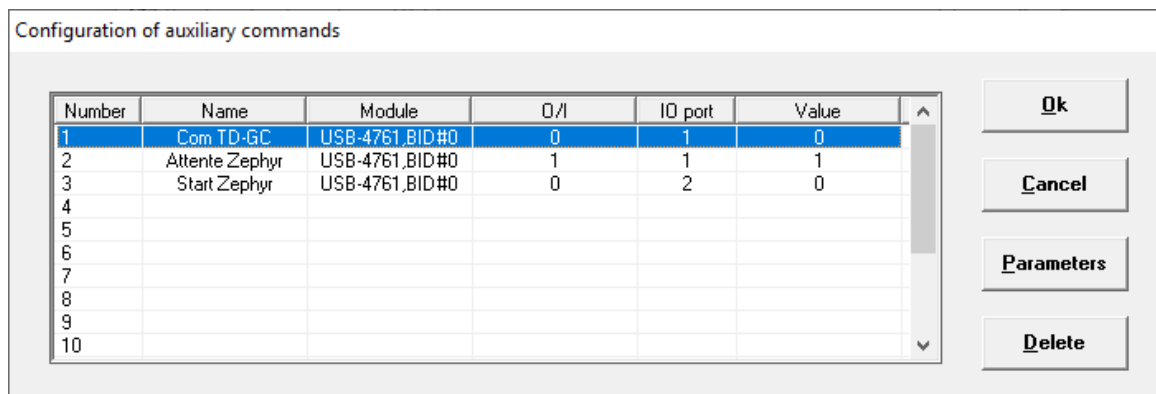


8.1.2 Sampling/Configuration menu

It is necessary to indicate to Prochem the same number of streams as there are analysis channels at the CIA Advantage level. The names of the streams must match the names of the channels.



8.1.3 Auxiliary commands menu



It is necessary to add a relay contact between the GC Ready output of the chromatograph and the input of the desorber so that Prochem can impose the start of the analyses.

Configuration of auxiliary command 1

Name :

Module :

Output/INput
 Output Input

ID port : Standby value

8.2 Using Prochem

In the Prochem software, it is necessary to use an event table which will allow to manage the relay control and to indicate to the desorber that the chromatograph is ready to perform an analysis.

8.2.1 Event table

Auxiliary commands - C:\Chem32\1\Sequence\robert.vnt

File Edit

0 Start GC

	Time (sec)	Command	Event
>	0	TD - GC	On
2	2	Read Marques channel	
3	5	Start GC	

Sort
Add
Modified
Delete
▲
▼

The 'Read Markes channel' command must be programmed to know the channel injected by the TD. Finally, it is necessary to add a 'Start GC' command to prepare the analysis.

8.2.2 Analysis sequences

If the launch of the analyses requires a sequence at the Markes software level, it is necessary to use a sequence also at the Prochem level in order to indicate the GC method and the event table that are used.

The screenshot shows a window titled 'Sequence table - C:\Chem32\1\Sequence\Perrier.seq'. It contains a table with the following data:

	Stream	Method	Sample Type	Cal Level	Event file
1	Gaz brut	méthode HC.M	Sample		Sra.vnt
2	Sortie Filtre N°1	méthode HC.M	Sample		Sra.vnt
3	Sortie Filtre N° 2	méthode HC.M	Sample		Sra.vnt
4	CO2 Source	méthode HC.M	Sample		Sra.vnt
5	Mix CO2	méthode HC.M	Sample		Sra.vnt
6	Gaz brut	méthode H2S.M	Sample		Sra.vnt
7	Sortie Filtre N°1	méthode H2S.M	Sample		Sra.vnt
8	Sortie Filtre N° 2	méthode H2S.M	Sample		Sra.vnt
9	CO2 Source	méthode H2S.M	Sample		Sra.vnt
10	Mix CO2	méthode H2S.M	Sample		robert.vnt

On the right side of the window, there are three buttons: 'Insert', 'Add', and 'Delete'.

Regarding the 'Sample Type' parameter, the type 'Sample' is to be used by default and it is not necessary to indicate the name of the channel, and therefore the number, because it will be retrieved when the desorber will inject.

However, in some cases, the user may want to impose the name of the sample if the analysis is not performed in the context of a standard sample but rather as part of a verification or calibration. The user must then change the type to either Calibration, Control or Blank and enter the name in the 'Sample name' field when starting the analysis.

8.2.3 Launching analyses

Before starting the analyses, the user must prepare the sequence in the Markes Instrument Control software and ensure that it contains the correct number of analyses.

9. Appendix V : Description of the Prochem database

Prochem uses a database to save the analysis results. This is a Microsoft Access compatible database saved as Resultsx.mdb where x represents the instrument number corresponding to the ChemStation session number.

At each end of analysis, the software checks the results stored in the database that were performed on the same stream as the analysis completed and erases the results prior to 31 days.

9.1 Definition of tables (information and common)

There are 2 information tables:

- **Version** containing the version number of the database (field and unique record)
- **Last analyse** containing 12 fields; this table contains the information of the last analysis performed and therefore has only one record.
 - o Stream : number of the sampling line
 - o Number : analysis number
 - o Vial : number of the vial or sampling line
 - o SampleAmount : injected quantity
 - o ISTDAmount : internal standard quantity
 - o Multiplier : multiplication coefficient
 - o Dilution : dilution factor
 - o InjVolume : Injected volume
 - o SampleType : sample type (sample, standard, blank)
 - o CalLevel : calibration level in case of calibration
 - o UpdateRF indicates if the response coefficients are refreshed after a calibration
 - o UpdateRT indicates if the retention times are refreshed after a calibration

There are 5 tables common to all streams.

- **Stream** containing three fields in reference to the sampling lines:
 - o IndStream : table index
 - o Name representing the stream name
 - o Etalon indicating whether the stream is a sample or a standard
- **Peak name** containing three fields referring to the analyzed components:
 - o IndName : table index
 - o Name representing the component name
 - o IdLims containing Lims number (not used)
- **Calcul name** containing 7 fields:
 - o IndName : table index
 - o Name corresponding to the name of the calculation
 - o Unit corresponding to the calculation unit
 - o IdLims corresponding to Lims number (not used)
 - o Value1

- Value2
- Value3

- **Input name** containing 4 fields with reference to analog inputs:
 - IndName : table index
 - Name corresponding to the name of the analog input
 - Unit corresponding to the unit of the analog input
 - IdLims corresponding to Lims number (not used)

- **Alarm** containing 6 fields with reference to the programmed alarms:
 - Number indicating the alarm number
 - Name corresponding to the followed parameter (peak or calculation)
 - Stream corresponding to the stream number to which the alarm is linked (0 for all sampling streams).
 - Value corresponding to the value followed for this alarm (surface, normalized surface, raw concentration, normalized concentration, retention time)
 - Valeur mini not to be exceeded
 - Valeur maxi not to be exceeded

9.2 Definition of the tables for each sample line (stream)

For each sampling line, there are 4 tables. In the following presentation X will correspond to the line number.

- **AnalyzeX**
 - IndAnal : table index
 - DateInject is the injection date
 - RawData is the name of the results file
 - Number : analysis number
 - Method is the name of the method used for the analysis
 - SampleName corresponds to the sample name
 - Operator is the name of the operator
 - IdLims is the Lims number of the component (not used)
 - Vial corresponds to the bottle or sample line number
 - FirstPeak : index of the first peak of the PeakX table for this analysis
 - LastPeak : index of the last PeakX table peak for this analysis
 - FirstCalcul : index of the first calculation in the CalculationX table for this analysis, if this value is zero, there are no calculations
 - Last Calcul : index of the last calculation in the CalculationX table for this analysis
 - FirstInput : index of the first analog input for this analysis, if this value is zero, there is no analog input
 - SampleAmount : injected quantity
 - ISTDAmount : internal standard quantity
 - Multiplier : multiplication coefficient
 - Dilution : dilution factor
 - InjVolume : injected volume
 - SampleType : sample type (sample, standard, blank)
 - CalLevel : calibration level in case of calibration
 - UpdateRF indicates if the response coefficients are refreshed after a calibration

- UpdateRT indicates if the retention times are refreshed after a calibration
- Flag (not used in reserve)

- **PeakX**
 - IndPeak : table index
 - Analyze corresponding to the analysis number
 - Number corresponding to the index of the Peak name table
 - RetTime corresponding to the retention time
 - Area corresponding to the surface
 - AreaNormal corresponding to the normalized surface
 - Concentration corresponding to the raw concentration
 - ConcUnit corresponding to the concentration unit
 - Normalize corresponding to the normalized concentration
 - Value corresponding to the calculated value (density)
 - ValueUnit corresponding to the unit of the calculated value
 - Average : average calculated during the analysis (depends on the value used for the calculation and the type of calculations per analysis or per time)
 - Signal corresponds to the chromatograph signal number
 - IsStd indicates if the component is an internal standard
 - Type corresponds to the type of peak (1 known peak, 2 group, 3 unknown, 4 total, 5 total of unknowns)
 - Group corresponds to the group number
 - Cal Amount corresponds to the standard concentration
 - Alarm indicates if the result of this component was in alarm
 - Low Limit corresponds to the minimum value programmed in the ChemStation
 - High Limit corresponds to the maximum value programmed in the ChemStation

- **CalculX**
 - IndCalcul : table index
 - Analyze corresponding to the analysis number
 - Number corresponding to the index of the Calculation name table
 - Value : the different values
 - Value1 "
 - Value2 "
 - Value3 "

- **AnalogInputsX**
 - IndInput : table index
 - Analyze corresponding to the analysis number
 - Number corresponding to the index of the Input name table
 - Value corresponding to the value of the analog input