

synthra



Synthra SynthraView

Software Manual



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Revision History

Revision	Date	Change
0.1	03.Mar.2011	First Draft
0.2	11.Jul.2012	Revised Format
0.21	12.Sep.2012	Typo removal and added explanation
0.22	14.Sep.2012	Final Revision
1.0	08.Feb.2022	Major revision and software update

Glossary

A:	Ampere
AC/DC:	Alternating Current / Direct Current
Click:	Pressing the left button of the computer mouse with the cursor in a certain position. Right-click is pressing the right mouse button with the cursor in a certain area.
.CSV:	Comma separated values (data format that can be opened by a spreadsheet application)
DAD:	Diode Array Detector
GUI:	Graphical User Interface
HPLC:	High Pressure Liquid Chromatography
LED:	Light Emitting Diode
PID:	Proportional-integral-derivative controller
.tcf:	Time Control File
USB:	Universal Serial Bus
UV:	Ultraviolet
V:	Volt

1 Introduction

As a preparative data and control system, SynthraView meets all the requirements of up-to-date software in radiochemical chromatography and synthesis control. Its superior flexibility and modular construction means that the program can be adapted to suit any user's requirements. The current version of SynthraView offers a simple user interface and an improved method construction. All the advantages of networks (LAN) can be exploited without restrictions. National and international regulations (such as 21 CFR Part 11) are fully supported.

The software allows isocratic elution of up to four solvents, gradient programming and gradient support. Switching valves, fraction collectors, heaters (reactor or column-oven) and syringe dosing pumps can be controlled by time, threshold values or automatic peak sampling. Programming can be carried out in units of time, units of supplied solvent volume or in units of column volume.

The screen is able to display the pump condition, flow rate, pressure, the solvent being pumped, solvent supply, detector signals, temperatures and valve positions. An entire synthesis run can be displayed in a visualization diagram of the system that can be individually formatted, and in a time control file that indicates the stage in progress at all times.

The screen keys and visualization diagram of the system allows manual control of the pumps and valves.

During a synthesis, the functions of the time control file can be adjusted using a graphic time control editor. This allows synthesis optimization and compensation for time shifts.

The resulting data of a synthesis include all the diagrams recorded (UV, radioactivity, temperature) with integration results, time control tables, sequence table, a protocol of the entire run and a fraction table with links to the appropriate chromatograms. Thus SynthraView allows the user to re-establish all the relevant information necessary to reproduce the synthesis only with the data recorded by the system.

1.1 This Manual's Audience

Prerequisites to use this manual are: Knowledge of how to use the operation system this software is installed on and training on the system this software operates to understand the activities of the software and interaction with the synthesis system. Knowledge of HPLC is also very helpful but not necessary to be able to configure the program. There is some information on how to handle some very basic tasks, this way even a user with little experience can use the software conveniently.

This is not meant to be the user guide for any Synthra synthesis system. All

the information a user needs to use the system for the predetermined task are found in the Operation Manual, delivered with the synthesis equipment. Any user reading this manual should be familiar with the Operation Manual of the system used.

Synthra synthesis systems are completely setup at customer's site and there is no necessity to modify the software, this is only an option.

A deeper reference to the setup structures will be given in the later chapters. They are meant for people who want to optimize their system for certain purposes. It will be explained what to do if the system is modified, how to tell the software that something on the machine has changed and incorporate it into the system visualization.

1.2 Overview of the Software Manual

This manual is not written for a specific system, it is concentrating on the software. This software is used on multiple standard and customized systems. Some of the information here may be about features that are not part of a system in question. If there are features described in this manual that are not part of the system in question, it is not because they are missing but they are no element of this configuration.

Most figures in this manual are examples of how something looks like. The real appearance is depending on the configuration of the system and the software version.

2 Starting the software

The software can be started by clicking the SynthraView Icon on the desktop or in the start menu.



Figure 1 (SynthraView) Icon

After an automated calibration a welcome window opens up.

To go on starting the software the welcome window has to be clicked on or enter has to be pressed to continue.



Figure 2 (Welcome Window)

3 The main window

The main window consists of:

- Title Bar
- Menu Bar
- Toolbar
- Display Bar

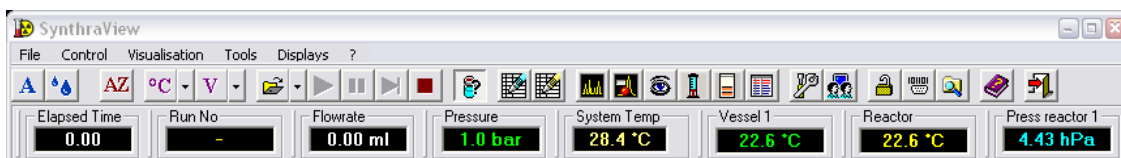


Figure 3 (Main Window)

3.1 Title Bar

The Title Bar shows the SynthraView icon and the name of the program on the left. In other windows the Title Bar doesn't always display the programs name; usually it is the name of the window that is displayed. This way it is easy to distinguish between different windows. On the right there are the usual buttons of most windows to:

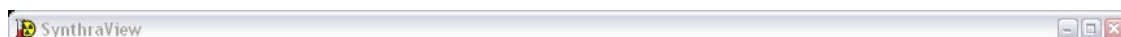


Figure 4 (Title bar)



Minimize the window



Maximize the window (if it isn't)



Restore Down the window (if it is maximized)



Close the window, that will end the program

One has also the possibility to move the window. Grabbing the Title Bar is done by a mouse click onto the Title Bar (not on the three buttons on the left but anywhere else). Holding the left mouse button and moving the mouse also moves the window. If the window has reached the destination desired the mouse button has to be released to drop it there.

Most windows can also be changed in size. The mouse cursor has to be moved onto the edge of the window to a position where the mouse cursor changes to an arrow pointing into opposite directions. Now it is possible to move the edge of the window by clicking the left mouse button and holding it down. Moving the mouse into the directions the arrows point changes the position of the edge. To release the grip on the frame, the mouse button has to be released. To change the window size in two directions at the same time, a window corner can be dragged similar to the edges.

3.2 Menu Bar

The Menu Bar is the access area to all possible actions you can perform with this software.



Figure 5 (Menu Bar)

Many of the menu items can also be accessed by the Toolbar (see chapter: 3.3 Toolbar). For the common actions available in the Menu and the Toolbar there is an explanation in both chapters to aid the reader who is looking for something specific. For Menu Items and Tools that many of the software's Menus and Toolbars have in common (e.g.: Open) there will be a special chapter called Common Actions (3.5). These are easy to understand actions that only need to be explained once.

We also show all the menus available for a better understanding if the program is not available to the reader at the moment.

3.2.1 File Menu

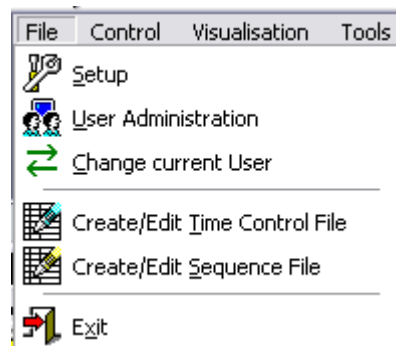


Figure 6 (File Menu)

3.2.2 Control Menu

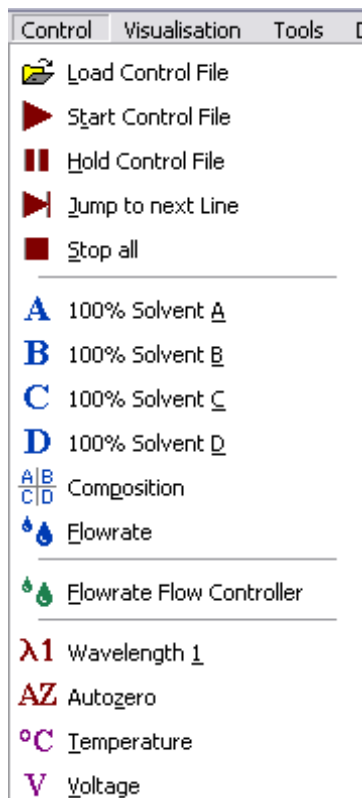


Figure 7 (Control Menu)

3.2.3 Visualization Menu

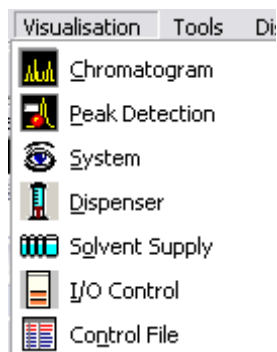


Figure 8 (Visualization Menu)

3.2.4 Tools Menu

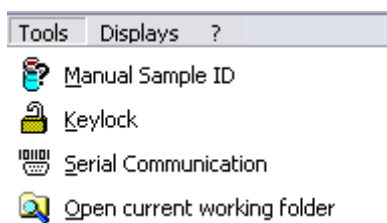


Figure 9 (Tools Menu)

3.2.5 Displays Menu

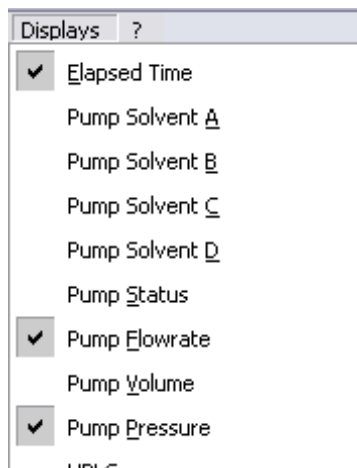


Figure 10 (Displays Menu)

3.2.6 ? (Help Menu)

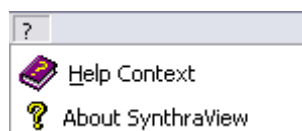


Figure 11 (Help Menu)

3.3 Toolbar

The Toolbar is a visual way to access the actions, which also can be accessed via the Menu Bar. The favorite way of working, either using the Menu Bar, the Toolbar or a mix is completely left to the user.



Figure 12 (Toolbar)

To change the Toolbar's contents double click in an empty space on the Toolbar, the "Customize Toolbar Window" will open. Here icons can be added and removed.



Figure 13 (Customize Toolbar)

All available icons are shown; those already displayed are checked in the checkbox underneath. If the icon's checkbox is empty it is not shown in the toolbar.

To add an icon the checkbox under the desired icon has to be checked by a single left mouse-click.

To remove an icon one has to un-check the checkbox under the undesired icon by a single left mouse-click on the checkbox to uncheck it that way.

3.4 Actions of the Menu- or Toolbar



100% Solvent A Major Pump: starts the pump with 100% eluent A and the currently set flow rate



100% Solvent B Major Pump: starts the pump with 100% eluent B and the currently set flow rate



100% Solvent C Major Pump: starts the pump with 100% eluent C and the currently set flow rate



100% Solvent D Major Pump: starts the pump with 100% eluent D and the currently set flow rate



Solvent composition Major Pump: starts the pumps with the solvent composition shown in the “Solvent Composition” window and the currently set flow rate



Flow Rate Major Pump: opens a window to show the flow rate. A change to the flow rate does not start the pumps, but will take immediate effect if the pump is running



Flow rate Flow Controller: opens a window to show the flow rate



Wavelength 1: opens a window in that the first wave length of a serial controlled detector can be entered



Auto zero: will set a serial controlled UV detector back to zero



Temperature: opens a window where the temperature for reactors and heaters can be seen



Voltage: opens a window where the voltages for flow regulators and pressure regulators can be set



Load Time Control File or Auto-sampler Control File: opens a file selection window in that a time control file or an auto-sample control file can be opened. In the file type box of that window one can see that *.tcf (Time Control File) or *.scf (Auto-sampler Control File) can be chosen. If the option “Start Pumps after loading Time Control File” is selected in the time control file, the pumps will begin at once, after the file is opened, with the flow rate and solvent composition programmed for time 0:00.



Start Time Control File or Auto-sampler Control File: starts the time control file or auto-sampler control file that has been loaded. If the function “Hold Time Control File or Auto-sampler Control File” was executed first, the run will resume by clicking this icon.



Hold Time Control File or Auto-sampler Control File: pauses the time laps of time of a time control file or auto-sampler table. If the option “Stop Pumps at Time Control Hold” is selected in the time control file, the pumps will have a flow rate of 0ml. If hold is active, the flow rate of the pumps can be adjusted manually using the “Flow rate” icon.



Jump to next Time Control Line: jumps forward in time to the next line programmed in the time control table. The first time this function is used one must confirm a dialogue box, here it is possible to use the option “Don’t ask again” for not being asked for confirmation anymore.



Stop All: stops the pumps and the time control file. It is not possible to resume a synthesis run when it was stopped.



Manual Sample ID: enables the user to enter a sample identifier starting a time control file. This option is not active if processing an auto-sampler control file, because the sampler identifiers are derived from the accompanying sample identifier file.



Create / Edit Time Control File: opens the Time Control File Editor to create or edit a time control file (see Chapter: 4 Time Control Files)



Create / Edit Sequence Control File: opens the Sequence Control File Editor to create or edit a sequence control file (see Chapter: 5 Sequence Control Files)



Chromatogram: opens the Chromatogram Window to show the Analysis, Reconstruct and Reprocess (see Chapter: 6 Chromatogram)



Peak detection: opens the window with the automatic peak sampling displays. (see Chapter: 7 Peak Detection)



System Visualization: opens the System Visualization Window (see Chapter 8: System Visualization)



Dispenser Visualization: opens the Dispenser Visualization Window for manual control of the dispenser (see Chapter 9 Dispenser Visualization)



Solvent Supply: opens the window with the Solvent Supply Display (see Chapter 10 Solvent Supply)



Event Box Control: opens the window with the Digital I/O Control (see Chapter 11 Event Box Control (Digital IO Control))



Time Control Visualization: opens the window with the visualization of the time control file and auto-sampler control file in table form. (see Chapter 12 Control File Visualization)



Setup: opens the Setup Window, in that communication settings, device parameter, descriptions etc. are set (see Chapter 13 Program Settings)



User Administration: opens the user Administration Window (see Chapter 14 User Administration)



Key-lock: enables the user to lock the program. After activation, a Key-lock Deactivation window appears on the task bar that will unlock the program if the user enters the password. The factory set password is: SCPA



Serial Communication: opens a terminal window showing the serial communication between the module and the notebook. It is possible to “manually” communicate over the serial ports here.



Open Current Working Folder: opens the folder in that all gathered data is saved



Online Help: opens up the program help



About SynthraView: opens the Welcome Window that contains the information what version of the software is used.



Exit: ends the program.

3.5 Common Actions

Some of the icons that already appear in the Main Window's Toolbar will also appear in the toolbars of other windows. Because their actions are useful in a great variety of contexts, those icons are summarized here and the principle of what they do is explained.



Open / Load: Opens up a window where a file can be chosen. Files show only the reasonable actions for the according context, all others are hidden. If no file should be opened this window can be closed by choosing *Cancel*.



Exit: Leaves the actual window by closing or if used on the Main Windows Toolbar ends the program.



Zoom: is used to enlarge parts of the display. To do this a frame has to be dragged around the area of interest with the left mouse button held down. The area that should be magnified should be included by this window. To return to the complete view right-click with the mouse.



Save: Writes changes of a file to the hard drive under a known file name. If a new file was created and the file name is not known the *Save As* window will open that the user can enter the location and name for the new file.



Save As saves the file with a new name and/or location (opens the Save As dialog)



Print: opens a print dialogue to print out the file

3.6 Display Bar

The Display Bar is used to visualize all important parameters of the system. Some of the system parameters may already be shown in the System Visualization but most systems have parameters that would be misplaced if showing up in that visualization. All of the parameters can be visualized in the display bar, no matter if already present in the visualization or not.

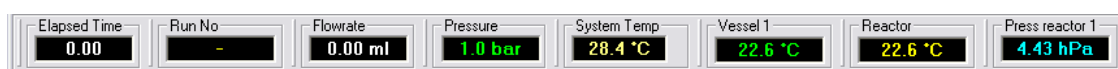


Figure 14 (Display Bar)

To add or remove displays the Displays Menu has to be opened on the Menu Bar. The Displays Menu is a list of all displays available. Some are checked and some are not. Those that are checked can already be seen in the Display Bar, those that are not checked cannot be seen in the Display Bar; to add or remove a display just click on its name.

To change the text color of a display, that display has to be right clicked, then chose *Edit Display Color* in the context menu opened, subsequently a color window opens and the color can be chosen by clicking on the desired color and finish by clicking the *OK* button.

Hint: If there is a display that is showing neither value nor line (a minus like symbol that is displayed if there is no value to display) check if the color of the display is set to black so that it isn't readable anymore.

The arrangement of the displays can also be changed. There is a vertical separation line between each neighboring display.

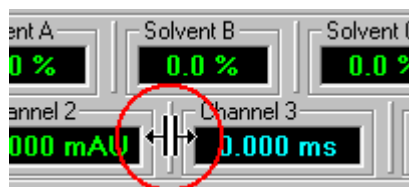
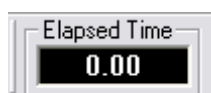


Figure 15

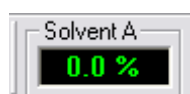
If this line is clicked on and pulled between two other displays, the one right to the line can be moved. While doing this, the mouse button may not be released. It is pulled along and is appearing between the two displays the line was pulled to. This is not only working horizontally but also vertically. If a display is pulled down a new display row appears where the display can be placed at.

3.6.1 Displays of the Display Bar

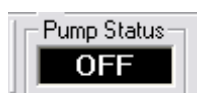
The displays look all quite similar so not all are explicitly shown here.



Elapsed Time: shows the time that has elapsed in a time control file. If the time control file is set on *hold* the display will flash between the elapsed time and “hold”. During the injection phase, the display flashes between the elapsed time and “Injection”. Following the time control file command “Wait for Input” the display will flash between the elapsed time and “Waiting”

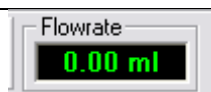


Solvent A: shows the current percentage of eluent A being pumped (also applies to the displays: Solvent B, Solvent C and Solvent D)



Pump status: shows the current pump status. ON = pump is running,

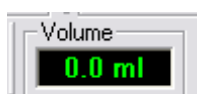
- OFF = pump has been stopped
- OVER= pump has stopped because the pressure was too high
- UNDER =pump has stopped because the pressure was too low



Flow rate: shows the pump’s current flow rate



Temperature: shows the heater’s current temperature



Volume: indicates the volume pumped since pumping has begun. If the pump is stopped, the volume display returns to 0. Depending on the volume pumped, the display unit changes automatically from μl through ml to l



Pressure: indicates the current pump pressure.

Collector Pos.: unnecessary for Synthra modules

Fraction Limit: unnecessary for Synthra modules




Valve Control: shows the current position of the selected valve and is also a way of switching the valve manually. To do this, select the desired valve and position; click the Set button to realize the change.

Vial No. : unnecessary for Synthra modules

Channel 1-Channelx: shows the values of the device connected to each of the analogue input channels. The names of the channels can vary, in a set up system most of the used channels get renamed so the channel names are more meaningful.

4 Time Control Files

Time control files are the ideal way to automatize a synthesis. It is something like a batch file that tells the synthesis module what to do at what time. The lines are not composed via a complicated programming language but by an intuitive modular interface.

The Time Control File Editor can be opened by the icon in the Main Window's Toolbar  or in the Menu Bar via File -> Create / Edit Time Control File.

The editor shows the time control file tabular as well as graphically. A chromatogram can be loaded as a background for the graphic section to check the functions of the time control file and adjust them along the time and intensity axes.

The graphic presentation of functions, especially the display of the gradient, provides improved perspicuity while programming and thus helps to avoid mistakes.

It is a basic principle that every time control file begins at the time of 0:00 with a set eluent composition and flow rate, this way the initial conditions of the pumps are known.

Because the time control file starts running after it has been loaded it is essential that all valves are set to the normal position and all event box exits set. In this way it is ensured that the system is in a defined state.

If a gradient should be programmed it needs to be taken care that all the angles of the gradient as eluent compositions are included in the time control file. A linear gradient will be calculated between two different eluent compositions at two different times. If a step is to be included into the gradient, a start and an end point are added with a delay of 0:01. The last eluent composition set will be isocratic until the time control file is ended (manually or automatic).

4.1 Editor window

The Time Control File Editor Window consists of multiple parts:

- Title Bar
- Menu Bar
- Toolbar
- Time Control Table
- Tab Area

There is an optional chromatogram area that has:

- Status Bar
- Graphic Time Control File Editor

- Toolbar

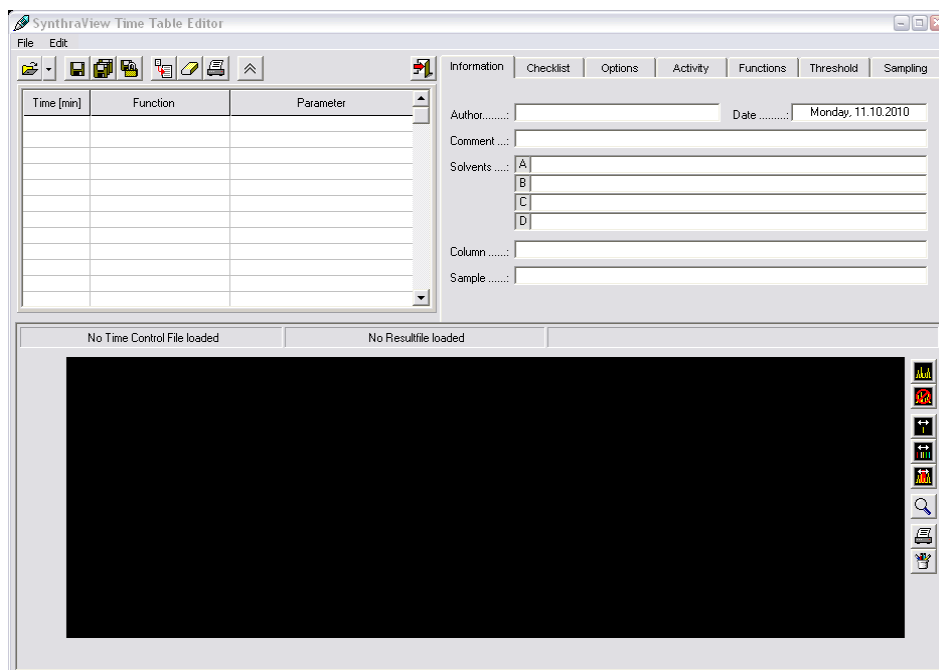


Figure 16 (Time Control File Editor)

4.2 Menu Bar

The menu bar works similar to the most known menu bars. The menus available are:

- File
- Edit



Figure 17 (The Time Control File Editor Menu)

Again most of the entries in the Menu match icons in the toolbar.

4.2.1 File Menu

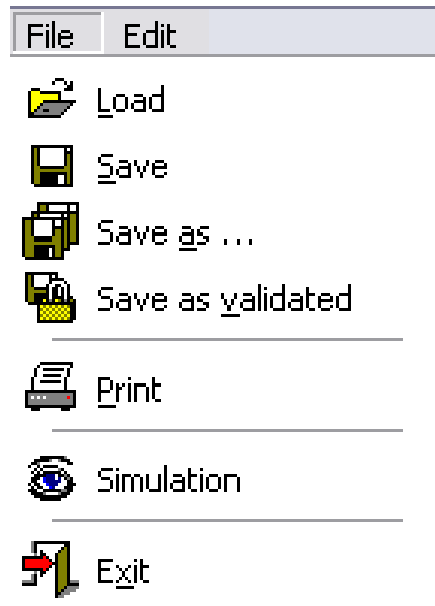


Figure 18 (File Menu of the Time Control File Editor)

Load: opens *.tcf

Save: Saves changes

Save As ...: Saves changes under new filename

Save As validated: Saves the time control file as a validated file that cannot be changed anymore.

Print: opens up a dialog to print

Simulation: Starts the simulation mode, during programming or editing of the synthesis file the valves are virtually switched in the visualization

Recent Files Section: the latest files opened are displays in the recent files section for easy access.

Exit: exits the time control editor

4.2.2 Edit Menu

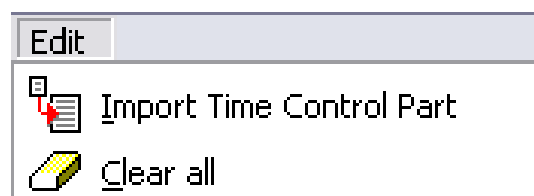


Figure 19 (Time Control Edit Menu)

Import Time Control Part: imports the information of the chosen tab on the

right side from another file.

Clear all: clears all information of this time control file but the name it has. Closing the editor after this will not save the changes.

4.3 Tool Bar

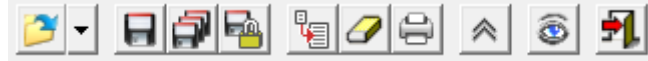


Figure 20 (Toolbar of the time control file editor)

Open Time Control File: loads an available time control file into the editor. The types of files you can select to load here are:



- Time control files *.tcf
- Result file *.rfp



Save Time Control File: saves the time control file



Save Time Control File As: saves the time control file with a new name



Save Time Control File As Validated: saves the time control file as a validated file, this file cannot be changed anymore.



Import Time Control Part: is used to import an element of a time control file. The content of the selected tab can be imported from an existing time control file.



Clear All: deletes the contents of a time control file. In order to prevent data being deleted accidentally a query window opens that asks for confirmation on this action. Leaving the program after this action won't cause the program to save the change or ask for it.



Print Time Control File: opens a print dialogue



Show more: Extend the time table list



Show Graphic: Shows the Graphic Time Control File Editor and the according Status- and Toolbar



Hide Graphic: Hides the Graphic Time Control File Editor and the according Status- and Toolbar



Simulation mode: Starts the simulation mode, during programming or editing of the synthesis file the valves are virtually switched in the visualization



Exit: closes the time control file editor.

4.4 Time Control Table

Time [min]	Function	Parameter
0.00	Composition Major Pump	100.0 , 0.0 , 0.0 , 0.0
0.05	Flowrate Major Pump	3.00 ml/min
0.20	Flowrate Major Pump	5.50 ml/min
0.25	Valve Position	V17 Helium Eluent 1 = Position 2
1.00	Valve Position	noop = Position 2
1.10	Valve Position	V15 Reactor out = Position 2
1.30	Dispenser ("Dispenser Reac	Aspirates 2000 µl from 1
2.00	Dispenser ("Dispenser Reac	Dispenses 1000 µl to 1
2.75	Dispenser ("Dispenser Reac	Dispenses 1000 µl to 2
3.49	Valve Position	noop = Position 2
3.50	Start Chromatogram	Ch. 17 (500 ms)
3.60	Valve Position	noop = Position 1

Figure 21 (Time Control Table)

The Time Control Table on the upper left shows all steps that a load time control file is programmed to perform. The information is displayed in a table, the first column shows the time code, the second the function and the third the parameter for the function in chronologic order.

4.5 Tab Area



Figure 22 (Time Control Editor Tabs)

The area right to the Time Control Table has various tabs that will be explained each in its own here.

4.5.1 Information Tab

Figure 23 (Time Control File Information)

In the Information Tab of a file are entered: the author, the eluents used, the column used, a sample identifier and comments. The date is automatically added if the file is saved. The sample identifier is not included if using an auto-sampler or if the Manual Sample ID option is activated. The information is saved in the results file generated and can be reviewed later.

4.5.2 Checklist Tab

Type	Requirement
Check Box	Fill up the HPLC solvents
Check Box	Install prepared SiOH and Thiosulphate cartridge
Check Box	Fill 5ml of CH ₂ Cl ₂ into vial A1
Check Box	Fill 18ml of Ether into vial A2
Check Box	Fill 0.9ml of HCL 5N into vial B3
Check Box	Fill 1 ml of NaOH 3N into vial B2
Check Box	Fill 1.1ml of Phosphate buffer into vial B1
Check Box	Fill 5ml of saline into vial C1
Check Box	Fill up the dewar with liquid nitrogen

Check Box

Insert Overwrite Delete

Figure 24 (Time Control File Checklist)

The Checklist Tab is used to make the later user of the .tcf check certain prerequisites before a synthesis is started. After starting the control file, the checklist is displayed. It has to be filled in and answered before the operation is started.

User Input: requires values or names e.g. production number

Check Box: has to be checked

4.5.3 Options Tab

Options

Programming Mode

Time min h

Volume µl ml l

Column Volume µl ml l

Volume Calculator

Length ...: [] [cm] [?]

Diameter: [] [cm] Calculate

Extended Pump Options

Start Pumps after loading Control File

Stop Pumps at Time Control "Hold"

Sampling Control

Disable Peaksampling

Disable Thresholds

Report Printing

Automatic Print

Resultfile

User defined name

Username Author Time Control File Sample Identifier

Vial + Injection Current Date Current Time Auto Increment

" 0001.rfp "

Figure 25 (Options Tab of the Time Control File Editor)

There are different sections in the Options Tab that will be explained one by one.

Programming Mode

In the area Programming Mode of the Options Tab allows to set the dimension of the x-axis. The choices are units of time, volume or column volume.

Volume Calculator

To help determining the column volume while programming in those units the volume calculator can be used. After entering the length [cm] and the diameter [cm] the *calculate* button has to be clicked and the calculated volume is put in the Column Volume field of the Programming Mode area.

Extended Pump Options

- **Start Pumps after loading Time control File:** If this option is checked, the result is that the pumps start after loading the file with the parameter set at the time 0:00 of the file.
- **Stop Pumps at Time Control Hold:** determines whether the pump should stop if a time control file is on hold.

Sampling Control

- **Disable Peak Sampling:** deactivates all peak sampling programmed.
- **Disable Threshold:** disables all thresholds programmed.

These two options allow disabling common functions without deleting every single entry of that kind in the programmed file (and saves the time to reinsert them).

Report Printing

The Automatic Print option determines whether a report should be automatically printed after the program run.

Result File

In this area the generation of the result file is configured. A custom filename can be set and additionally the following information can be added to the filename (if checked):

Username: Adds the name of the current user to the filename (if only one user is configured in the user setup despite multiple operators it makes no sense to use this)

Author: Adds the name of the time control file author to the filename

Time Control File: Adds the name of the time control file to the file name of the report

Sample identifier: Adds the sample identifier to the file name

Vial + Injector: Adds the number of the current sample vial and the current injector to the file name

Actual Date: Adds the current date to the filename

Actual Time: Adds the current time to the filename

Auto Increment: Adds a four digit consecutive number to the end of the file name in order to prevent result files with the same name to be overwritten.

It has to be taken care that no two filenames are same if former results should remain available and not be overwritten!

4.5.4 Activity Tab

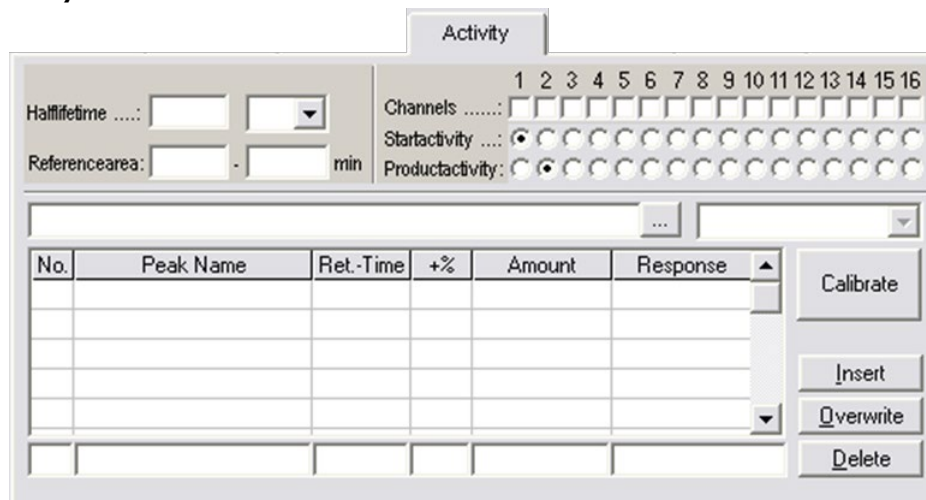


Figure 26 (Activity Tab of the Time Control File Editors)

The parameters of half-life correction and calibration are defined in the Activity Tab. The half-life of the radionuclide and the corresponding dimension have to be entered in half-life-time. Either time or area can be chosen as reference area for baseline correction of half-life-time corrected chromatograms selected by channels.

The setting of data channels to Start-activity and Product-activity allows the calculation of recovery with the following equation:

$$Recovery[\%] = \frac{Product\ activity}{Start\ activity} * 100$$

In the lower area of the Activity Tab all parameters for calibration can be entered. Above the table the calibration chromatogram and the channel are selected.

The table is used for input of peak name, retention time and peak-window in time-percent and amount value in the standard. With that information the system calculates the response factors that are used for analyzing peaks with similar names in the following chromatograms.

4.5.5 Functions Tab (Creation of Time Control Files)

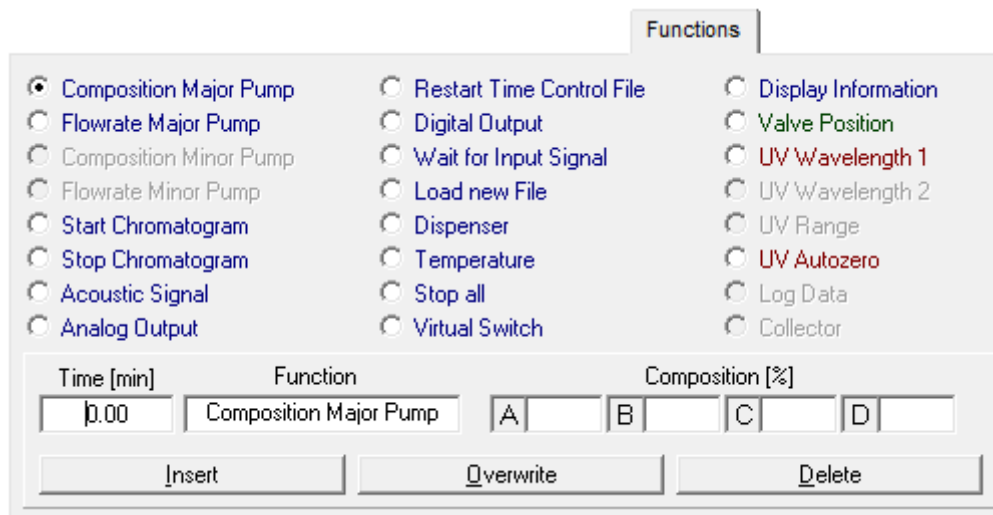


Figure 27 (Functions Tab of the Time Control File Editor)

In the Functions Tab all programmable functions for a time control file can be found. The editor bar is at the bottom of the tab; all the program steps are entered here together with the time and parameters. The parameter boxes in the Editor Bar change depending on the function *selected*.

It has to be taken notice that time is not entered in a hexadecimal way. The time in these programs is counted in decimal numbers.

(e.g. hexadecimal counting of units smaller than minutes: ...0:58; 0:59; 1:00; 1:01... Counting in this program ...0.58; 0.59; 0.60; 0.61; 0.62; ... 0.98; 0.99; 1.00; 1.01; 1.02 ...)

The Insert button adds the current command set to the time control file. The order of entering the steps is not of relevance; they are sorted by the time code they get if entered.

The overwrite button exchanges the contents of the line in the table, that is selected, with the contents of the Editor Bar.

The Delete button deletes the line that is selected in the table.

Most function's times can be changed by selecting the already inserted function in the table and then right-clicking on them. A context menu appears that the only menu item is Cut / Insert Time. Choosing this menu item by clicking on it with the left mouse button will cause a small time selection arrow to pop-up. Here a time offset can be entered: A negative one if the execution should begin earlier, a positive one if later; this changes the execution of the selected and all following program steps, it shortens or lengthens the break where the arrow has been.

The functions are explained in the chapter 4.6 Time control file commands.

4.5.6 Threshold Tab

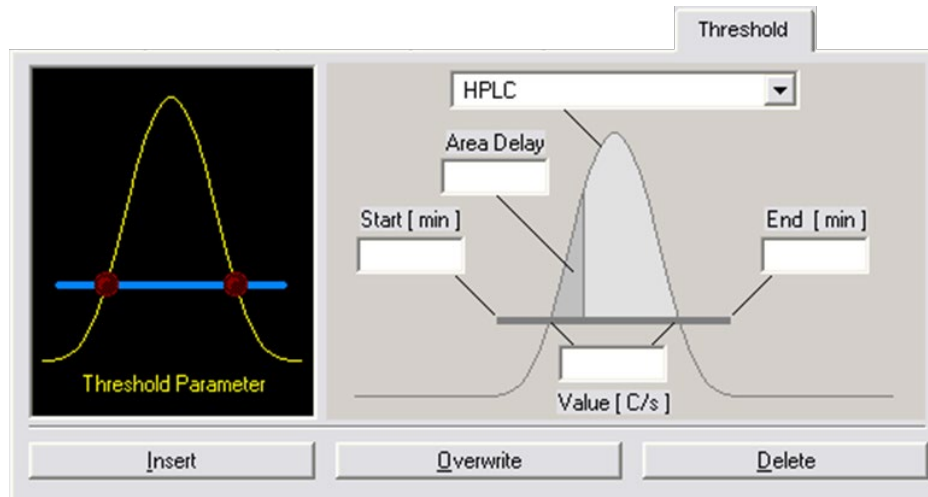


Figure 28 (Threshold Tab of the Time Control File Editor)

The Threshold tab allows programming of threshold events: This way a set of device control functions can be executed if an observed parameter exceeds or drops below a certain value. The threshold allows individual fractioning and system monitoring possibilities by the aid of selectable data source, programmable time frames for activities and programmable threshold levels. Up to 50 threshold observations can be active at any time.

The graph on the left of the tab is used to select the threshold parameter. Click anywhere on the graph (except on to the red dots LEDs) and the general threshold parameters show up on the right side of the tab.

In the upper selection box the input channel can be chosen, this determines the channel to observe. Available are the analogue channels, the system pressure and the event box inputs. The boxes *Start Time [min]* and *End Time [min]* are used to set the time frame for the activity of the threshold. In the value box the parameter's thresholds value is entered. If using an event box or game port input, this parameter is not available, since the data source only has two possible states (Low = Threshold Under Even; High = Threshold Over Event)

Area delay describes a delay time for the threshold event that is depending on the integrated area the observed parameters function creates.

Clicking on the left LED (red dot) on the graph, the "Over Event Functions" table opens up. Here the functions can be entered that should be carried out, if a threshold over event happens. The desired function can be selected in the boxes *Device* and *Operation* beneath the table. Clicking on the *Insert* button the set device operation is being inserted into the time control file. If *Overwrite* is clicked the selected (red) line is replaced by the settings of device operation set. If *Delete* is clicked the selected line is removed.

Similar to this a "Threshold Under Event" is configured by clicking on the right LED of the graph.

4.5.7 Peak Sampling Tab

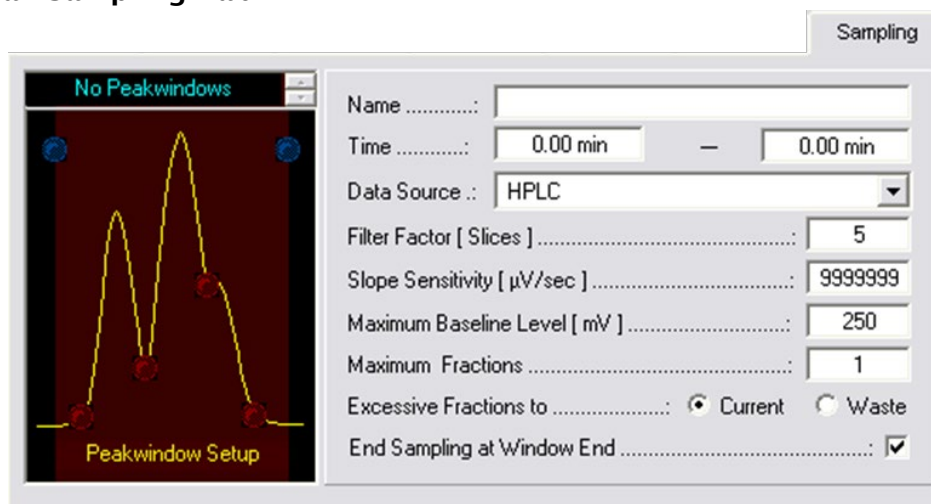


Figure 29 (Peak Sampling Tab of the Time Control File Editor)

The Sampling Tab allows the programming of peak sampling. Peak sampling makes it possible to carry out a set of device control functions triggered by an automatically recognized peak situation. Peak sampling takes place in so called peak windows, whose start and end time can be set by the user. The data source, sensitivity of peak recognition and functions to be carried out are set for each peak window individually. This empowers to react to single peaks separately on an individual basis. If fractioning in combination with threshold values, the thresholds and peak samples always combine to form one fraction event. This means that as long as the threshold is still exceeded or the peak sampling has not yet recognized the end of a peak, fractioning continues.

The graph of peak situations is used to select the peak sampling parameters and peak situations. Click anywhere on the graph except of the red or blue dots (LED), the peak-window set-up will appear to the right of the graph. The following parameters can be entered here:

Name:	Peak Windows get individual names to be able to differentiate them.
Time:	Start and end time of the peak window.
Data Source:	The source of data can be selected here
Filter Factor:	indicates the number of data points used for the first derivation if calculating the gradient
Slope Sensitivity:	indicates the size of the gradient above which the start of the peak is recognized.
Max. Baseline Level:	is used as a threshold value for peak sampling. No peak end is recognized above the value entered.
Max. Fractions:	is only relevant to the defined by Peak Window setting that is a possible position setting for

motorized switching valves. It indicates the maximum number of fractions that can arise in this peak window.

Excessive Fractions to: option determines where the fractions that exceed the maximum number of fractions should be pumped. The 'Current' setting pumps them into the current position; the 'Waste' setting pumps them into the waste.

End Sampling at Window End: indicates whether fractioning should continue after the end of the time period of a peak window or whether the system should switch to waste.

To program peak sampling events click on the LED at the desired location. A function table will appear on the right side that can be filled with functions.

The possible peak sampling situations are:

Peak window start: the blue LED on the left, is the time the peak window "opens"; starts observing the parameter

Peak window end: the blue LED on the right side is the time the peak window "closes"; it stops observing the parameter

Red LEDs from left to right:

Peak Start: start of a peak as recognized by the peak sampling

Peak Valley: dip in a peak recognized by the peak sampling

Peak Shoulder: shoulder of a peak recognized by the peak sampling

Peak End: end of a peak recognized by the peak sampling

The desired event can be selected in the boxes *Device and Operation* beneath the table. Clicking on the *Insert* button the set device operation is inserted into the time control file. If *Overwrite* is clicked, the selected (red) line is replaced by the settings of device operation set. If *Delete* is clicked the selected line is removed.

The following rules apply to the sensitivity of peak sampling:

- The smaller the data point density, the faster and more sensitive the peak sampling. (However it has to be mentioned that very small slice widths lead to large results files.)
- The smaller the Filter Factor, the faster and more sensitive the peak sampling. (The range of this factor is 5 to 15 and the value entered has to be odd.)
- The smaller the Slope Sensitivity, the more sensitive is the peak sampling.

4.6 Time control file commands

Composition Major Pump: determines the eluent composition for the primary pump of the system. Entries are made in percent and switching into the following box the entry will automatically have the missing difference to 100 % entered (e.g. if entering 80% for eluent A leaving this field automatically fills in 20 % into the field of eluent B).

Flow rate Major Pump: determines the flow rate of the primary. Changes are made in discrete steps; a flow rate gradient for example cannot be entered. Values are entered in ml/min.

Start Chromatogram: starts plotting the chromatogram for the analogue channels selected, with the data point density entered in *Slice Width*.

Stop Chromatogram: stops plotting the chromatogram for the selected analogue channels or if *all active* is selected, stops plotting the chromatogram for all the analogue channels.

Acoustic Signal: initiates a sound reproduction of the *.wav file selected with an interval of 4 seconds. The test button plays the file. The sound will end if the time control file is stopped.

Analog Output: is used to control external instrumentation according to the specifications.

Restart Time Control File: is used to restart the time control file. It is possible to select the parameter 'Loop' for an endless loop or "Repeats" in order to enter a certain number of repeats. Once all the iterations have been performed this command will be ignored for this program run.

Digital Output: is used to switch one of the 12 digital outputs. The required digital output and the state to be switched to [On, Off, Pulse] has to be selected as parameters.

Wait for Input Signal: puts the actual time control file on hold until the selected event box input or the game port has the state programmed [On, Off, Pulse]. (This function can be used e.g. if injecting with a manual

injection valve.)

- Load new File:** is used to load and start the time control file selected. This allows linking several time control file.
- Dispenser:** controls the installed dispenser of the system. For each selected dispenser (1-4) one of four operations can be selected:
- *Aspirate* to fill the syringe
 - *Dispense* to discharge
 - *Dose* for the delivery of solvents (aspirates and dispenses)
 - *Initialize* to initialize the dispenser
- The speed of the syringe is entered in $\mu\text{l}/\text{min}$ filled syringe. In Source and Destination the ports of the dispenser valve have to be set.
- Temperature:** sets a temperature for a heater; the parameter is temperature in $^{\circ}\text{C}$.
- Stop all:** is used to end the run and stop the pumps.
- Virtual Switch:** is a program variable that can be set and read.
- Display Information:** is used to manually add text annotations to the chromatograms.
- Valve Position:** is used to switch valves. Select the Valve and the final position as parameter. To set all valves into the same position select *All Valves*.
- UV Wavelength 1:** is used to select the wavelength of the UV detector.
- UV Autozero:** automatically returns the UV detector to zero.

4.7 Graphic Time Control File Editor

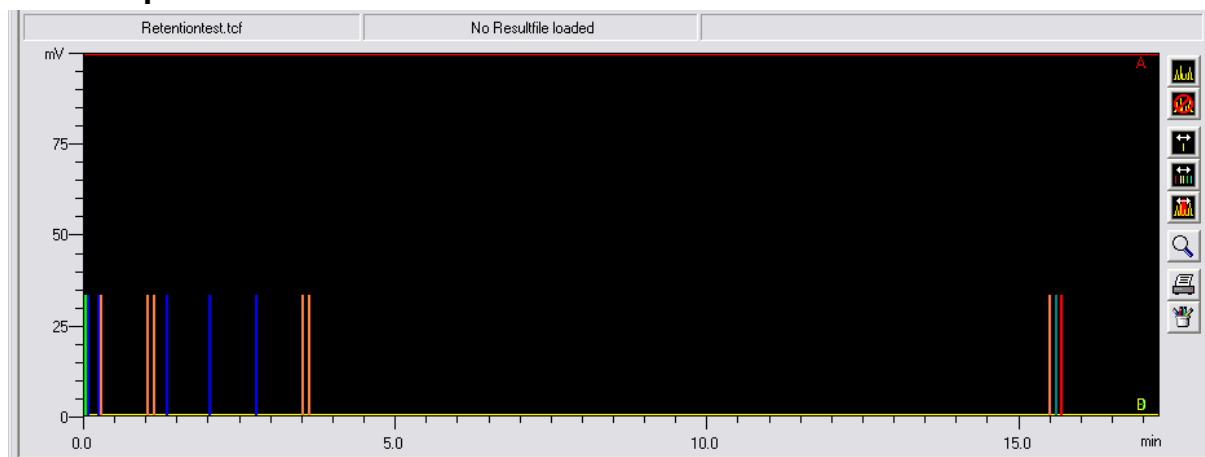


Figure 30 (Graphic Time Control File Editor)

The Graphic Time Control File Editor is used to create a graphic representation of a time control file and allows visual editing. All the functions of the time control file are shown as colored lines that can be moved horizontally (movement in time) and vertically (changing the threshold value or peak limit) with the mouse. A selected function in the table of the time control file will flash the graph belonging to that function. Peak windows are also represented graphically and can be created and edited with the mouse.

A programmed gradient development is also represented by colored lines. The y-axis minimum is 0% and the y-axis maximum is 100%.

A chromatogram can be opened as background; it can be used to adjust the functions of the time control file. The display colors of all the functions can be selected in the Graphic Time Control File Editor color setup, and any functions that should not be visible can be deactivated.

4.8 Status Bar

The Status Bar in the Graphic Time Control File Editor shows the name of the time control file open, the name of the chromatogram and an information box open up indicating:

- The time control function that the mouse cursor is hovering over or that is moved by the aid of Single Function Moving.
- The time by that the function is shifted using the Multi-Function Moving
- The name and times of the peak window that the mouse cursor is hovering over using the Create / Edit Peak Window function.

4.9 Graphic Time Control File Editor Tool Bar



Load Chromatogram: opens a dialogue to choose a chromatogram that is used as background



Clear Chromatogram: removes the chromatogram in the background



Single Function Moving: allows to move single functions



Multi-Function Moving: allows moving multiple functions. To do this begins by drawing a time window with the left mouse button held down. All the functions within the window are then moved with the mouse at the same time. Holding down the right mouse button will adopt the time shift.

Create / Edit Peak Window: allows editing and creating peak windows. To create a peak window, hold down the left mouse button and draw a new window on the screen. Releasing the mouse button triggers a query window for the name of the new peak window.



An existing peak window can be edited by moving the mouse over it, the cursor will change depending on its position on the window. An arrow points left on the left hand side of the window to an arrow pointing right and left in the center of the window. By holding down the left mouse button the peak window can be moved or extended depending on the position the mouse cursor was while pressing the mouse button. Right clicking on a peak window a context menu opens up where the window can be renamed or deleted.



Zoom Graphic: is used to enlarge parts of the graph.



Print Graphic prints the graph

5 Sequence Control Files

The editor shows the Sequence Control File as a table. A sequence control file is in principle a series of time control files.

The sequence control file editor can be opened by the icon in the Main Window's Toolbar or in the menu bar via File -> Create / Edit Sequence File.



Figure 31 (Sequence Editor)

The runtime programmed into the sequence control table determines the time the actual time control file ends and the next begins.

5.1 Sequence Editor Toolbar



Load Sequence Control file: opens a Load time control Sequence window to choose the file to be opened.



Save Sequence Control File: Writes changes to a sequence control file to the hard drive



Save Sequence Control File As: saves sequence control file under new name.

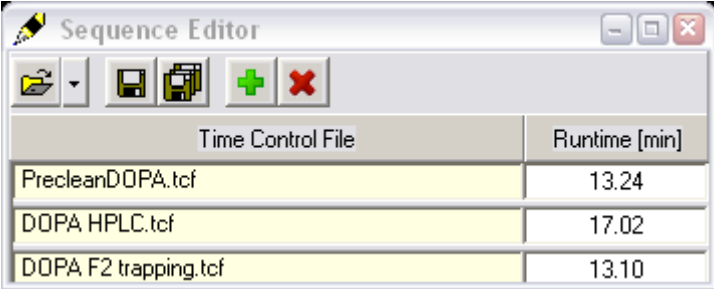


Add Time Control File: opens the add control file window. Here the time control file to be added can be chosen



Delete Selected Time Control File: will delete the selected time control file from the sequence run list.

5.2 Creating Sequence Control files



The screenshot shows a window titled "Sequence Editor" with a toolbar containing icons for file operations and a table with two columns: "Time Control File" and "Runtime [min]". The table contains three rows of data.

Time Control File	Runtime [min]
PrecleanDOPA.tcf	13.24
DOPA HPLC.tcf	17.02
DOPA F2 trapping.tcf	13.10

Figure 32 (Sequence Control File)

For creating a sequence control file the Time Control Files that should be chained must already exist. Pressing the *Add Time Control File* button a dialogue opens to choose a time control file. After pressing *OK* in that dialogue it is added to the sequence. The order of the files is the order that was added, a new added file is put at the end of the sequence.

If the order of files should be changed, every row can be dragged into a new position. The mouse cursor has to be placed on the item to replace it. Then the left mouse button has to be pressed down. Without releasing the mouse button the item has to be moved to the new location in the table. Releasing the mouse button places the item.

The editor evaluates the last step of the file and sets it as runtime for this sequence step. The run time can be changed manually. If the runtime is shorter than the real time needed for a time control file to process the file will be stopped and the next one starts. If the runtime is longer than the time to process the time control file, the additional time is waiting time.

6 Chromatogram

The Chromatogram window can be opened by the icon in the Main Window's Toolbar or in the menu bar via Visualization -> Chromatogram.

The Chromatogram window has four modes available, selectable by the first four leftmost toolbar icons.

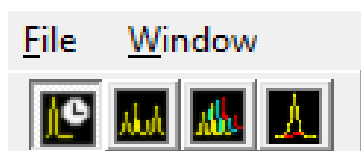


Figure 33 (Tool bar of chromatogram window)



Analysis Window: records and visualizes analog signals



Reconstruction Window: opens and visualizes saved synthesis run data



Compare Window: opens multiple saved synthesis run data to compare single channels



Integration Window: is used to reintegrate chromatograms

6.1 Data Recording (Analysis Window)

The Chromatogram Window can be opened by the icon in the main window's toolbar or in the Menu Bar via Visualization -> Chromatogram.



This window is also called the data-recording window, it is used to display and record analogue signals (like UV, radioactivity or temperature).

Data recording is started in the time control file with the command Start Chromatogram and stopped by the command Stop Chromatogram. Chromatograms can start simultaneously or with delay.

While a time control file is running, the graphic display of the time control file, the current chromatogram trace, the programmed peak windows, the gradient and the current chromatogram labels are displayed in the data recording windows. Just like in the Graphic Time Control File Editor there is the possibility to edit control file functions and peak windows in the data recording window. These changes take effect in the current run and can also be saved in the time control file opened. This way it is possible to intervene in a running process. However, if a gradient is moved, this will not take effect until the next time the time control file starts.

After performing a change in the File of a currently running program there will always be a query if the changes should be saved to the file.

6.1.1 Toolbar



Channel: is used to open or close a data channel window. Only the buttons for the channels that can be selected are shown. The *U* button belongs to a user defined channel. Data channels which are programmed into a time control file are automatically opened upon loading. If no data recording is active, the data track selected runs in base line mode, i.e. from the left to the right edge in about 8 minutes as an endless loop.



[...]



Show Peak Windows: is used to show or hide the peak windows.



Show Gradient: is used to show or hide the programmed gradients.



Show Annotations: Is used to show or hide the current annotations.



Show Last Chromatogram: automatically loads the last chromatogram as background image in the data channel window



Show Elapsed Time Line: is used to show or hide the vertical line indicating the elapsed time.



Open last Chromatogram: is used to load the last chromatogram manually, as a background image for the data channel window.



Channel Setup: opens the window with the settings for the individual data channels. The different parameters are described in chapter 6.1.3 Data channel settings.



Automatic Print: activates or deactivates the automatic printing of the report after the recent run.

6.1.2 Status Bar

The Status Bar of the chromatogram window has three information areas.

The leftmost one is a visualization of the actual status:




Baseline: baseline is displayed



Ready: data channel is in use, but has not yet started.

 **Chromatogram running:** data recording is active.

 **Chromatogram finished:** data recording has finished.

The box to its right shows the chromatogram runtime and the rightmost box shows the current status with the name of the result file.

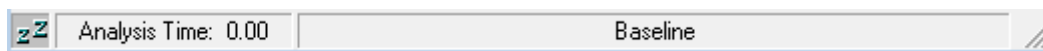


Figure 34 (Status bar of chromatogram window)

6.1.3 Data channel settings

The window always shows the data of the selected channel, i.e. the analysis window in focus. In the Name box the name of the channel can be changed. The data source of the channel is determined by the checkbox A/D Converter or DAD for data of the A/D conversion cards and DAD for the data of the DAD. The DAD's range of wavelength is set in the boxes adjacent to the DAD. The Offset parameter can be entered to compensate for a detector offset. The value entered will be added to the analogue signal (it can be positive or negative). The Factor Parameter is used to correct the size of the analogue signal. A factor of 1 shows the analogue signal at its original size. The Y-Maximum and Y-Minimum parameter determine the scale of the y-axis. The Auto Scaling option automatically corrects the scaling if these values exceed the corresponding minimum or maximum signal. The measurement unit of each channel can be set in the Dimension box. Clicking the Color 1 or Color 2 box opens up a color selection dialogue that can be used to set the color of each chromatogram trace. Color 1 is the color of the current chromatogram; Color 2 is the color of the last chromatogram that is displayed if the "Show last Chromatogram" function is used. The Apply button applies the settings, and the OK button applies the settings and closes the window.

Choose the type of the display spectrum in the setup window for the DAD spectrum in the area Spectrum Type.

Dark Current is the remaining current without exposing the diode array.

Reference Spectrum is a saved lamp spectrum. A reference spectrum can be set manually by the Set Spectrum function key. Otherwise it is set automatically at the time SynthraView starts.

Absorption Spectrum of DAD is the logarithm of the reference spectrum minus the logarithm of the actually measured lamp spectrum.

The refreshing parameter defines after what time the spectrum display is actualized. Y-Maximum and Y-Minimum values define the scaling of the y-axis. The Auto Scaling option automatically fits the scaling according to the signal's maximum and minimum.

6.2 Reconstruction

Result files can be opened and displayed in the reconstruction window. Chromatograms, time control file functions, peak windows, gradients,

chromatogram labels and the protocol of the synthesis run can be displayed.

The chromatograms can be displayed individually or in the case of multiple channel data recording, superimposed. To enhance the visibility of certain areas it is possible to drag a zoom window. To perform a zoom place the mouse cursor inside the chromatogram area. Hold down the left mouse button. Dragging it makes appear a rectangle. One corner sticks on the point where the left mouse button was pushed down and the other corner is still connected to the mouse cursor. Capture the area of interest in this frame. Releasing the left mouse button will cause an automatic zoom in the area chosen. To return to the total view the right mouse button has to be clicked onto the chart.

6.2.1 Toolbar of the Reconstruction Window



Open Result File: opens the Open Results File window



Previous Results File: loads the result file that is located directly before the already open file if ordered by name.



Next Results File: loads the result file that is located directly behind the already open file if ordered by name.



View Sample Information: opens a window containing the sample information of the run protocol



View Protocol: opens a window that displays the run protocol ordered by time.



View Peak results: opens a table that shows the results of the integrations.



View Peak Value: is used to register the peak values. After selecting this function, a crosshair will appear on the graph that can be moved along the chromatogram trace. The time and intensity will be displayed on the cross hair lines. In a multiple channel result file, only one chromatogram can be selected to register peak values.



Export Chromatogram: is used to export one or more chromatograms. The export formats can be selected in the file section window as file types. Possible export formats are **.CSV** if to import the data in a spreadsheet application or a slice file to import the data into ChromStar.

Print Results File: is used to print the result file loaded. After selecting this function the Report Options window opens up with different options to choose:



Chromatogram prints the chromatogram as it is on the screen

Peak Results prints the table of peak results

Fraction Table prints the result file's fraction table

Run Protocol prints the protocol of the run



Show Channel: shows or hides each chromatogram. Hidden chromatograms are not displayed on screen and do not appear on a printout either.



Show Peak Window: shows or hides Peak Windows.



Show Gradient: shows or hides Gradient.



Show Annotations: shows or hides Annotations.

6.2.2 Status Bar

The status Bar at the bottom of the window shows the complete path and name of the result file opened.

6.3 Compare Chromatograms

Chromatograms from multiple runs can be loaded at ones and the chromatograms can be compared.



Open Result File: opens the Open Results File window. The .tcf files must be selected by selecting them with left mouse click and holding "ctrl" on the keyboard.



Show Channel: shows the selected chromatogram. Non selected chromatograms are not displayed on screen and do not appear on a printout either.



Chromatogram Offset: an offset to separate the chromatograms can be defined by using the arrow keys of the keyboard.



Chromatogram History: opens a new window with the chromatogram history



Print Resultfiles: Prints the selected channel of the compared synthesis files and the chromatogram history.

6.4 Integration Window

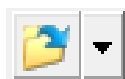
The fourth option of the Chromatogram window is the reintegration. It is possible to reintegrate the chromatograms of result files into the integration window.

The chromatograms can be reintegrated individually or in groups in case of multiple channel data recording. Once reintegration has been performed it is saved automatically. The original integration remains in the result file, this way it is always possible to return to the original data.

Reintegration allows optimizing the integration of your chromatograms at a later time. If the time control file is loaded from a reintegrated results file into the time control file editor, the program will recognize the reintegration and ask if reintegration parameter should be loaded. This time control file is identical to the one that completed the last run but contains the integration parameter of the reintegration.

To magnify certain areas of the chromatogram on the display it is possible to drag a zoom box. To perform a zoom place the mouse cursor inside the chromatogram area. Hold down the left mouse button. Dragging now let appear a rectangle that one corner sticks on the point where the left mouse button was pushed down and the other corner is still connected to the mouse cursor. Capture the area of interest in this frame. Releasing the left mouse button will cause an automatic zoom in the area chosen. To return to the total view the right mouse button has to be clicked onto the chart.

6.4.1 Toolbar of the reintegrating window



Open Result File: opens the Open Results File window where the file to integrate can be chosen



Channel: is used to select the chromatogram shown in the reintegration window.



View Peak Results: opens the window with the display of the integration results in table form.



Integration Tools: opens a window with the function buttons and parameter boxes for reintegration.

The Integration Tools window contains the tools necessary for reintegration. As described in chapter 6.4, the integration parameters are saved with the peak windows. Performing reintegration always concerns the part of the

chromatogram with the selected peak window. The parameters of the first peak window apply from the beginning of the chromatogram.

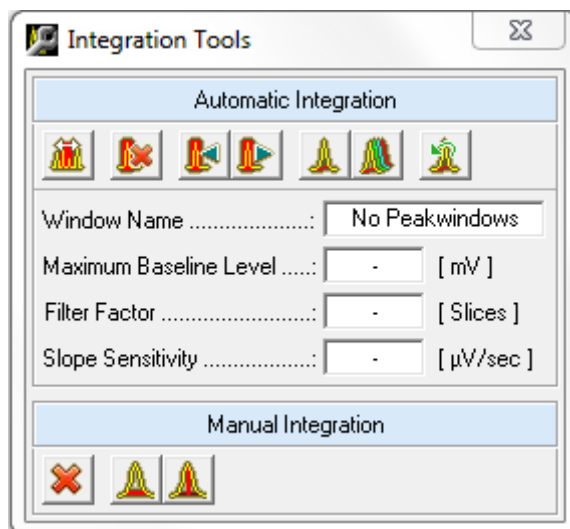


Figure 35 (Integration Tools)

Until the time the next window begins, these parameters remain standard for integration. The buttons in the toolbar provide the following functions.

Automatic integration



Create / Edit Peak Window: enables you to create and edit peak windows (see chapter 4.5.7 Peak Sampling Tab).



Delete PeakWindow: is used to delete the selected peak window.



Previous Peak Window: is used to select the previous peak window. The peak window selected is framed in the graph in the reintegration window. The name of the window is displayed in the box below the toolbar.



Next Peak Window: is used to select the next peak window (see previous window).



Integrate Selected Channel: reintegrates the selected chromatogram.



Integrate All Channels: reintegrates the selected channels the chromatograms of the results file loaded.



Original integration: reverts to the original integration.

Manual Integration



Clear Integration: is used to delete all integrations.



Set Manual Baseline: is used to integrate peaks manually. By activating this function you can select the start and end of the peak by left click each in the chromatogram. With deselecting this function the new peak is fixed.



Set Manual Drop: by activating this function you can split a peak by left click in an integrated peak. This way one peak in the chromatogram is split into two peaks. With deselecting this function the setting is fixed.

The reintegration parameters have the following meanings:

Maximum Baseline Level – functions as a threshold for peak sampling. No more peak ends are recognized above the value entered [mV]

Filter Factor – Shows the number of slices used to form the first derivate of the gradient calculation.

Slope Sensitivity – indicates the size of the gradient where a peak beginning is recognized [$\mu\text{V/s}$]

6.4.2 Status Bar of the Reintegration Window

The Status Bar at the bottom of the window shows the path and name of the results file opened.

7 Peak Detection

The Peak Detection Window shows the actual status of peak detection. The Peak Detection Window can be opened by the icon in the Main Window's Toolbar or in the Menu Bar via Visualization -> Peak Detection.

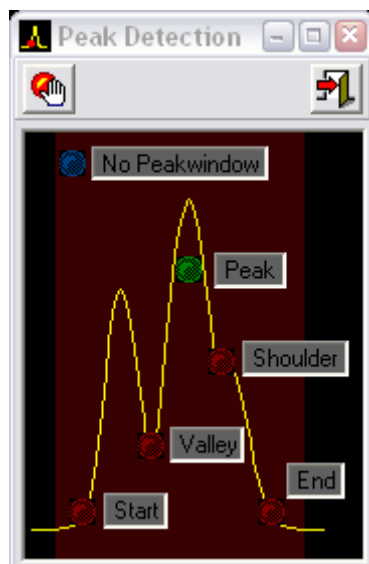


Figure 36 (Peak Detection Window)

The peak detection window visualizes the status of peak detection during any synthesis run. It shows the name of the peak window as well as all other information of the peak. (For further information on peak sampling see chapter 4.5.7 Peak Sampling Tab.)



Disable Peak Sampling: disables all peak sampling

8 System Visualization

The System Visualization window can be opened by the icon in the Main Window's Toolbar or in the Menu Bar via Visualization -> System.

The System Visualization is used to display the process flow graphically, as well as operation interface all the devices that can be controlled manually by means of the visualization. The visualizations can also show data relating to the detector signals, auto-sampler vial numbers, fraction collector position and temperature.

A library of graphic objects and the use of background images in BMP format, allows creating individually configured system visualizations.

Each of the active devices that can be visualized displays the current position or state all the time. The visualization window can be scaled using the Zoom menu or dragging the borders of the window.

8.1 Functions

All the active devices visualized can be controlled online, some with the aid of context menus.

Two state devices can be switched on by double clicking on their representation in the visualization.

The menu is opened by clicking the right mouse button onto a device that should be controlled. The first level of the menu always contains the element's name that was chosen. Hover the mouse cursor over the area with the name opens the options menu. The option that is active at the moment is checked. By left clicking a different option the device is switched.

A right click on a box (value label) shows its data source.

8.2 System Visualization Setup

The System Visualization Setup Window can be opened via the menu File -> Setup in the System Visualization Window.

8.2.1 Toolbar of System Visualization Setup



Load Visualization: opens a previously created visualization.



Save Visualization: saves the visualization to the hard drive.



Load Background Picture: opens the Load Background Window where a background file, in BMP format for the visualization, can be chosen. All the background images are located in the Visualization Backgrounds subfolder of the visualization folder of the SynthraView installation folder.



Clear Visualization: deletes all loaded visualization elements. To avoid accidental deletion pressing this button opens a confirmation dialogue that asks the user if the visualization should really be cleared.



Rotate Object 90°: rotates the object selected 90° clockwise.



Flip Object: flips the object selected horizontally.



Insert Object: adds the object selected to the visualization window. All objects are inserted in their basic position and need to be moved to the correct destination and place.



Place Object: fixes the inserted object at the current location in the visualization.



Move Object: enables you to move a placed object to a different location.



Delete Object: removes a placed object.



Exit Setup: closes the Visualization Setup Window.

8.2.2 Creating / Modifying a Visualization

To create a new visualization the first step is to draw a background image that corresponds to the device's tubing system. This image has to be of the file type **.BMP**. A program of choice can be used for that. In the subfolder Bitmap Library of the Visualization folder of the SynthraView installation folder a number of models for the elements can be found. The finished background itself has to be saved to the subfolder Visualization Backgrounds of the Visualization folder of the SynthraView installation folder.

The background picture has to be opened in the Visualization Setup with the Load Background Picture function. Now the active visual elements have to be placed on top of that background picture. On the left of the Setup Window there is a table containing all possible graphical representations for the active and passive elements. The chosen element is displayed in the center of the Visualization Setup window. On the right hand side of the Visualization Setup window there is a table of all devices of the system that can be visualized. If

choosing the object Value Label the table to the right changes and only shows devices whose values can be visualized.

In the devices section of the setup window the state of every device is also mentioned. There are two different states concerning the visualization setup:

- **Free:** The device is not in the visualization yet.
- **Selected:** the device is already part of the visualization, adding it a second time will open a window asking if it is intended to create a multiple visualization object. Answering with *yes* creates a copy that shows the same state as all its clones (the maximum number of clones is 5).

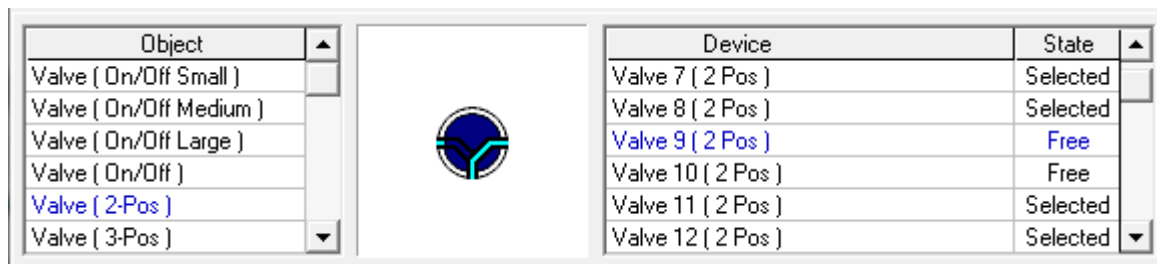


Figure 37 (the object, preview and device window of the Visualisation Setup)

As already mentioned, the graphic chosen is shown in the central preview window. It should be taken care to give the object the right orientation corresponding to the element of the background image. Elements can be oriented by using the Rotate Object 90° and the Flip Object functions. Subsequent to this, the object is transferred into the visualization area by using the Insert Object function. The object will appear in the top left corner of the visualization. It can be dragged into the right position by placing the mouse cursor over it, holding the left mouse button and moving it into the desired position. The object can also be positioned by using the arrow keys on the keyboard. If the object is in position the Place Object function has to be used to fix it there.

8.3 Simulation, Simulation mode

The system visualization and the programming of time control files is linked in a way that simplifies programming .tcf files.

After activating the simulation mode, if selecting a line of a time control file with a valve operation, the valve incorporated in this operation is displayed with a pulsing red frame that highlights the valve that is affected by the selected line of the time control file.

9 Dispenser Visualization

The Dispenser Visualization Window can be opened by the icon in the main window's toolbar or in the Menu Bar via Visualization ->Dispenser.

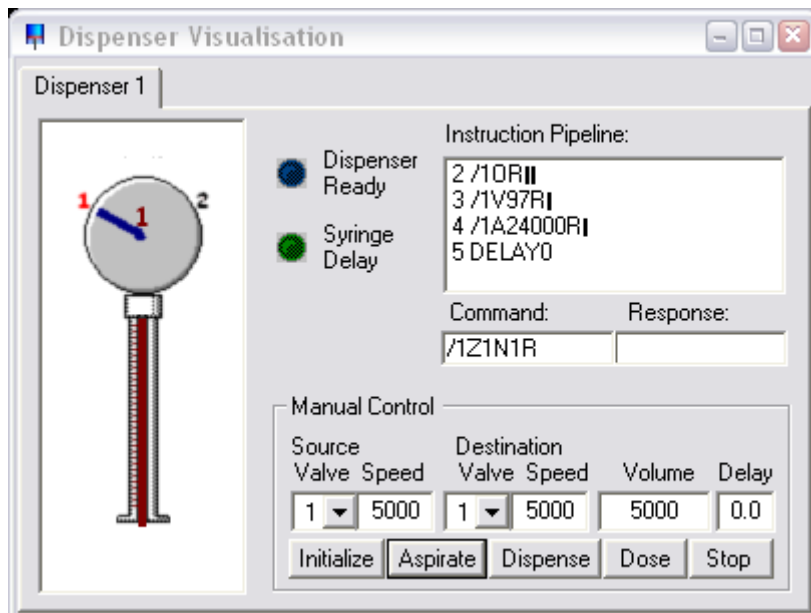


Figure 38 (Dispenser Visualization)

Depending on how many dispenser the system has there will be one tab for each. On the left a scheme of the dispenser is shown. (Please note that the dispenser will not show upside down even if it is installed that way in your system.)

Dispenser Ready: this indicator shows that the dispenser is ready to receive commands

Syringe Delay: this indicator shows that the dispenser is on a delay that was set, not ready to receive commands

Instruction pipeline: shows all commands for the dispenser that are given but not executed yet like a command cue.

Command: shows the actual command that is sent to the dispenser

Response: shows the response of the dispenser, the dispenser response can tell if a command could be executed successfully or not.

Manual control: this area allows manual control over the dispenser

Source Valve: sets the valve number that will be the source

Speed: sets the speed that the dispenser will use to fill

	itself [$\mu\text{l}/\text{min}$]
Destination Valve:	sets the valve number that will be the drain
Speed:	sets the speed that the dispenser will use to drain itself [$\mu\text{l}/\text{min}$]
Volume:	Sets the volume that is either taken from the source or pumped to the train, or both depending on the operation performing
Delay:	is the time delay between aspiration and dispense if a dose is performed
Initialize:	pushing this button the dispenser will check its own positioning by going from one positive stop to the other and checking the valves
Aspirate:	the dispenser fills itself with the parameter set in Source Valve at the according speed
Dispense:	the dispenser discharges itself with the parameter set in Destination Valve at the according speed
Dose:	will cause the dispenser to charge and discharge itself and pumps the amount set in <u>Volume</u> from source to destination with a certain <u>Delay</u> if applicable.
Stop:	ends all dispenser actions at once and clears the instruction pipeline.

10 Solvent Supply

The Solvent Supply can be opened by the icon in the Main Window's Toolbar or in the Menu Bar via Visualization -> Solvent Supply.

The solvent supply display is used to control the supply of solvents. To save the column from running dry one has the possibility of setting two volume limits in [percent]. If the volume drops below the first limit an acoustic warning will sound and dropping below the second limit the pumps will be stopped.

The values displays are based on the calculated used volume of solvent at the current flow rate and time passed. This means that there is no provision for pump tolerance in this calculation. For this reason the volume limits for the warning and pump shut down should allow a certain leeway. Regular control of the supply containers also helps to prevent that the column runs dry.

10.1 Solvent Visualization

The supply of solvents A to D and the level of the waste container are shown as a graphic on the left of the window. They are intended to allow the user to make instant checks.

A solvent that has dropped below the minimum percent level set or a waste volume that has exceeded the maximum percentage level will be marked with a red exclamation mark. The right of the window can be expanded with the *More Info* button. It can be collapsed again with the *Less Info* button. The right of the window displays the solvent names and the numerical solvent quantities. It also shows the solvent consumption for the current run. The values are shown as absolute volumes and as percentage of the total volume.

On the right the solvent names are displayed with the current values as volumes and percentages next to them.

The values next to Actual Run Uses show the solvent consumption of the time control file loaded as a volume and percentage. This display is intended as a check of whether the solvent supplies are sufficient for the current run.

10.2 Solvent Supply Display Settings

In the Volume Settings Tab, names for the solvents A to D can be entered in the name section. The total volume of the individual solvent container has to be noted in the boxes below *Total[l]* and the actual volume in the fields below *Current[l]*. The pumps should be stopped if the current solvent volume is entered, since the fields - where they ought to be entered - are updating all the time if the pumps are running and every try to enter a value is immediately overwritten. With the [l] button in the bottom right the units can be switched between [l] and [ml]. The *Refill All* button returns all solvent containers to 100 % and the waste to 0 %. The *Save* button applies and saves changes. The second threshold has the option "Stop all" or "Hold with Pump stop" is used to

stop the pumps in order to prevent the column from running dry.

Stop all: stops the time control file and the pumps (a stopped time control file cannot be resumed)

Hold with pumps stop: pauses the time control file and sets the pumps to a flow rate of 0ml. After the solvent containers have been refilled it is possible to resume the time control file with Continue.

11 Event Box Control (Digital IO Control)

The Digital IO Event Box shows the 12 outputs that are used to control system components and 12 inputs that are used to capture system signals.

The outputs are depending on channel mapping.

The inputs are low active, i.e. they are considered to be active if they are connected to ground or if the input voltage is around 0V. In this example only digital input No 5 is used, for the digital input of the fluid detector. Examples of other applications for the inputs are:

- Feedback from an injection valve
- Controlling devices with TTL input
- Etc. etc.

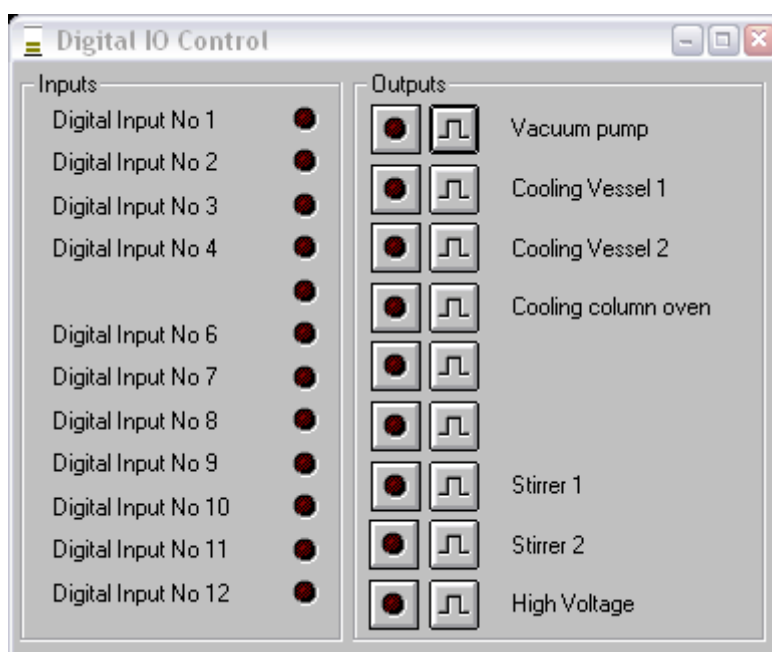


Figure 39 (Digital IO Control)

The first four outputs are solid state relays that can switch pumps for example at 24V up to 6A. The seventh and eighth switches control the magnetic stirrers. Output nine controls the high voltage used for the Geiger-Müller counter.

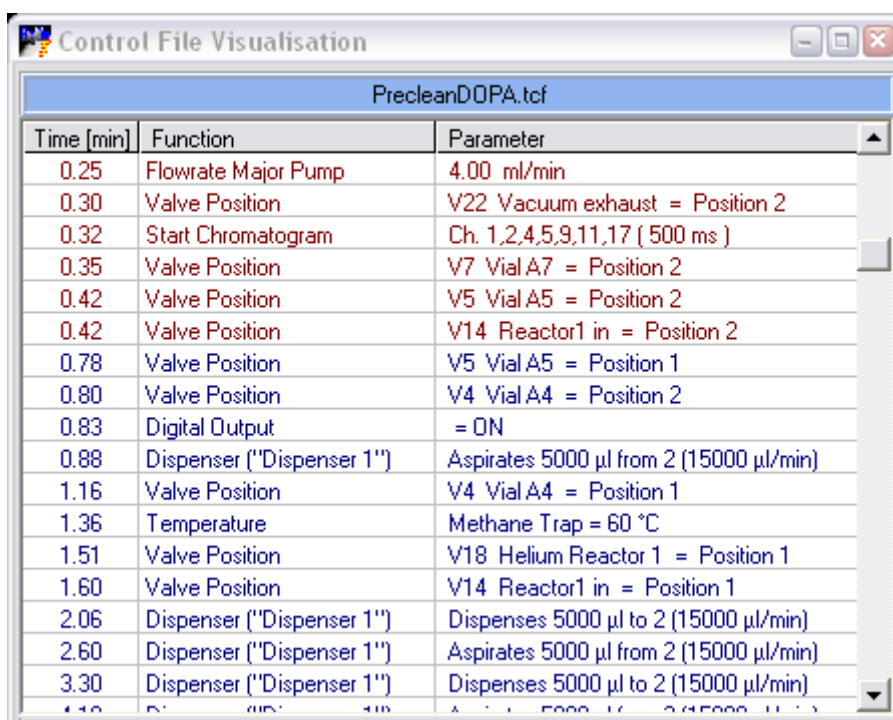
The Digital inputs are visualized by the LED representations in the window. The Outputs can be activated manually. One way is to use the switch with the red LED in the output section. It activates the channel and shows that it is activated by its red light. The other way is to send a pulse to the output; this is a short signal that activates the device only for an instant. This can be done to check if the vacuum pump is running e.g. but won't work very well to find out if the stirrers are working properly.

12 Control File Visualization

The Control File Visualization can be opened by the icon in the main window's Toolbar or in the Menu Bar via Visualization -> Control File Visualization.

If running a time control file it is displayed as a table. All the rows that have already been performed will be displayed in red; all those rows that still have to be performed are displayed in blue. The blue field above the table shows the name of the time control file loaded.

If running a sequence control file one can observe an additional table above the time control table. In this additional table the time control files and the assigned runtimes can be seen. The files that already have been performed are red; those still to perform are blue. In the additional yellow field at the top you can see which sequence control file has been loaded.



The screenshot shows a window titled "Control File Visualisation" with a sub-header "PrecleanDOPA.tcf". Below the header is a table with three columns: "Time [min]", "Function", and "Parameter". The rows are color-coded: red for completed steps and blue for pending steps. The current step shown is at 1.16 minutes.

Time [min]	Function	Parameter
0.25	Flowrate Major Pump	4.00 ml/min
0.30	Valve Position	V22 Vacuum exhaust = Position 2
0.32	Start Chromatogram	Ch. 1,2,4,5,9,11,17 (500 ms)
0.35	Valve Position	V7 VialA7 = Position 2
0.42	Valve Position	V5 VialA5 = Position 2
0.42	Valve Position	V14 Reactor1 in = Position 2
0.78	Valve Position	V5 VialA5 = Position 1
0.80	Valve Position	V4 VialA4 = Position 2
0.83	Digital Output	= ON
0.88	Dispenser ("Dispenser 1")	Aspirates 5000 µl from 2 (15000 µl/min)
1.16	Valve Position	V4 VialA4 = Position 1
1.36	Temperature	Methane Trap = 60 °C
1.51	Valve Position	V18 Helium Reactor 1 = Position 1
1.60	Valve Position	V14 Reactor1 in = Position 1
2.06	Dispenser ("Dispenser 1")	Dispenses 5000 µl to 2 (15000 µl/min)
2.60	Dispenser ("Dispenser 1")	Aspirates 5000 µl from 2 (15000 µl/min)
3.30	Dispenser ("Dispenser 1")	Dispenses 5000 µl to 2 (15000 µl/min)

Figure 40 (Control File Visualisation)

Each table scrolls itself so the actual step can always be seen.

13 Program Settings

The Setup Window can be opened by using the setup icon on the Toolbar or via the Menu Bar: File -> Setup

WARNING: CHANGING SETTINGS IN THE SETUP OF THE SOFTWARE CAN HAVE GREAT IMPACT ON THE FUNCTION OF YOUR MACHINE. THE SETTINGS ARE NOT TO BE CHANGED UNLESS THE PERSON IS QUALIFIED FOR THIS TASK.

The setup window has several tabs, the function of each will be described now one after the other.

13.1 Communication Tab

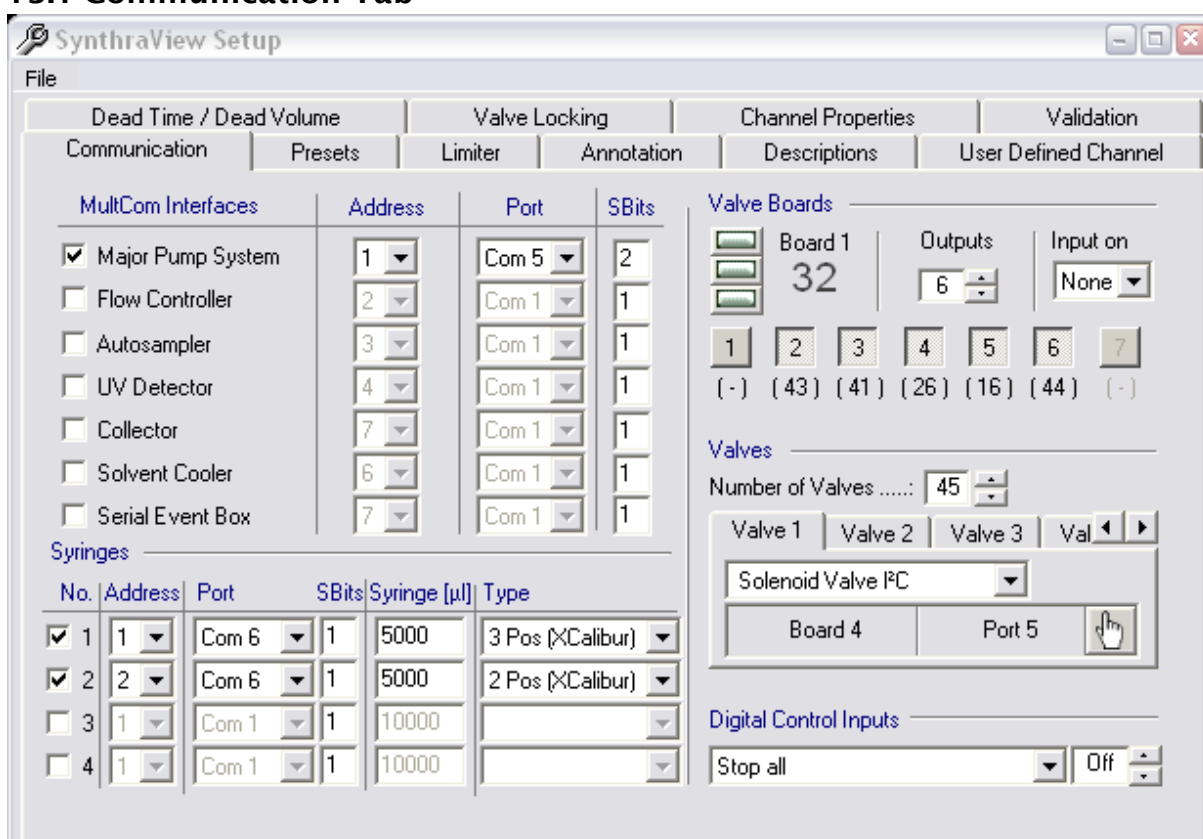


Figure 41 (Setup Communication Tab)

The Communication Tab is used to configure the system's serial controlled interfaces and valves. There are different sections in this tab that are taking care about different communication tasks.

13.1.1 MultCom Interfaces Section

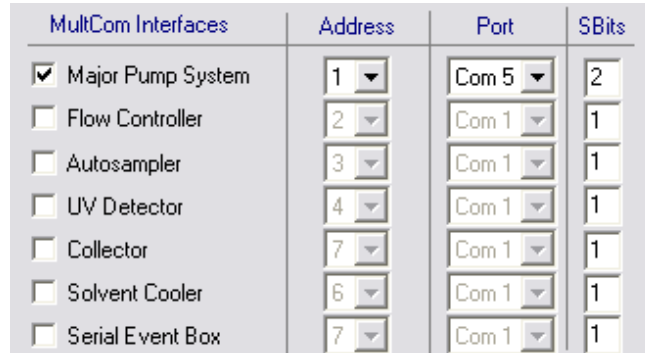


Figure 42 (Setup Communication MultiCom Section)

MultCom Interfaces Section lists all the controllable interfaces which are communicating via a COM port that can be activated or deactivated in this area of the window (Figure 42). In the address column it can be seen to which address the device is set. The Port column shows to which serial port or Winsock port the interface is connected.

13.1.2 Syringes

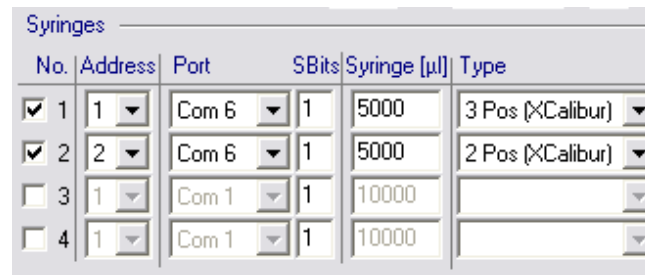


Figure 43 (Setup Communication Syringes Section)

The Port column shows to which serial port or Winsock port the device is connected to. The dispenser is also connected to COM ports. In the Syringe [µl] column the volume of the syringe is entered and the type column needs to know the kind of dispenser sending the data to.

13.1.3 Valve Boards and Valves

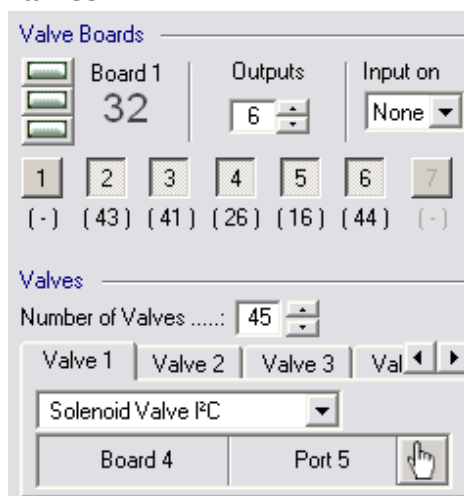


Figure 44 (Setup Communication Valve Boards and Valves Section)

In the right section the serial controlled valves are managed. *Number of valves*

shows how many valves are to manage. Each valve has its own tab; the valves are operated by *Valve Boards* that are managed in the upper area. You know from the look at the valve's fab the kind of valve and on which port on what board the valve is assigned to.

The valves are grouped on boards; this way not all valves have to be plugged into the mainboard of the system but get remote connection boards that are linked into the systems bus.

The Valve Boards are similarly configured; in the left area the three jumpers that are representing the address of the board in binary code can be seen. For better understanding there is also a decimal board number displayed depending on the configuration of the three jumpers. A jumper can be changed from 1 to 0 or vice versa by clicking it and below the board number with address is displayed. Beside the numbers and addressing the number of in- and outputs of the valve board has to be specified. This can be different from board to board.

After all these specifications it may be necessary to remove a valve assignment from a board or add a new one.

Removing is easily done by clicking on an assigned port of a board (assigned ports are the impressed grey squares)

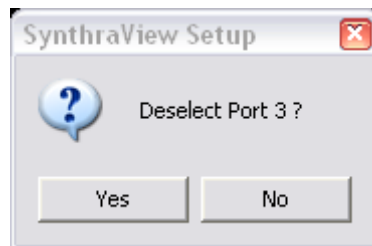


Figure 45

A query window opens to get a confirmation that the assignment should be deleted.

If such an assignment of a valve to a board needs to be created, this can be done by choosing the tab of the valve that has to be assigned. Click on the pointing hand icon beside the port and board addresses. The mouse cursor changes in shape. Pointing on the actual boards ports above it shows the pointing hand. Just click with the finger on the port you want to assign it to. The board number can easily be adjusted even while the mouse cursor is the pointing hand. One thing to take care of is that the port needs to be "existing" before starting the assignment. If a board has only 4 outputs you cannot assign a valve to port no. 5. And you cannot change the number of output ports while having a pointing hand mouse cursor.

If you don't want to assign anything but already clicked on the pointing hand, just go in an area where the mouse cursor shows a not allowed symbol. If clicking there the mouse cursor will turn to "ordinary" one again.

Summary

MultCom Interfaces	Select the peripheral instrumentation and the Com-Port to that it is connected
Valve Boards	If an I ² C-bus-board is connected, it can be configured with the jumper positions. The jumpers allow to configure up to 8 I ² C-bus-boards, each with up to 7 valves.
Valves	Need to be assigned to a Board. <i>Warning: if a valve is assigned to more than one board it is possible that the valve is not working correctly, or the whole setup or software stops working</i>
Dispenser	Up to 4 dispensers can be controlled. If the dispensers are connected to one serial port (system is then one master-syringe and all others are slave syringes) the syringe assigned to address 1 is the master-syringe, addresses 2 - 4 are slave syringes. If there are several master syringes they all need to be assigned to address 1, but then the com-port has to differ. For each dispenser the syringe volume is defined.
Digital Control Inputs	The control-functions <i>Stop all</i> , <i>Time Control Start</i> and <i>Time Control Hold</i> can be selected and addressed. This allows external use of those functions.

13.2 Presets

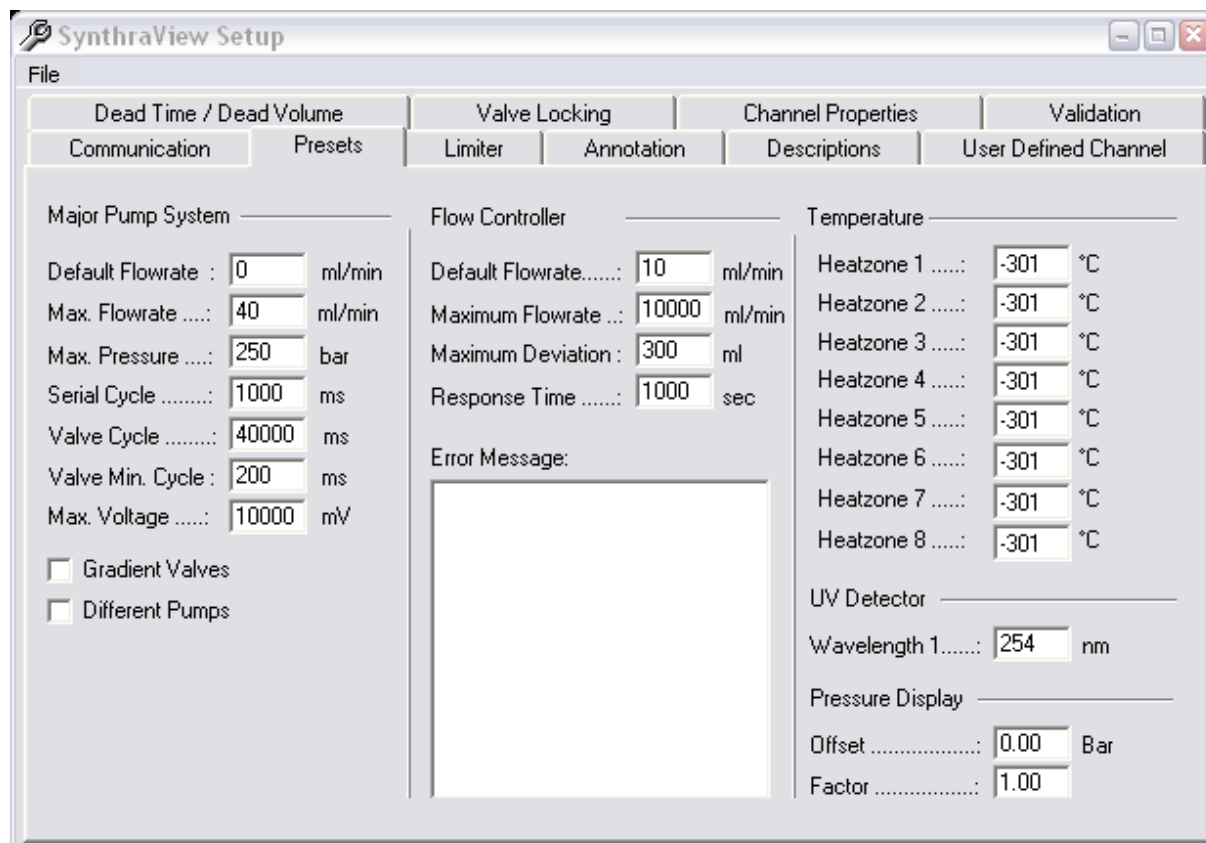


Figure 46 (Setup Presets Tab)

The Presets Tab also has different areas to configure; the explanation will be given one by one.

13.2.1 Major Pump System

In the *Major Pump System* area of the *Presets* tab (Figure 46) the standard and maximum values for the Primary Pump is set:

- Default Flow-rate:** the standard flow-rate set for the pump at the start of the program
- Max. Flow-rate:** maximum flow-rate for the pump
- Max. Pressure:** maximum pressure, the pump will stop if reaching this pressure
- Serial Cycle:** time interval of status requests to the pump
- Valve Cycle:** time for a mix cycle of a low pressure gradient system at a flow rate of 10ml/min
- Valve Min. Cycle:** minimum permitted switching time for the gradient mix valves in use
- Max. Voltage:** maximum controlling voltage for voltage controlled pumps

Gradient Values: has to be checked if a low pressure gradient system is used

Different Pumps: can be activated if different voltage controlled pumps with different maximum flow-rates are set up. The control voltage and the maximum flow rate for each pump can be set separately.

13.2.2 Temperature

Heat-zone X: Here the default temperature of the heaters at program start are set. [X=1-10]

13.2.3 UV-Detector

Wavelength: shows the wavelength the UV detector is set to at the start of the program.

13.2.4 Pressure Display

To calibrate the pressure display the according factors can be entered in this section. This changes the display of the HPLC pump pressure

Offset: The offset the pressure sensor has

Factor: should not be changed

13.3 Limiter Tab

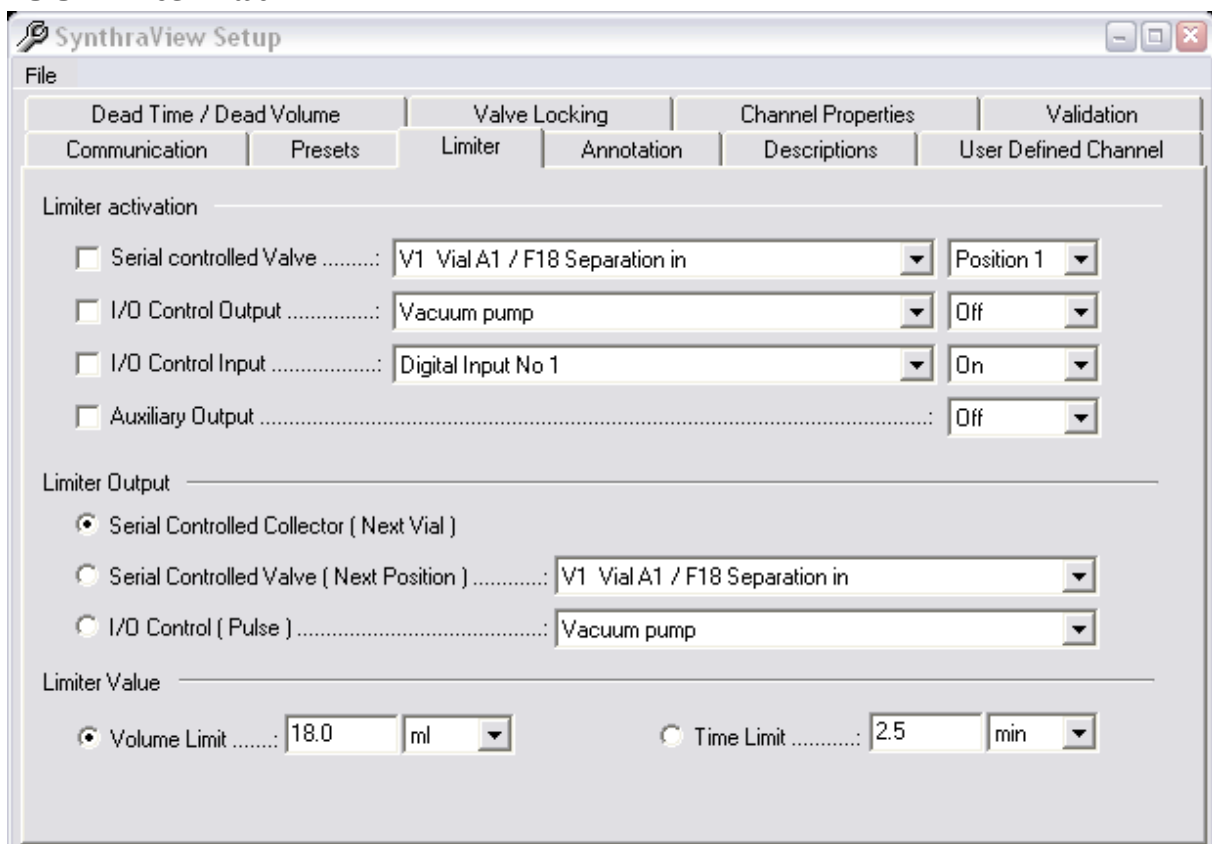


Figure 47 (Setup Limiter Tab)

The fraction limiter is configured in the *Limiter* Tab of the Setup.

13.3.1 Limiter activation Section

In this section the condition that activates the limiter is defined, it defines the point of switching between waste and fraction.

Serial controlled Valve: has to be activated if using a serial controlled valve to switch between waste and fraction. The position following must be the fraction position of the valve.

I/O Control Output: has to be activated if using an I/O control output to switch between waste and fraction. The setting that is following must be the fraction state of the I/O Control output.

I/O Control Input: has to be activated if using an I/O control input to switch between waste and fraction. The setting that is following must be the fraction state of the I/O Control input.

Auxiliary Output: has to be used if using an auxiliary output of the pump interface to switch between waste and fraction.

13.3.2 Limiter Output Section

In the Limiter Output Section it is set how the limiter should act if reaching the fraction limit.

Serial Controlled Collector: has to be activated if using a serial controlled fraction collector. If the fraction limit is reached a "Step" is carried out.

Serial Controlled Valve: has to be activated if using a serial controlled motor switching valve. If the fraction limit is reached, it switches to the next position.

Event Box Output: has to be activated if using a fraction collector controlled by the event box. If the fraction limit is reached, there is a pulse at the indicated output.

13.3.3 Limiter value

Volume Limit: the volume limit for the fraction limiter is entered here.

Time Limit: the time limit for the fraction limiter is entered here.

13.4 Annotation

The automatic annotations of the chromatograms are configured in the *Annotations* tab.

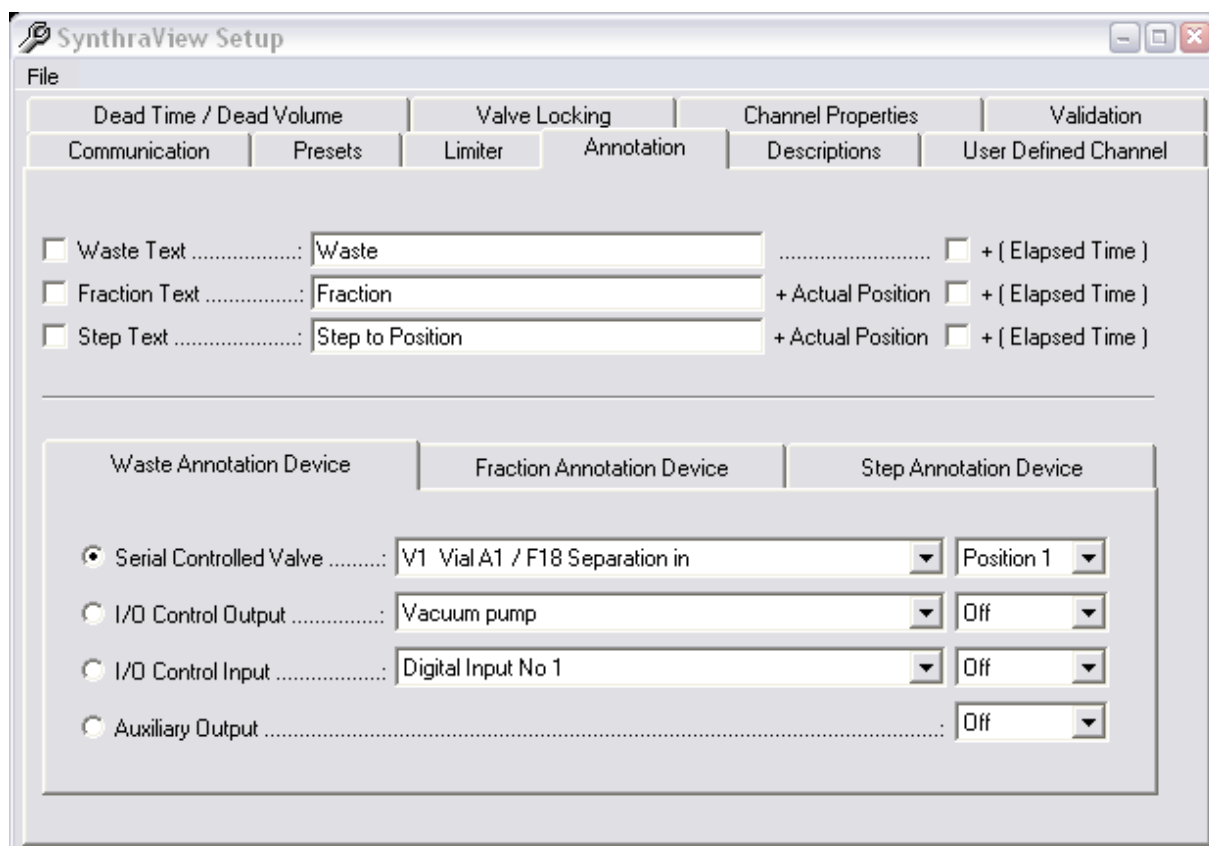


Figure 48

Waste Text: allows activating or deactivating annotation if switching to the waste position. The text can be chosen by entering it into the text box of Waste Text. The option + (Elapsed Time) add the elapsed time to the text.

Fraction Text: allows activating or deactivating annotation if switching to the fraction position. The text can be chosen by entering it into the text box of Fraction Text. The fraction number is automatically appended to the text. The option + (Elapsed Time) add the elapsed time to the text.

Step Text: allows activating or deactivating an annotation if switching a position. The text can be chosen by entering it into the text box of Step Text. The fraction number is automatically appended to the text. The option + (Elapsed Time) add the elapsed time to the text.

The *Waste Annotation Device* Tab and the *Fraction Annotation Device* Tab are quite similar in their options, one corresponding to waste and the other with the same settings corresponding to fraction.

13.4.1 Waste Annotation Device Tab

Serial controlled Valve: has to be activated if using a serial controlled valve to switch to waste. The position following must be the waste position of the valve.

I/O Control Output:	has to be activated if using an I/O control output to switch to waste. The setting that is following must be the waste state of the I/O Control output.
I/O Control Input:	has to be activated if using an I/O control input to switch to waste. The setting that is following must be the waste state of the I/O Control input.
Auxiliary Output:	has to be used if using an auxiliary output of the pump interface to switch to waste

13.4.2 Fraction Annotation Device Tab

Serial controlled Valve:	has to be activated if using a serial controlled valve to switch to fraction. The position following must be the fraction position of the valve.
I/O Control Output:	has to be activated if using an I/O control output to switch to fraction. The setting that is following must be the fraction state of the I/O Control output.
I/O Control Input:	has to be activated if using an I/O control input to switch to fraction. The setting that is following must be the waste state of the I/O Control input.
Auxiliary Output:	has to be used if using an auxiliary output of the pump interface to switch to fraction.

13.5 Descriptions Tab

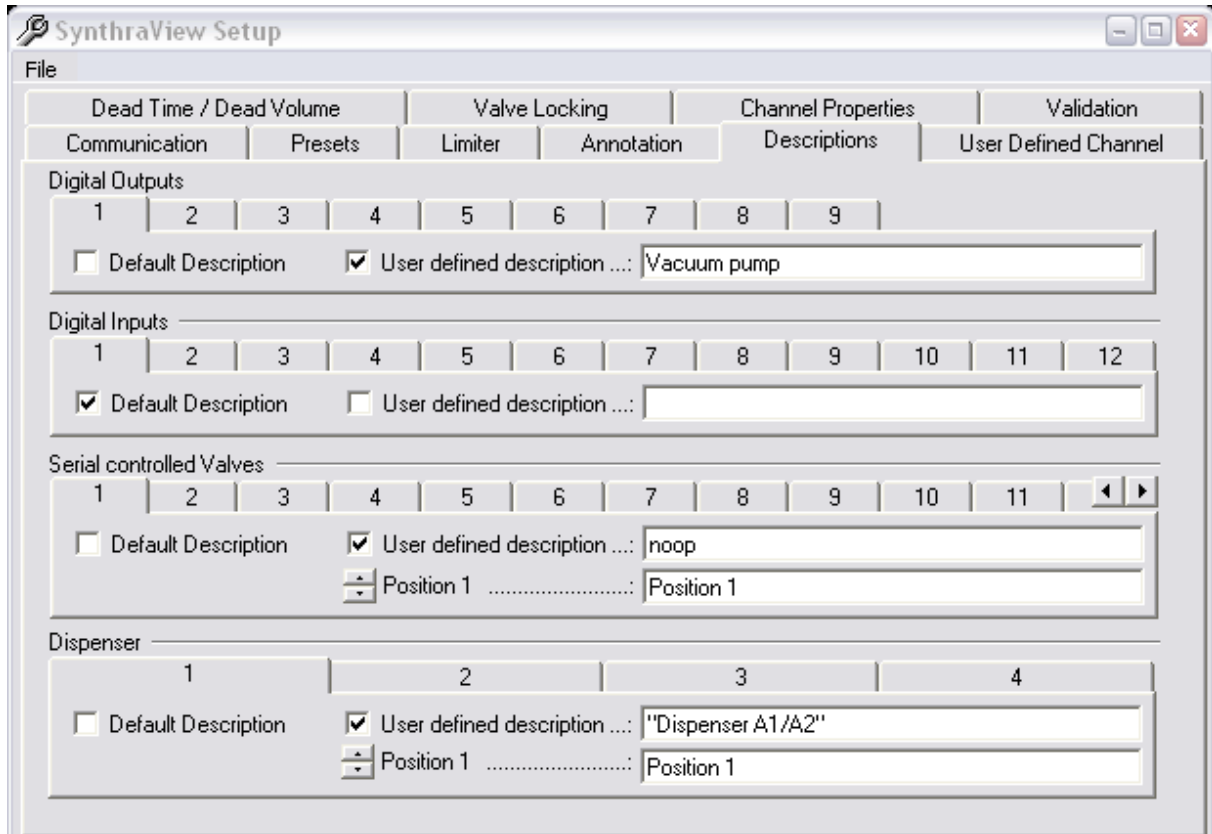


Figure 49 (Setup Description Tab)

All digital outputs, digital inputs, serial controlled valves and dispensers can be given customized names.

Using customized names for all these parts makes it much easier to program time control files. Also the visualizations are clearer because the inputs, outputs and valves can be listed by function.

Each element has its own register card in the section it belongs to, there are two choices:

Default Description: this element gets a standard description consisting of the group name (e.g. valve) and the number of the element.

User defined description: It is possible to enter a user defined description for the element into the textbox.

Also the different positions of the elements can be named, for a valve e.g. the positions can be renamed to Position 1 = open; Position 2 = closed.

13.6 User Defined Channel

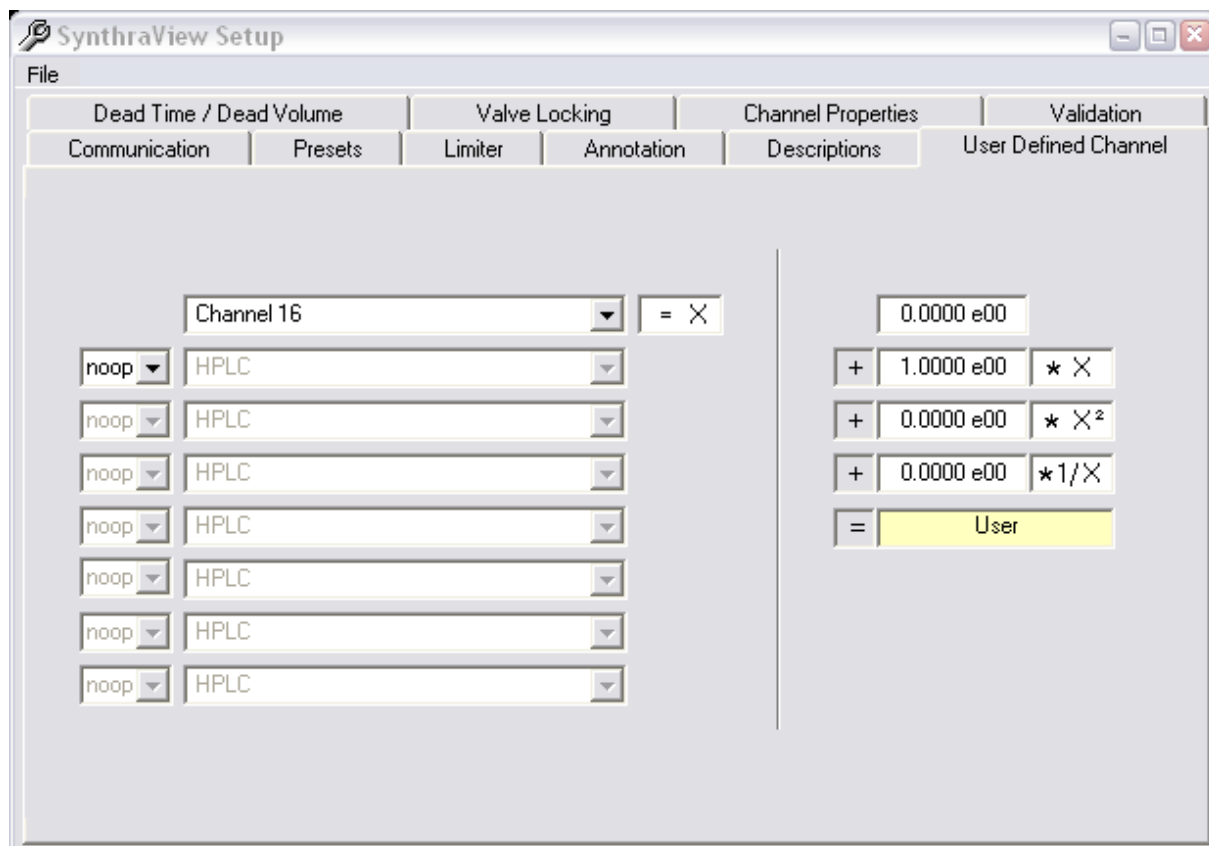


Figure 50 (User Defined Channel)

It is possible to set up a user-defined data channel in the *User Defined Channel Tab*. This data channel is used similar to any analogue channel and is labeled “U”.

The channel is calculated by means of other channels and/or calculations. On the left side one can activate one or more analogue signals as a source of data. The possible operations are:

- NOOP No operation
- + Adds the channel mentioned in the same row
- Subtracts the channel mentioned in the same row
- * Multiplies with channel mentioned in the same row
- / Divides by the channel mentioned in the same row

The result of these operations is available on the right side as value X for further calculations. Here an offset-, linear-, square- and reciprocal coefficient can be entered (top to bottom). The sum of the four lines results in the final value of the user defined channel.

13.7 Dead Time / Dead Volume

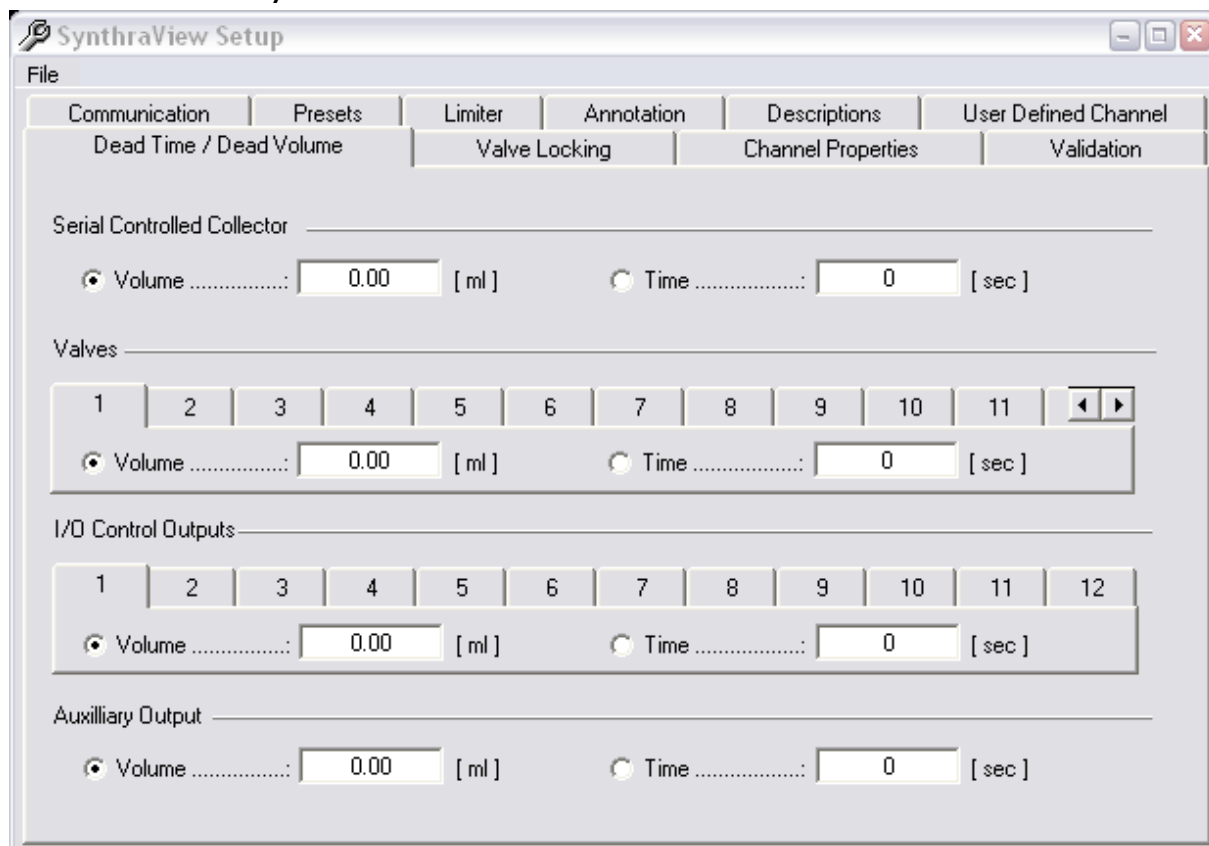


Figure 51 (Dead Time / Dead Volume)

If fractioning it can happen that a dead time or -volume has to be taken into account, especially at low flow rates. This can be done automatically if the software knows those values.

If a dead volume is entered the software calculates the dead time for each device according to the current flow-rate. Actions triggered by threshold values or automatic peak detection are also carried out with this delay. If a dead time is entered these are carried out in real-time. Annotations are logged in a chromatogram without the delay.

- Serial Controlled Collector
- Serial Controlled Valves
- Event Box Outputs
- Auxiliary Output

13.8 Valve Locking

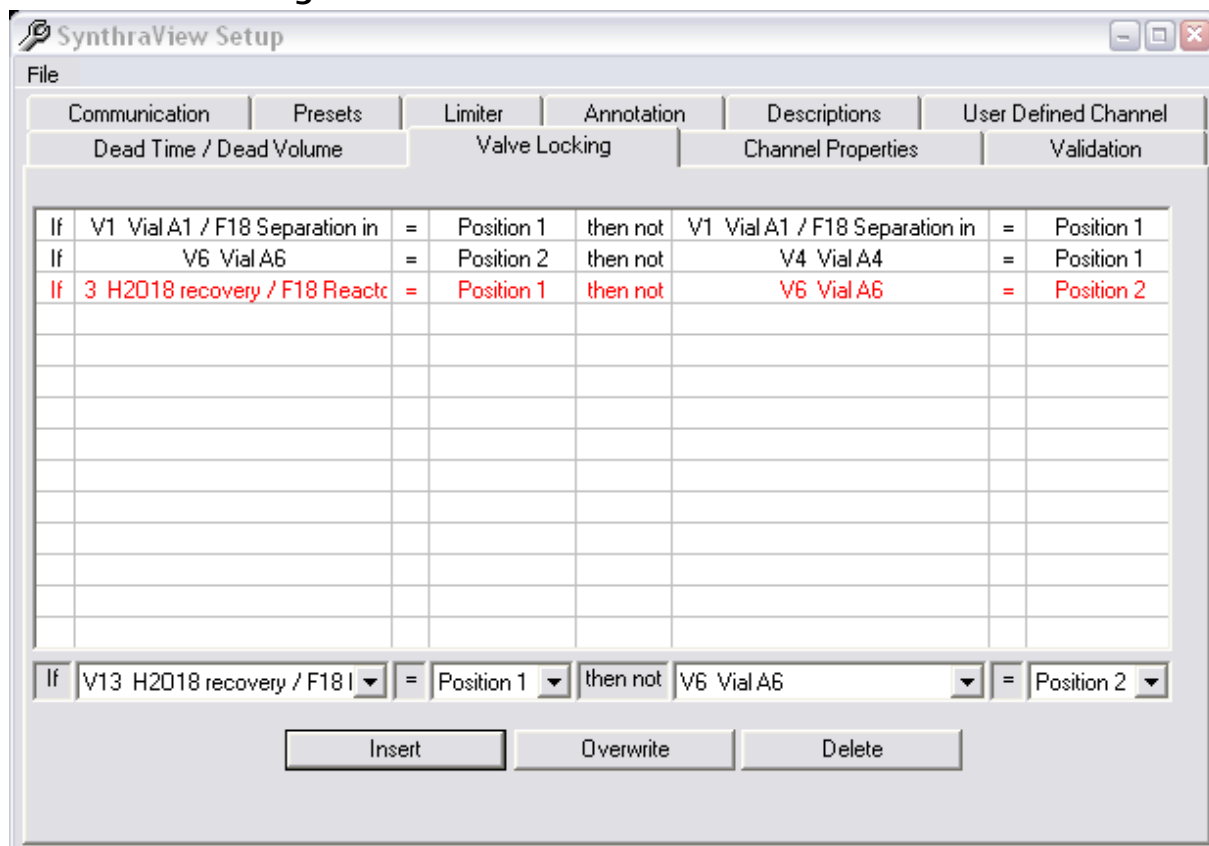


Figure 52 (Valve Locking)

If working with a system that has a considerable amount of valves it is possible to switch to non-permitted valve settings, this can cause closing off the flow through the system without intention. In order to prevent this it is possible to enter a list of non-permitted valve positions into the software. This is done in the Valve Locking Tab.

The software will constantly check for these combinations and prevent them being carried out. If one of these non-permitted valve positions is ordered, a message appears on the screen.

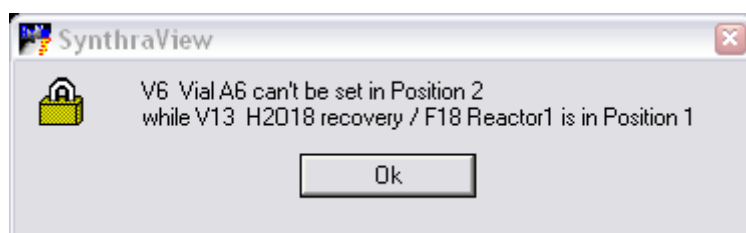


Figure 53 (Valve locking message)

To enter the non-permitted valve positions one has to set the parameters in the rule row (beneath the table) and then hit the *Insert* button. The new non-permitted combination of valve settings appears in the table-

If one of those rules should be changed, first it has to be selected by clicking on it with the mouse, then the selected row turns red. After that the new rule has to be set like you would enter a new rule. *Overwrite* has to be clicked with

the mouse. Subsequently the old setting is overwritten with the new.

If a non-permitted valve position should be deleted first it has to be selected by clicking on it with the mouse, the selected row turns red. Clicking on Delete with the mouse removes the rule.

13.9 Channel Properties

	Description	Dimen.	Offset	Factor
1	HPLC	C/s	0.0000e+00	1.0000e+00
2	Starting activity	GBq	0.0000e+00	3.0000e+00
3	Reactor 1	GBq	0.0000e+00	2.8100e-03
4	Product Activity	GBq	0.0000e+00	3.0000e-03
5	Product	GBq	0.0000e+00	3.0000e-03
6	Channel 6	GBq	0.0000e+00	1.0000e+00
7	Vessel 1	°C	0.0000e+00	1.0000e+00
8	Reactor	°C	0.0000e+00	1.0000e+00
9	Channel 9	°C	0.0000e+00	1.0000e+00
10	Press reactor 1	hPa	0.0000e+00	1.0000e+00
11	Channel 11	hPa	0.0000e+00	1.0000e+00
12	Channel 12	hPa	0.0000e+00	1.0000e+00
13	Channel 13	hPa	0.0000e+00	1.0000e+00
14	Channel 14	°C	0.0000e+00	1.0000e+00
15	Channel 15	°C	0.0000e+00	1.0000e+00
16	Channel 16	°C	0.0000e+00	2.8100e-03
17	Serial UV	mAU	0.0000e+00	1.0000e+00
User	User	mV	0.0000e+00	1.0000e-01

Figure 54 (Channel Properties)

In the Channel Properties tab each ADC- and GM-tube-input of the control box can be given a custom name. This helps in programming time tables and in a better arrangement of visualizations.

The order of the channels is depending on their mapping.

13.10 Validation Tab

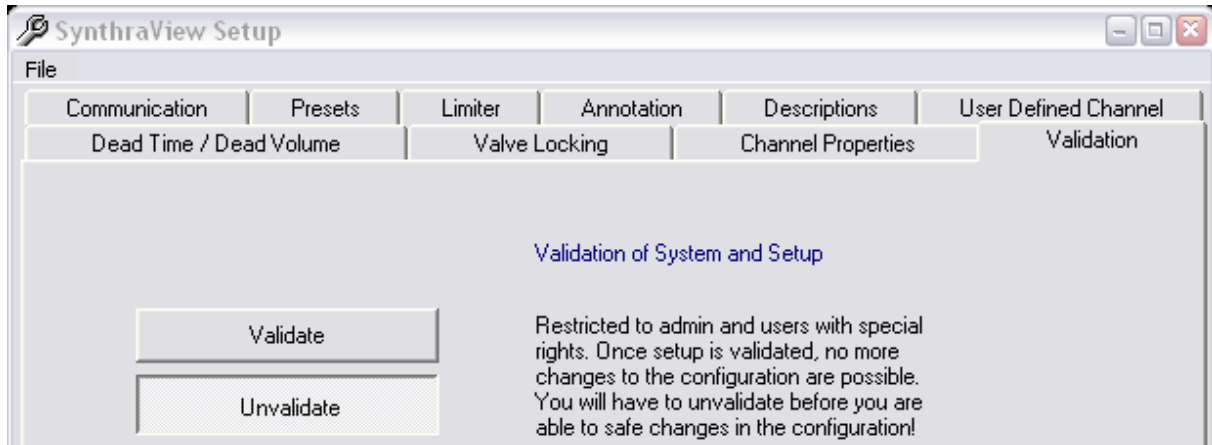


Figure 55 (Validation)

To be able to confirm certain regulatory it might be necessary that to ensure that changes are not made accidently. This can be done in the Validation Tab of the setup.

If validated once; no more changes to the program configuration can be realized without un-validating. If trying to save new settings in the setup the following query appears:

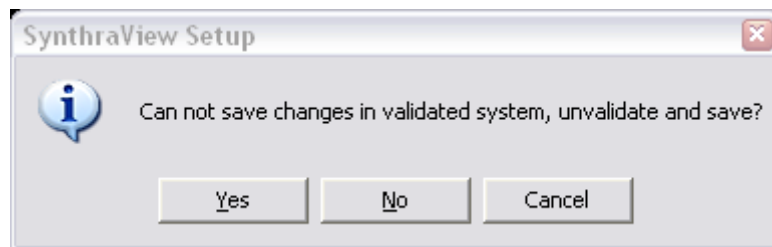


Figure 56 (Validation message)

Now the user has the choice to leave the system validated as it is or de-validate it save the changes and revalidate it.

Warning: Revalidation is a process that follows certain rules and is not only done by pushing the Validate button again!

14 User Administration

The User Administration allows creating profiles for multiple users and managing of their permissions.

The User Administration Window can be opened by using the icon on the Toolbar or via the Menu Bar: File -> User Administration

Once one or more users have been set up a login window appears at the start of SynthraView. Here the user has to enter the username he has been given and the password. This also has to be done if un-locking the program with the key-lock function.

14.1 Settings

The *User Administration* window can be opened via the menu *File -> User Administration* or by pressing the corresponding icon in the toolbar.

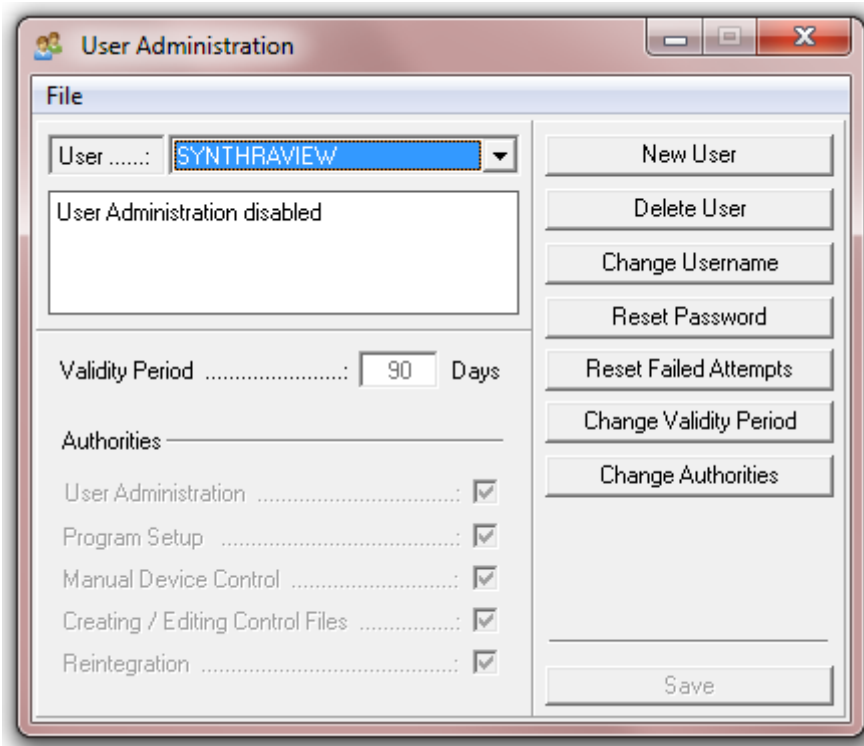


Figure 57 (User Administration Window)

To activate the “User Administration” the password of the first user, usually SYNTHRAVIEW needs to be assigned a password via “Reset Password”

14.1.1 Creating a user

To create a new user, click on the “New User” button. Now the user name can be put in and in the Authorities section in the lower part the access level can be configured.

Press the “Save” button to confirm creation

14.1.2 Delete User

By pressing this button the selected user is deleted

Warning: Deleted users cannot be recovered in any way and have to be recreated, if desired.

The first user cannot be deleted.

14.1.3 Change Username

The username of the selected user can be changed by pressing "Change Username" the change needs to be confirmed by pressing the "Save" button.

14.1.4 Reset Password

To activate a created user the password has to be reset by pressing the "Reset Password" button

An initial password is displayed in the information section of the User Administration window. This Password has to be used for the first login of the user into the SynthraView Software.

If the user logs in the first time he is asked for a new password and a confirmation. After that password change only the new password, the user has assigned is working.

Passwords cannot be looked up in any way, if they get lost they have to be reset.

14.1.5 Reset failed attempts

This button resets the counter that is keeping track of failed password requests

14.1.6 Change Validity Period

The period till the password has to be changed again can be changed here.

14.1.7 Change Authorities

Here the authorities of an existing user can be changed.

14.1.8 Authorities

User Administration: provides the user with the power to create new user

Program Setup: provides access to the setup windows

Manual device control: allows manual operation of the system using the control functions of the main, the visualization and the Digital IO Control e.g.

Creating / Editing Control Files: allows the creation and modification of time and sequence control files.

Reintegration: allows reintegration of result files

15 Troubleshooting

15.1 Temperature calibration

In the case that a thermometer is changed in the machine it has to be recalibrated to show the correct results.

For temperature calibration an external reference thermometer is necessary.

The values to calibrate the temperature are not changed via the user interface; they are changed in the SynthraView.ini. The SynthraView.ini is located in the installation directory of SynthraView (usually "c:\SynthraView"). It can be opened by a simple text editing program, usually it is opened the editor by just double-clicking.

WARNING

BEFORE CHANGING ANYTHING BACK-UP THE SYNTHRAVIEW.INI THAT IT CAN BE RESTORED, IF NECESSARY

There are multiple temperature channels in the machine, not all necessarily used.

In the SynthraView.ini there is a section starting with [Calibration] (see chapter 16.1 Settings in the SynthraView.ini). The offset and gain are set for the channel number that is following the expression (e.g. gain4 is gain for channel 4).

Start SynthraView to see the temperature display of the internal temperature sensor.

15.1.1 Set offset

To set the offset compare the displays of SynthraView and the external thermometer to calculate the new offset.

$$\text{New offset} = (\text{external Temp} - \text{SynthraView Temp}) + \text{Actual offset}$$

Change the actual "offsetX=" to the new. Save SynthraView.ini.

15.1.2 Set gain

To set the gain you have to heat up the oven, the temperature is depending on the oven to be calibrated (e.g. reaction vessel 120°C).

Wait for the temperature to stabilize.

If the temperature is stable read the SynthraView display and the external thermometer to calculate the new gain.

$$\text{New gain} = \left(\frac{(\text{external Temp} - \text{Offset})}{(\text{SynthraView Temp} - \text{Offset})} \right) * \text{Actual gain}$$

Change the actual "gainX=" to the new. Save SynthraView.ini.

After changing the parameters SynthraView.ini has to be saved and SynthraView has to be restarted.

16 Appendix

16.1 Settings in the SynthraView.ini

[Main Window]

AlwaysOnTop=0	[0; 1]	Should the main window stay on top of all other windows open?
SolventConfirm=0	[0; 1]	Should the starting of the pump by the eluent buttons be confirmed by the user?
DataPathSelection=0	[0; 1]	Should the user be able to choose a folder for result files after opening a time control file?

[User Company]

Name=Company	Text	User defined company name that appears on reports.
FontName=Braggadocio	Text	Name of the font for the company name
FontSize=18		Font size of the printed company name
FontBold=0	[0; 1]	Should the company name be printed bold?
FontItalic=0	[0; 1]	Should the company name be printed italic?
FontColor=128	[0-128]	Font color of the company name.

[PUMPS]

MajorControl=SERIAL_MULTCOM	[Serial; Voltage]	Is the pump connected to a serial interface or voltage?
MinorControl=SERIAL	[Serial; Voltage]	Is the pump connected to a serial interface or voltage?
OnlineMoving=0	[0; 1]	Should the pump system support online gradient shift?

[WINSOCKPORTS]

Port1=192.168.0.106,100 [IP address] IP address of the Winsock board with the extension for the ports.

[Ethernet]

URL=192.168.0.105 [IP address] IP address of the mainboard.

[Detector]

S3245=1 [0; 1] Does the module contains a S3245 UV/Vis detector?

Risetime=1000

Wavelength [190; ...; 800] Set the wavelength for the S3245 on start of the software.

Range=1000

[Peakcut]

ValveNumber=X [1; ...] Select the valve number for the manual peak cut with F11 and F12.

[F7], [F8], [F9]

Vavnumber=X [1; ...]
VirtualSwitch=X [1; ...; 10]
Function=on ON, OFF, TOGGLE

Declares the

[EVENTBOX]

PulsLength=0.1 [0.1; ...] Pulse length of the digital outputs in [ms]

[ChromatogramPrinting]

Orientation=Portrait [Portrait; Landscape] Page orientation of the printed chromatogram

Monochrom=0 [0; 1] Should the chromatogram be printed black and white?

DrawWidth=1.5 [1.0; ...] Printing weight of the chromatogram

[IntegrationPresets]

IntegrateInhibit=2,3,4,..16,18 [0; 'see description'] Data channels that should not be automatically integrated are entered as parameter, separated by commas if multiple

MaxBaselineLevel=250	[...]	Preset values for integration outside
FilterFactor=5	[5 - 15]	Peak windows (see chapter 6.4 Integration Window)
SlopeSensitivity=9999999	[...]	
[TempZones]		
Name 1="Zone 1"	"Text"	Name of the temperature zone that should be displayed in the visualization
up to		
Name 10="Zone 10"	"Text"	Name of the temperature zone that should be displayed in the visualization
[AnalogOutputs]		
Name 1="Analog Output 1"	"Text"	Name of the analog output that should be displayed in the visualization
up to		
Name 8=" Analog Output 8"	"Text"	Name of the analog output that should be displayed in the visualization
[Heater1]		
Name="Sample Oven"	"Text"	Name of the component corresponding to the given name of the [TempZones]
P=8		P-term of the PID controller
I=0.3		I-term of the PID controller
D=4		D-term of the PID controller
PMAX=100	[0-100]	Maximum percentage the P-Term may get in controlling the heater.
IMAX=40	[0-100]	Maximum percentage the I-Term may get in controlling the heater.

DMAX=20	[0-100]	Maximum percentage the D-Term may get in controlling the heater.
ADC=1	[1-10]	Temperature input of the heating zone (1-8 are PT100; 9+10 are thermocouples)
Precision=3	[1; ...]	+/- Range in that the oven is considered ready. (setting in oven to 50°C with Precision=3 the program considers it ready from 47 to 53°C)
Switch=3,5	[Power Switch, Tolerance]	Power switch for cooling, max. Temperature deviation till cooling. (Power Switch 3 will be activated if actual temperature exceeds set temperature by 5°C)
I2C=14,5	[I2C Port, Tolerance]	I2C interface for cooling, max. Temperature deviation till cooling. (I2C port 14 will be activated if actual temperature exceeds set temperature by 5°C)
Limit=200	[1-...]	Maximum temperature this heater can be set to.
[Calibration] Range=2		
Offset1=0		Offset factor for linear approximation of the sensor signal of channel 1 (Channel can go from 1 to 22)
Gain1=0.2		Gain coefficient for linear approximation of the sensor signal of channel 1 (Channel can go from 1 to 22)
[Valve] Type=0		
[Counter] Bunching=3		
[Detector]		

Port=1

[Boardtemp]

Chip=CGA

[I2CBus]

Speed=5

[2-7]

I2C bus speed, 2 is fastest 7
is slowest

synthra



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