

ProMISE 2 user manual

Probabilistic model for immiscible separations and extractions (ProMISE) 2 developed by Joost de Folter, is available as Open Source software under the [GNU GPL-3.0 License](http://www.gnu.org/licenses/gpl-3.0.html).

The model software can be downloaded here:
<http://joostdefolter.info>

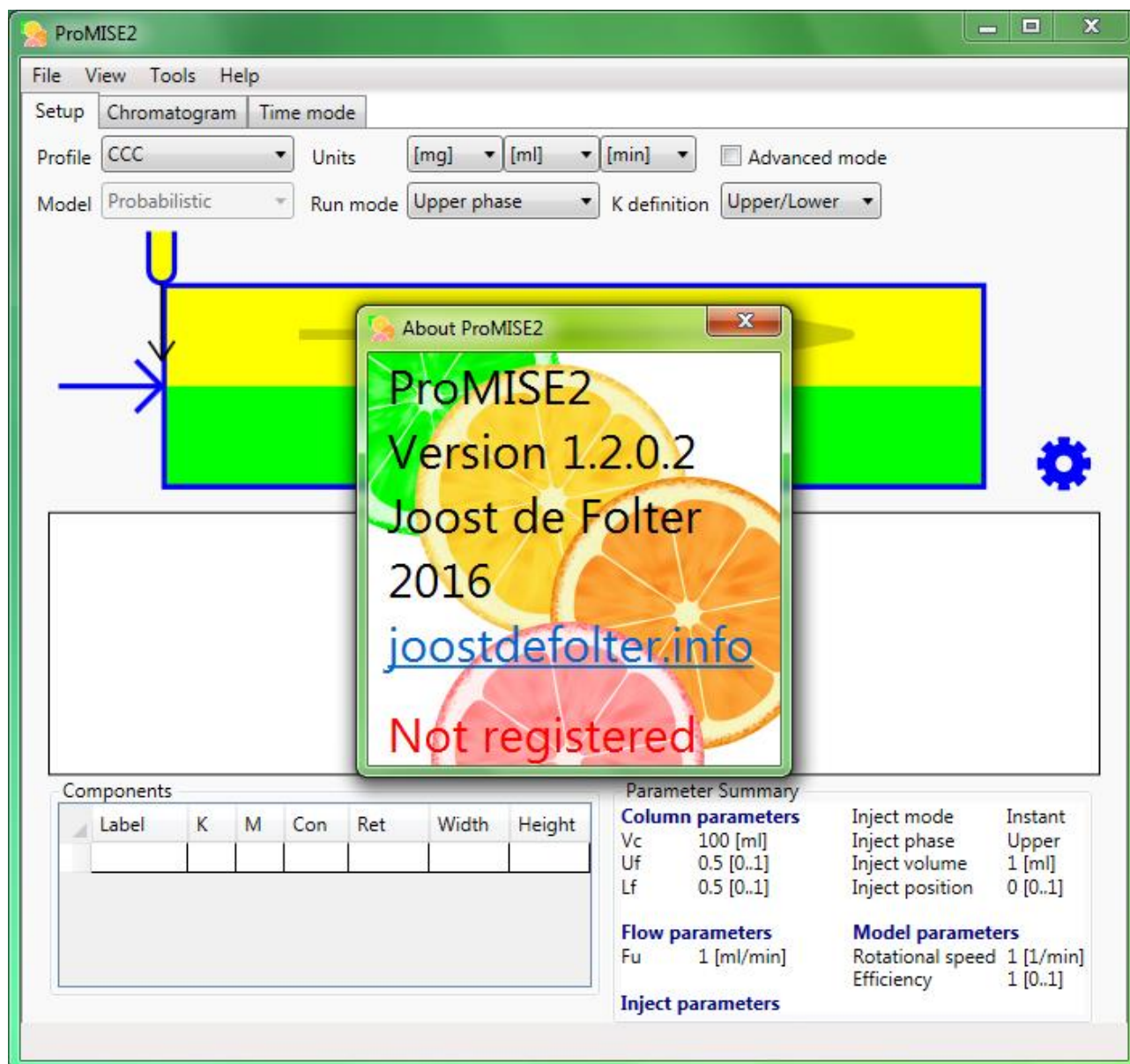
System requirements

Minimum requirements

- Operating system: Windows XP or higher

Recommended

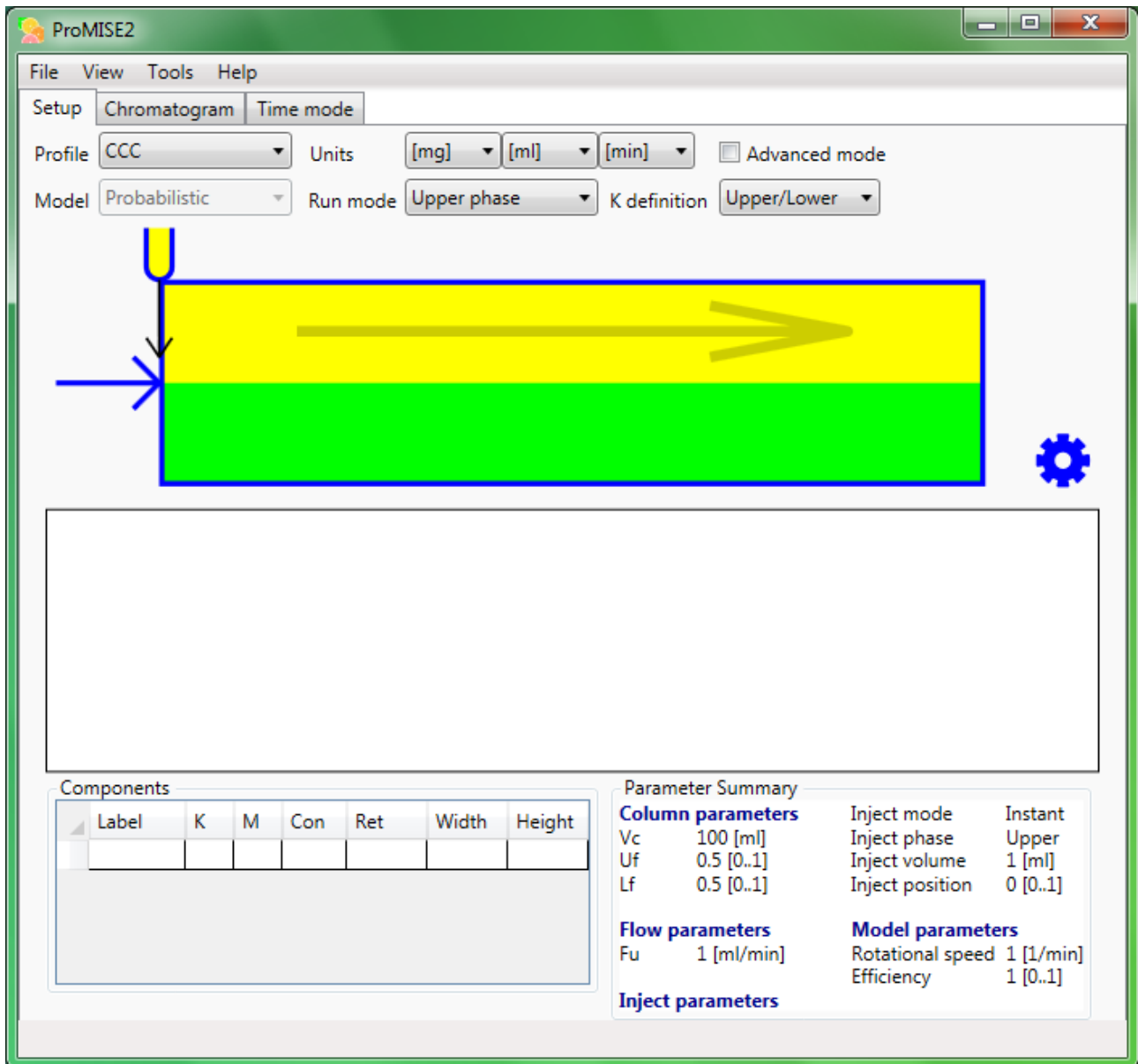
- CPU: Multi core (e.g. dual core)
- RAM: 2 GB (or more)
- Internet connection



Using ProMISE 2

Model Setup

When ProMISE 2 starts, the integrated setup view will automatically be shown.



The main window has various tabs which contain different views. Selecting the Chromatogram or Time mode views will run the model. Model execution can be aborted by returning to the Setup tab. Various instances of the model can be started concurrently.

The model setup view contains a number of interactive elements. At the top, a number of general input parameters is shown. Immediately below that, a visual representation of the selected separation profile that is selected.

Below that, a preview of the model output is displayed in a chromatogram style view. At the bottom left, a table is visible, allowing input parameters of sample components to be entered (Label, K-value, Mass, Concentration), and showing preview output parameters (Retention / Position, Width, Height) for these same components.

The bottom right shows a summary of all the input parameters.

the input parameters for the model which are shown in a number of parameter groups. The input controls contain tool tips which are displayed by hovering the mouse over a particular control. The model window title shows a summary of the main input parameters currently selected.

General input parameters

The general input parameters shown at the top of the screen are as follows.

The Profile sets the desired separation type profile, and will automatically select the most suitable model type.

The units for the different input parameters can be set for mass values, volume values and time values.

The Run mode can be set:

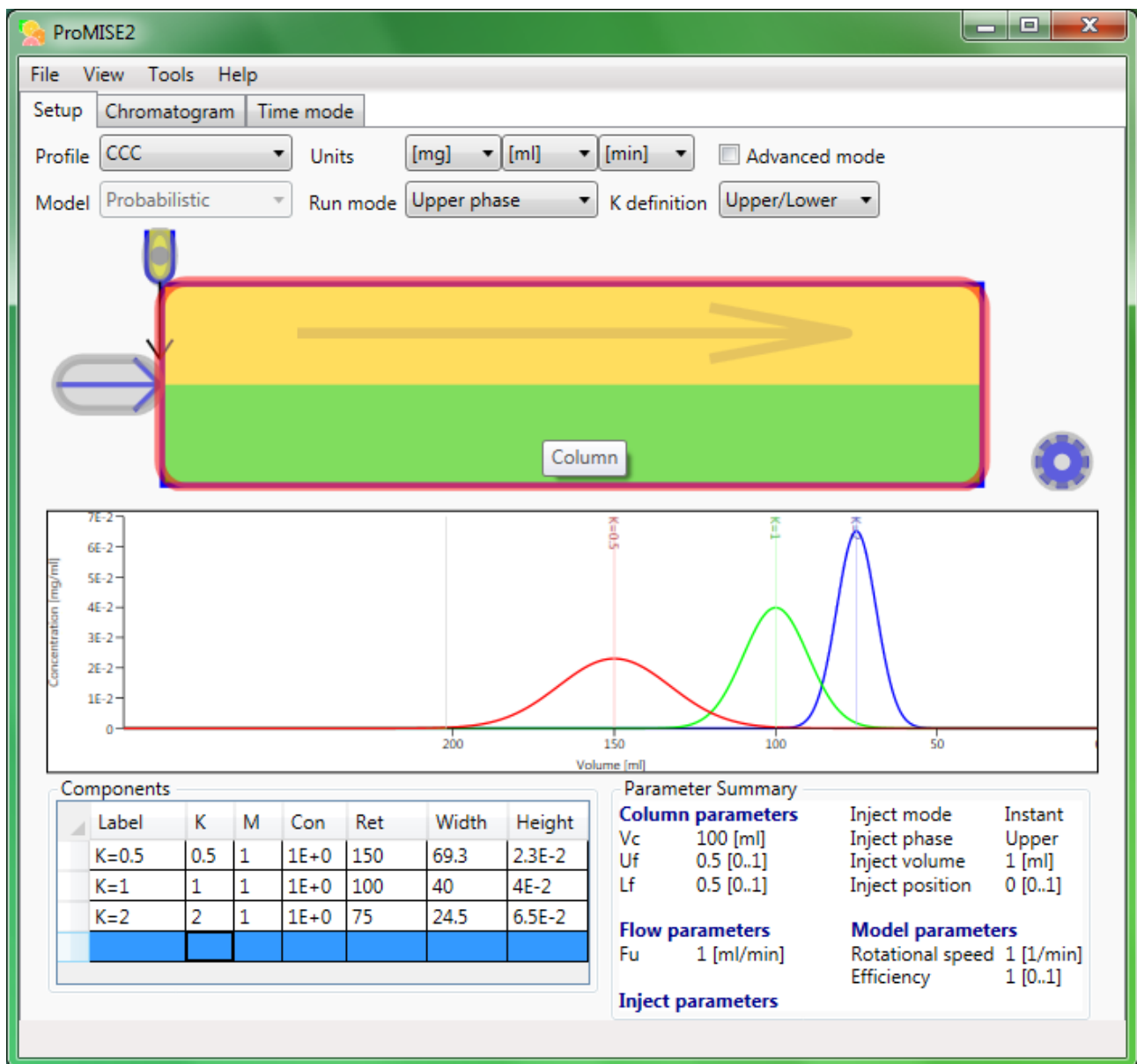
- Upper phase is mobile
- Lower phase is mobile
- Dual mode: Both phases move in opposite direction
- Intermittent mode: Both phases alternatively move (in opposite direction)
- Co-current: Both phases move in same direction

Advanced options enables modifying options for more expert users (disabled by default).

The K Definition sets the definition for the K-values:

Upper/Lower means $K = C_U / C_L$ (default)

Lower/Upper means $K = C_L / C_U$



Hovering the mouse over the visual representation will show the interactive areas, each overlaid with a grey coloured ellipse. The area the mouse is directly over will be shown with a red coloured ellipse and additionally a tool tip is shown with a description.

Column parameters

Each of these areas can be selected by subsequently selecting it using the mouse button. This will show the specific input parameter group corresponding to the visual element.

The screenshot displays the ProMISE2 software interface. The main window shows a chromatogram setup with a yellow and green column. A 'Column parameters' dialog box is open, showing the following settings:

- Vc: 100 [ml]
- Vdead: inlet 0 [ml], outlet 0 [ml], inject 0 [ml]
- Vtot: 100 [ml]
- Phase ratio: Uf [0..1] 0.5, Vu 50 [ml], Lf [0..1] 0.5, Vl 50 [ml]
- X: 1

The dialog box also includes a 'Components' table and a 'Model parameters' section.

Label	K	N
K=0.5	0.5	1
K=1	1	1
K=2	2	1

Model parameters:

- Mode: Instant
- Phase: Upper
- Volume: 1 [ml]
- Position: 0 [0..1]

Column parameters:

- Rotational speed: 1 [1/min]
- Frequency: 1 [0..1]

The column parameters are as follows.

Vc stands for the column volume, which is the active volume of the separation column.

Vdead stands for the dead volume, and can be enabled and specified for various locations.

Upper phase and lower phase ratio can be set, representing the volume ratio of the upper and lower phase.

The corresponding upper phase, lower phase and total volume are also displayed.

Flow parameters

The screenshot displays the ProMISE2 software interface. At the top, the 'Setup' tab is active, showing 'Chromatogram' and 'Time mode' sub-tabs. The main configuration area includes:

- Profile: CCC
- Units: [mg], [ml], [min]
- Advanced mode:
- Model: Probabilistic
- Run mode: Upper phase
- K definition: Upper/Lower

 Below this is a schematic of a column with a yellow upper phase and a green lower phase. A red oval on the left indicates the injection point. A 'Flow parameters' dialog box is open in the foreground, showing:

- Phase flow:** Fu = 1 [ml/min], FI = 0 [ml/min]. A circular gauge is visible for Fu.
- Partial phase transfer:** Upper = 1, Lower = 1. An 'Enabled' checkbox is present.
- Conditions:** Limit system volumes, value: 10.
- Intermittent switching:** Mode: Time, Start: Upper. Upper: 0 [min], Lower: 0 [min]. Max iterations: 10. Final elution.

 In the background, a chromatogram shows two peaks: a green peak at approximately 100 minutes and a blue peak at approximately 50 minutes. A 'Parameter Summary' table is also visible:

Parameter Summary		
Injection parameters	Inject mode	Instant
	Inject phase	Upper
	Inject volume	1 [ml]
	Inject position	0 [0..1]
Flow parameters	Model parameters	
1 [ml/min]	Rotational speed	1 [1/min]
	Efficiency	1 [0..1]

The main flow parameters are the upper and lower phase flow rates (F_u and F_l). The flow rates can be set here, depending on which phase(s) is / are mobile.

Next, the Elution-Extrusion mode can be enabled. The following options are available:

- None: Normal elution (default)
- EE: Elution – Extrusion
- BEE: Back Elution – Extrusion

Limit iterations: limits number of model iterations to x times the column volume.

Partial phase transfer mode is only enabled when using the CCD model, with advanced mode enabled. This mode enables partial transfers of the cell content, as opposed to a normal transfer where the entire cell content is transferred between cells. This mode is by default disabled.

Upper / Lower: The transfer factor for each respective phase; set to a value less than 1 (default: 1)

Intermittent switching parameters are only enabled having selecting intermittent mode in the Run mode parameter. These are as follows.

Mode: sets the type of intermittent switch criteria (default: time). This can also be set to 'Component', where a component can be selected that is allowed to elute (switching before other components elute).

Upper / Lower: switch amount (or component) for upper phase and lower phase flow.

Start: The first phase used in the intermittent switch (default: upper phase).

Max iterations: The number of intermittent switches (for both phases) (default: 10).

Final elution: Can only be changed in advanced options mode. Enables final elution after intermittent switches have completed (default: enabled).

Inject parameters

The screenshot displays the 'Inject parameters' dialog box and the main software interface. The dialog box is open, showing the following settings:

- Inject mode: Instant
- Inject phase: Upper
- Sample volume: 1 [ml]
- Sample feed: 0 [ml]
- Position: 0

The main interface shows a schematic of a column with an injector at the top left. Below the schematic is a chromatogram showing Concentration [mg/ml] on the y-axis (ranging from 0 to 7E-2) and Volume [ml] on the x-axis (ranging from 200 to 50). Three peaks are visible, labeled with their retention times: K=0.5 (red peak at 150 ml), K=1 (green peak at 100 ml), and K=2 (blue peak at 75 ml).

Below the chromatogram is a table of components and a parameter summary.

Label	K	M	Con	Ret	Width	Height
K=0.5	0.5	1	1E+0	150	69.3	2.3E-2
K=1	1	1	1E+0	100	40	4E-2
K=2	2	1	1E+0	75	24.5	6.5E-2

Parameter Summary:

Column parameters		Inject parameters	
Vc	100 [ml]	Inject mode	Instant
Uf	0.5 [0..1]	Inject phase	Upper
Lf	0.5 [0..1]	Inject volume	1 [ml]
		Inject position	0 [0..1]
Flow parameters		Model parameters	
Fu	1 [ml/min]	Rotational speed	1 [1/min]
		Efficiency	1 [0..1]

Inject mode:

- Instant: instantaneous (ideal) sample injection in first model step (default)
- Batch: More realistic sample injection enabling specific sample feed amount
- Continuous: continuous sample feed. (Use in combination with limit system volumes, in flow properties.)

Position: The relative column position; from 0 (start of column) to 1 (end of column). Only enabled in advanced mode. (Default 0.5 for dual flow and intermittent modes, and otherwise 0).

Phase: This is the phase initially containing the sample components. Only enabled in advanced mode.

Units: set units for sample feed (default: volume).

Sample volume: Sample volume used to calculate component mass / concentration.

Sample feed: feed amount for sample components.

Model parameters

ProMISE2

File View Tools Help

Setup Chromatogram Time mode

Profile CCC Units [mg] [ml] [min] Advanced mode

Model Probabilistic Run mode Upper phase K definition Upper/Lower

Concentration [mg/ml]

Volume [ml]

Components

Label	K	M	Con	Ret	Width	Height
K=0.5	0.5	1	1E+0	150	69.3	2.3E-2
K=1	1	1	1E+0	100	40	4E-2
K=2	2	1	1E+0	75	24.5	6.5E-2

Parameter Summary

Column parameters

Vc 100 [ml]
Uf 0.5 [0..1]
Lf 0.5 [0..1]

Flow parameters

Fu 1 [ml/min]

Inject parameters

Model parameters

Rotational speed 1 [1/min]
Efficiency 1 [0..1]
Density steps 200
Probabilistic units 10000

These parameters are specific to the used model.

CCD model parameters

Transfer steps: Number of CCD system cells or (transfer) steps (default: 100).

Efficiency: Mixing efficiency (only enabled in advanced mode). Value must be between 0 and 1, where 1 represents perfect distribution of components. (default: 1).

Probabilistic model parameters

Mixing speed: Rotational speed in CCC (or equivalent) (default: 1). [Suggested units: rotations / min]

Efficiency: Mixing efficiency (only enabled in advanced mode). Value must be between 0 and 1, where 1 represents perfect distribution of components. (default: 1).

Density steps: The base amount of histogramical density bins (default: 200).

Probabilistic units: The number of representative probabilistic units used (default: 10000).

Transport model parameters

Transfer steps: Number of transport model steps (default: 100).

Mass transfer coefficient: the overall volumetric mass transfer coefficient (k_0a) (default: 0.01) [units: 1/s]

Sample component parameters

Label	K	M	Con	Ret	Width	Height
K=0.5	0.5	1	1E+0	150	69.3	2.3E-2
K=1	1	1	1E+0	100	40	4E-2
K=2	2	1	1E+0	75	24.5	6.5E-2

Sample components can be set by either entering a K-value; remaining columns will be filled in automatically. A component can be modified directly by selecting the desired field. A component can be removed by selecting the desired row and pressing the Delete key.

The columns are defined as follows:

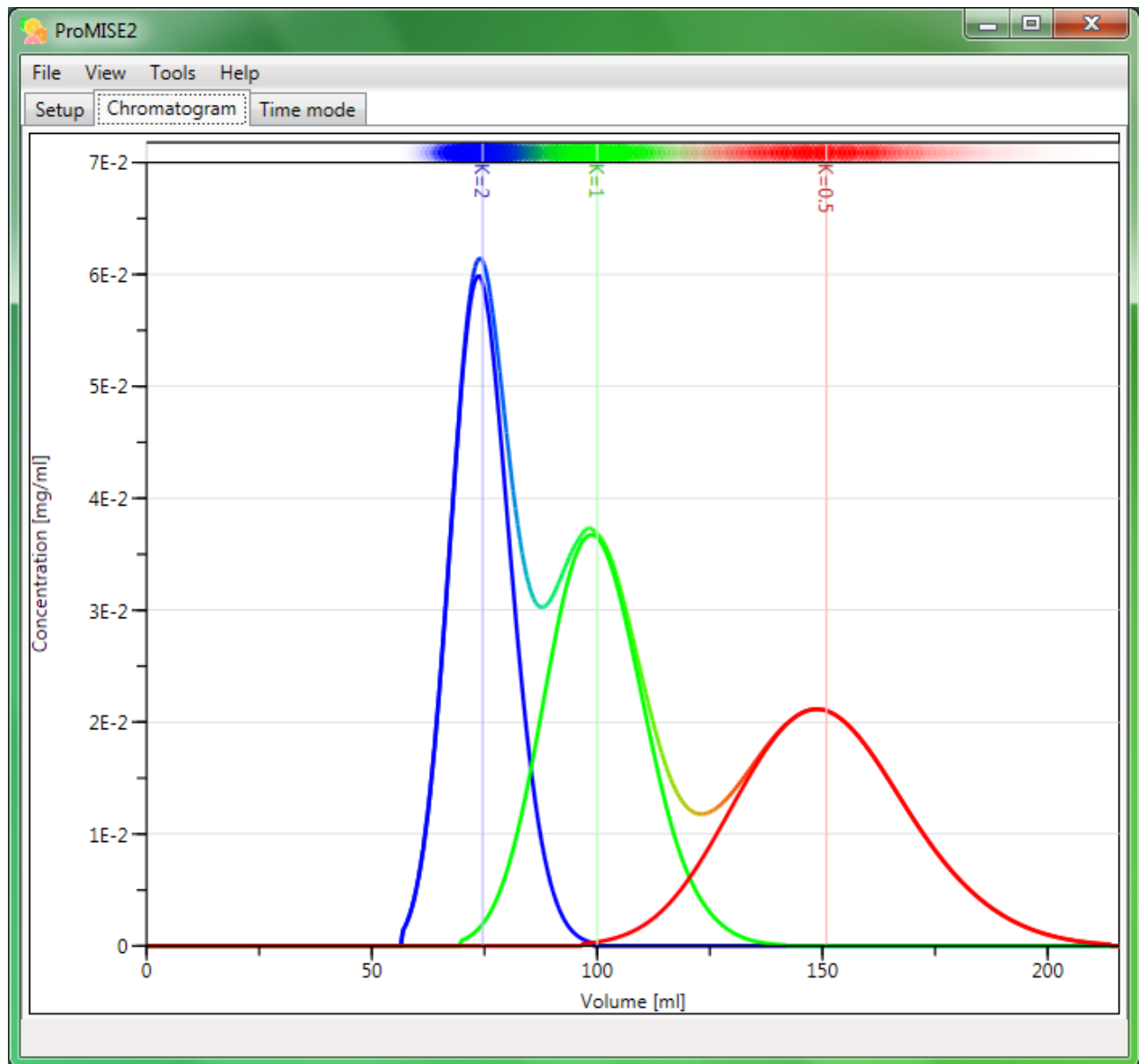
- Label: Custom text, displayed in chromatogram at peak position (set by default when entering K-value)
- K: K-value of sample component
- M: Mass of sample component (default 1). This value is automatically recalculated when the concentration field is modified, also using the sample volume
- Con: Component concentration. This field is automatically calculated when changing the component mass, also using the sample volume

Additional columns display the following preview output values:

- Ret: Component retention / elution position
- Width: Base width of component peak
- Height: Height of top value of component peak

Chromatogram view

Selecting the Chromatogram tab will run the model. Model execution can be aborted by returning to the setup tab.



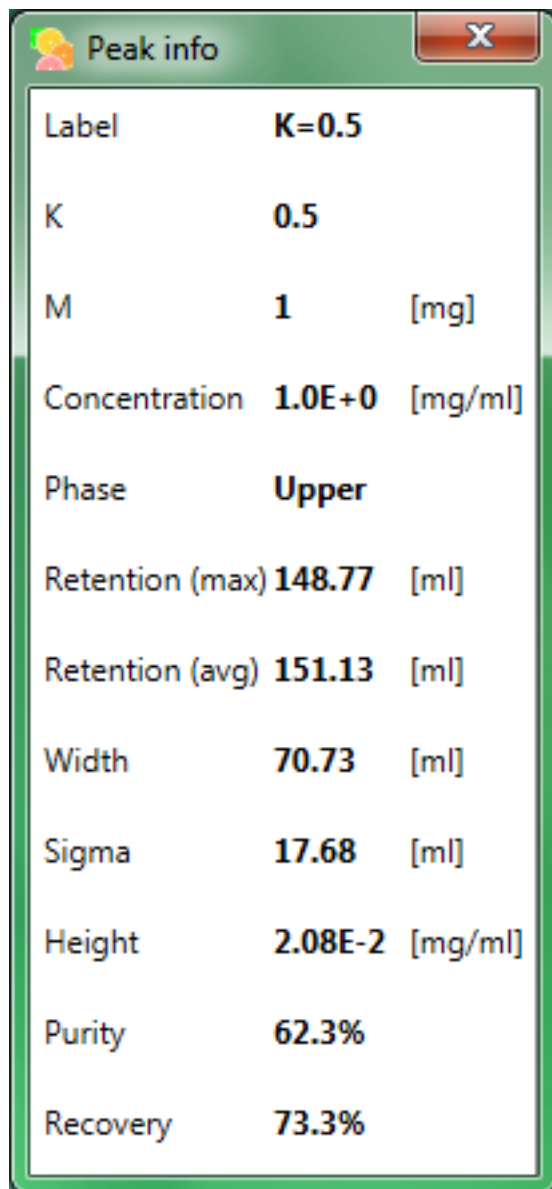
This view shows a graphical output of the model results, in this case showing the eluted upper phase content. For the probabilistic model an additional unit density graph is displayed at the top of the screen.

The chromatogram view is highly customisable, using the View menu (see the Menu section).

Peak information can be displayed by selecting a single peak, or by selecting multiple peaks (using the Shift key).

Peak information

The peak information window shows key properties of each component / peak.



The image shows a software window titled "Peak info" with a close button (X) in the top right corner. The window contains a list of peak properties and their values. The properties are listed on the left, and the values are on the right. Some values include units in brackets.

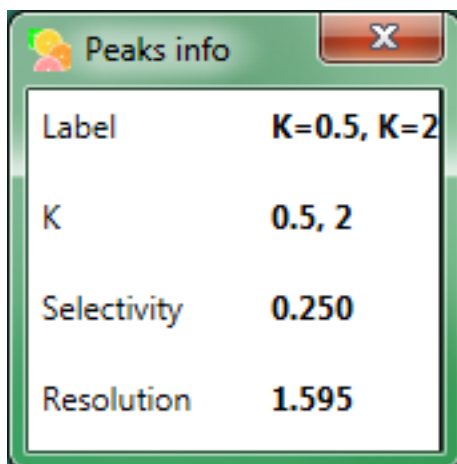
Label	K=0.5	
K	0.5	
M	1	[mg]
Concentration	1.0E+0	[mg/ml]
Phase	Upper	
Retention (max)	148.77	[ml]
Retention (avg)	151.13	[ml]
Width	70.73	[ml]
Sigma	17.68	[ml]
Height	2.08E-2	[mg/ml]
Purity	62.3%	
Recovery	73.3%	

The values shown are:

- Label: The component label
- K: K-value of sample component
- M: Mass of sample component
- Concentration: Sample component concentration
- Upper / Lower: The phase the component eluted in (a '-' symbol indicates component not eluted)
- Retention: The retention / elution time or peak position (max: using peak maximum; avg: using average over total peak).
- Width: Peak width
- Sigma: The peak σ value (relates to peak width)
- Height: Peak height or maximum concentration
- Purity: Purity of eluted component (cut off at concentration = 0.1%)
- Recovery: Recovery of eluted component (cut off at concentration = 0.1%)

Information for two peaks

After selecting a component peak, if a second peak is selected while holding the Shift key, the resolution between eluted peaks is calculated.



The image shows a software dialog box titled "Peaks info" with a close button (X) in the top right corner. The dialog contains a table with four rows of data:

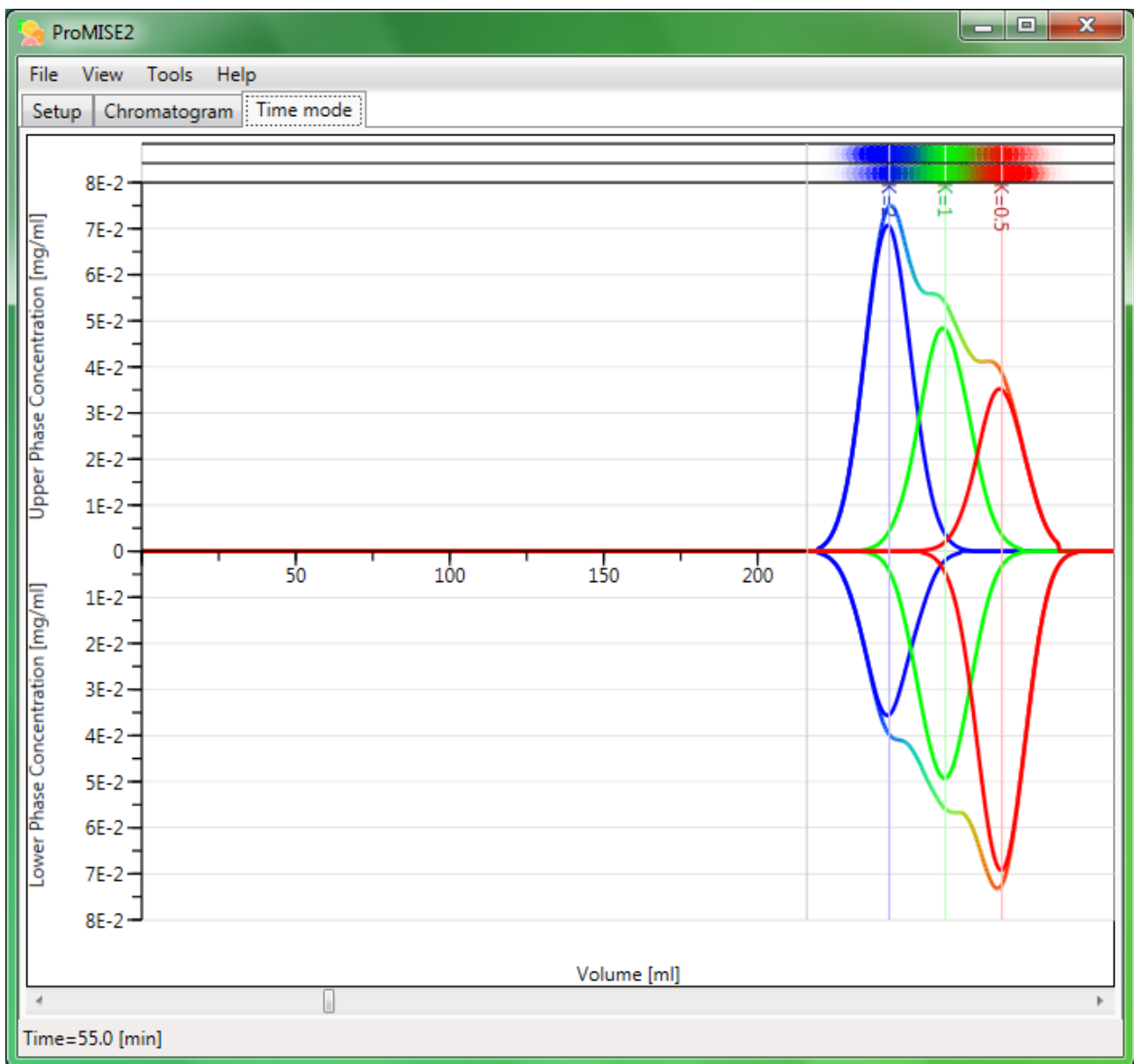
Label	K=0.5, K=2
K	0.5, 2
Selectivity	0.250
Resolution	1.595

The values shown are:

- Label: The labels of the selected components
- K: The K-values of the selected components
- Selectivity: The selectivity calculated between the K-values of the selected components
- Resolution: The resolution between eluted peaks

Time mode chromatogram view

Selecting the Time mode tab will show the time mode chromatogram view. This is an interactive view, allowing appreciating the chromatography process as the components travel through the column and separate.



Using the scrollbar at the bottom of the screen, any point in the chromatography process between injection and elution can be viewed.

Report window

Main parameters

Profile	CCC	Uf	0.5	[0.1]	Inject phase	Upper
Model	Probabilistic	Lf	0.5	[0.1]	Inject volume	1 [ml]
Run mode	Upper phase	Flow parameters			Inject position	0 [0.1]
K definition	Upper/Lower	Fu	1	[ml/min]	Model parameters	
Column parameters		Inject parameters			Rotational speed	1 [1/min]
Vc	100 [ml]	Inject mode	Instant		Efficiency	1 [0.1]

Output parameters

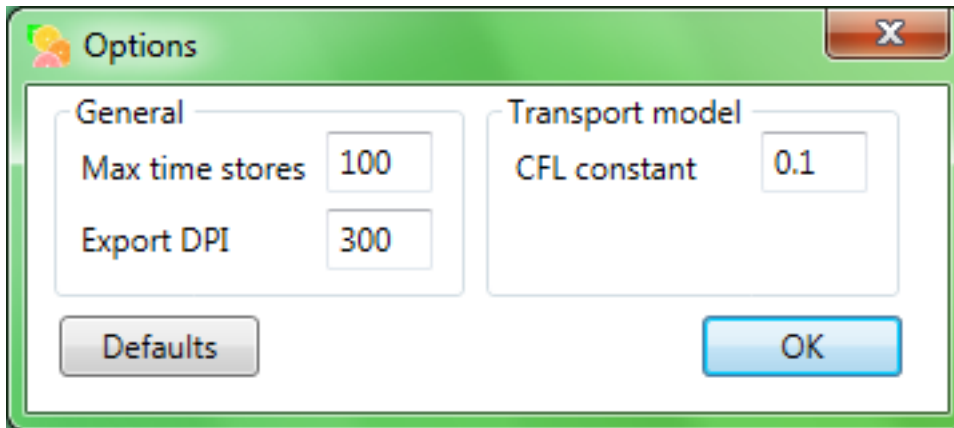
Label	K	M [mg]	Con [mg/ml]	Phase	Ret (max) [ml]	Ret (avg) [ml]	Width [ml]	Sigma [ml]	Height [mg/ml]	Purity	Recovery	Resolution
K=0.5	0.5	1	1.0E+0	Upper	148.77	151.13	70.73	17.68	2.08E-2	62.3%	73.3%	
K=1	1	1	1.0E+0	Upper	98.35	100.02	40.41	10.1	3.65E-2	48.5%	0.0%	0.9074
K=2	2	1	1.0E+0	Upper	73.39	74.56	24.88	6.22	5.78E-2	66.3%	20.3%	0.7646

Copy to clipboard

The report window shows a report of the model input and output parameters. The Copy to clipboard button copies the report content to the clipboard as text.

Options window

The options window is accessed from the main menu: Tools -> Options. Various global settings can be set here which are stored. Use caution changing these. Use the Defaults button to restore default values.



General

- Max time stores: The number of time store point for time mode chromatogram view (default: 100)
- Export DPI: The DPI used when exporting an image (default: 300)

Transport model

- CFL constant: the stability condition constant (default: 0.1)

Menu

- **File**
 - **Clear** : Clear all input parameters
 - **Load** : Open existing input parameters
 - **Save As** : Save input parameters
 - **Export data** : Export data in (text based) .CSV format (for spreadsheet applications)
 - **Export image** : Export chromatogram image
 - **Show report** : Show report window of model input and output parameters
 - **Print Preview** : Open Print preview window to print chromatogram and report
 - **Print** : Open Print dialog to print chromatogram and report
 - **Exit** : Exit application

- **View**
 - **Phases** : How sample concentrations in upper / lower phase are displayed
 - **Upper/Lower Time** : Upper / Lower phase on same scale
 - **Upper/Lower** : Upper / Lower phase separately
 - **All** : Upper / Lower phase combined
 - **Upper** : Only upper phase
 - **Lower** : Only lower phase

 - **Peaks**
 - **Peaks** : Component peaks separately
 - **Peaks & Sum** : Component peaks + sum of all component peaks
 - **Sum** : Sum of all component peaks
 - **Totals (Intermittent)** : Show accumulated totals (Intermittent mode only)
 - **Units (Probabilistic)** : Show probabilistic units (probabilistic model only)

 - **X Scale**
 - **Steps** : Set units to steps
 - **Volume** : Set units to volume
 - **Time** : Set units to time
 - **Normalised** : Normalised to system volume
 - **ReS** : Reciprocal Symmetry Plots (K-value) scale
 - **Sync scales** : Synchronise phase scales

 - **Y Scale**
 - **Automatic** : Automatic scale according to maximum concentration
 - **Normalised** : Each component peak normalised
 - **Absolute** : Absolute concentration scale with maximum 1
 - **Logarithmic** : Use logarithmic scale

- **Tools**
 - **Options** : Open options window

- **Help**
 - **Check for updates** : Check if a newer version of the software exists
 - **Stats** : Show model time statistics
 - **About** : Show about window