

Getting started with Simulis® Thermodynamics

Use Case 4: Calculating thermodynamic properties on a
pure component or on a mixture

Software & Services In Process Simulation

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ProSim

Introduction

Calculation of Thermodynamic properties and fluid phase equilibria can be performed from Simulis Thermodynamics. The user can also edit tables and graphs and export them to other applications.

This document presents in details the different steps to follow in order to perform these types of calculation.

The following steps are described in this document

-  Step 1: Select the components
-  Step 2: Calculate properties of a pure component
-  Step 3: Calculate properties of a mixture
-  Step 4: Calculate fluid phase equilibria

The example is based on a mixture of Benzene, Toluene and o-Xylene.

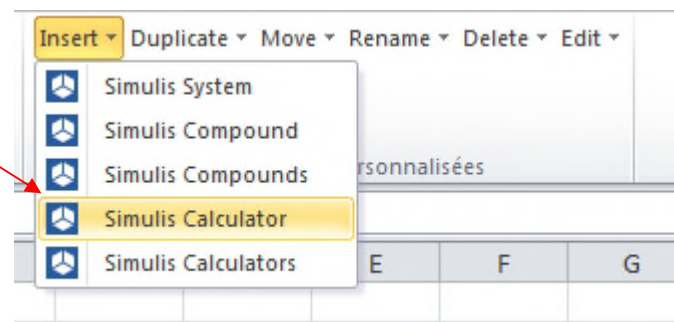
Before studying this chapter, it is recommended to consult “Getting Started with Simulis Thermodynamics: Use Case 1” that explains the method to select components and configure a thermodynamic profile.

Step 1: Select the components

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- If you are using Simulis Thermodynamics in Excel:

Create the calculator object in a spreadsheet



- If you are using Simulis Thermodynamics within another ProSim environment (ProSimPlus, BatchReactor, BatchColumn etc...):

Click on the thermodynamic icon to open the calculator editor:

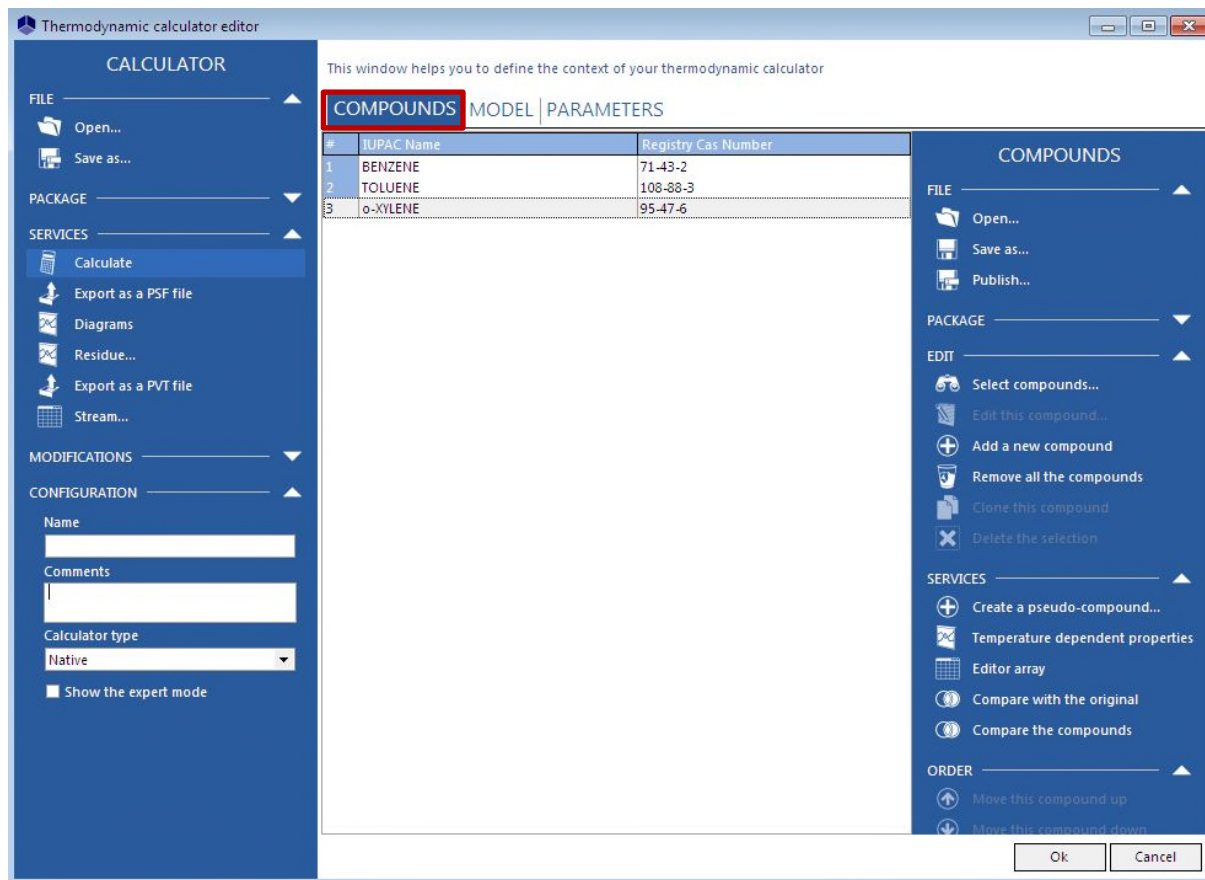


or



Simulis Thermodynamics is a « software component » that you can integrate into different applications: ProSim software, Excel, Matlab, your own software, etc...

Step 1: Select the components



Select the following components:

- Benzene (CAS 71-43-2)
- Toluene (CAS 108-88-3)
- o-Xylene (CAS 95-47-6)

(Refer to “Getting Started with Simulis

Thermodynamic: Use case 1” for details on these operations)

Step 2: Calculate properties of a pure component

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The screenshot shows two windows from the ProSim software. The top window is the 'Thermodynamic calculator editor' with a 'CALCULATOR' tab. It contains a table of compounds:

#	IUPAC Name	Registry Cas Number
1	BENZENE	71-43-2
2	TOLUENE	108-88-3
3	o-XYLENE	95-47-6

A red arrow points from the 'o-XYLENE' row to the 'Compound Editor' window below. The 'Compound Editor' window shows the details for 'o-XYLENE' (ID: 48C4832B-88B1-4ABE-B8FF-C4D5928B5A8C). It includes a list of properties to be calculated, such as Identification, Group contribution model, Atomic, Phase change, Combustion, security, toxicity, Condensed phase, Phase thermochemistry, Interaction, gas phase reaction, User properties, PPC-SAFT, NRTL-SAC, and Temperature dependent properties. A 3D ball-and-stick model of the o-xylene molecule is displayed in the center.

Double click on the component you want to analyze (in this example, the o-Xylene).

The component description window opens. It presents all the properties that are available in the database for this component.

You can expand the different categories in order to view the details of the properties.

Step 2: Calculate properties of a pure component

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Expand the folder “*Temperature Dependent Properties*”. When you select a temperature dependent property, a graph appears on the right side of the window.

The screenshot shows the 'Compound Editor' window for 'o-XYLENE'. The left sidebar contains 'FILE', 'TOOLS', 'VIEW', and 'MODIFICATIONS' menus. The main panel displays a tree of properties under 'Temperature dependent prop...'. 'Liquid viscosity' is selected, showing its correlation equation and coefficients. On the right, a graph titled 'Liquid viscosity (Pa.s)' plots viscosity against temperature (K). Below the graph, a 'Tools' panel allows for parameter adjustments and visualization options.

Property	Value
Correlation	Equation # 101
TMin	247,98 K
TMax	418,1 K
Coef A	-15,489
Coef B	1393,5
Coef C	0,63711
Coef D	0
Coef E	0
Coef F	0

Tools panel details:

- Temperature Min: 247,98 K
- Temperature Max: 418,1 K
- Points: 20
- Refresh button
- Temperature: 247,98 K
- Property: 1,73459E-003 Pa.s
- Buttons: Copy, Print, Regression

Units can be modified.

The property can be visualized as a graph or a grid of values. The formulation can also be displayed.

Scales can be changed.

The calculation parameters are defined here. You can change the units, the number of steps etc... After each change, click on “*Refresh*” to obtain the new values and charts.

Click on “*OK*” or “*Cancel*” to go back to the thermodynamic calculator editor.

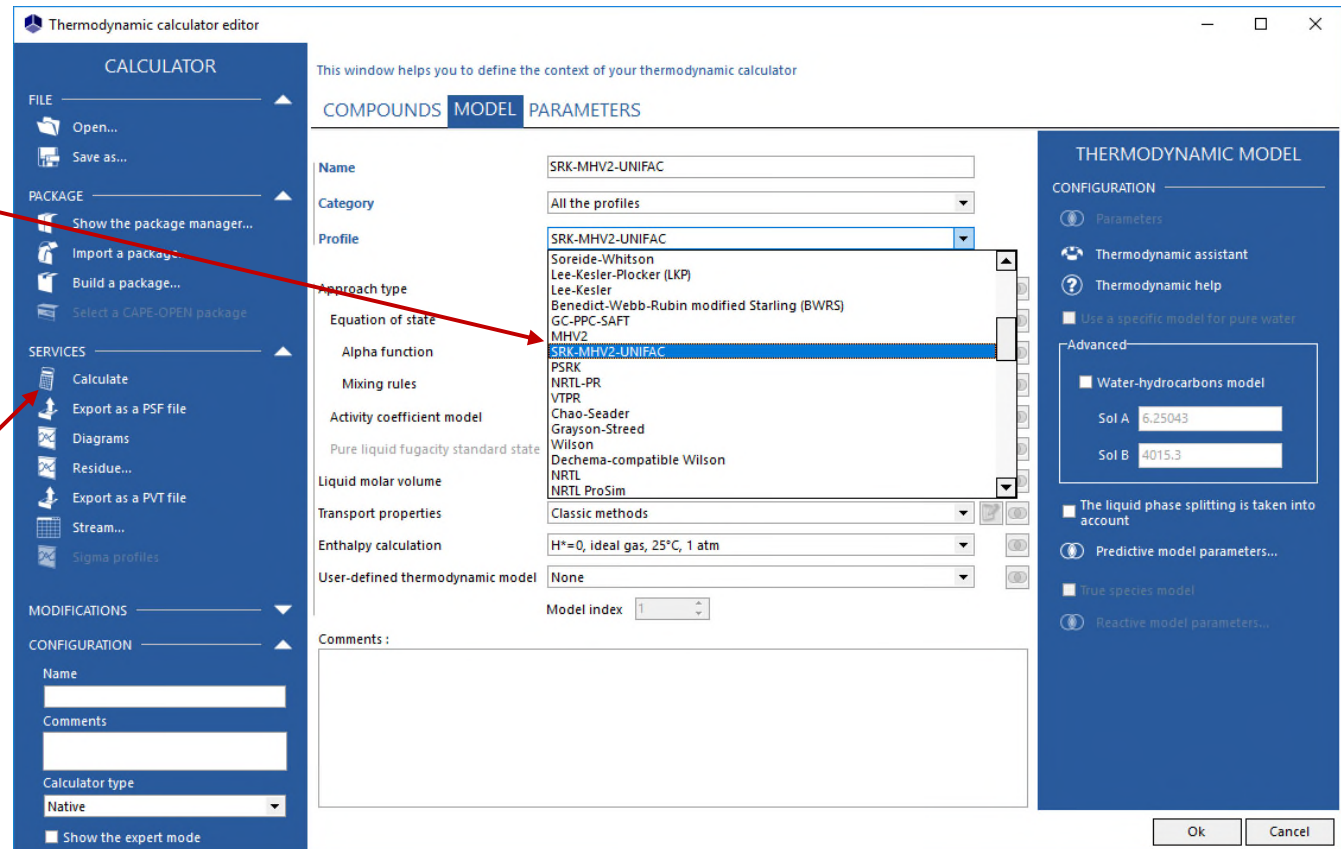
Step 3: Calculate properties of a mixture

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In order to calculate thermodynamic properties of a mixture, it is necessary to configure the thermodynamic profile.

1- For the mixture used in this example, select the **SRK-MHV2-UNIFAC** thermodynamic profile in the pull-down menu.

2- Click on **"Calculate"** to open the **Calculation service window**.



Step 3: Calculate properties of a mixture

1- You can chose the type of calculation to run (calculation of mixture properties or fluid phase equilibria). Select “*ThermoPhysical properties*”.

Calculation service

SESSSIONS

+ Add a new session...

- Delete the current session

Session list

New session

Calculate the current session

Calculate all the sessions

UNIT SYSTEM (RESULTS)

For the calculation conditions

For the calculated properties

MODIFICATIONS

OPTIONS

Hide the constant results

Automatically plot the results

HELP

Help

This window helps you to define the context of your calculations

Type of calculation: ThermoPhysical properties

Session name: New session

Physical state: Automatically determined

System: Vapor - Liquid

Property	Unit	Initial	Final	Step	Points
Pressure	atm	1	1	0	1
Temperature	K	298.15	298.15	0	1

Values: Fractions (selected), Quantities

Type: Molar (selected), Mass

Total: 0 kmol

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	BENZENE	0	0	0	1
<input type="checkbox"/>	TOLUENE	0	0	0	1
<input checked="" type="checkbox"/>	p-XYLENE	Auto	Auto	Auto	Auto

Results type: Molar (selected), Mass

Show the error messages

Same compositions whatever the calculation type

To calculate:

Quit

2- Select the properties to calculate (in this example, “*Dynamic viscosity*”).

Step 3: Calculate properties of a mixture

1- Specify the operating conditions:

- Pressure: 1 atm.
- Temperature: from 20°C to 80°C with a step of 1°C.
- Mixture composition: 50% mol of benzene, 10% mol of toluene, “auto” (in order to get a global composition of 100%) for o-Xylene.

2- You can change the unit system that is used for the presentation of the results.

3- Select the option “Automatically plot the results”.

Calculation service

Calculation service

SESSIONS

- Add a new session...
- Delete the current session

Session list

- New session

UNIT SYSTEM (RESULTS)

- For the calculation conditions
- For the calculated properties

MODIFICATIONS

OPTIONS

- Hide the constant results
- ☒ Automatically plot the results

HELP

- Help

This window helps you to define the context of your calculations

Type of calculation: ThermoPhysical properties

Session name: New session

☐ Allow the calculation of derivatives

Physical state: Automatically determined

System: Vapor - Liquid

Property	Unit	Initial	Final	Step	Points
Pressure	atm	1	1	0	1
Temperature	°C	20	80	1	61

Values: Fractions (selected), Quantities

Type: Molar (selected), Mass

Total: 0 kmol

Au...	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	BENZENE	0.5	0.5	0	1
<input type="checkbox"/>	TOLUENE	0.1	0.1	0	1
<input checked="" type="checkbox"/>	o-XYLENE	Auto	Auto	Auto	Auto

Mixture compositions

Results type: Molar (selected), Mass

☐ Show the error messages

☐ Same compositions whatever the calculation type

To calculate:

Quit

Step 3: Calculate properties of a mixture

Click on “**Calculate the current session**”.

Click on « **Add a new session** » if you want to run multiple sessions in parallel.

Calculation service

Calculation service

SESSIONS

- + Add a new session...
- 🗑 Delete the current session

Session list

- New session

Calculate the current session

Calculate all the sessions

UNIT SYSTEM (RESULTS)

- 📄 For the calculation conditions
- 📄 For the calculated properties

MODIFICATIONS

OPTIONS

- Hide the constant results
- ☑ Automatically plot the results

HELP

- 🔍 Help

This window helps you to define the context of your calculations

Type of calculation: ThermoPhysical properties

Session name: New session

Data Results

☐ Allow the calculation of derivatives

Physical state: Automatically determined

System: Vapor - Liquid

Property	Unit	Initial	Final	Step	Points
Pressure	atm	1	1	0	1
Temperature	°C	20	80	1	61

Values: Fractions Quantities

Type: Molar Mass

Total: 0 kmol

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	BENZENE	0.5	0.5	0	1
<input type="checkbox"/>	TOLUENE	0.1	0.1	0	1
<input checked="" type="checkbox"/>	o-XYLENE	Auto	Auto	Auto	Auto

Results type: Molar Mass

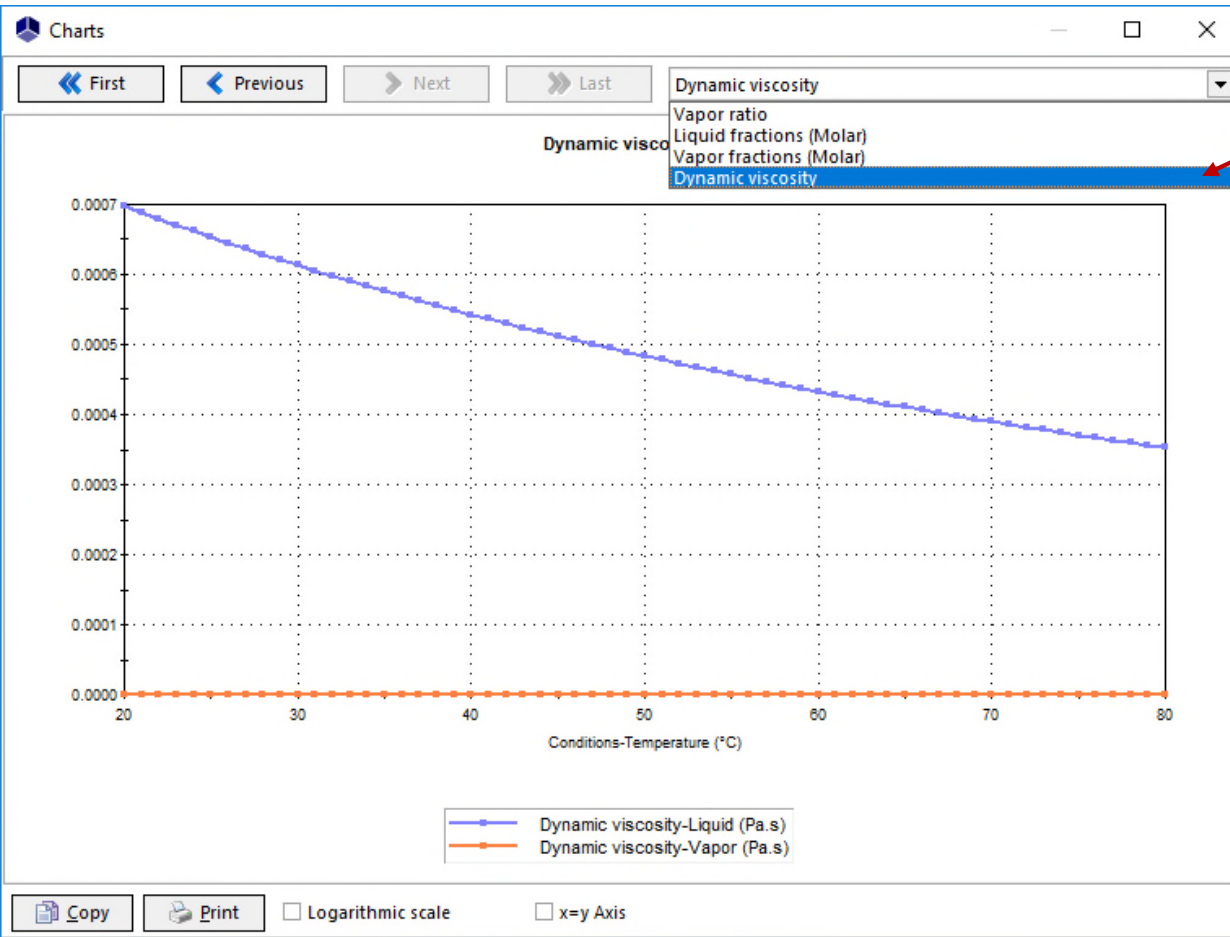
☐ Show the error messages

☐ Same compositions whatever the calculation type

To calculate:

Quit

Step 3: Calculate properties of a mixture



If the option **“Automatically plot the results”** has been checked, this window appears. Several graphs are available, select **“Dynamic Viscosity”** from the drop-down list.

Graph can be copied into other documents.

Step 3: Calculate properties of a mixture



The « *Export to Excel* » button is active if you are using Simulis from another application than Excel.

Results are tabulated in the “*Results*” tab.

The values of liquid and vapor dynamic viscosity of the mixture are displayed in this column.

Click on “*Plot the points*” if you want to manually plot the results.

You can copy the results into other applications.

Calculation service

This window helps you to define the context of your calculations

Type of calculation: ThermoPhysical properties Session name: New session

Data Results

Results

Conditions		or-Liquid k-values			Dynamic viscosity	
Pressure	Temperature	ZENE	TOLUENE	o-XYLENE	Liquid	Vapor
1 atm	20 °C	000	0.00000	0.00000	0.000697605 Pa.s	0.000000 Pa.s
1 atm	21 °C	000	0.00000	0.00000	0.000688419 Pa.s	0.000000 Pa.s
1 atm	22 °C	000	0.00000	0.00000	0.000679408 Pa.s	0.000000 Pa.s
1 atm	23 °C	000	0.00000	0.00000	0.000670566 Pa.s	0.000000 Pa.s
1 atm	24 °C	000	0.00000	0.00000	0.000661891 Pa.s	0.000000 Pa.s
1 atm	25 °C	000	0.00000	0.00000	0.000653377 Pa.s	0.000000 Pa.s
1 atm	26 °C	000	0.00000	0.00000	0.000645021 Pa.s	0.000000 Pa.s
1 atm	27 °C	000	0.00000	0.00000	0.00063682 Pa.s	0.000000 Pa.s
1 atm	28 °C	000	0.00000	0.00000	0.000628769 Pa.s	0.000000 Pa.s
1 atm	29 °C	000	0.00000	0.00000	0.000620864 Pa.s	0.000000 Pa.s
1 atm	30 °C	000	0.00000	0.00000	0.000613104 Pa.s	0.000000 Pa.s
1 atm	31 °C	000	0.00000	0.00000	0.000605483 Pa.s	0.000000 Pa.s
1 atm	32 °C	000	0.00000	0.00000	0.000597999 Pa.s	0.000000 Pa.s
1 atm	33 °C	000	0.00000	0.00000	0.000590648 Pa.s	0.000000 Pa.s
1 atm	34 °C	000	0.00000	0.00000	0.000583428 Pa.s	0.000000 Pa.s
1 atm	35 °C	000	0.00000	0.00000	0.000576336 Pa.s	0.000000 Pa.s
1 atm	36 °C	000	0.00000	0.00000	0.000569367 Pa.s	0.000000 Pa.s
1 atm	37 °C	000	0.00000	0.00000	0.000562521 Pa.s	0.000000 Pa.s
1 atm	38 °C	000	0.00000	0.00000	0.000555793 Pa.s	0.000000 Pa.s
1 atm	39 °C	000	0.00000	0.00000	0.000549182 Pa.s	0.000000 Pa.s
1 atm	40 °C	000	0.00000	0.00000	0.000542684 Pa.s	0.000000 Pa.s

Results visibility... Copy the results Export to excel... Plot the points

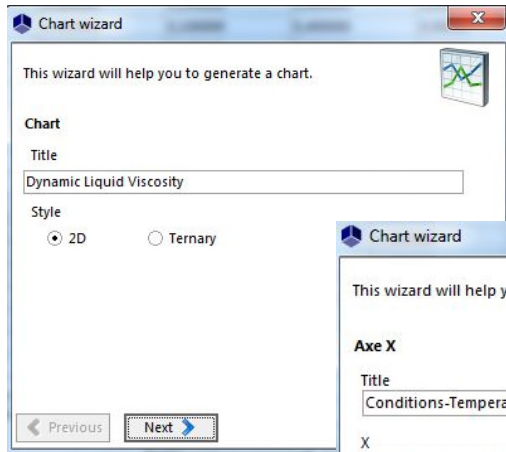
☐ Show the error messages ☐ Same compositions whatever the calculation type

To calculate:

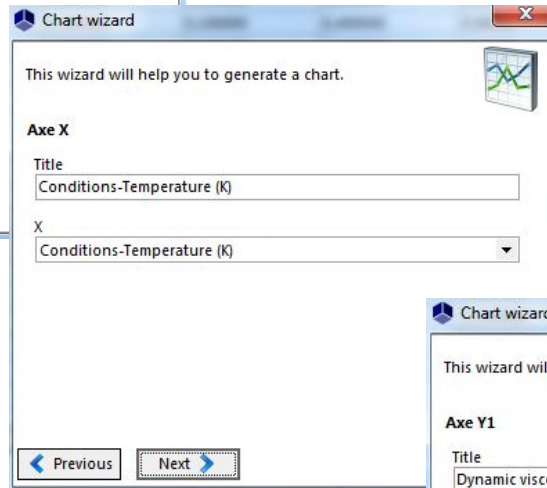
Quit

Step 3: Calculate properties of a mixture

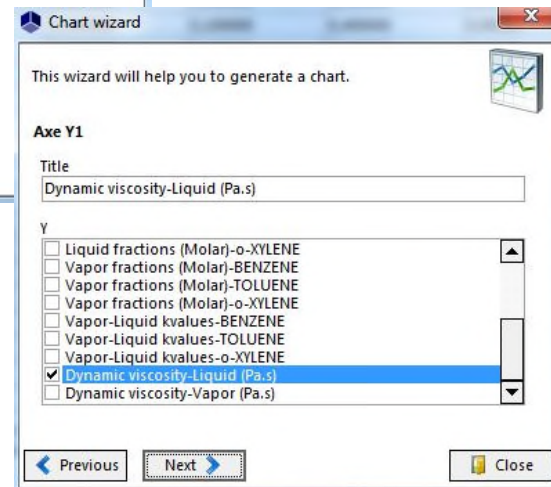
If you want to plot the graph manually (after selecting “*Plot the points*”), follow the instructions from the Chart wizard:



1- Specify the title of the chart.



2- Define the X-axis (the temperature in this example).



3- Define the Y-axis (the dynamic liquid viscosity in this example).



You can plot multiple curves on the same graph by selecting several properties in the chart wizard.

Step 4: Calculate fluid phase equilibria

In order to calculate fluid phase equilibria, go back to the *Calculation service* window.

1- Select “*Equilibria*” from the drop-down list.

The screenshot shows the 'Calculation service' window. On the left is a sidebar with sections: SESSIONS, UNIT SYSTEM (RESULTS), MODIFICATIONS, and HELP. The main area has a title bar and a description: 'This window helps you to define the context of your calculations'. Below this, there's a 'Project' field, a 'Type of calculation' dropdown menu, and a 'Session name' field. The 'Type of calculation' dropdown is open, showing a list of options. A red box highlights 'Flash at given temperature and pressure' under the 'Vapor - Liquid' category. A red arrow points from the text '1- Select “Equilibria” from the drop-down list.’ to the 'Equilibria' option in the dropdown menu. Another red arrow points from the text '2- Here are displayed the different types of flash that can be calculated. Select “Flash at given temperature and pressure”.' to the highlighted option. The right side of the window shows a table for 'Property' with columns: Property, Unit, Initial, Final, Step, Points. Below this is a 'Values' section with radio buttons for 'Fractions' and 'Quantities', and a 'Type' section with radio buttons for 'Molar' and 'Mass'. There is also a 'Mixture compositions' table with columns: Auto, Compound, Initial, Final, Step, Points. The table lists BENZENE, TOLUENE, and o-XYLENE. At the bottom, there's a 'Results type' section with radio buttons for 'Molar' and 'Mass', and an 'Automatic initialization' checkbox. A 'Compound' dropdown menu is also present. A 'Quit' button is at the bottom right.

Calculation service

This window helps you to define the context of your calculations

Project: C:\dde

Type of calculation: Equilibria

Session name: New session

Vapor - Liquid

- Flash at given temperature and pressure
- Flash at given temperature and volume
- Flash at given pressure and volume
- Flash at given enthalpy and temperature
- Flash at given enthalpy and pressure
- Flash at given enthalpy and volume
- Flash at given enthalpy and energy
- Flash at given enthalpy and entropy
- Flash at given entropy and temperature
- Flash at given entropy and pressure
- Flash at given entropy and volume
- Flash at given entropy and energy
- Flash at given energy and temperature
- Flash at given energy and pressure
- Flash at given energy and volume
- Henry constant

Liquid - Liquid

- Flash at given temperature and pressure

Vapor - Liquid - Liquid

- Bubble temperatures
- Flash at given temperature and pressure
- Flash at given enthalpy and pressure

Property table:

Property	Unit	Initial	Final	Step	Points
Pressure	atm	1	1	0	1

Values:

☒ Fractions ☐ Quantities Total: 0 kmol

Type:

☒ Molar ☐ Mass

Mixture compositions:

Auto	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	BENZENE	0	0	0	1
<input type="checkbox"/>	TOLUENE	0	0	0	1
<input checked="" type="checkbox"/>	o-XYLENE	Auto	Auto	Auto	Auto

Results type:

☒ Molar ☐ Mass

☐ Automatic initialization

Compound:

Show the error messages

To calculate:

Quit

2- Here are displayed the different types of flash that can be calculated. Select “Flash at given temperature and pressure”.

Step 4: Calculate fluid phase equilibria

1- Specify the operating conditions:

- Pressure: 1 atm.
- Temperature: from 115°C to 130°C with a step of 1°C.
- Mixture composition: 50% mol of benzene, 10% mol of toluene, “auto” for o-Xylene.

2- Click on “Calculate the current session”.

Calculation service

SESIONS

- Add a new session...
- Delete the current session
- Calculate the current session
- Calculate all the sessions

Session list

Session name
New session

UNIT SYSTEM (RESULTS)

- For the calculation conditions
- For the calculated properties

MODIFICATIONS

- Undo
- Redo

OPTIONS

- ☐ Hide the constant results
- ☒ Automatically plot the results

HELP

- Help

This window helps you to define the context of your calculations

Project: C:\dde

Type of calculation: Equilibria

Session name: New session

Data | Results

Vapor - Liquid

- Bubble and dew temperatures
- Bubble and dew pressures
- Flash at given vaporization ratio and pressure
- Flash at given vaporization ratio and temperature
- Flash at given temperature and pressure
- Flash at given temperature and volume
- Flash at given pressure and volume
- Flash at given enthalpy and temperature
- Flash at given enthalpy and pressure
- Flash at given enthalpy and volume
- Flash at given enthalpy and energy
- Flash at given enthalpy and entropy
- Flash at given entropy and temperature
- Flash at given entropy and pressure
- Flash at given entropy and volume
- Flash at given entropy and energy
- Flash at given energy and temperature
- Flash at given energy and pressure
- Flash at given energy and volume
- Henry constant

Liquid - Liquid

- Flash at given temperature and pressure

Vapor - Liquid - Liquid

- Bubble temperatures
- Flash at given temperature and pressure
- Flash at given enthalpy and pressure

Property	Unit	Initial	Final	Step	Points
Temperature	°C	115	130	1	16
Pressure	atm	1	1	0	1

Values

☒ Fractions

☐ Quantities Total: 0 kmol

Type

☒ Molar

☐ Mass

Mixture compositions

Auto	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	BENZENE	0,1	0,1	0	1
<input type="checkbox"/>	TOLUENE	0,5	0,5	0	1
<input checked="" type="checkbox"/>	o-XYLENE	Auto	Auto	Auto	Auto

Results type

☒ Molar

☐ Mass

☐ Automatic initialization

Compound: [dropdown]

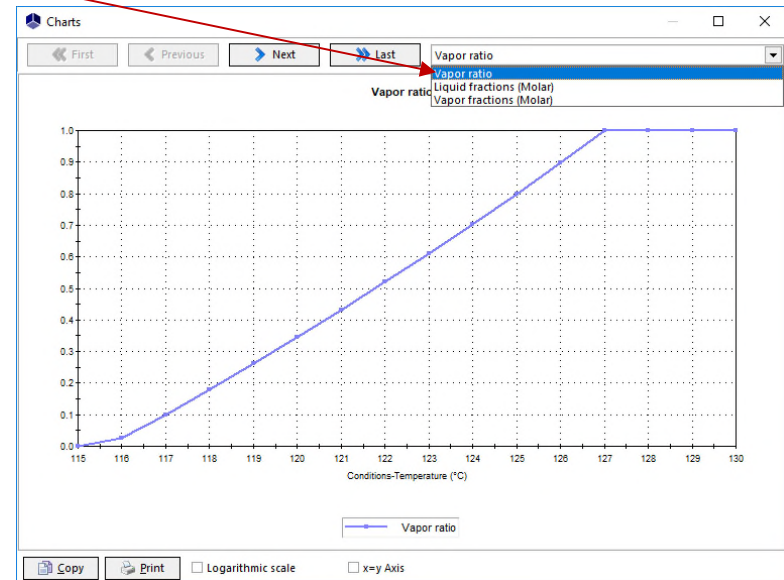
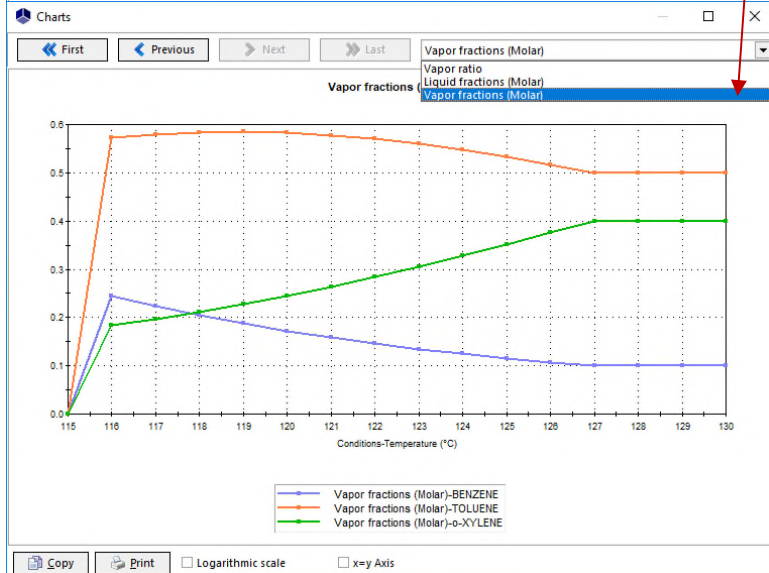
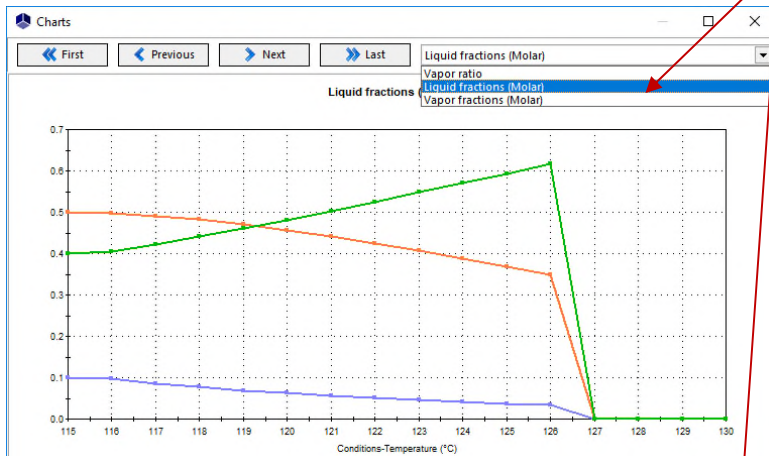
☐ Show the error messages

To calculate: [text box]

Quit

Step 4: Calculate fluid phase equilibria

If the option “*Automatically plot the results*” has been checked, you can select from the drop-down list the graph you want to display.



Step 4: Calculate fluid phase equilibria

Results are tabulated in the
“Results” tab.

Calculation service

SESIONS

+ Add a new session...

Delete the current session

Session list

New session

Calculate the current session

Calculate all the sessions

UNIT SYSTEM (RESULTS)

For the calculation conditions

For the calculated properties

MODIFICATIONS

OPTIONS

Hide the constant results

Automatically plot the results

HELP

Help

This window helps you to define the context of your calculations

Type of calculation: Equilibria

Session name: New session

Data Results

Results

Conditions		Liquid fractions (Molar)			Vapor fractions (Molar)	
Temperature	Pressure	BENZENE	TOLUENE	o-XYLENE	BENZENE	TOLUENE
115 °C	1 atm	0.100000	0.500000	0.400000	0.000000	0.000000
116 °C	1 atm	9.64164E-002	0.498179	0.405405	0.243665	0.573008
117 °C	1 atm	8.63235E-002	0.491121	0.422555	0.223078	0.579900
118 °C	1 atm	7.72966E-002	0.481739	0.440964	0.204221	0.583827
119 °C	1 atm	6.92927E-002	0.470150	0.460557	0.187138	0.584704
120 °C	1 atm	6.22374E-002	0.456564	0.481199	0.171785	0.582571
121 °C	1 atm	5.60351E-002	0.441249	0.502716	0.158046	0.577565
122 °C	1 atm	5.05800E-002	0.424505	0.524915	0.145753	0.569892
123 °C	1 atm	4.57671E-002	0.406625	0.547608	0.134722	0.559781
124 °C	1 atm	4.14988E-002	0.387878	0.570623	0.124767	0.547466
125 °C	1 atm	3.76891E-002	0.368498	0.593813	0.115714	0.533162
126 °C	1 atm	3.42642E-002	0.348681	0.617055	0.107412	0.517061
127 °C	1 atm	0.000000	0.000000	0.000000	0.100000	0.500000
128 °C	1 atm	0.000000	0.000000	0.000000	0.100000	0.500000
129 °C	1 atm	0.000000	0.000000	0.000000	0.100000	0.500000
130 °C	1 atm	0.000000	0.000000	0.000000	0.100000	0.500000

Results visibility...

Copy the results

Export to excel...

Plot the points

Show the error messages

Same compositions whatever the calculation type

To calculate:

Quit

You can copy the
results and
manually plot the
points.

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