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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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.

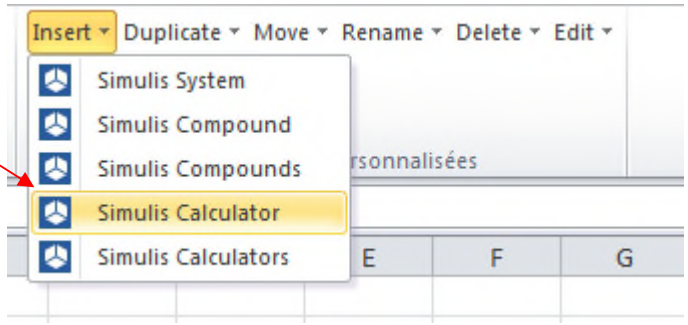
Before studying this chapter, it is recommended to consult "Getting Started with Simulis Thermodynamics: Use Case 1" that explains the method to select components and configure a thermodynamic profile.

Step 1: Select the components

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- **<u>If you are using Simulis Thermodynamics in Excel</u>:**

Create the calculator object in a spreadsheet



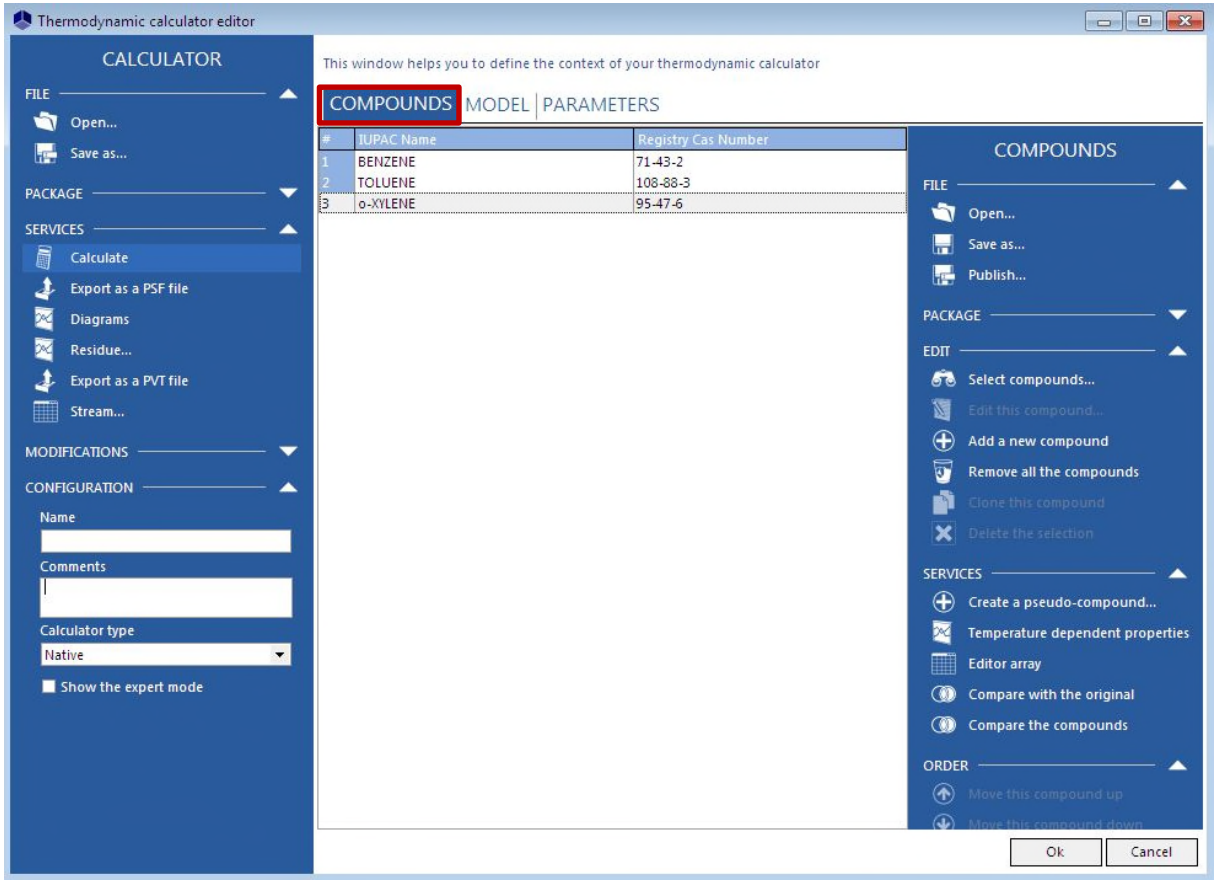
- **<u>If you are using Simulis Thermodynamics within another ProSim environment</u> (ProSimPlus, BatchReactor, BatchColumn etc…):**

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:

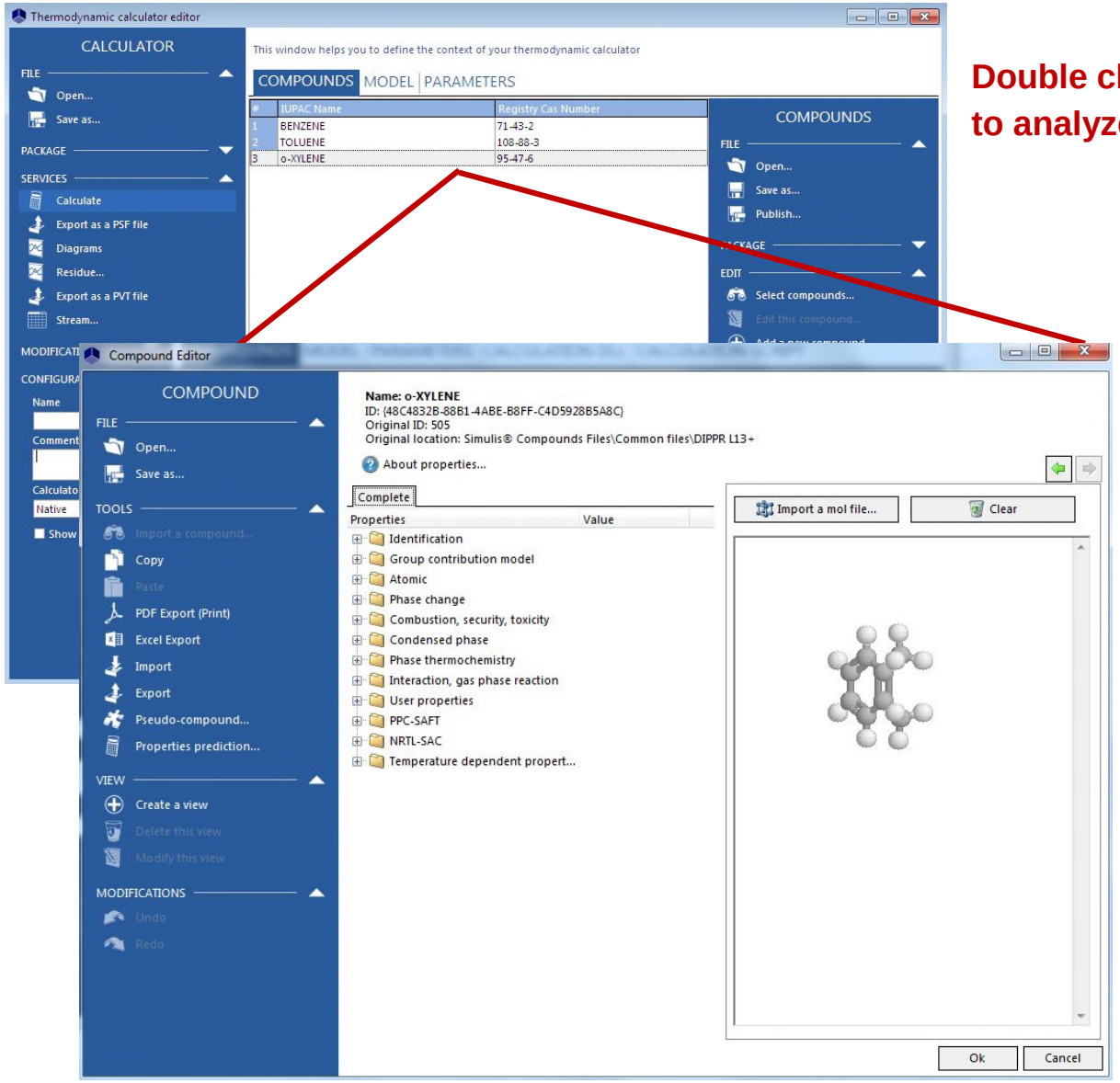
- Benzene (CAS 71-43-2)

- 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



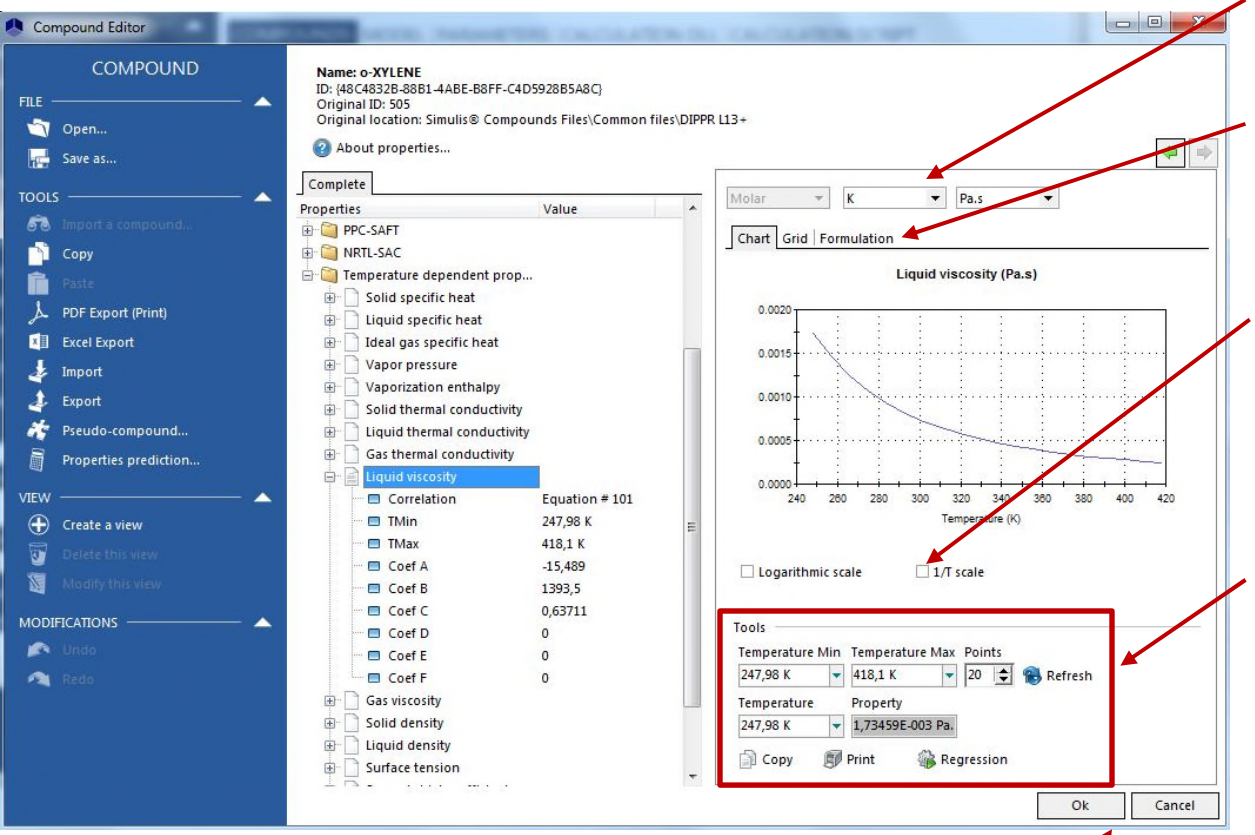
Double click on the component you want to analyze (in this example, the o-Xylene).

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

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



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.

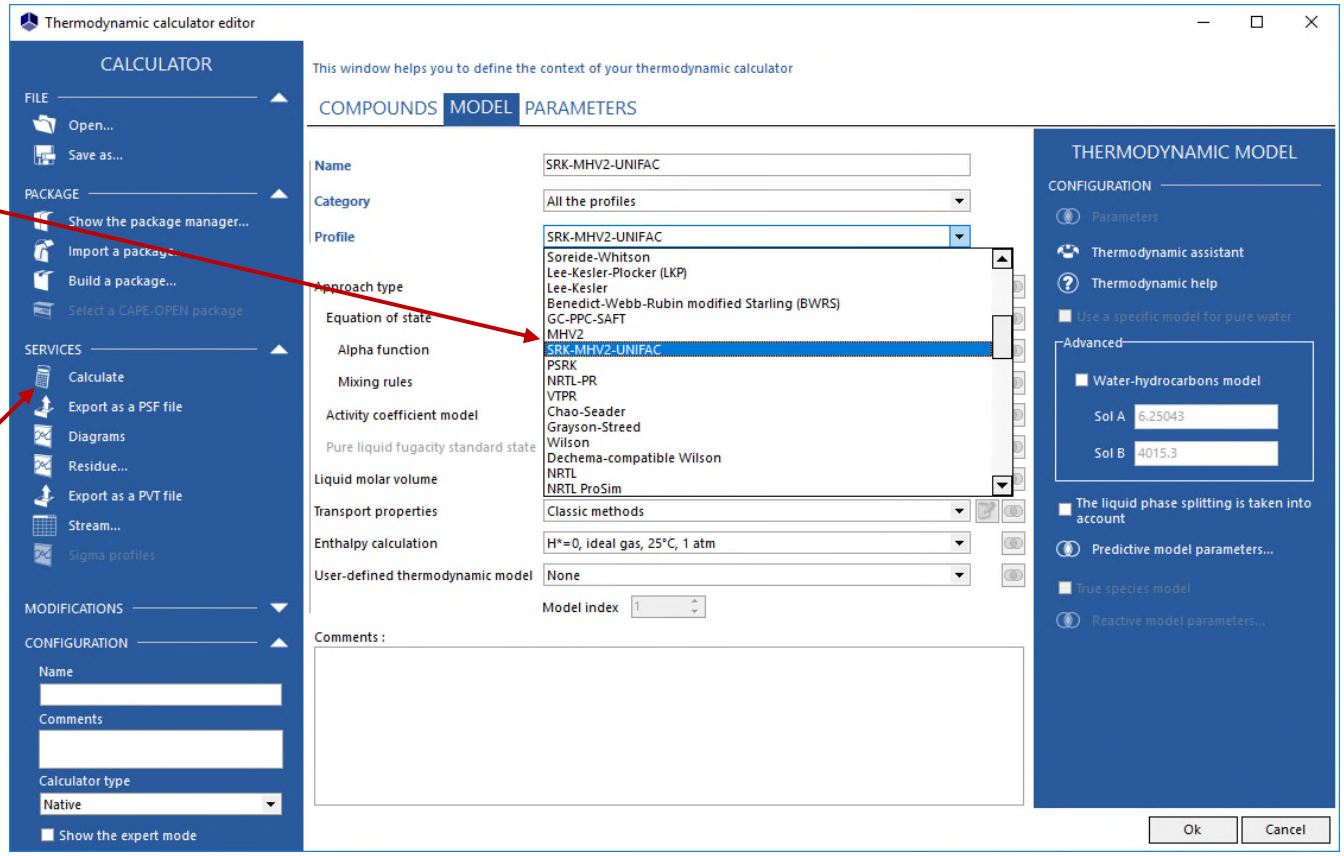
Click on "*OK*" or "*Cancel*" to go back to the thermodynamic calculator editor.

Step 3: Calculate properties of a mixture

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.

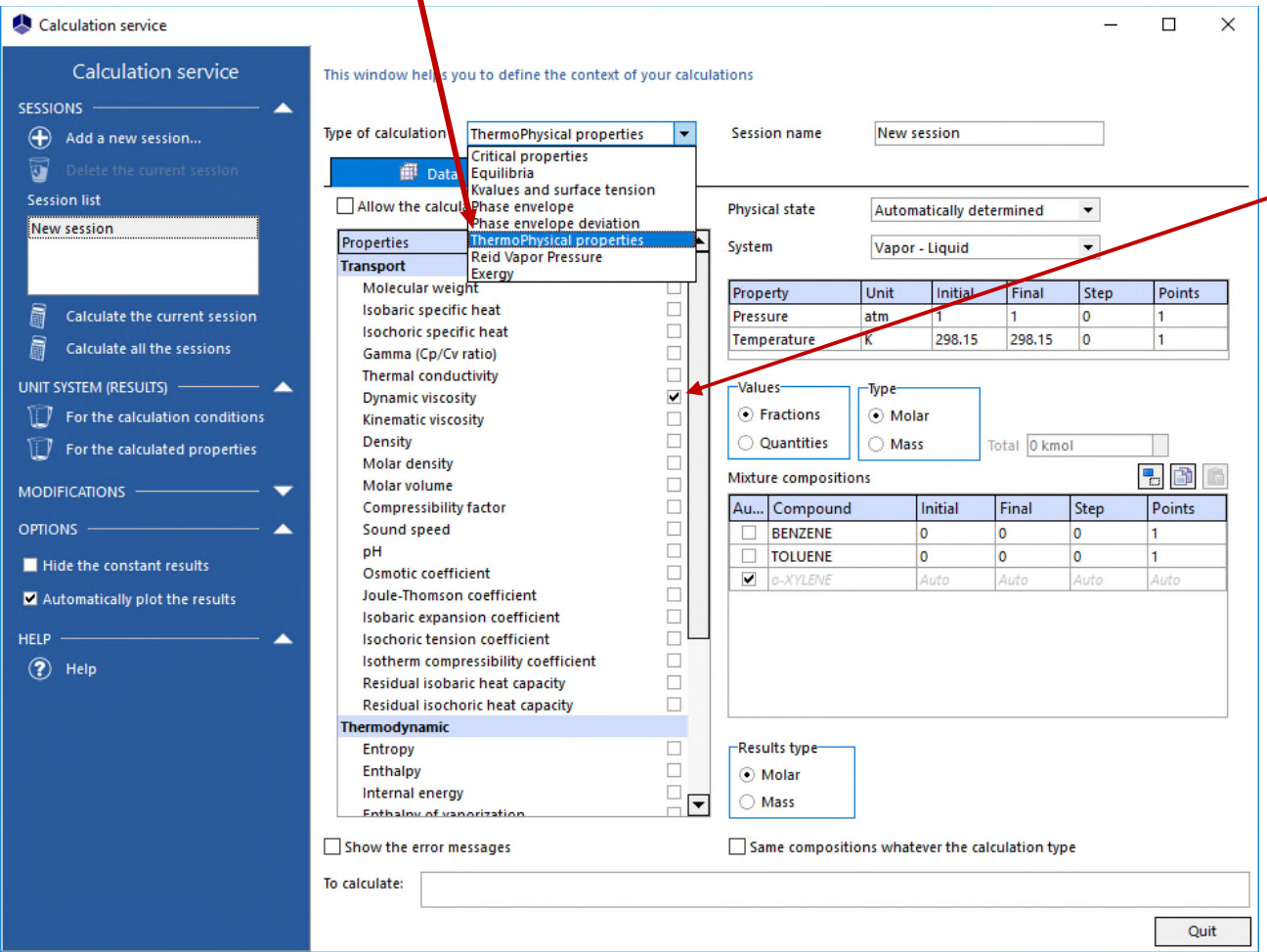
2- Click on "*Calculate*" to open the *Calculation service* window.



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*".

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



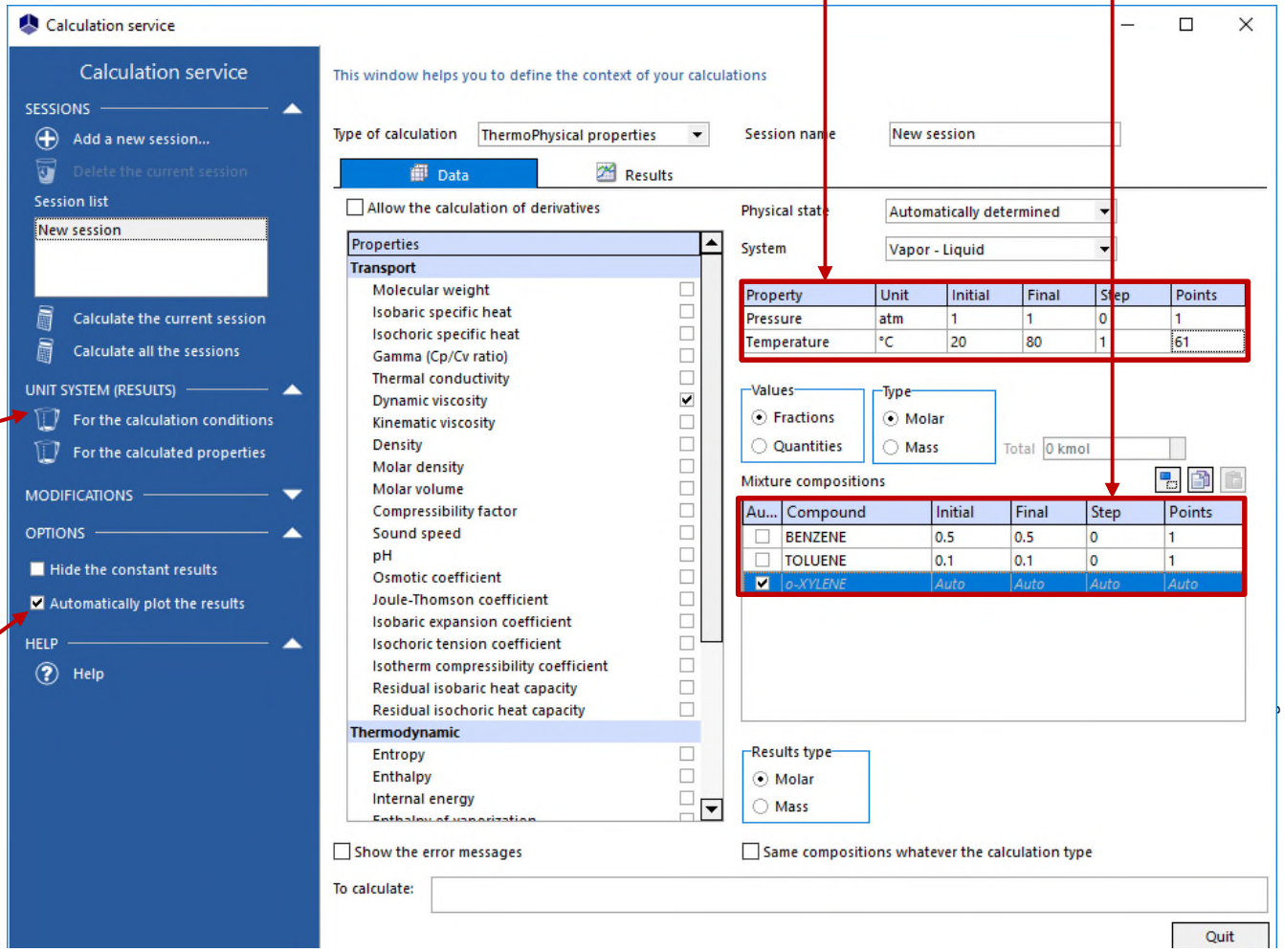
Step 3: Calculate properties of a mixture

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.

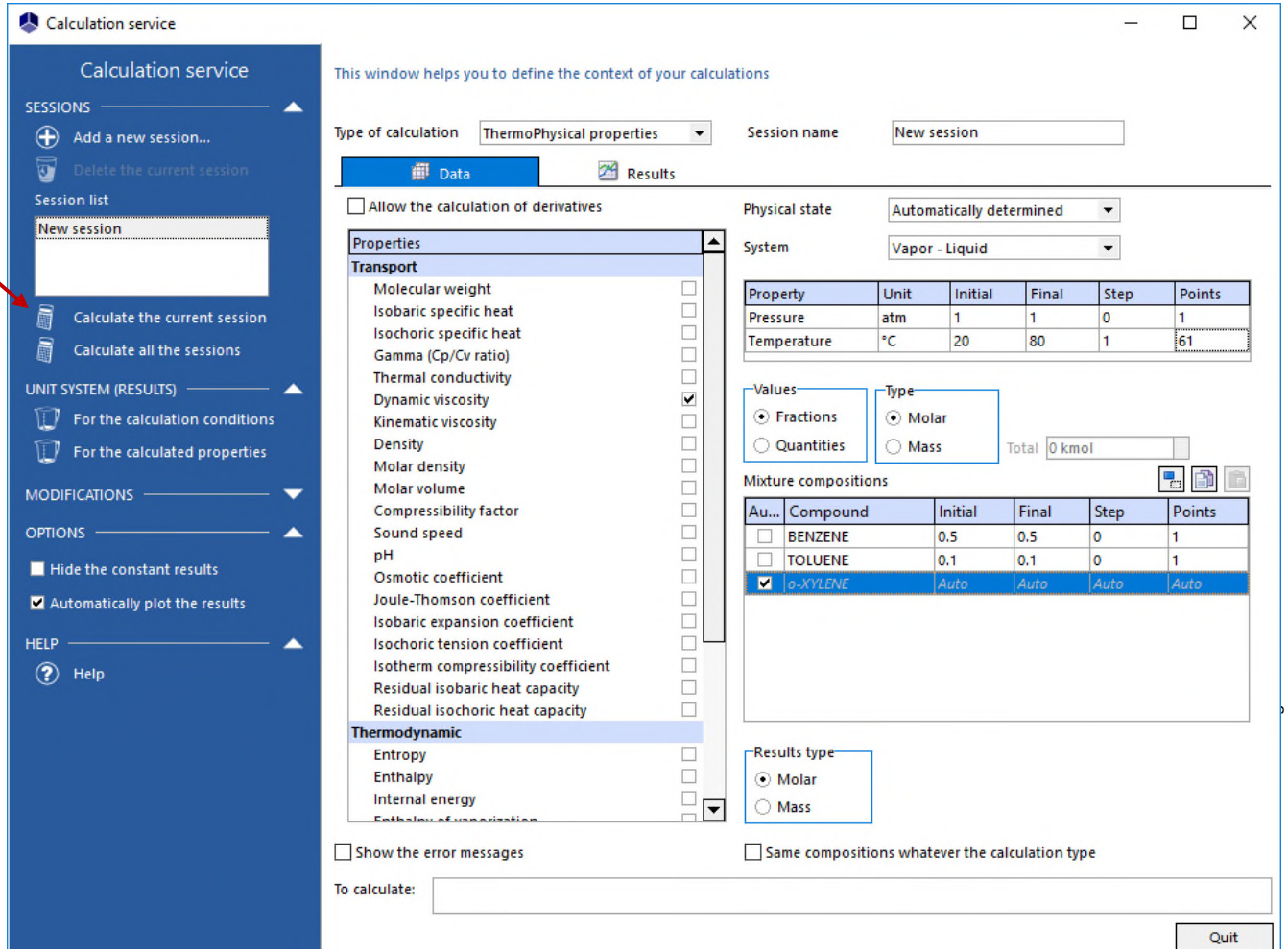
2- You can change the unit system that is used for the presentation of the results.

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



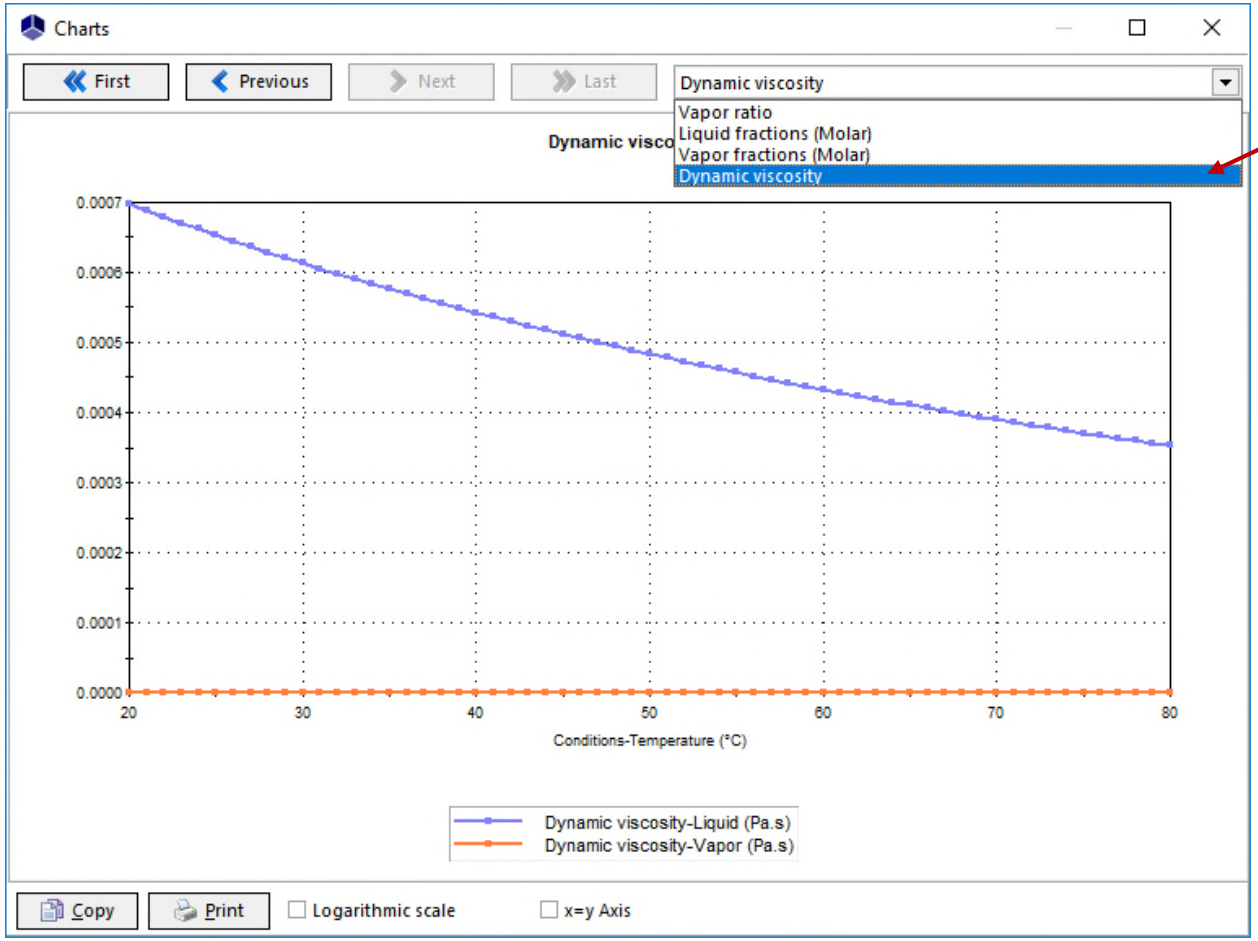
Step 3: Calculate properties of a mixture

Click on "*Calculate the current session*".



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

Step 3: Calculate properties of a mixture



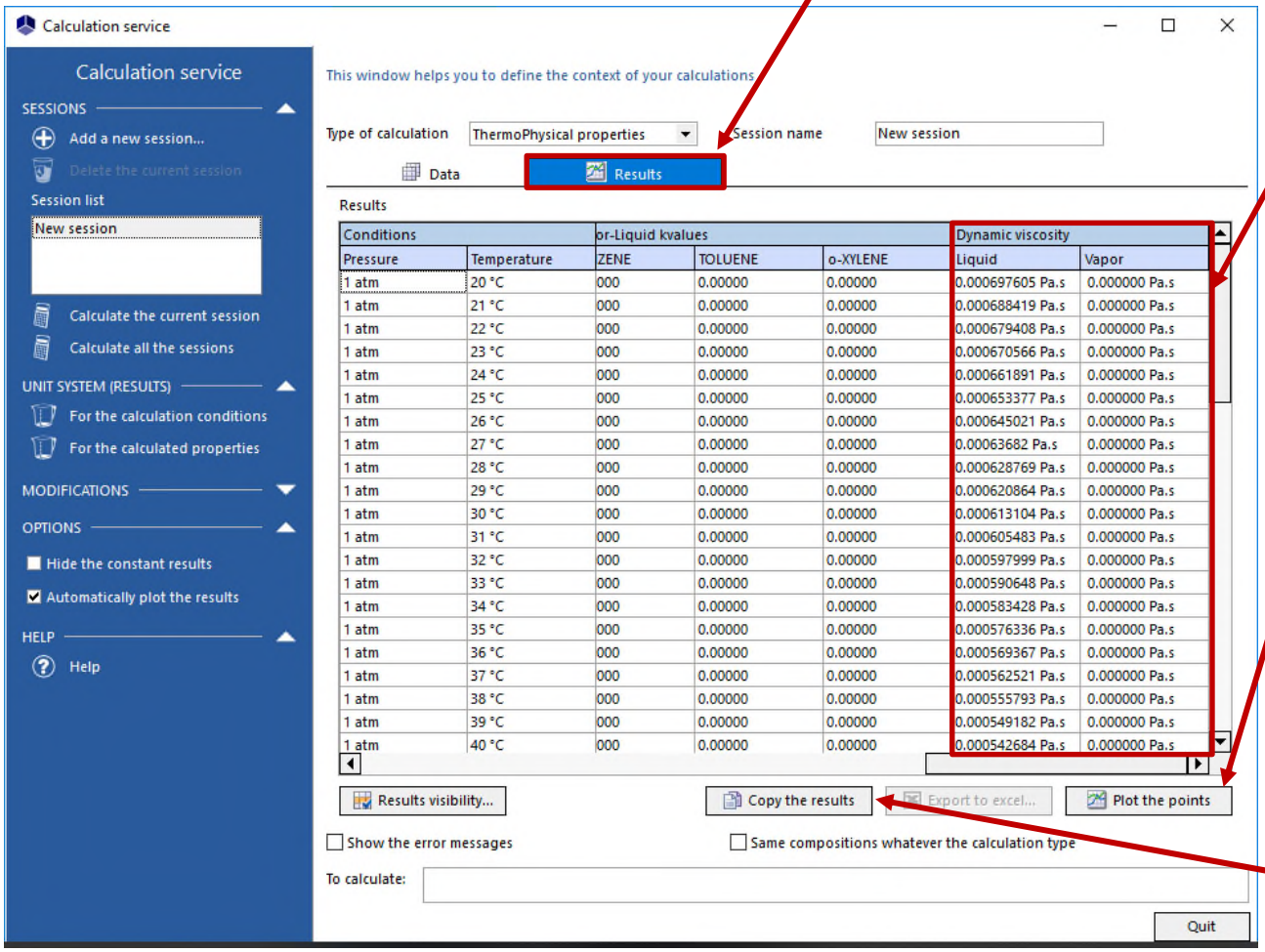
If the option "*Automatically plot the results*" has been checked, this window appears. Several graphs are available, select "*Dynamic Viscosity*" from the drop-down list.

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.



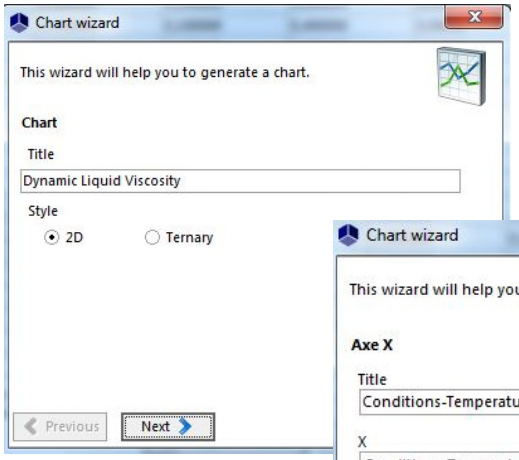
The values of liquid and vapor dynamic viscosity of the mixture are displayed in this column.

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

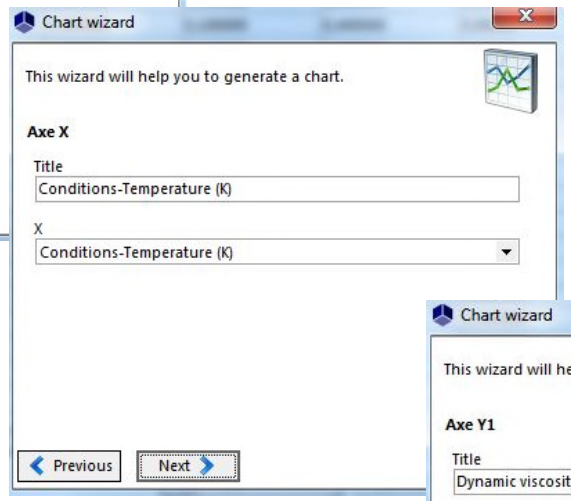
You can copy the results into other applications.

Step 3: Calculate properties of a mixture

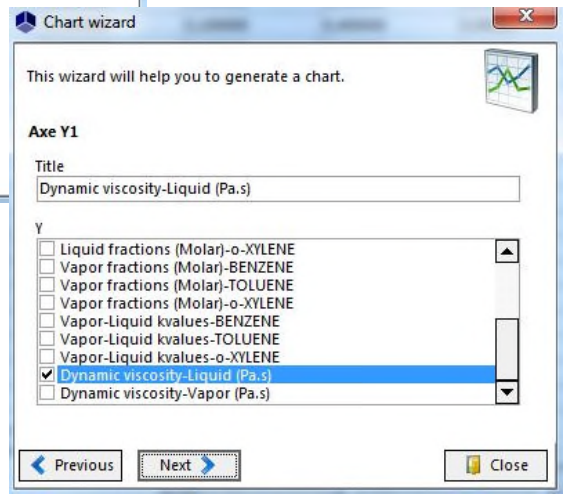
If you want to plot the graph manually (after selecting "*Plot the points*"), follow the instructions from the Chart wizard:



1- Specify the title of the chart.



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



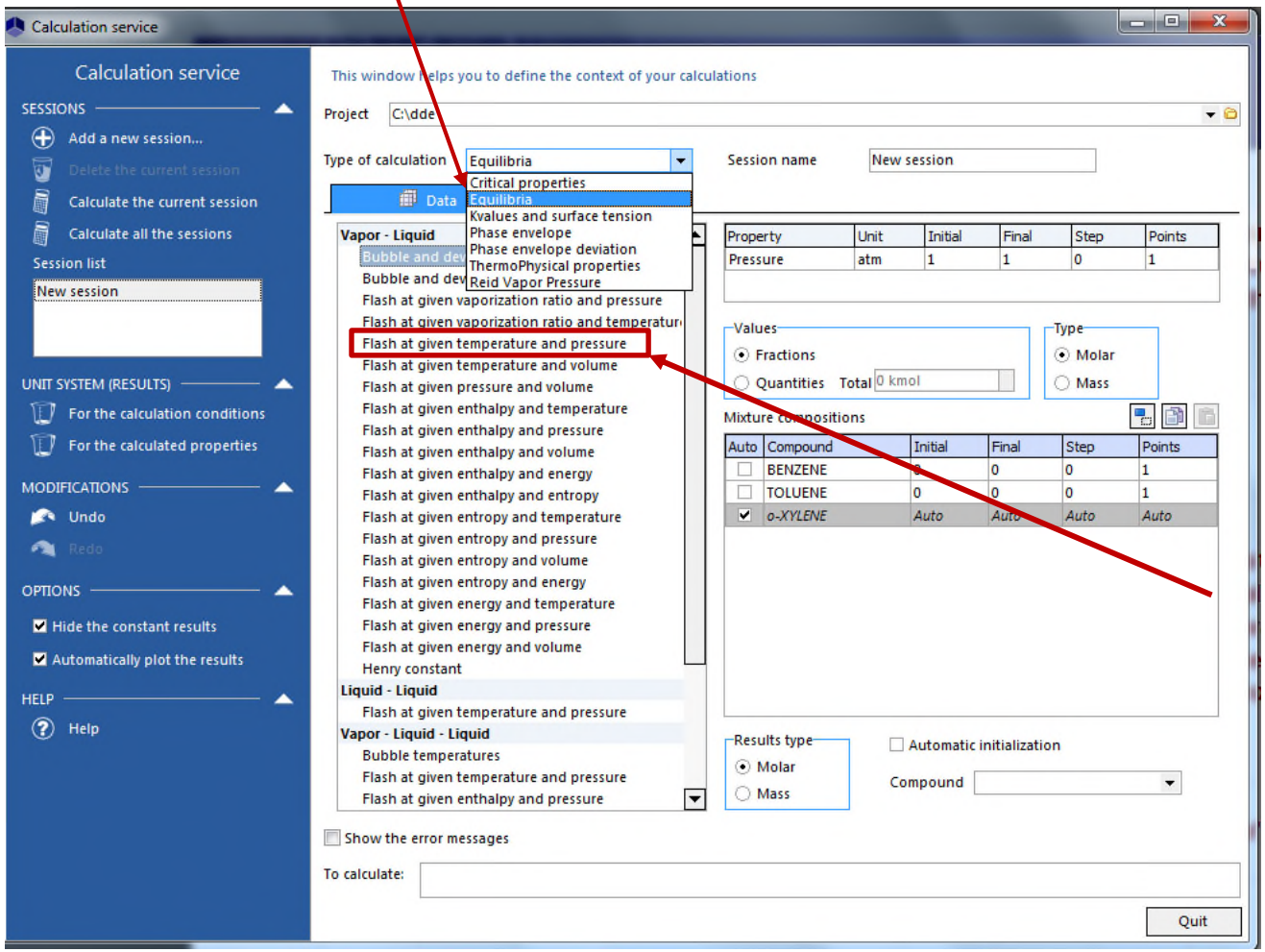
3- Define the Y-axis (the dynamic liquid viscosity in this example).

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.



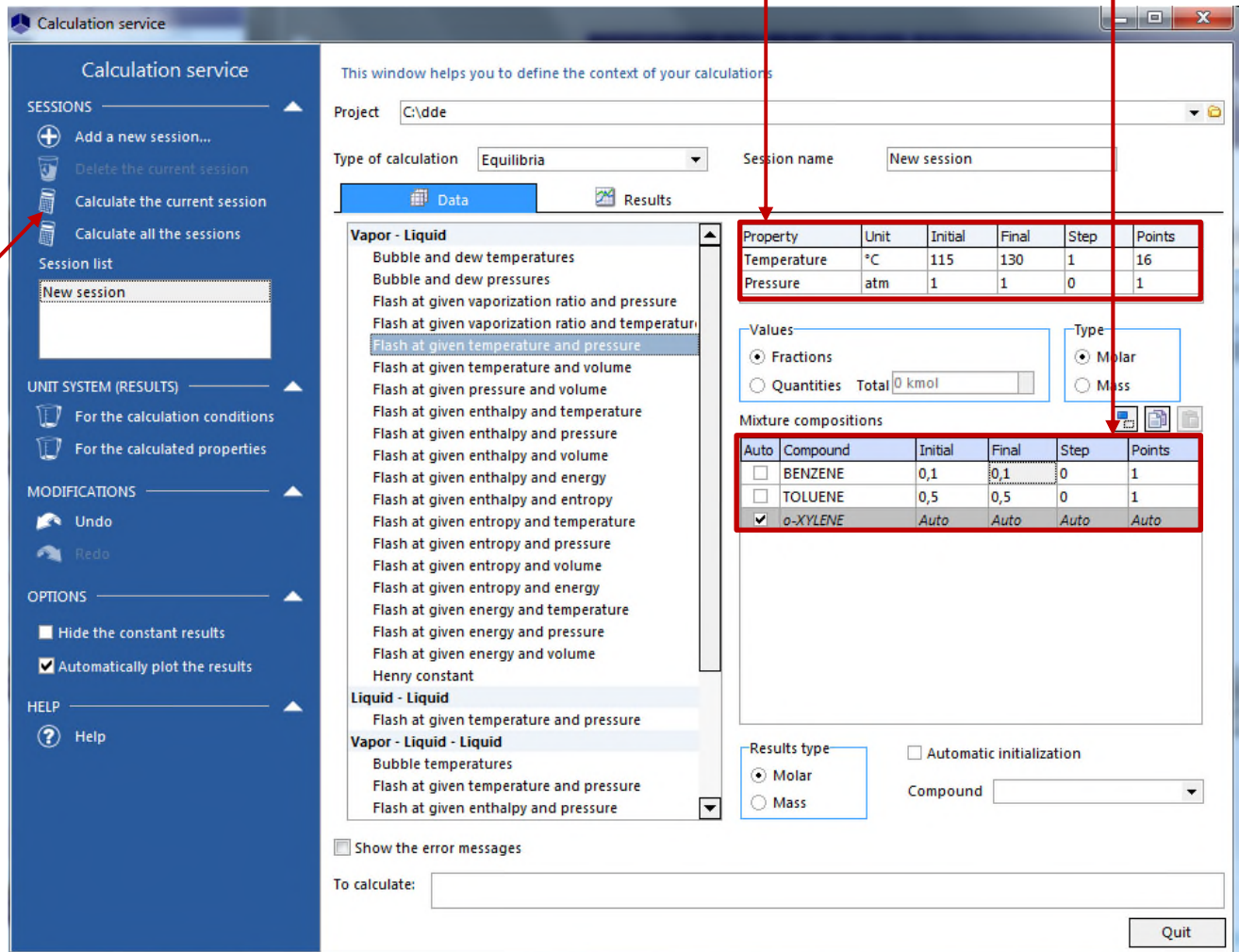
2- Here are displayed the different types of flash that can be calculated. Select "*Flash at given temperature and pressure*".

Step 4: Calculate fluid phase equilibria

1- Specify the operating conditions:

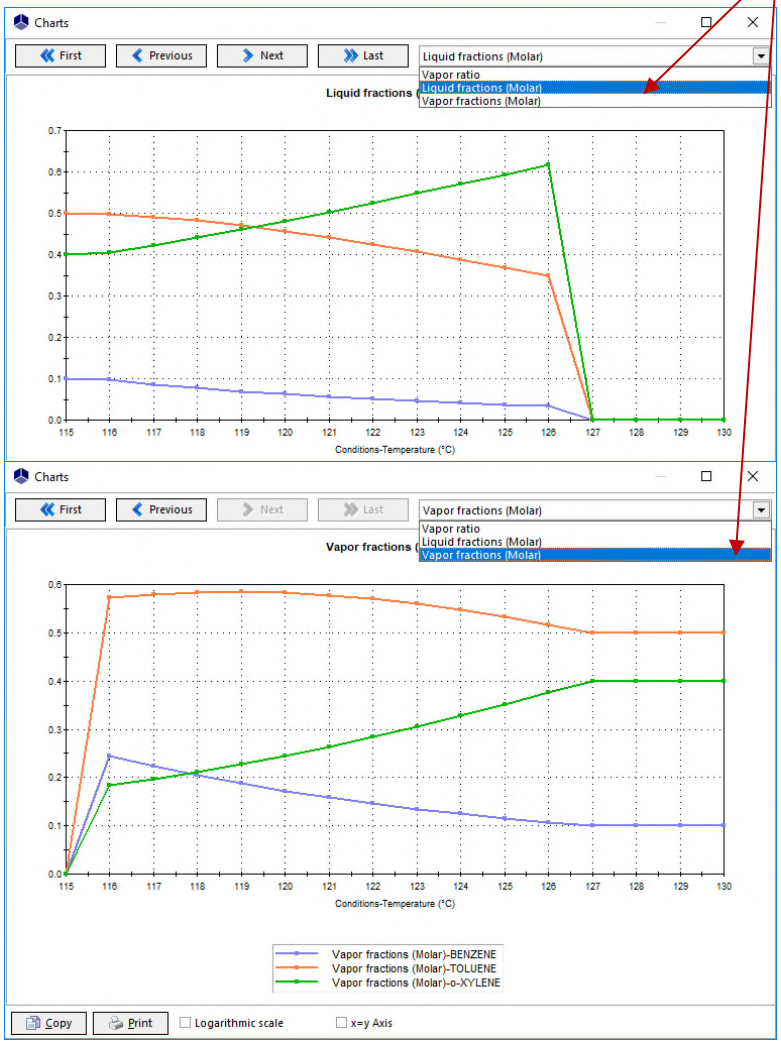
- Pressure: 1 atm.
- Temperature: from 115°C to 130°C with a step of 1°C.
- Mixture composition: 50% mol of benzene, 10% mol of toluene, “auto” for o-Xylene.

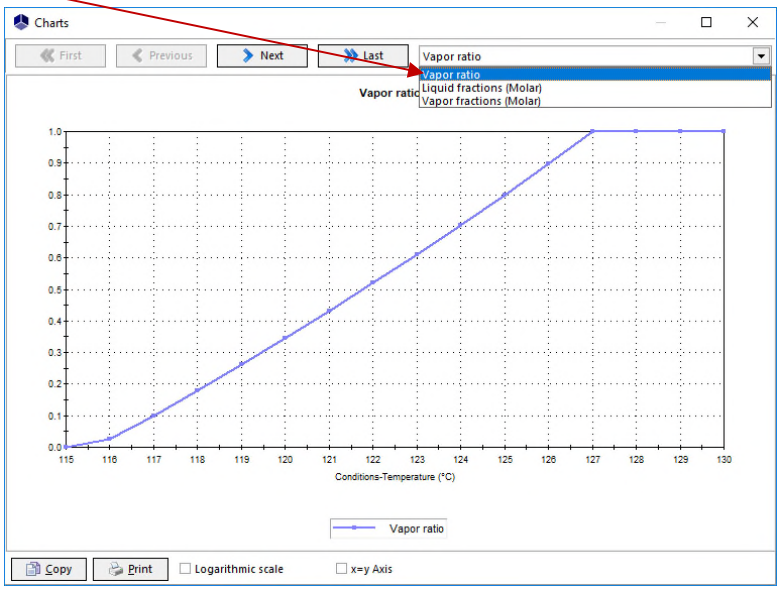
2- Click on “*Calculate the current session*”.



Step 4: Calculate fluid phase equilibria

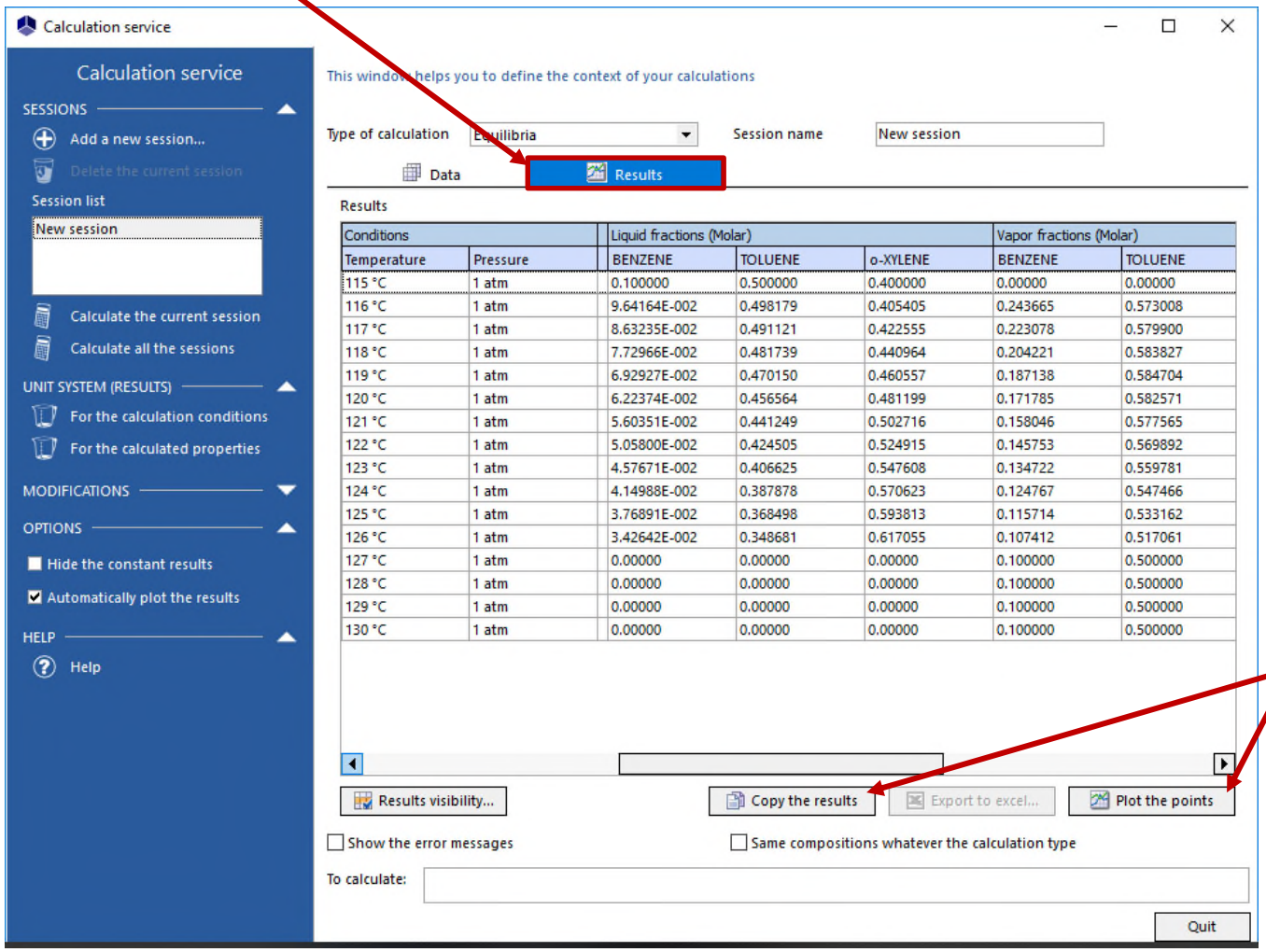
If the option "*Automatically plot the results*" has been checked, you can select from the drop-down list the graph you want to display.





Step 4: Calculate fluid phase equilibria

Results are tabulated in the "*Results*" tab.



You can copy the results and manually plot the points.

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