Getting started with ProPhyPlus®

Use Case 1: Main features overview

Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

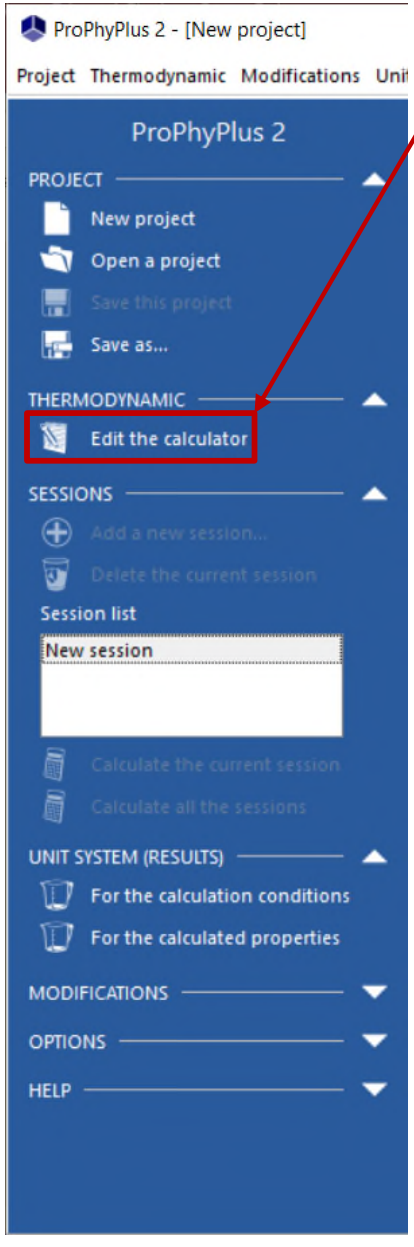
Based on Simulis Thermodynamics software, ProPhyPlus is a stand-alone software to compute mixture properties and fluid phase equilibria without any programming efforts. This document gives an overview of ProPhyPlus main features. It is based on a practical example: the calculation of bubble and dew temperatures for a mixture of water and ethanol.

The steps are the following:

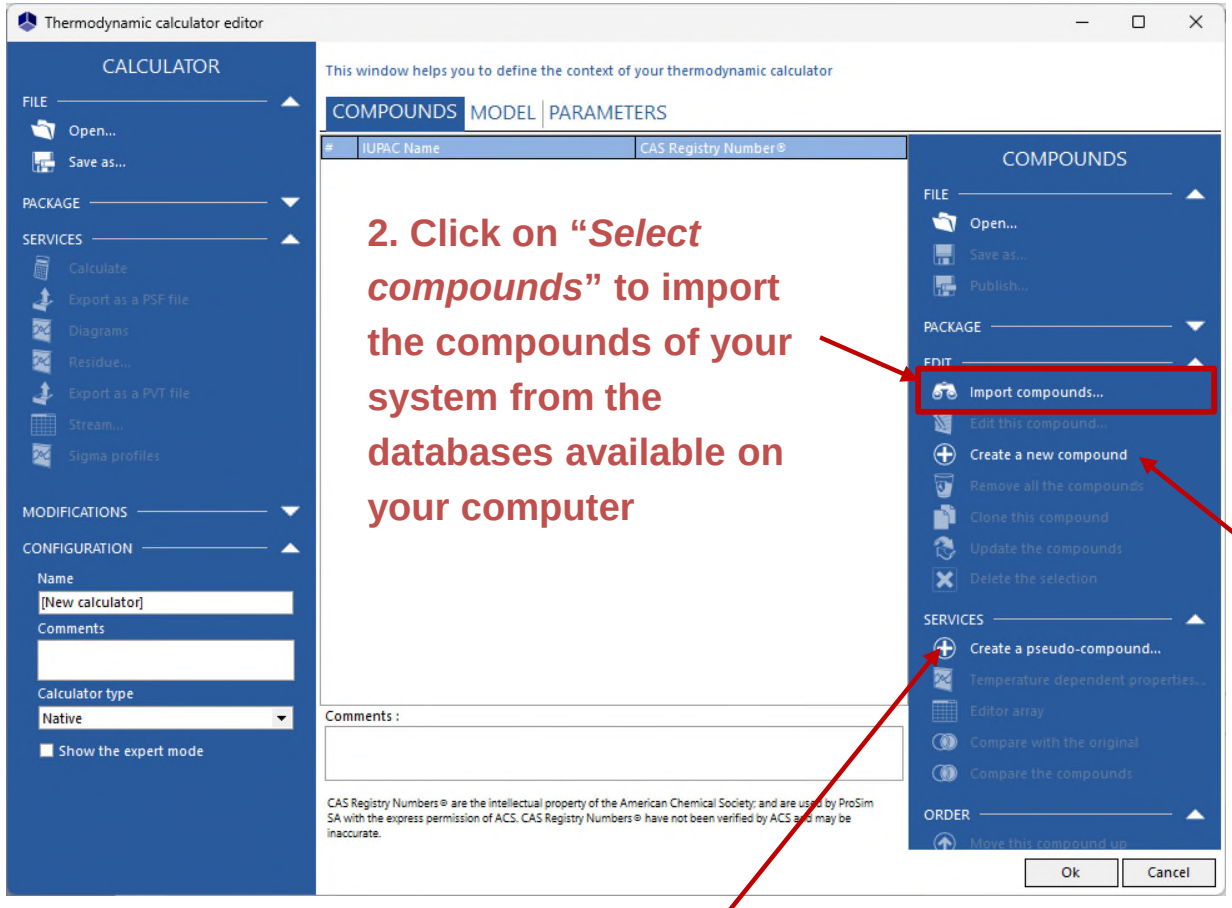
- **Step 1: select the compounds**
- **Step 2: select the thermodynamic model**
- **Step 3: manage the unit system**
- **Step 4: define calculation conditions**
- **Step 5: generate the results**

For additional tutorials, please consult « Getting started with Simulis Thermodynamics » documents.

Step 1: select your compounds



1. Click on "*Edit the calculator*" to open the calculator configuration window



2. Click on "*Select compounds*" to import the compounds of your system from the databases available on your computer

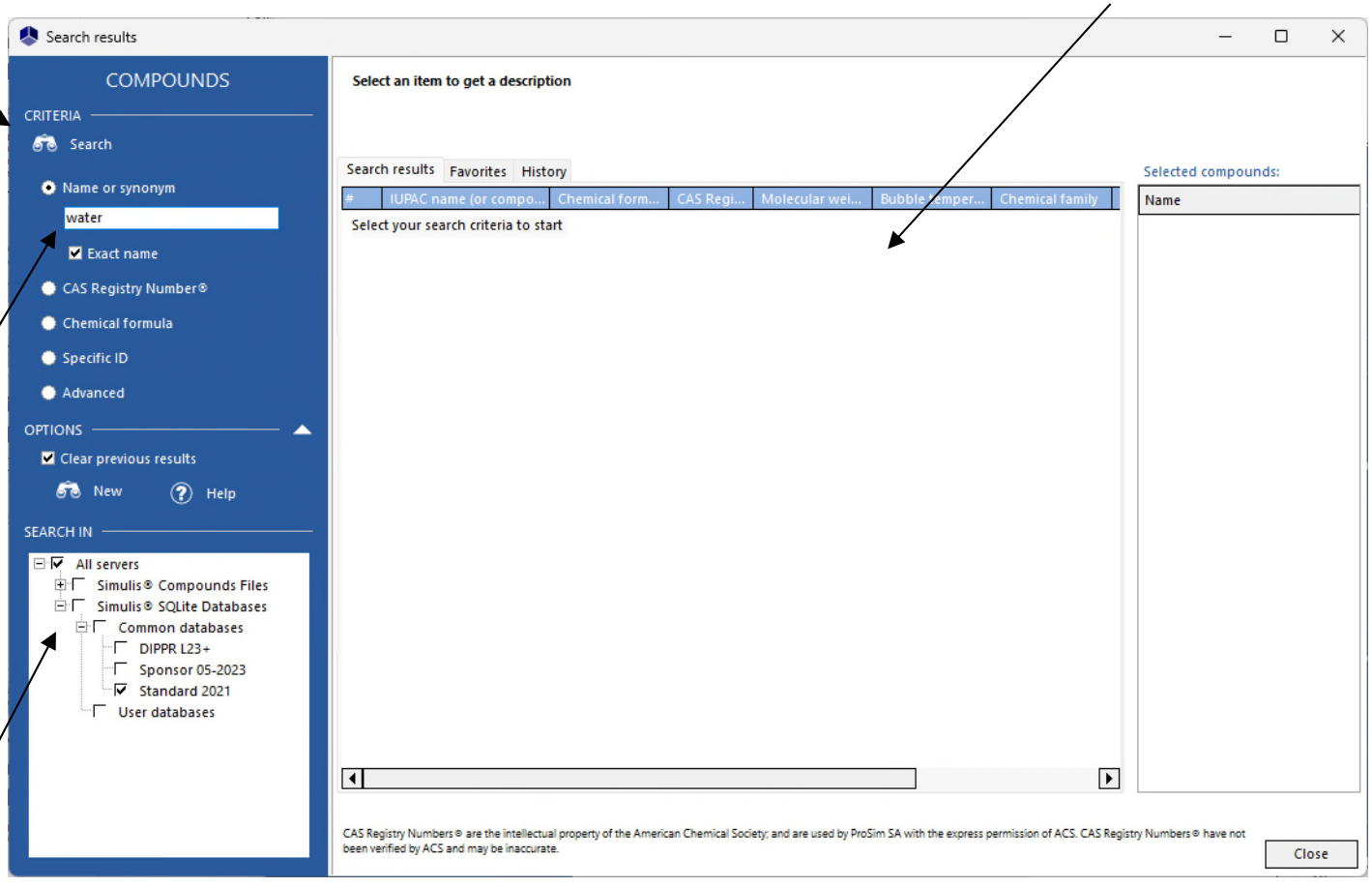
You can create your own compounds, by clicking on "*Import compound*"

You can create pseudo-compounds corresponding to a petroleum cut, by clicking on "*Create a pseudo-compound*"

Step 1: select your compounds

3. Press "*Enter*" or click on the "*Search*" button to get the list of compounds that match your criteria

4. The search results are shown in this area



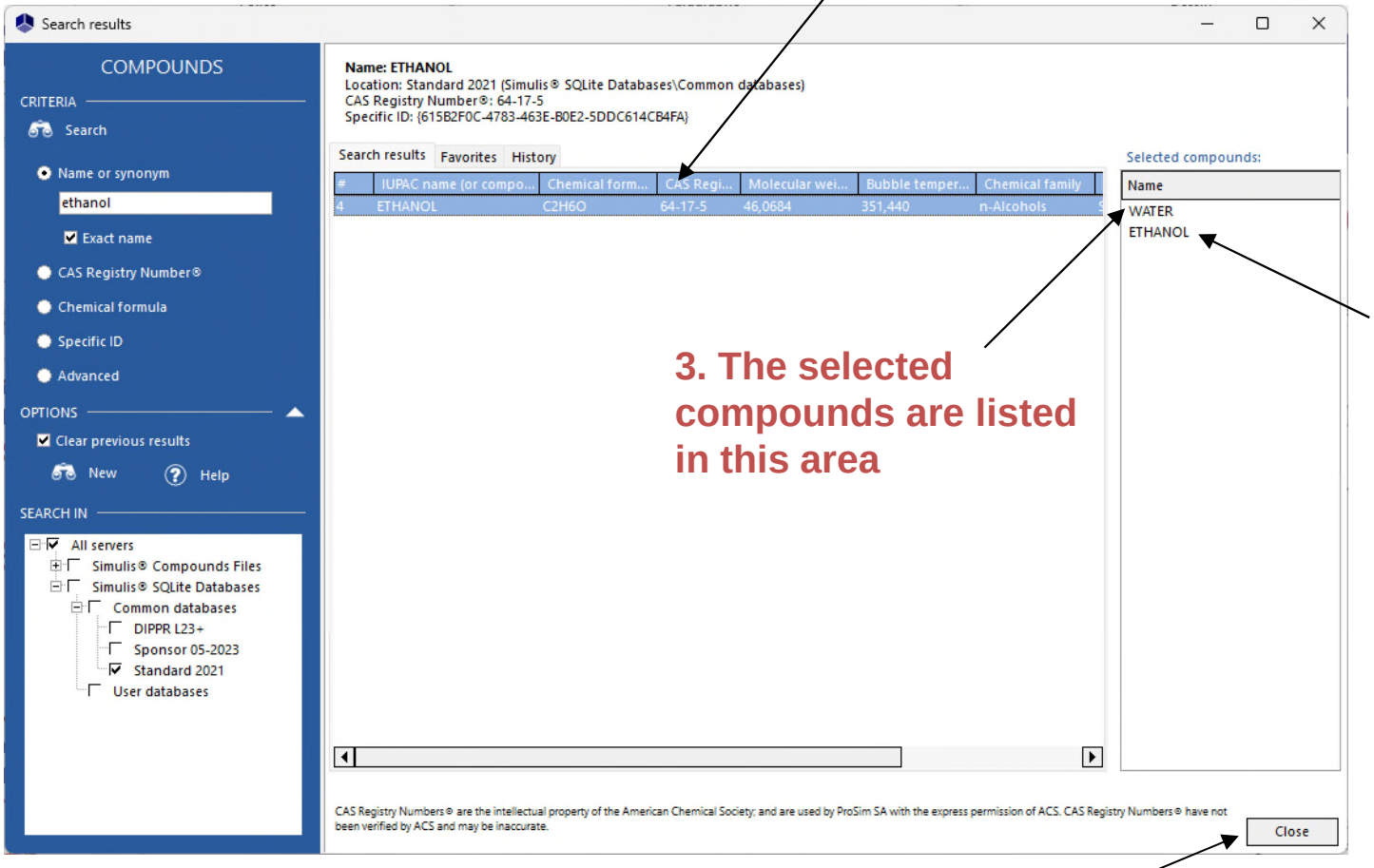
2. You have access to multiple search criteria (in this example, search "*Water*" by name)

1. Select the compounds server(s) (databases or packages) in which you want to search the compounds (by default, select the most recent one)

You can run multiple searches without closing this window

Step 1: select your compounds

1. Double click to add the compound (Water) to your final selection, on which you will run the calculations

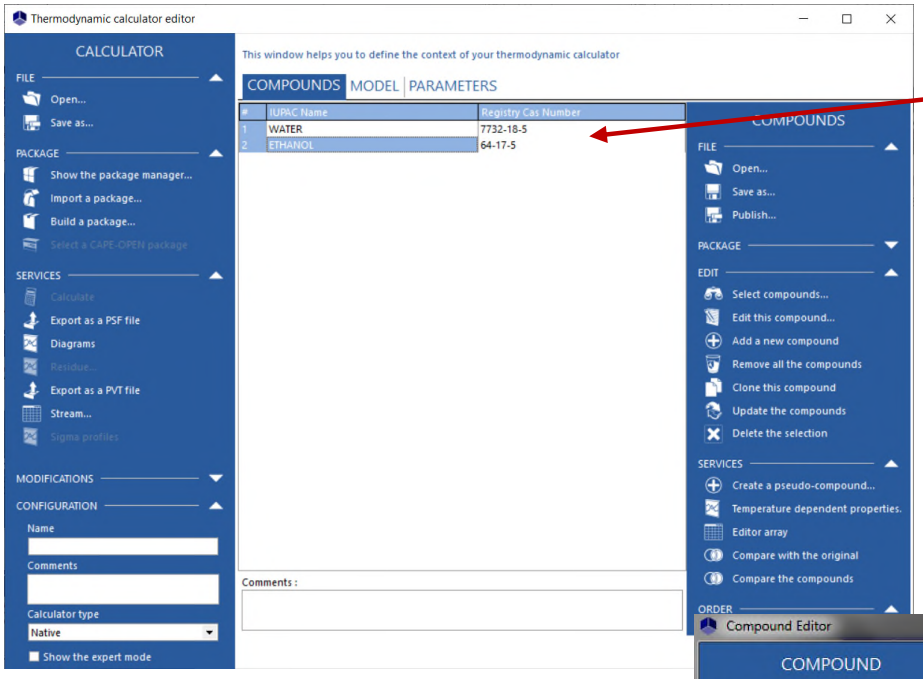


2. Repeat this operation for the other compound (Ethanol)

3. The selected compounds are listed in this area

4. Click on *"Close"* to end the compounds selection process

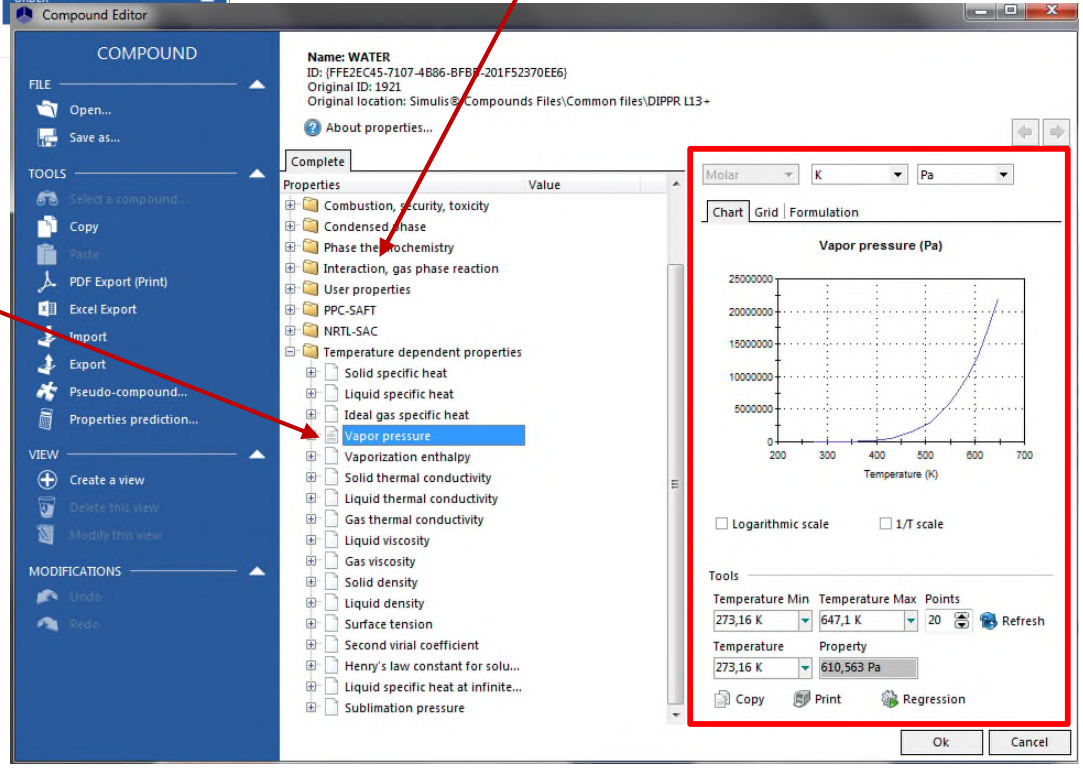
Step 1: select your compounds



1. Double click on a compound to access the compound configuration window

2. All of the compound properties are organized into different folders. Expand the folders to view details of each property

3. Click on a temperature dependent property to access its correlation and diplay the graph



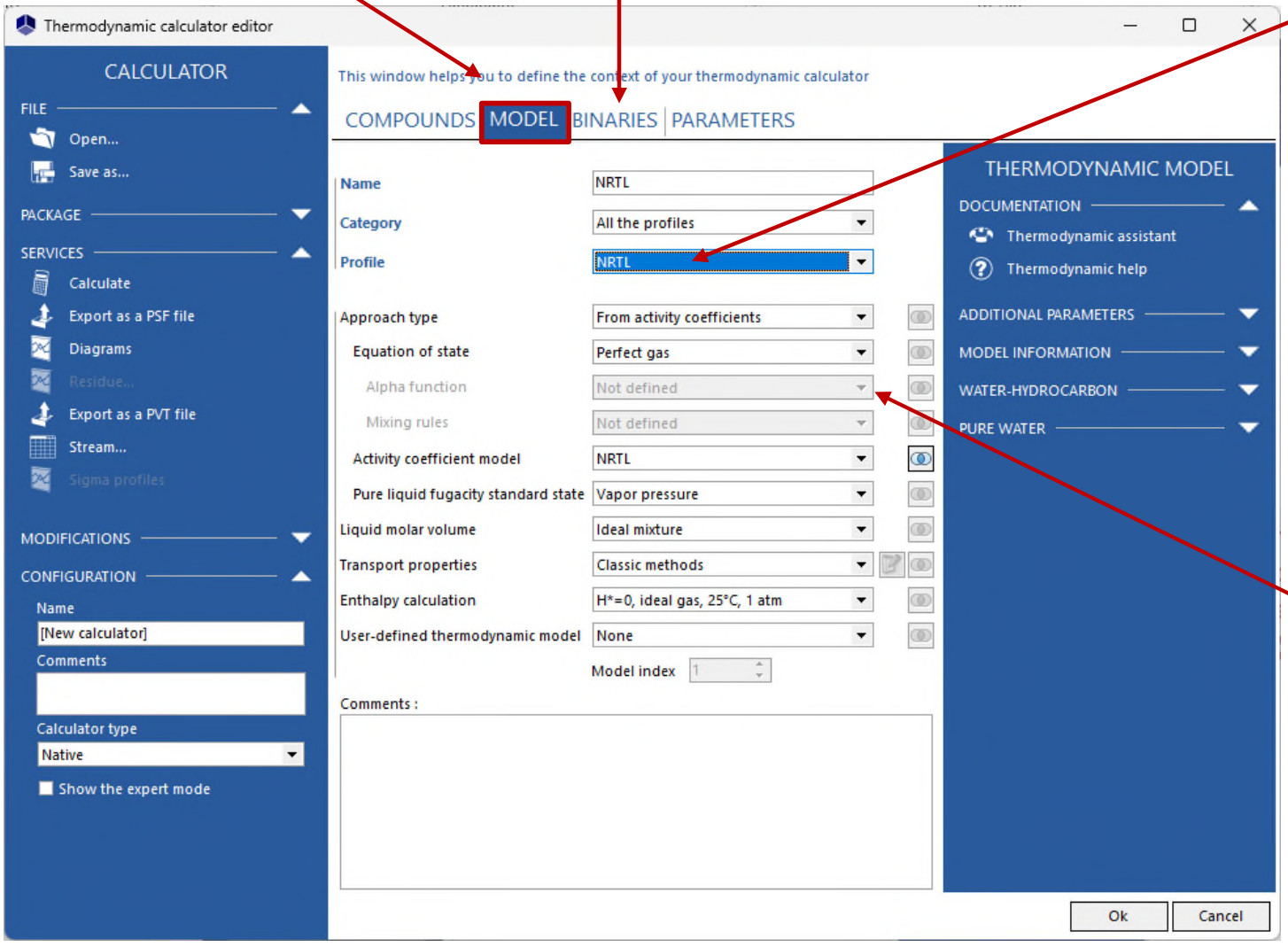
For more details about pure components properties, please consult “Getting started with Simulis Thermodynamics, use case 4”

Step 2: select the thermodynamic model

1. Click on the "*Model*" tab to enter the thermodynamic models editor

The "*Binaries*" tab appears automatically when you select a model that requires binary interaction parameters

2. Select the Thermodynamic profile

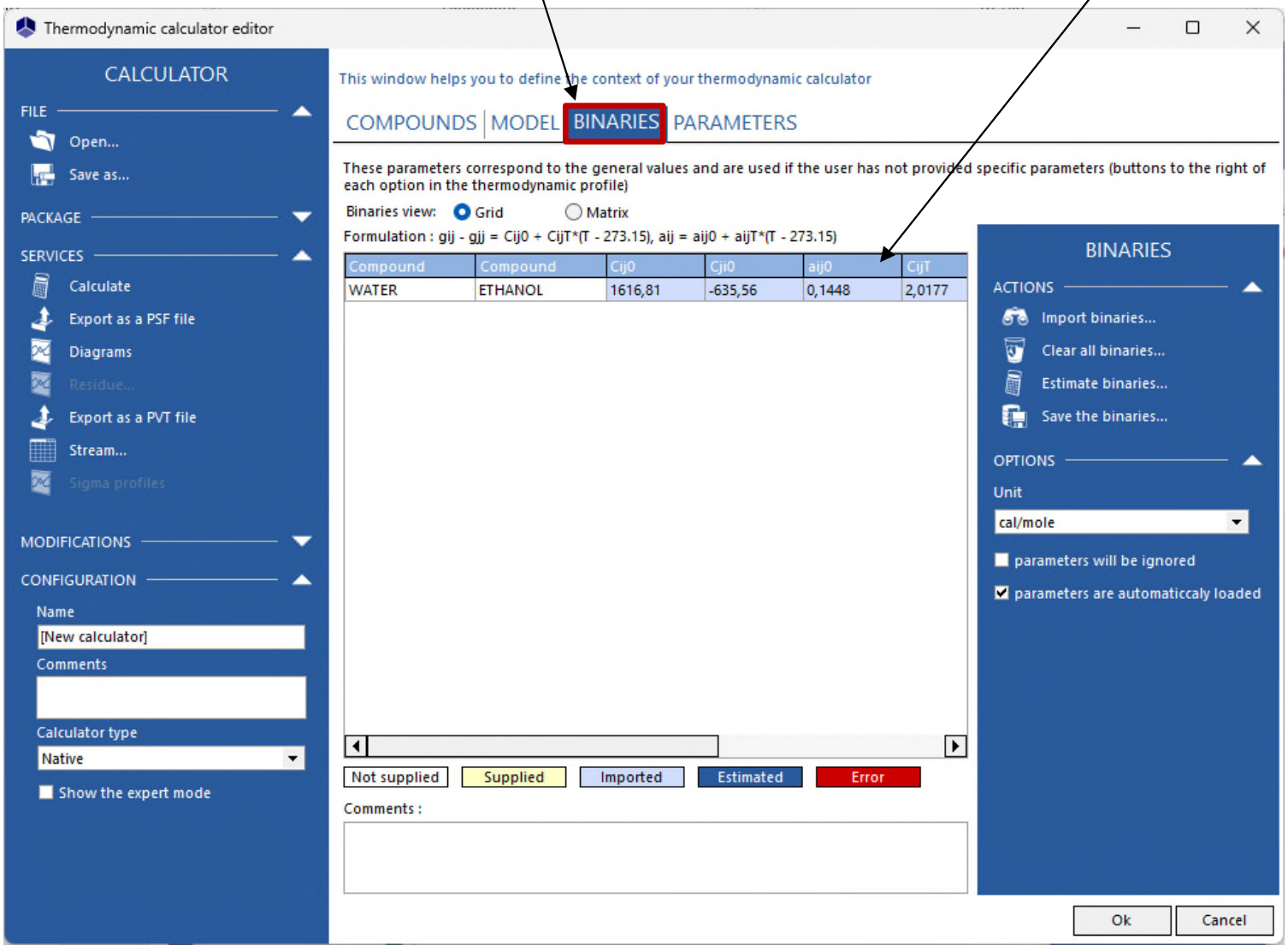


3. Adjust the thermodynamic profile if it is necessary

Step 2: select the thermodynamic model

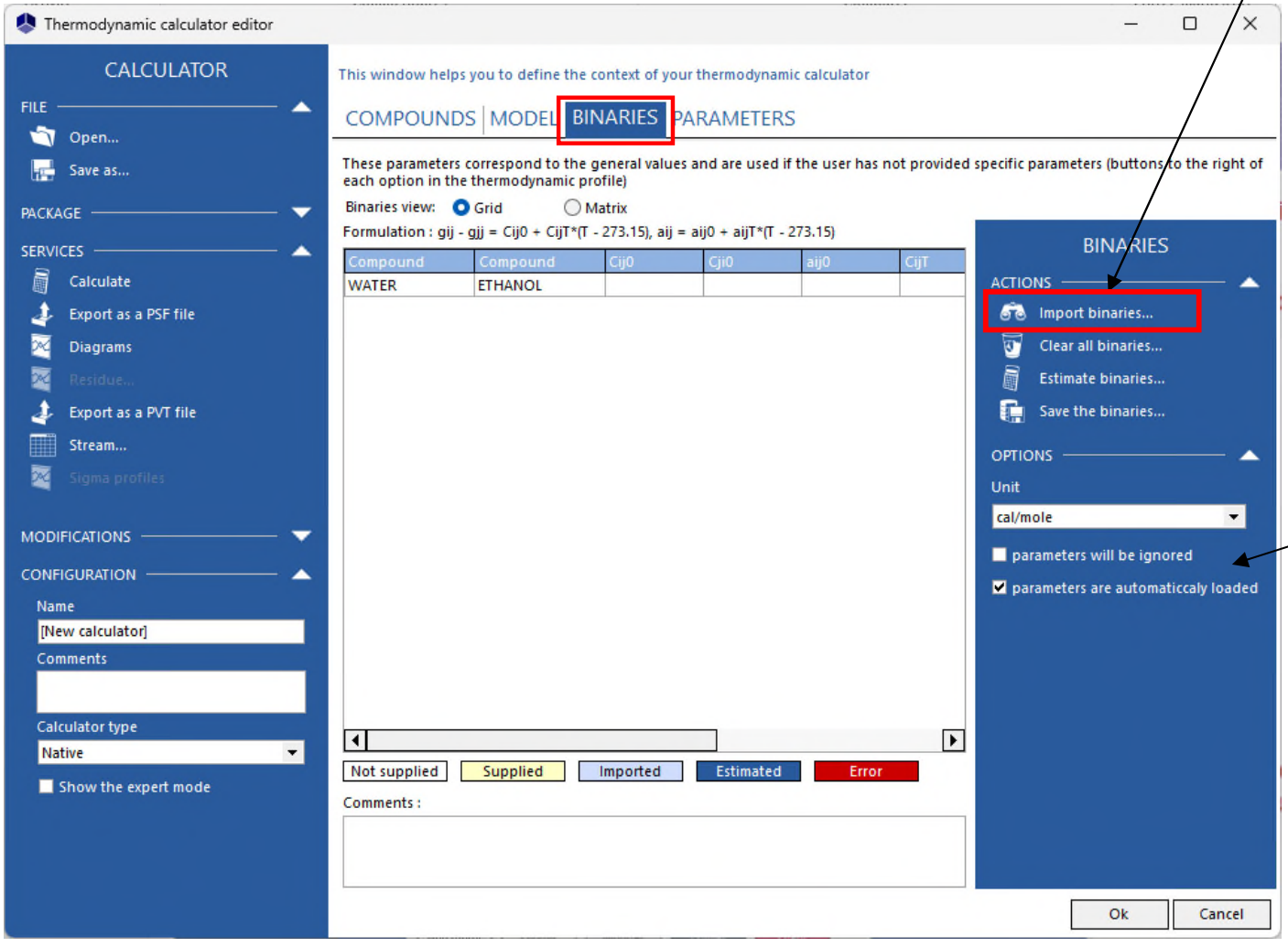
1. Click on the *"Binaries"* tab to enter the binaries search window (if required by the model)

2. Automatic load if the binaries are available in Standard database



Step 2: select the thermodynamic model

For the calculator that is already defined in a simulation, if parameters are missing, if the loading is nor activated: Import binaries
Import binaries from a private database

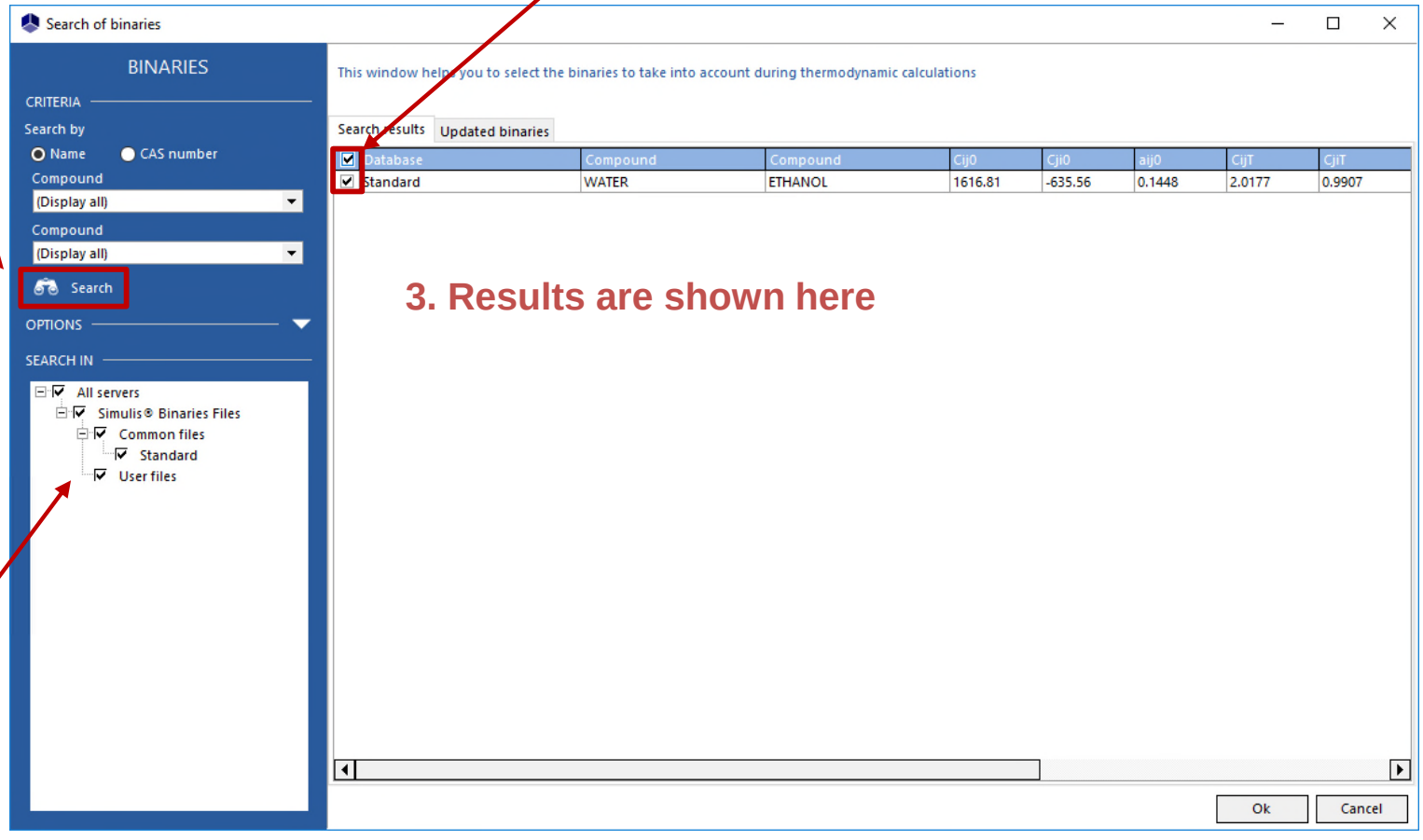


Automatic load is not activated

Step 2: select the thermodynamic model

4. Select the binary interaction parameters to be used and click on *"OK"*

2. Click on *"Search"*

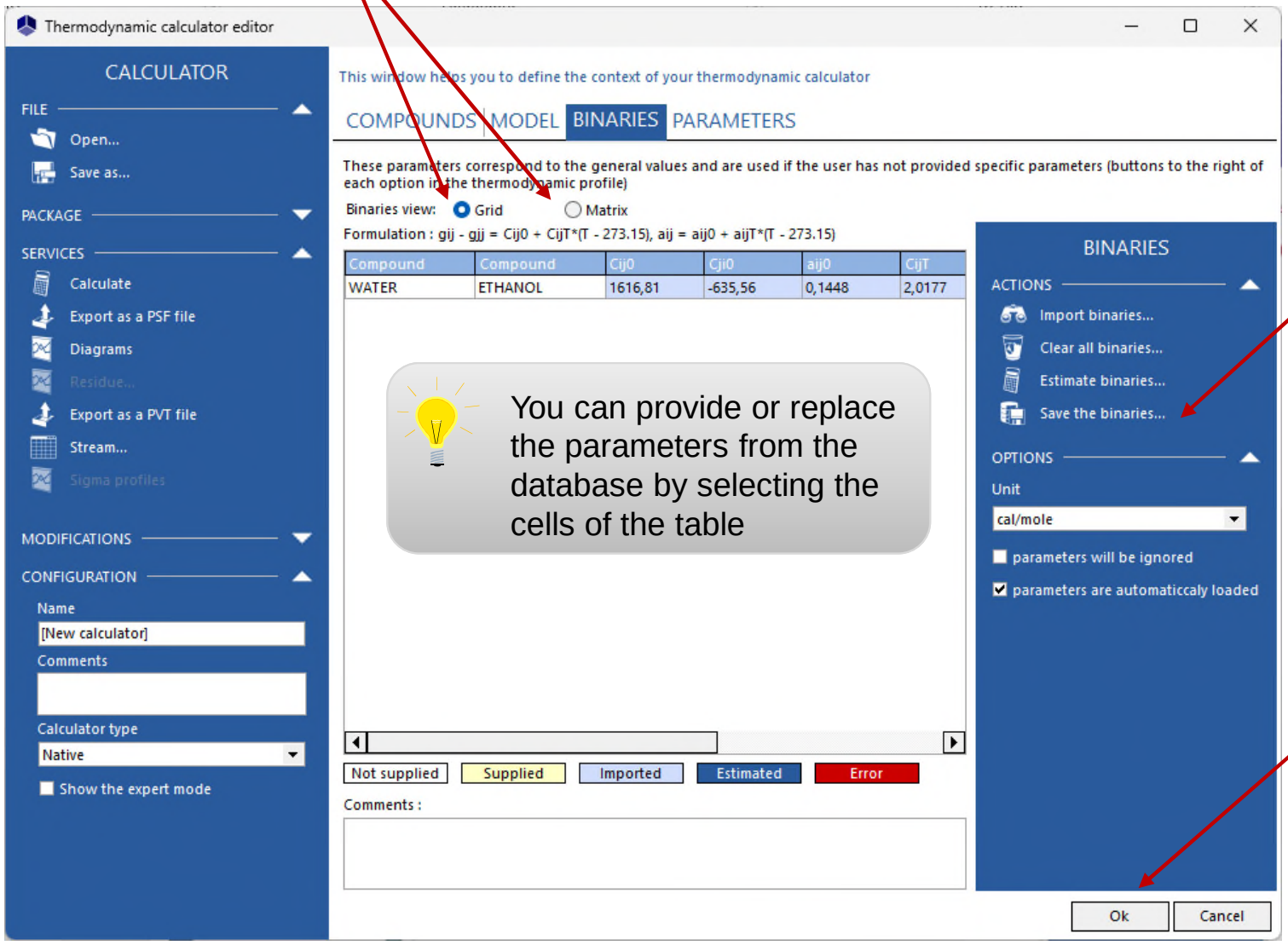


3. Results are shown here

1. Select the binaries server(s) that you want to use for your research

Step 2: select the thermodynamic model

You can display the binaries as a grid or a matrix



You can save the binaries in "*user databases*"

Click on *"OK"* to validate your inputs and return to the main window

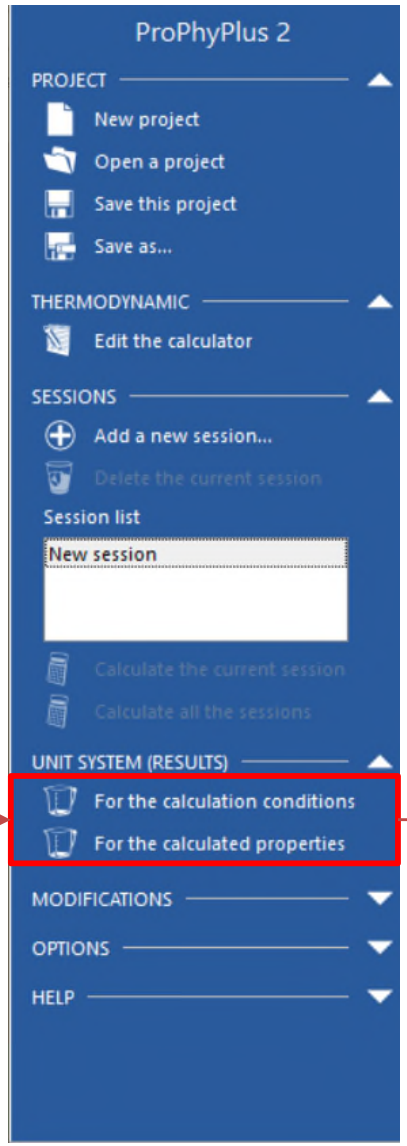
Step 3: manage the unit system

Different unit systems can be used for the:

- **calculation conditions**
- **calculated properties**

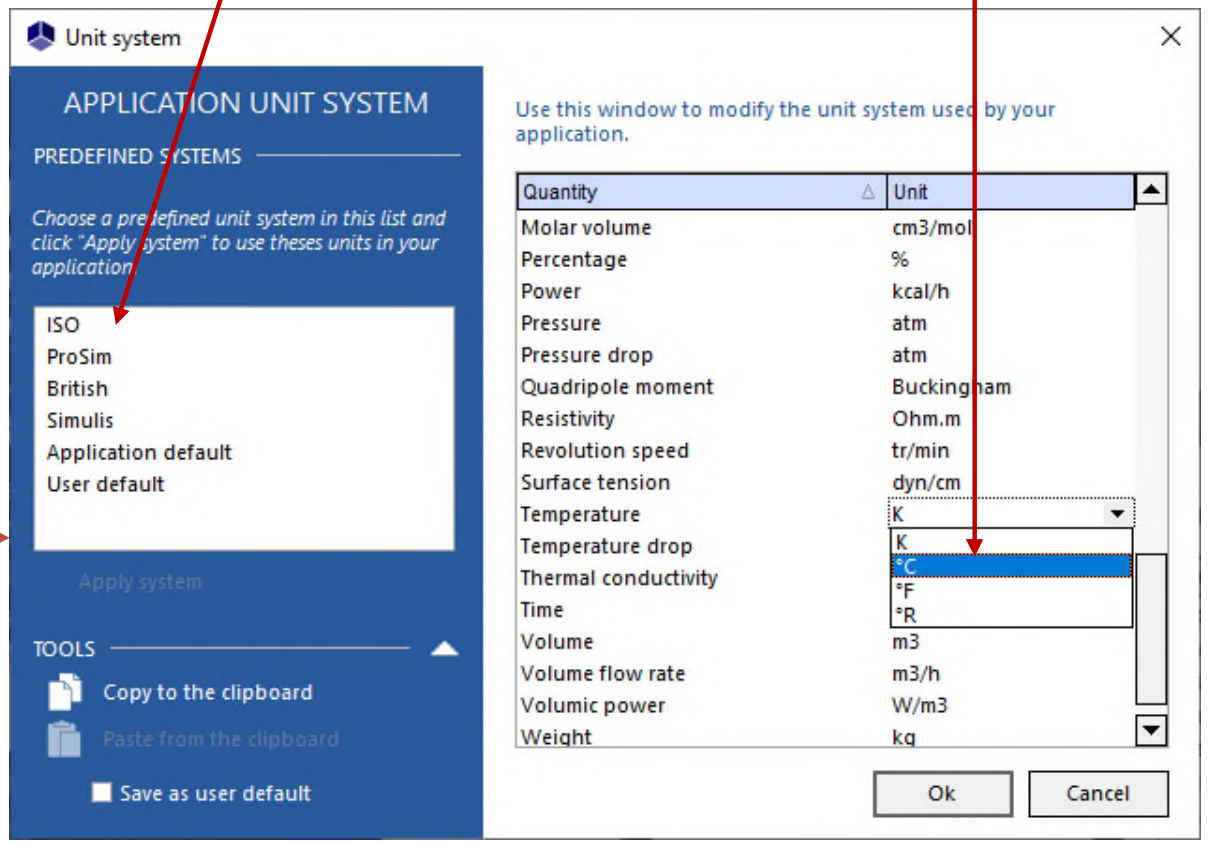
- Both input and output unit systems can be customized.
- You can choose different unit systems for the input and for the output

Click



You can select predefined unit systems…

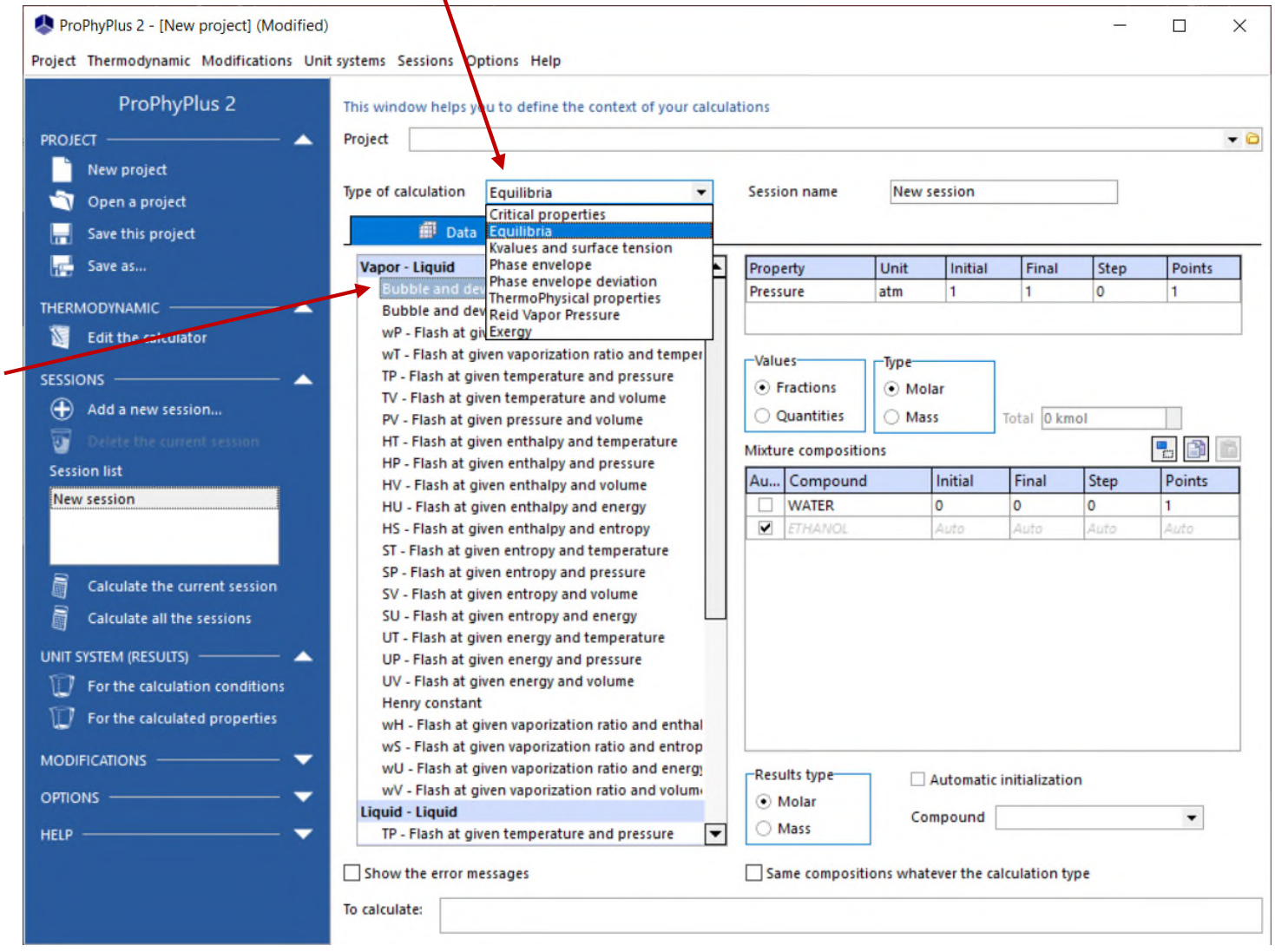
…or customize your unit system, quantity per quantity, with the scroll down menu



Step 4: define calculation conditions

1. You can chose the type of calculation to run (calculation of mixture properties or fluid phase equilibria). Select "*Equilibria*"

2. Select the properties to calculate (in this example, "*Bubble and dew temperature*")



Step 4: define calculation conditions

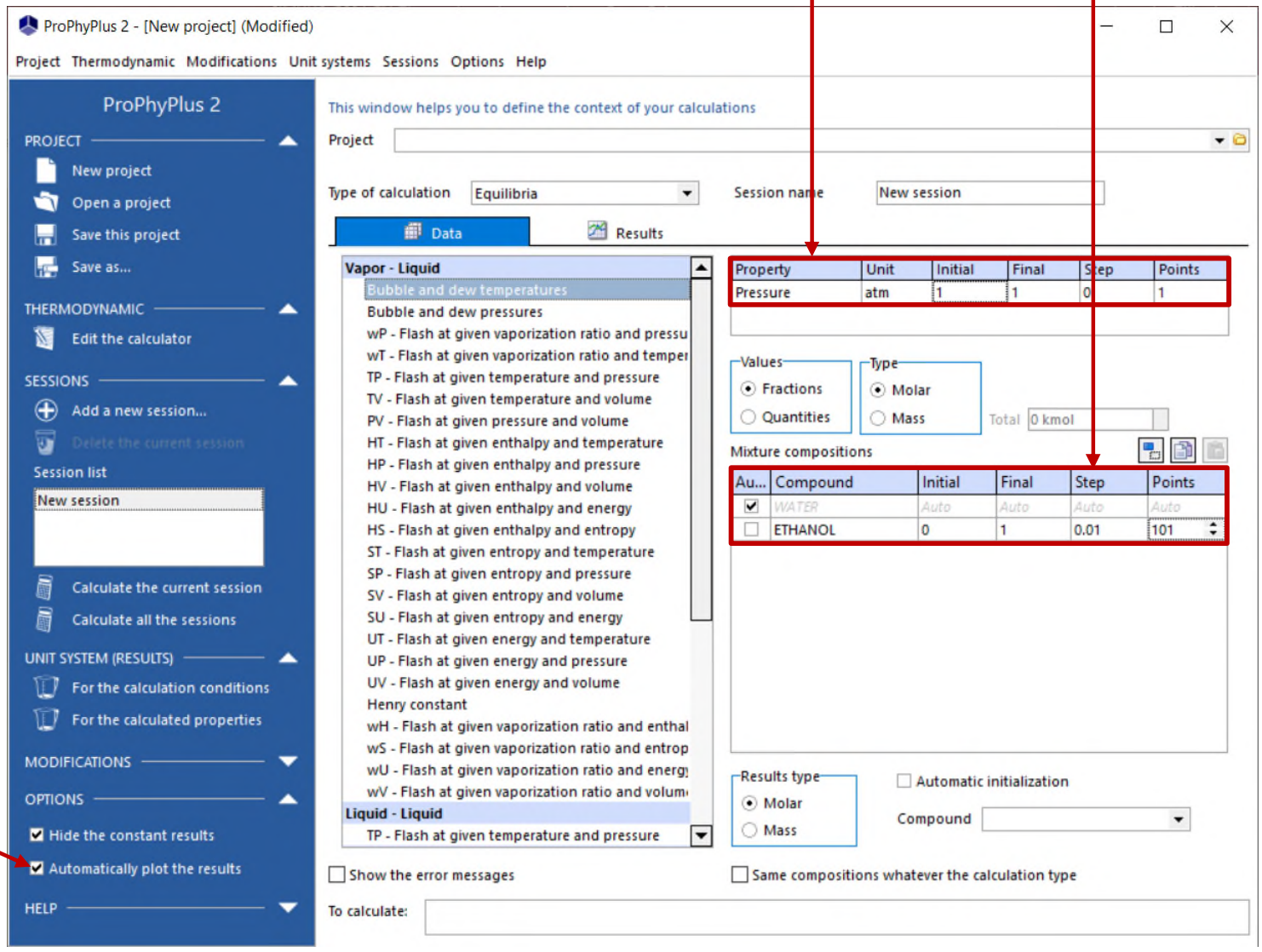
1. Specify the operating conditions:

Pressure: 1 atm.

Mixture composition:

- From 0% mol to 100% mol of Ethanol
- "Auto" for Water (in order to get a global composition of 100%)
- Specify a step of 0.01 (corresponding to 101 points)

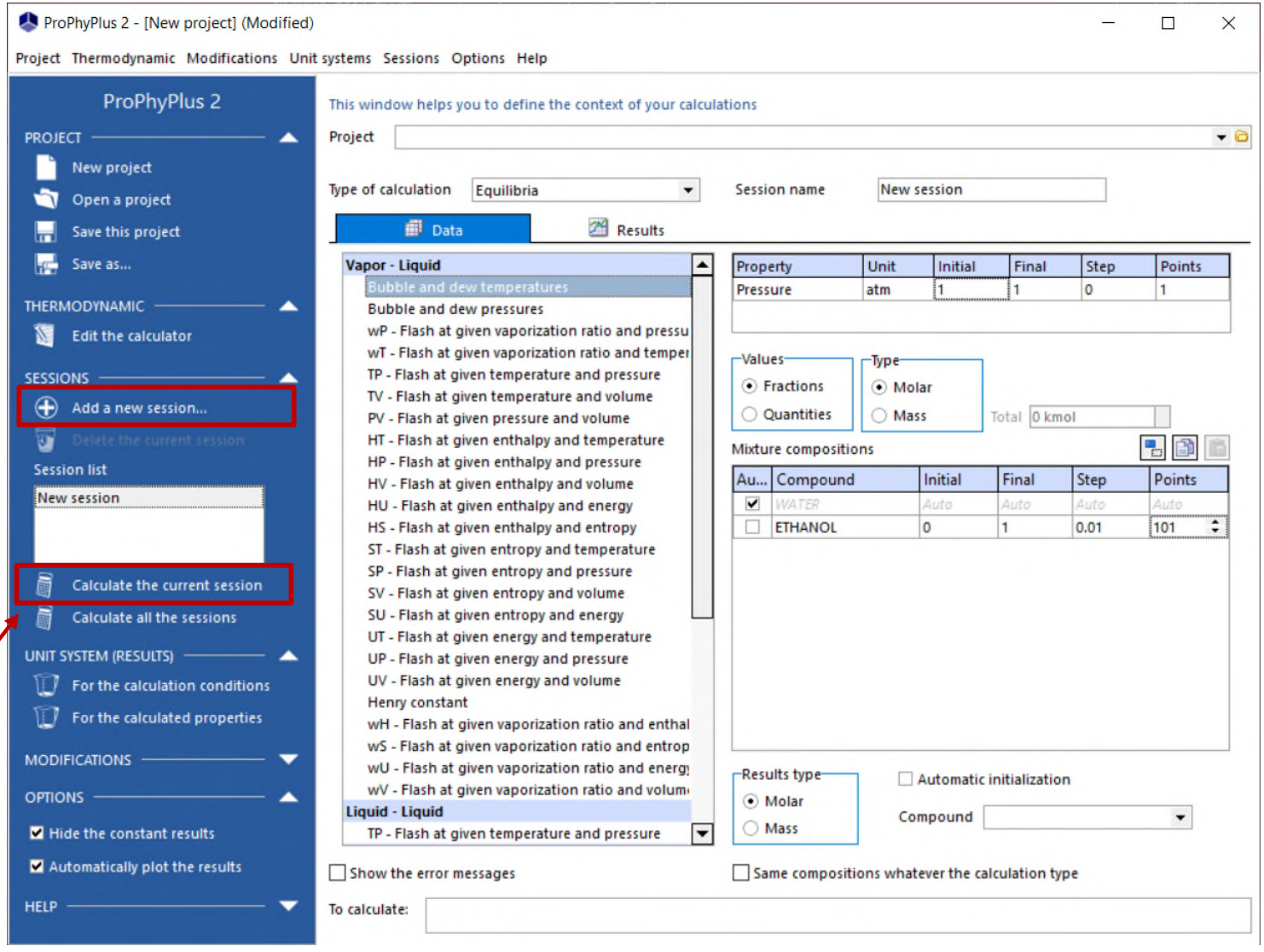
2. Select the option "*Automatically plot the results*"



Step 4: define calculation conditions

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

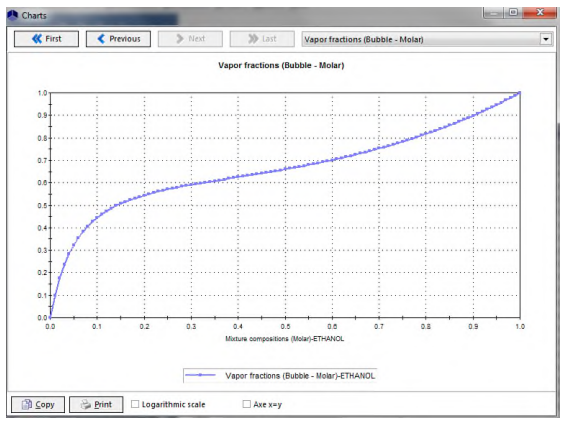
Click on "*Calculate the current session*"

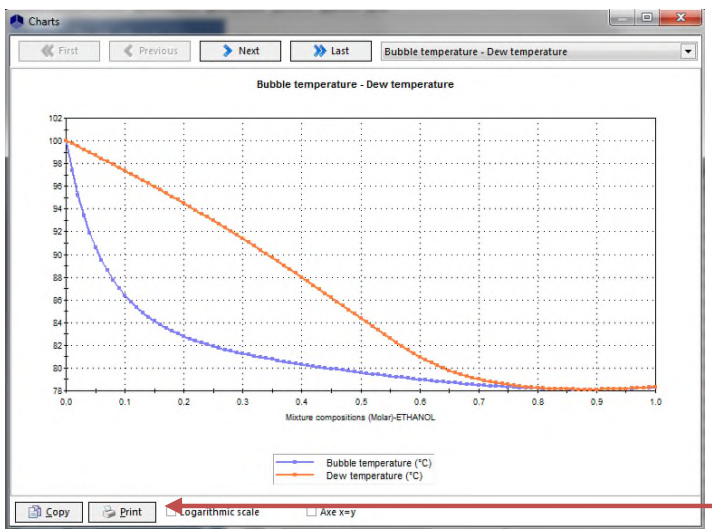


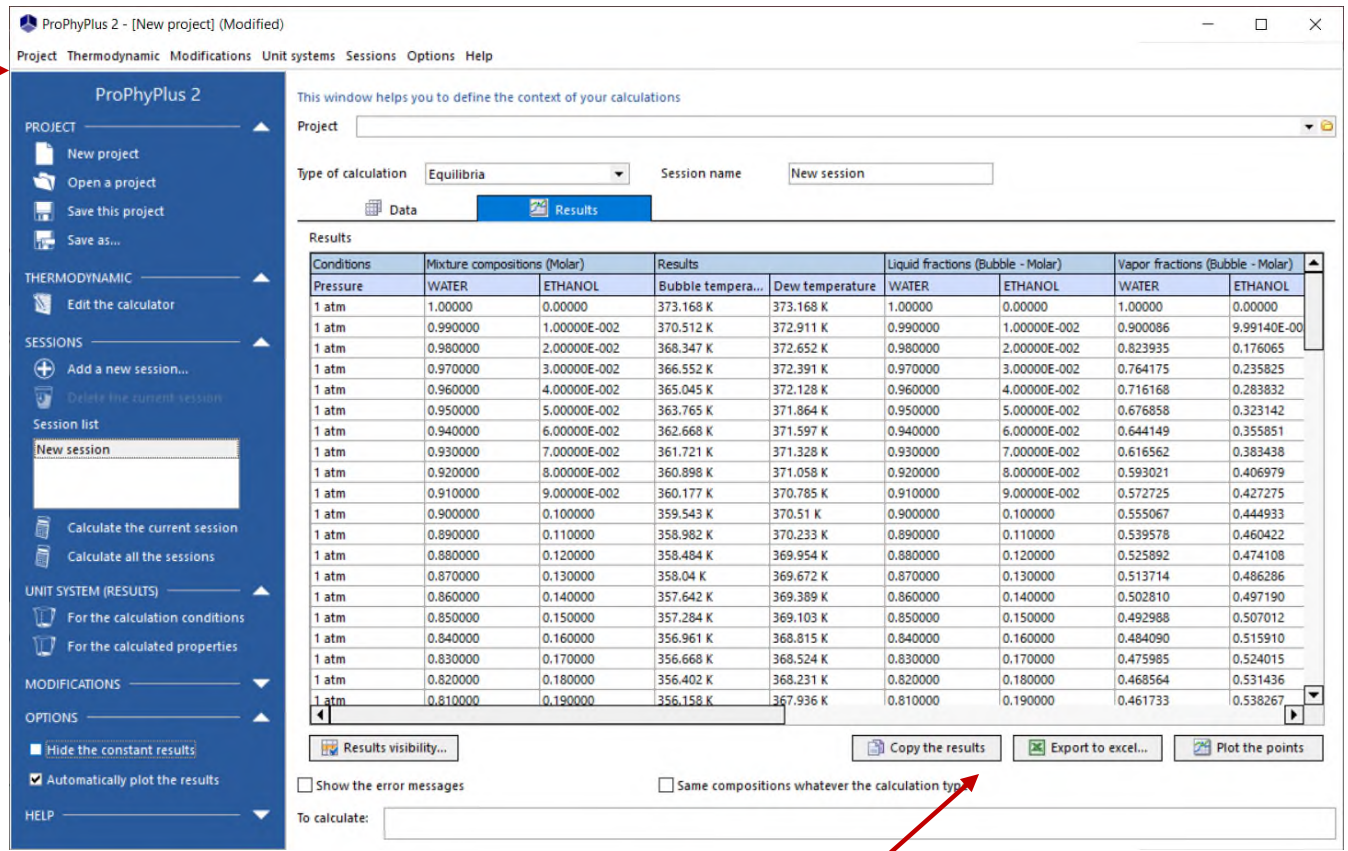
Step 5: generate the results

Results are displayed in a table…

… and charts are automatically generated.





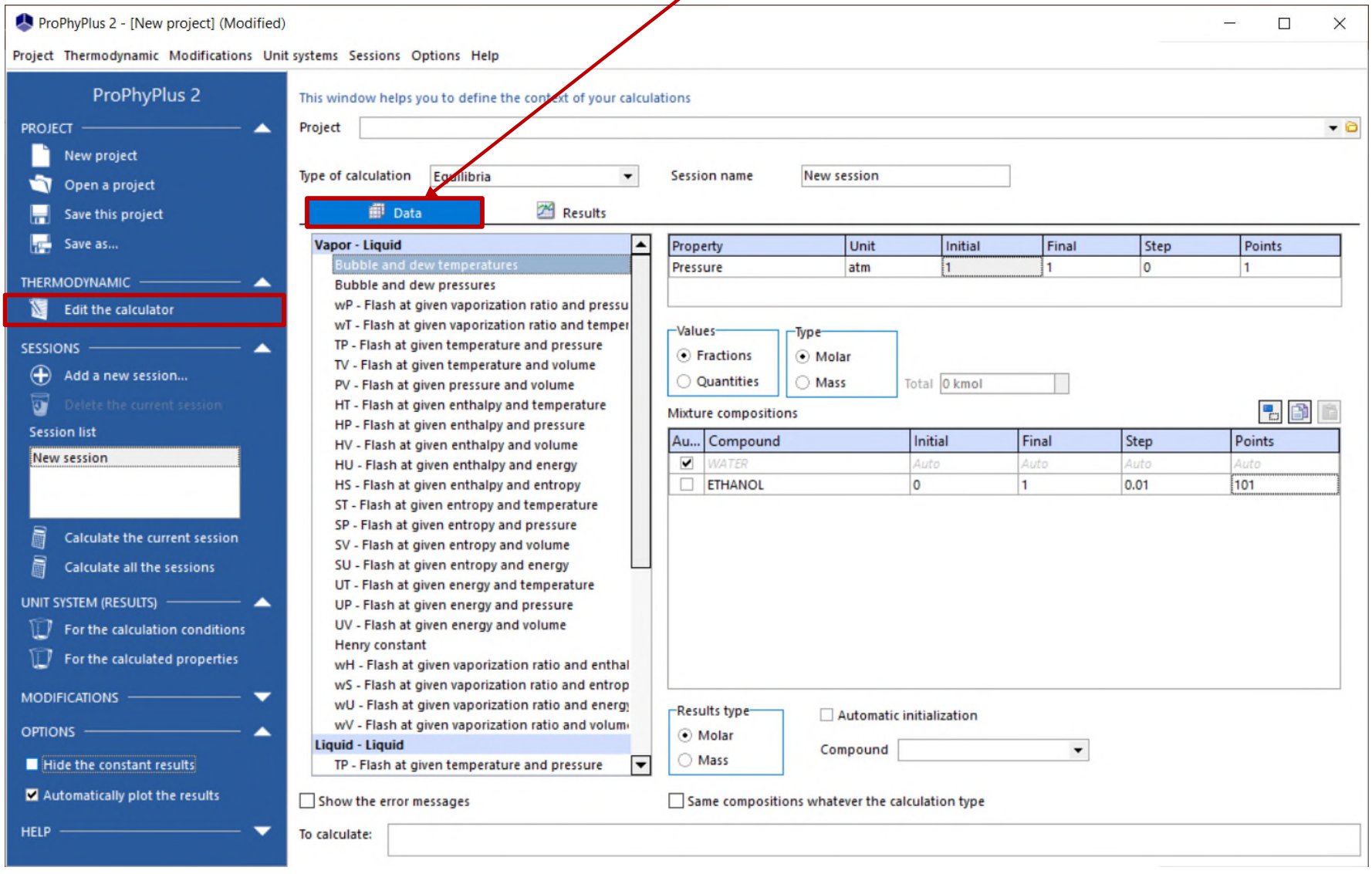


You can copy the table and graphs into other applications

Set up the next calculation…

You can return to the calculator configuration window at any time by clicking on "*Edit the calculator*"

To modify the calculation conditions, click on the "*Data*" tab



ProSim

Software & Services In Process Simulation

ProSim SA
51, rue Ampère
Immeuble Stratège A
F-31670 Labège
France

☎: +33 (0) 5 62 88 24 30

www.prosim.net

info@prosim.net

ProSim, Inc.
325 Chestnut Street, Suite 800
Philadelphia, PA 19106
U.S.A.

☎: +1 215 600 3759