Getting started with Simulis® Thermodynamics

Use Case 1: Main features overview

Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

This document gives an overview of Simulis Thermodynamics features, and describes the steps to follow in order to configure it. As an example, a vapor – liquid equilibrium calculation is performed at a given temperature and pressure and for a mixture of water and ethanol.

Simulis Thermodynamics is a "software component" that you can integrate into different applications

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Case 1: if you are using Simulis Thermodynamics within ProSim environment (ProSimPlus, BatchReactor, etc…)

Case 2: if you are using Simulis Thermodynamics Add-in (in Excel, Matlab, etc...)

The steps are the following:

- Step 1: Accessing the thermodynamic calculator editor
- Step 2: Selecting the compounds
- Step 3: Selecting the thermodynamic model
- Step 4: Calculation of the flash using the calculation service
- Step 5: Calculation of the flash in Excel (only for the "case 2", this step requiring to have Simulis Thermodynamics Excel Add-in)

Step 1: Accessing the thermodynamic calculator editor

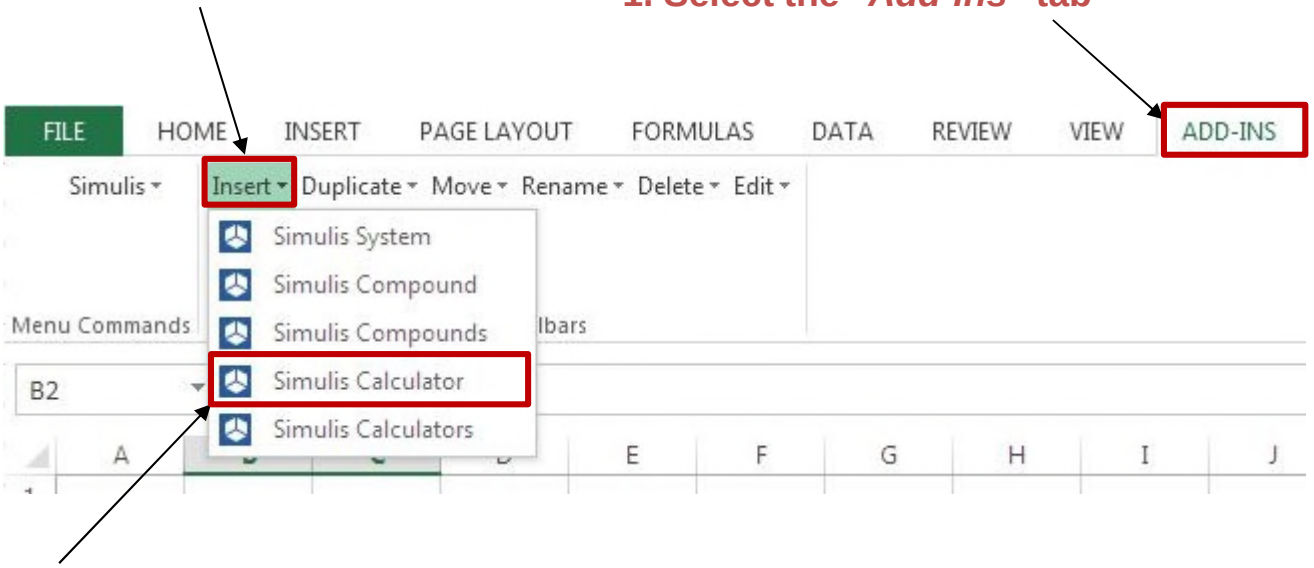
- **Case 1:** If you are using Simulis Thermodynamics within ProSim environment (ProSimPlus, BatchReactor, BatchColumn etc…):

Click on the thermodynamic icon to open the calculator editor:  **or** 

- **Case 2:** If you are using Simulis Thermodynamics in Excel

2. Click on the *"Insert"* menu

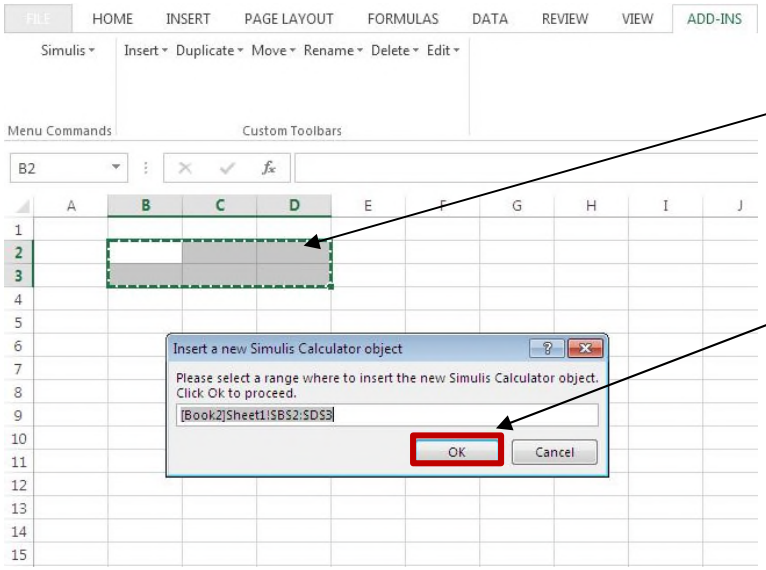
1. Select the *"Add-Ins"* tab



3. Select the *"Simulis Calculator"* object

Step 1: Accessing the thermodynamic calculator editor

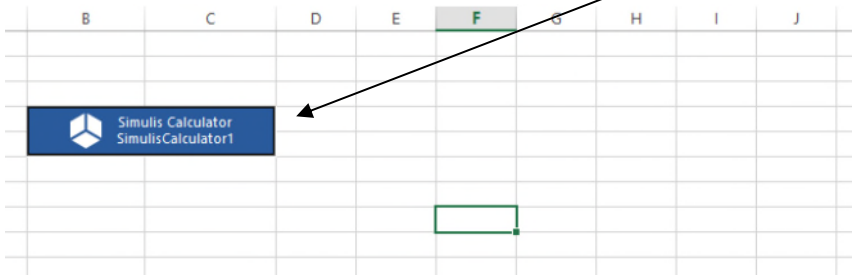
- **Case 2:** If you are using Simulis Thermodynamics in Excel



4. Select the cells in which will be inserted the *Simulis Calculator* object

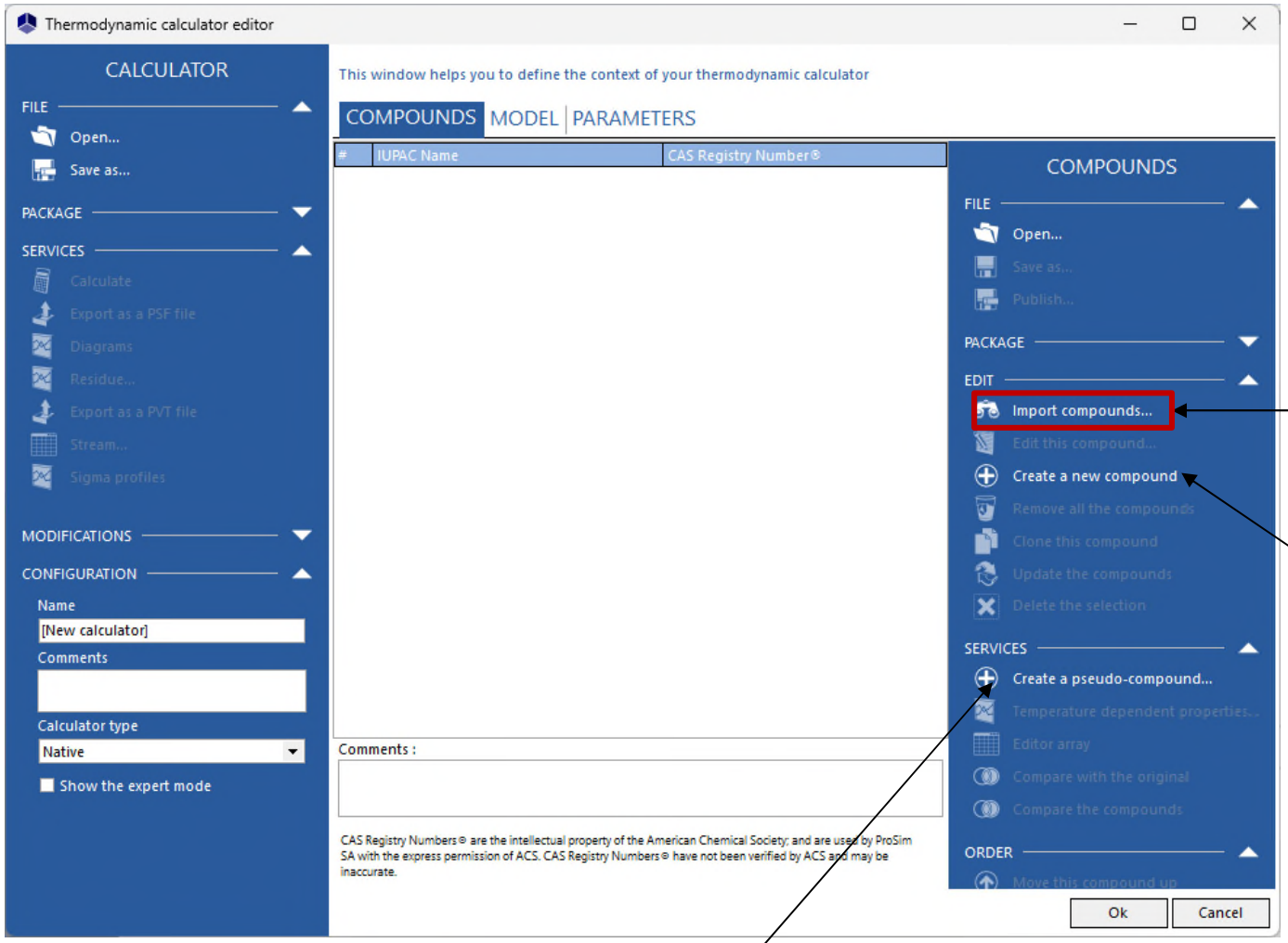
5. Click on *"OK"*

6. A new *Simulis Calculator* object is created. Click on it to access the calculator editor



You can insert multiple Simulis objects in the same spreadsheet

Step 2: Selecting your compounds



1. Click on "*Import compounds*" to import the compounds of your system from the available databases

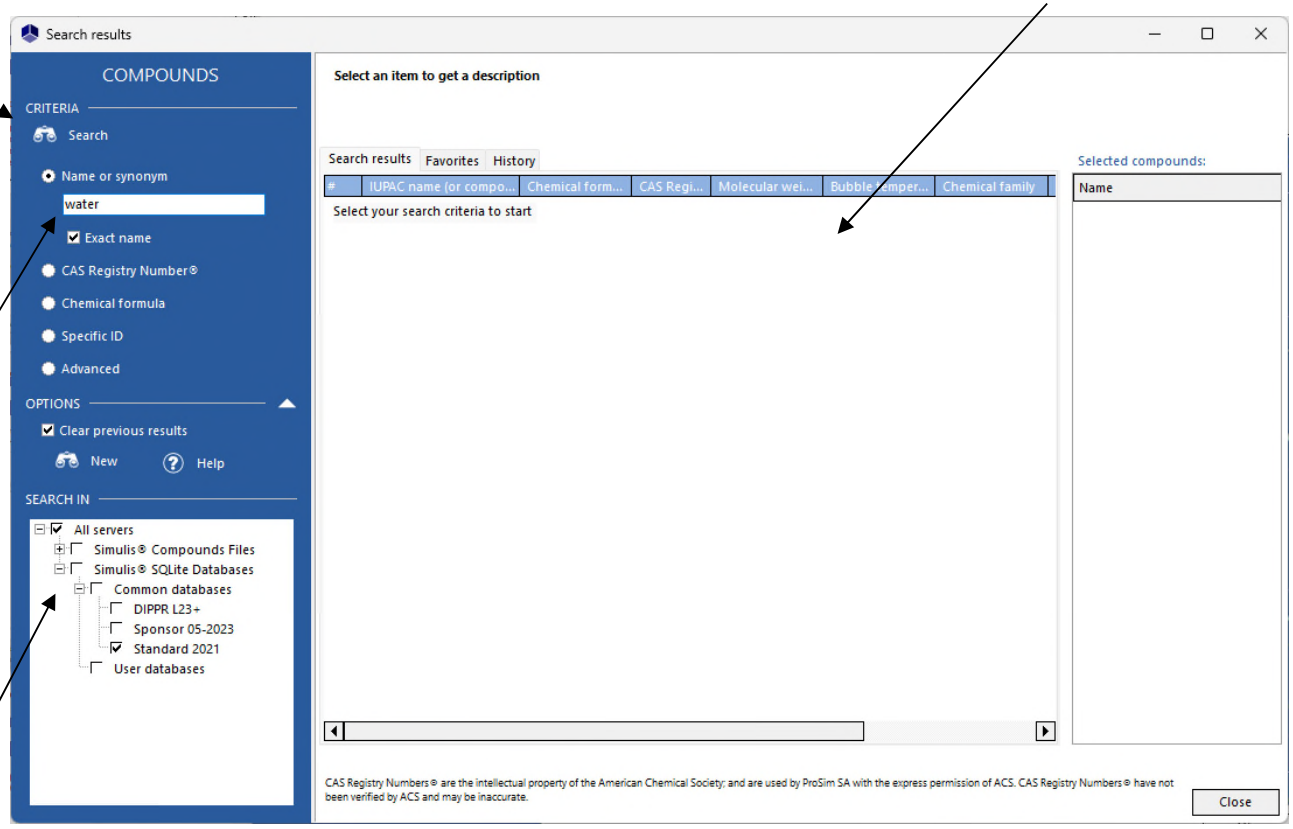
To create new compounds, please consult "*Getting Started with Simulis Thermodynamics, use case 9*"

To create pseudo-compounds corresponding to a petroleum cut, please consult "*Getting Started with Simulis Thermodynamics, use case 5*"

Step 2: Selecting 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



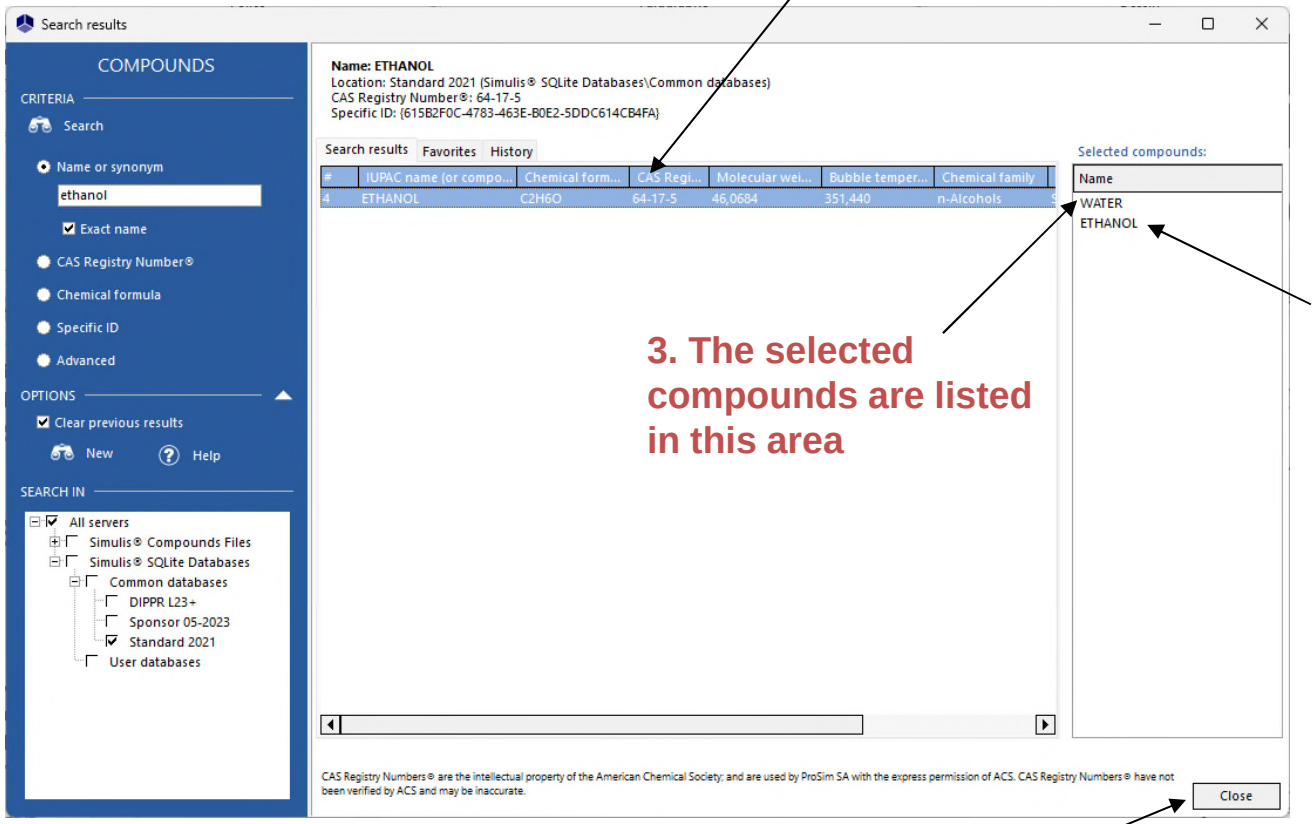
2. You have access to multiple search criteria (in this example, search "*Water*" by name)

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 2: Selecting your compounds

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

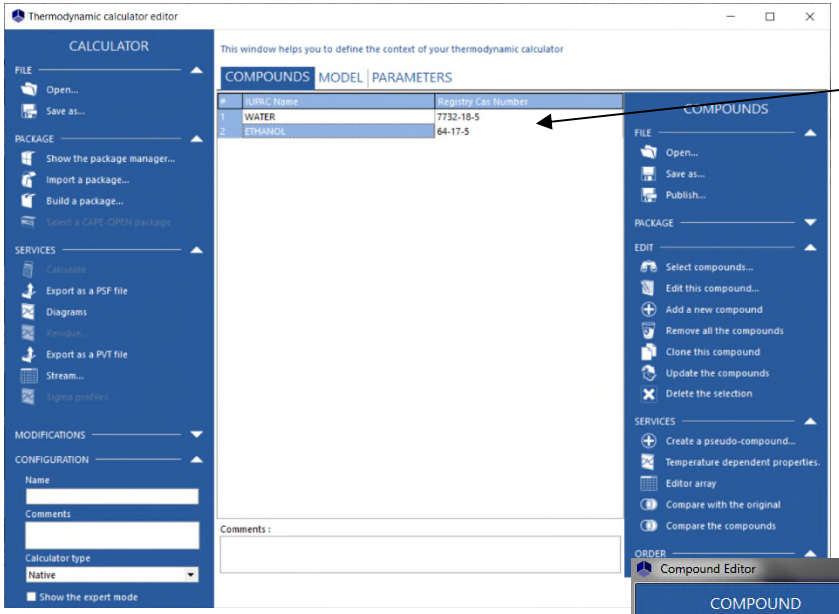


2. Repeat this operation for the other compound (Ethanol)

3. The selected compounds are listed in this area

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

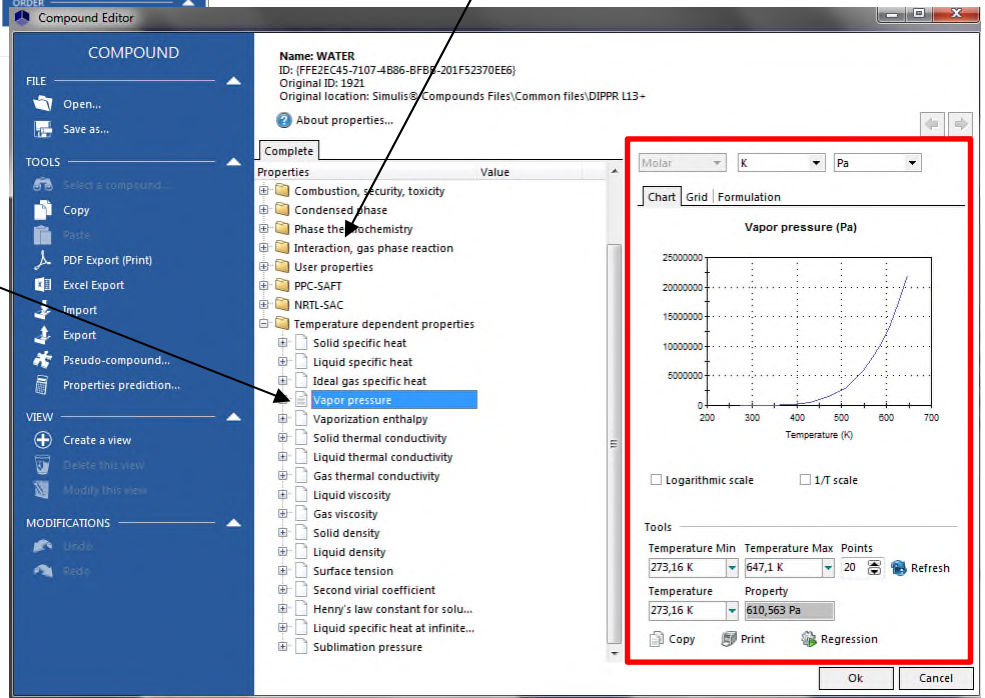
Step 2: Selecting your compounds



1. Double click on a compound to access the compound editor

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

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

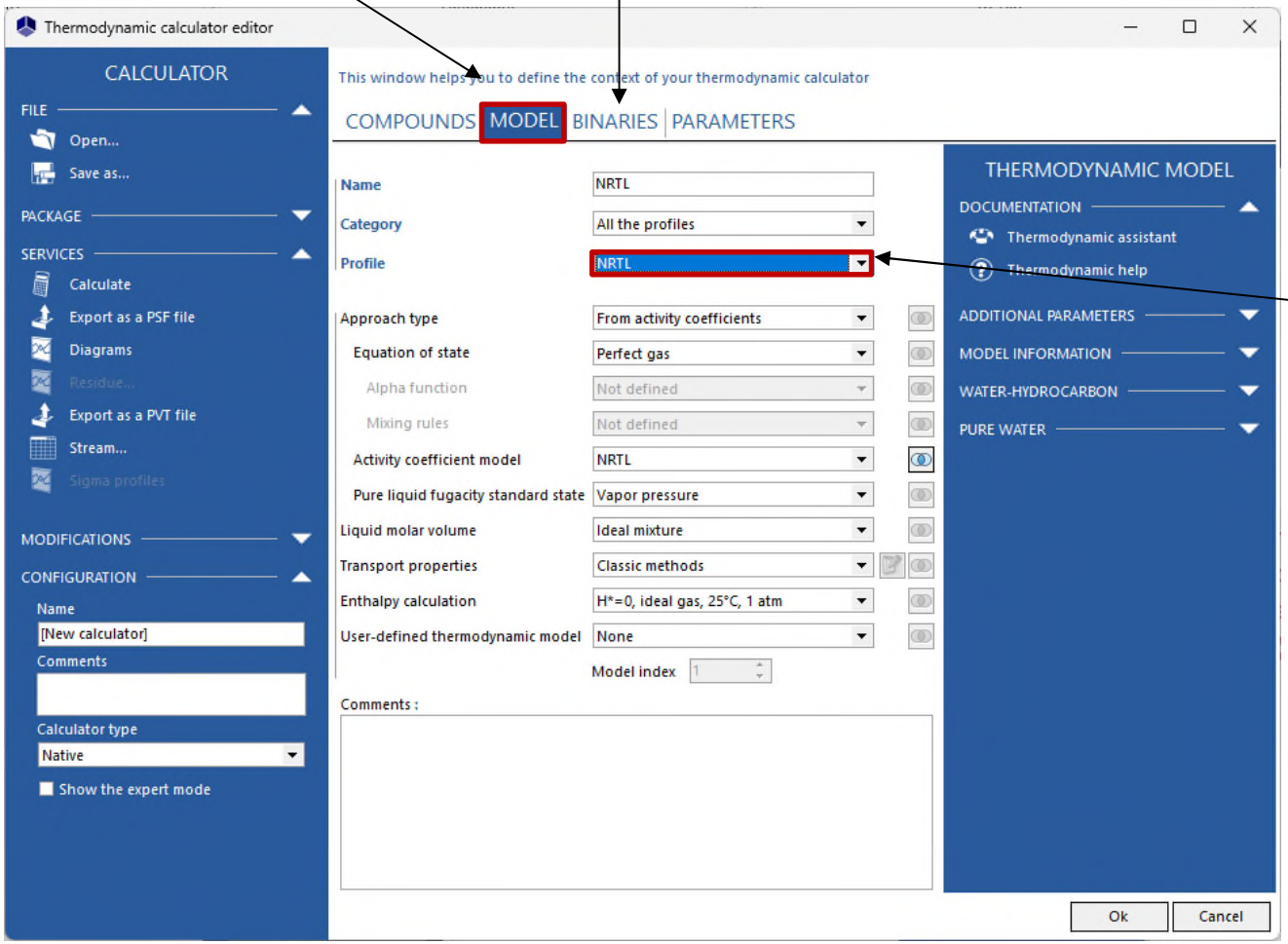


For more details about pure components properties, please consult "*Getting started with Simulis Thermodynamics, use case 4*"

Step 3: Selecting 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

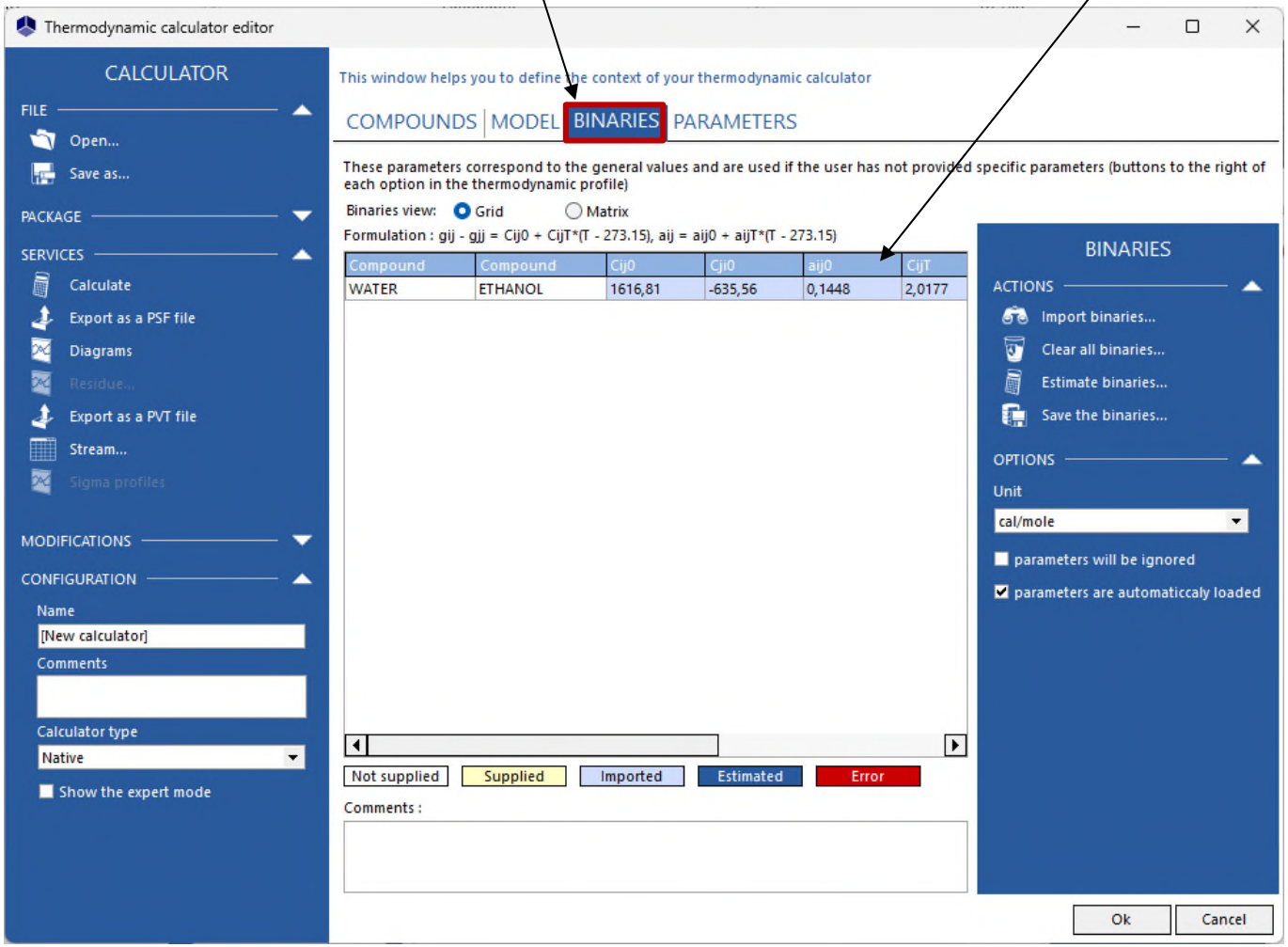


2. Select the thermodynamic profile (in this example, select "*NRTL*")

Step 3: Selecting the thermodynamic model

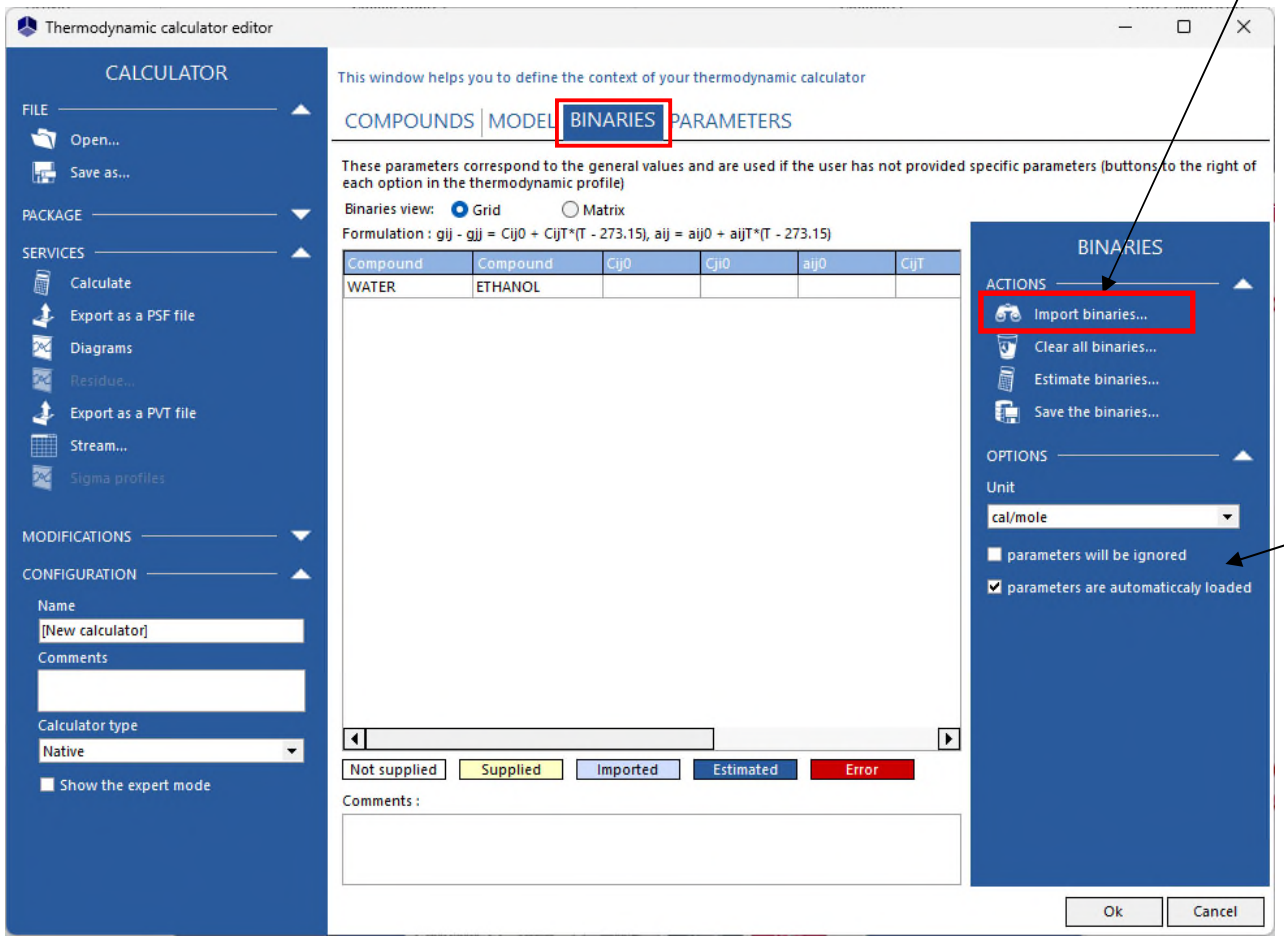
1. Click on the *"Binaries"* tab to enter the binaries search window (if required by the model)

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



Step 3: Selecting 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

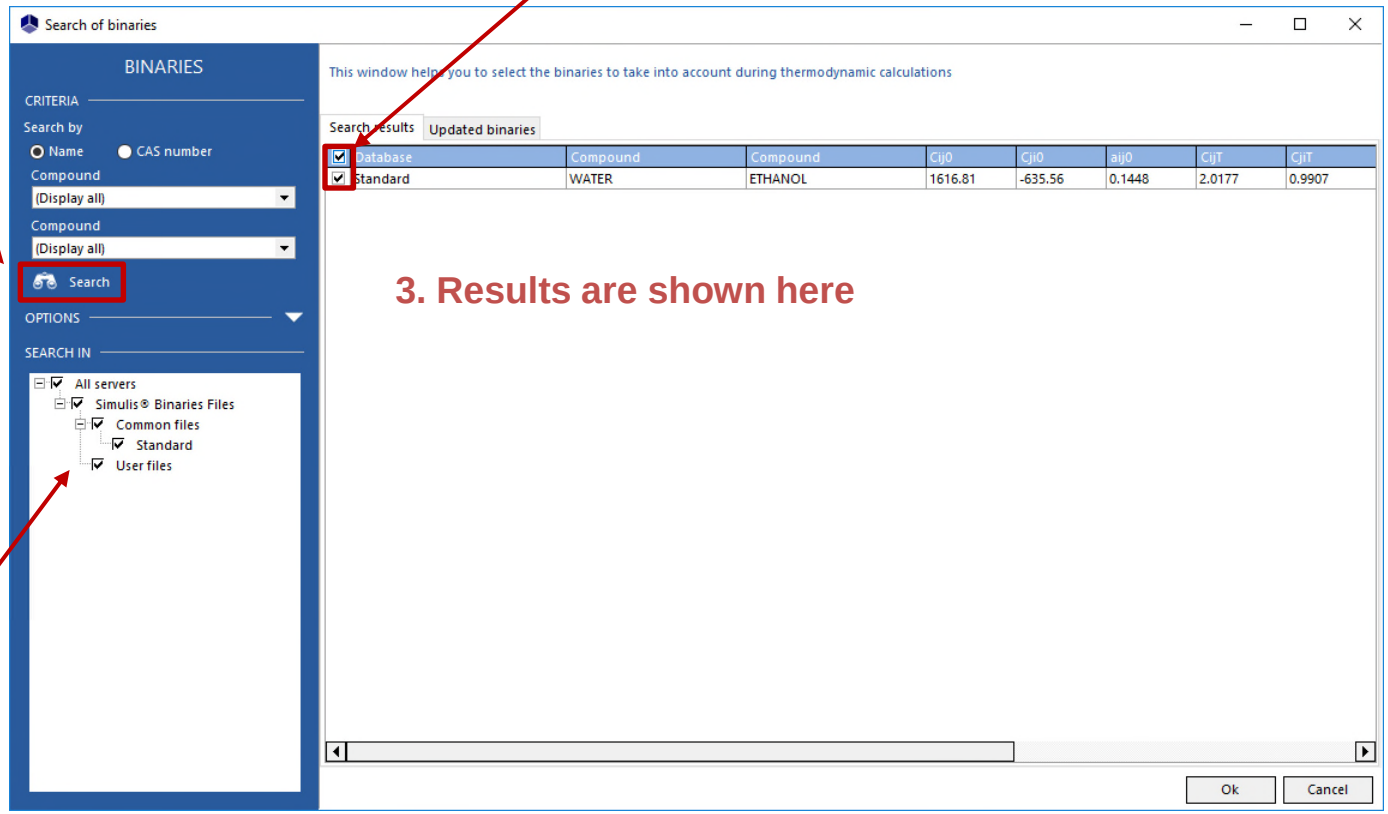


Automatic load is not activated

Step 3: Selecting the thermodynamic model

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

2. Click on *"Search"*

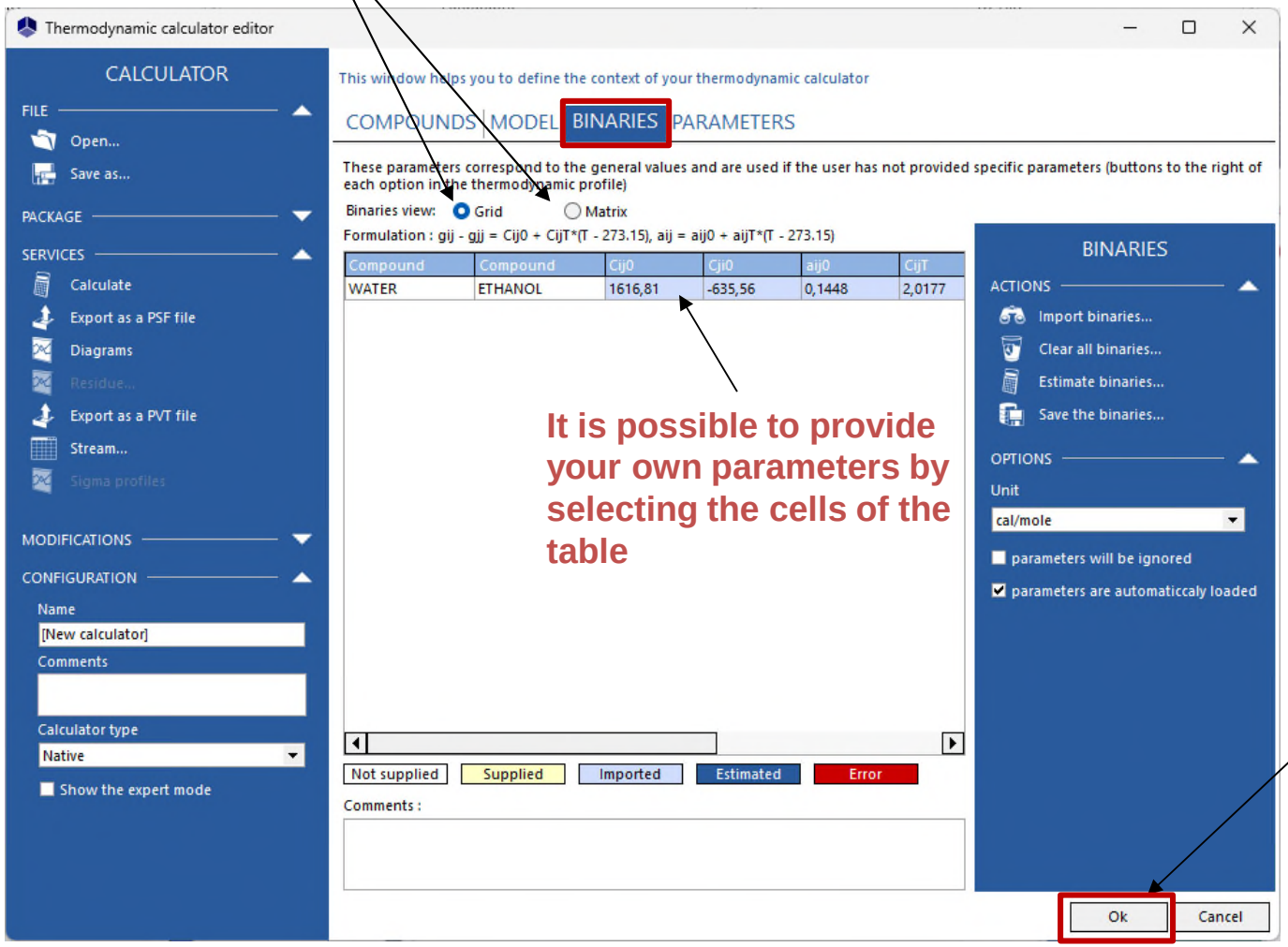


3. Results are shown here

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

Step 3: Selecting the thermodynamic model

It is possible to display the binaries as a grid or a matrix

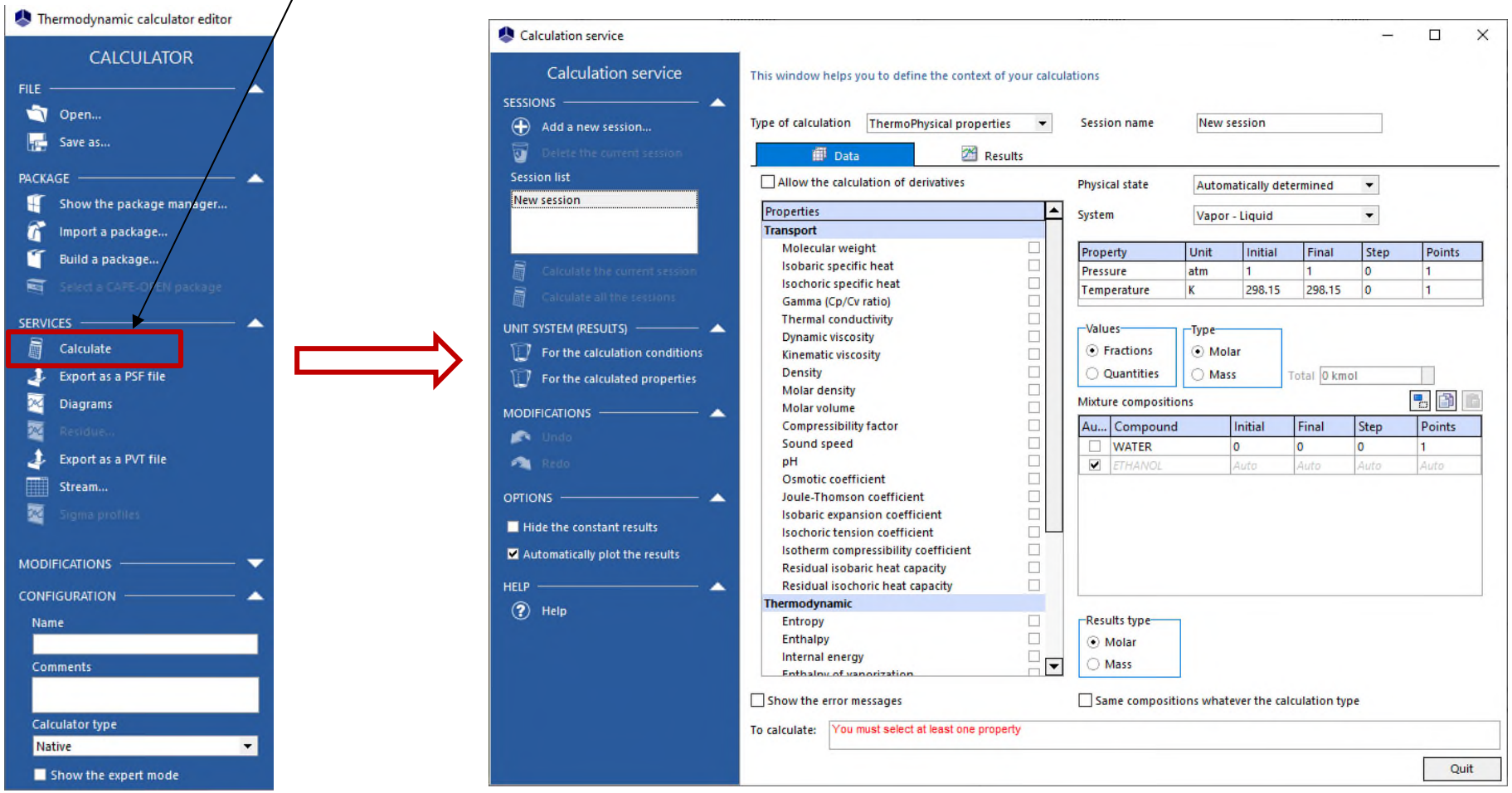


It is possible to provide your own parameters by selecting the cells of the table

Click on *"OK"* to validate your inputs and return to the main application (ProSim software, Excel, etc...)

Step 4: Calculation of the TP flash using the calculation service

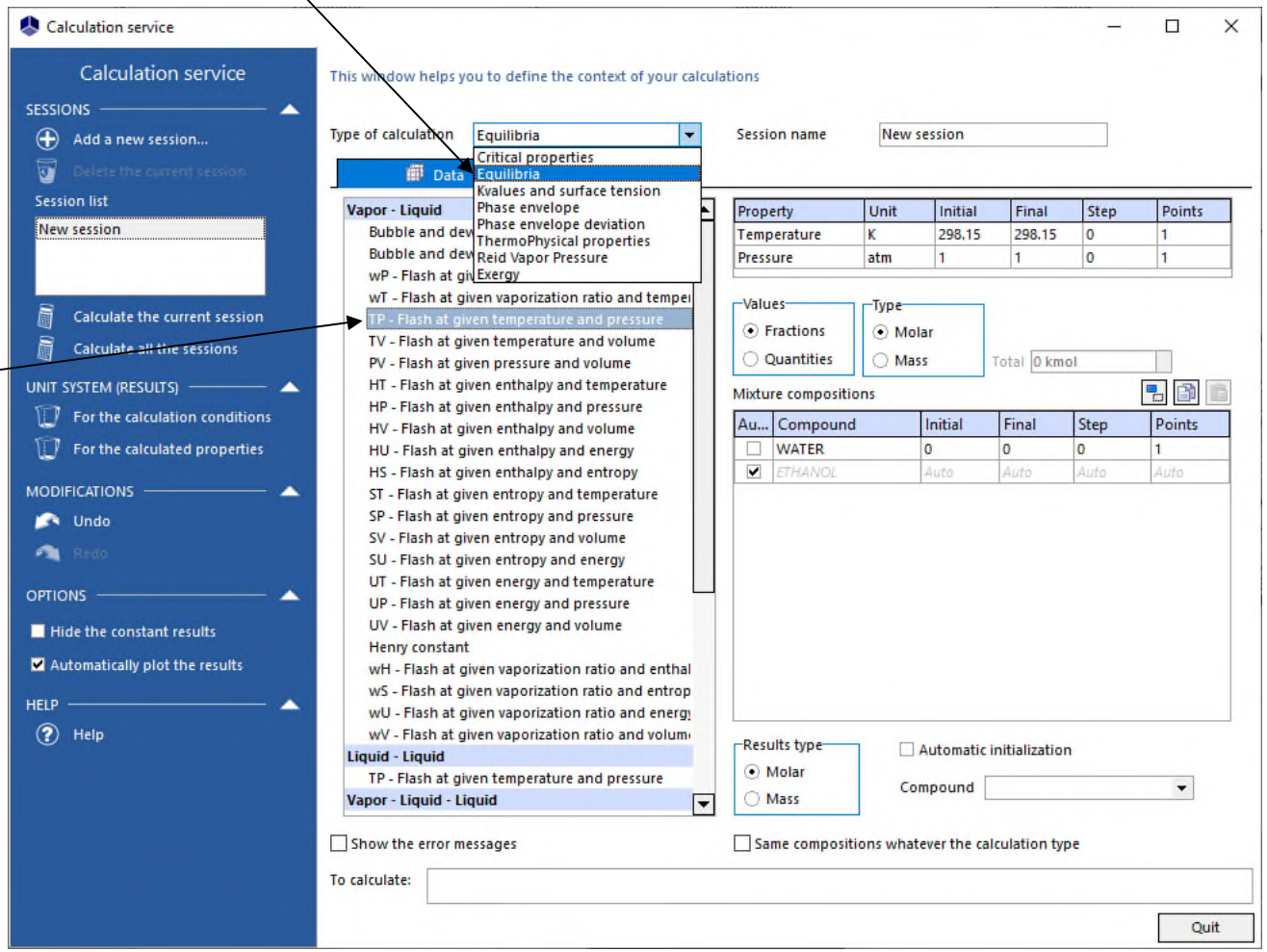
To access the calculation service: open the calculator editor and click on "*Calculate*"



Step 4: Calculation of the TP flash using the calculation service

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, "*flash at given temperature and pressure*")



Step 4: Calculation of the TP flash using the calculation service

1. Specify the operating conditions:

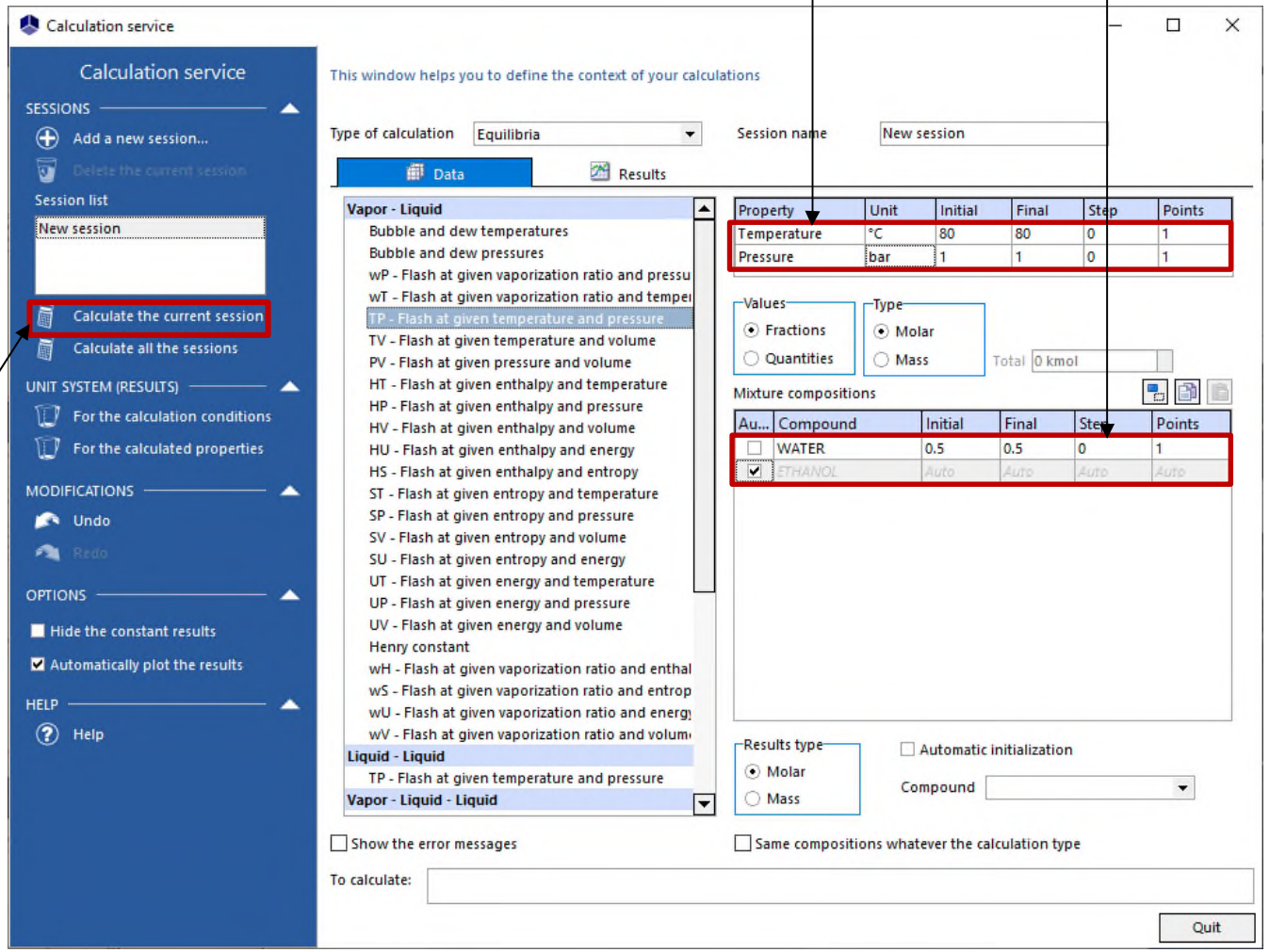
Pressure: 1 bar

Temperature: 80°C

Mixture composition:

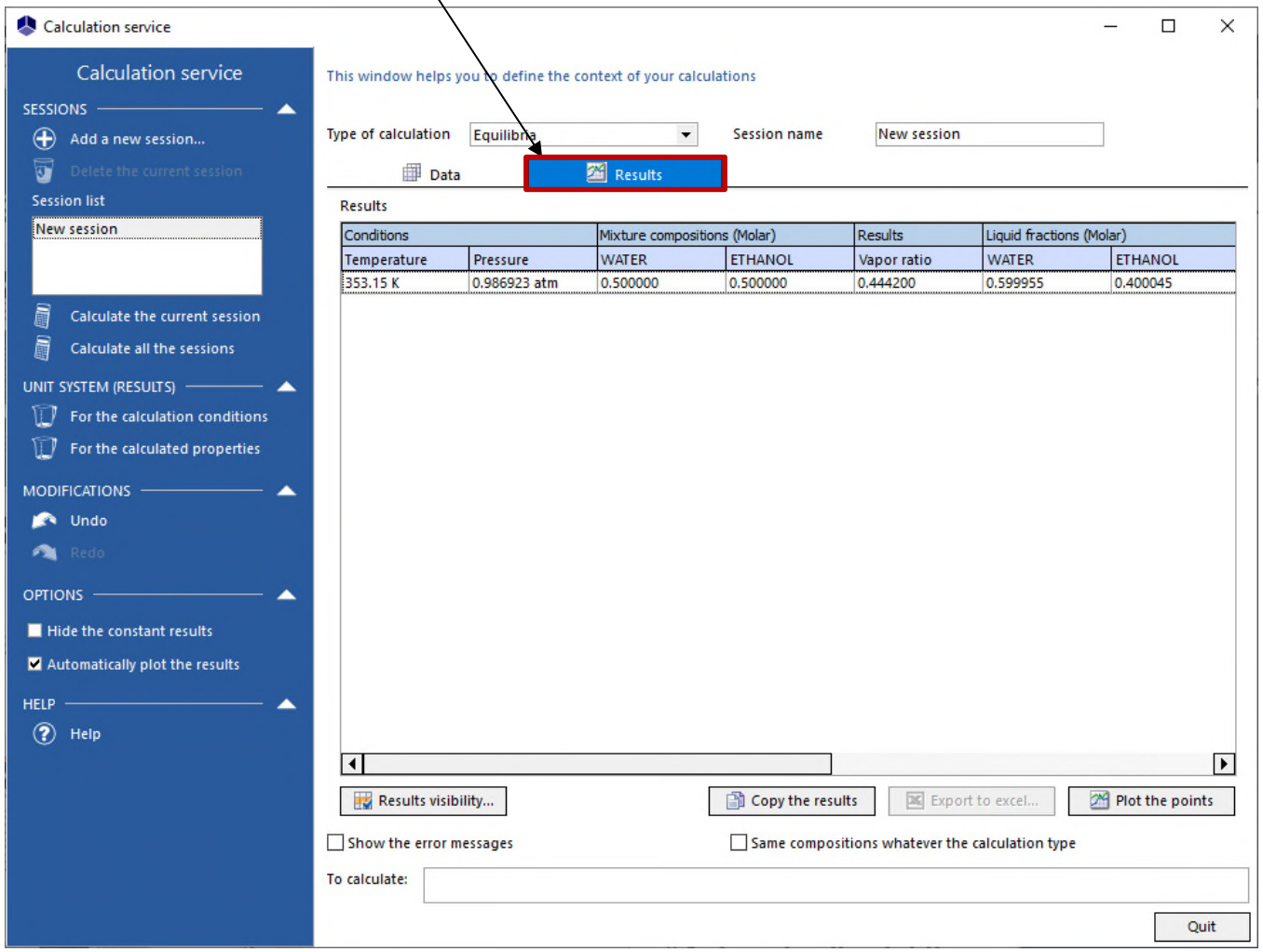
- 50% mol of Ethanol
- "Auto" for Water (in order to get a global composition of 100%)

2. Click on "*Calculate the current session*"



Step 4: Calculation of the TP flash using the calculation service

The results are displayed as a table in the "*Results*" tab



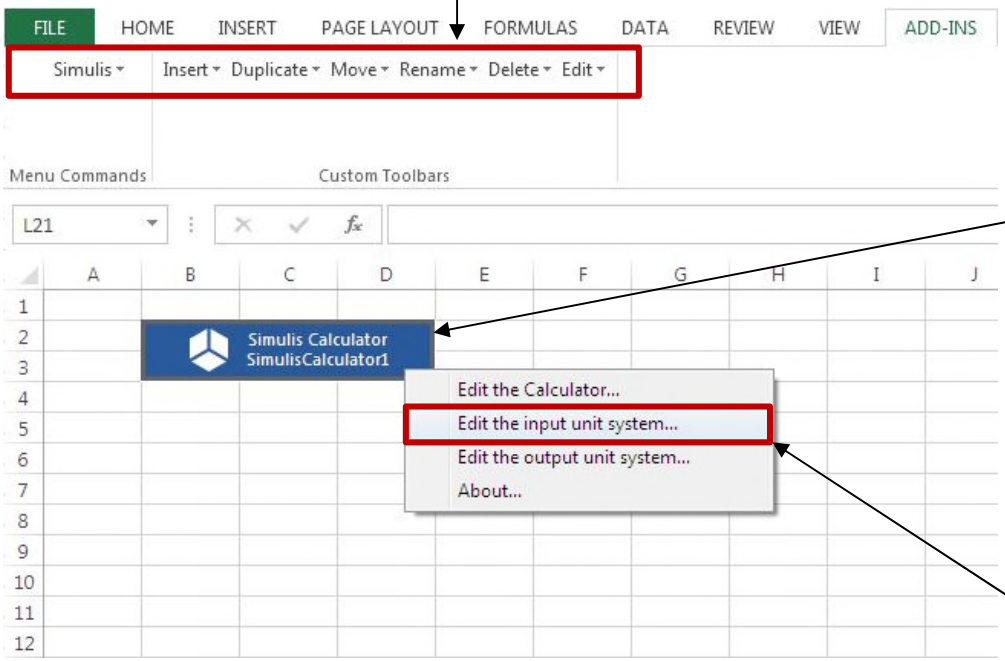
For more details about mixture properties calculation, please consult "*Getting started with Simulis Thermodynamics, use case 4*"

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

Only in the case 2: if you are using Simulis Thermodynamics in Excel

Features of Simulis Thermodynamics Excel Add-in are accessible from the main toolbars



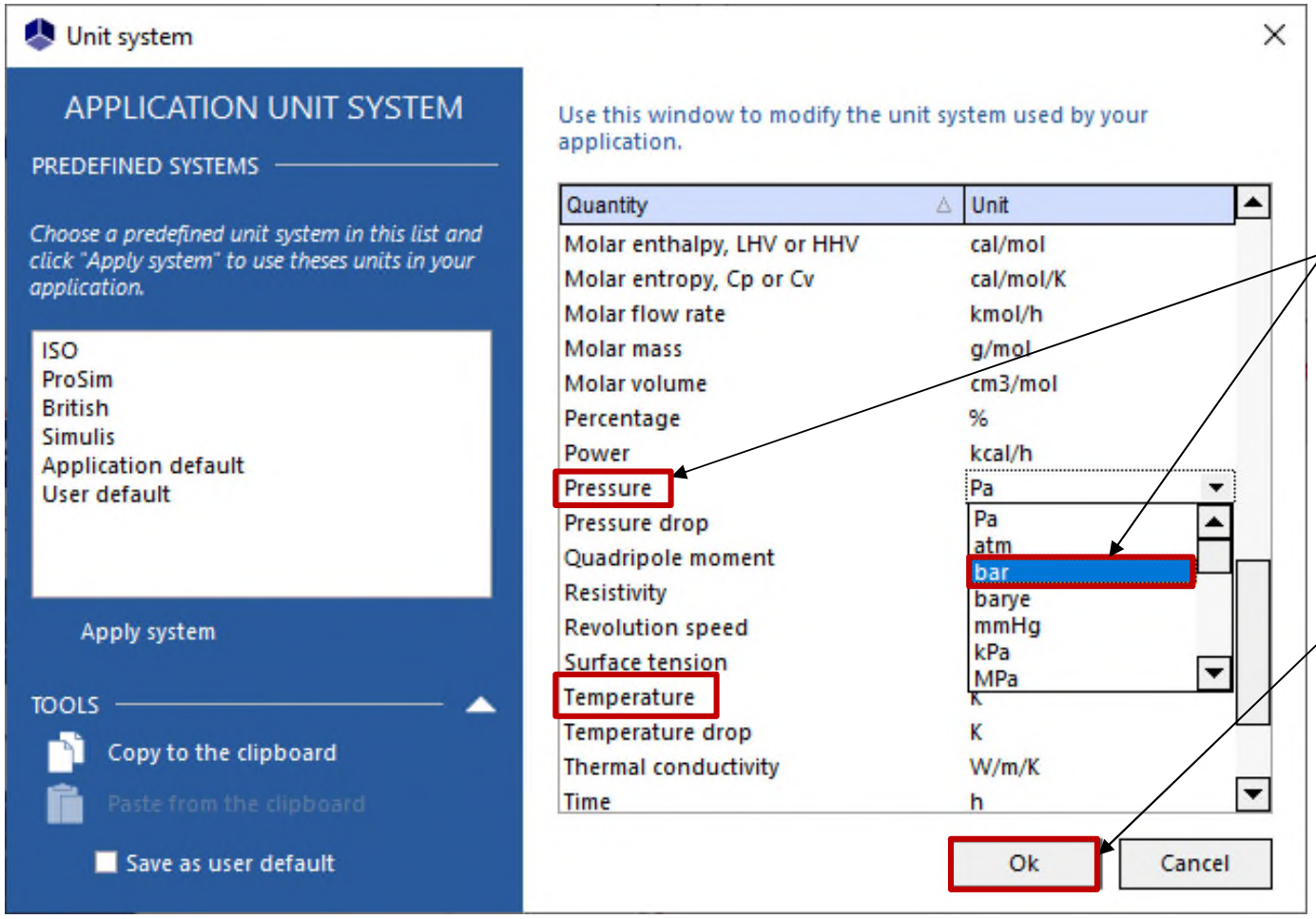
1. Right click on the *Simulis Calculator* object

2. Select *"Edit the input unit system"* to customize the input unit system

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

The default units system is in “Pa” and “K”, but the input data provided in this example are in “bar” and “°C”. Therefore, you need to adapt the unit system to avoid any conversion calculation.



1. Scroll down to find “*Pressure*”, then select “*Pa*” and change it to “*bar*”

2. Repeat the operation for the temperature (replace “*K*” by “*°C*”)

3. Press “*OK*” to confirm

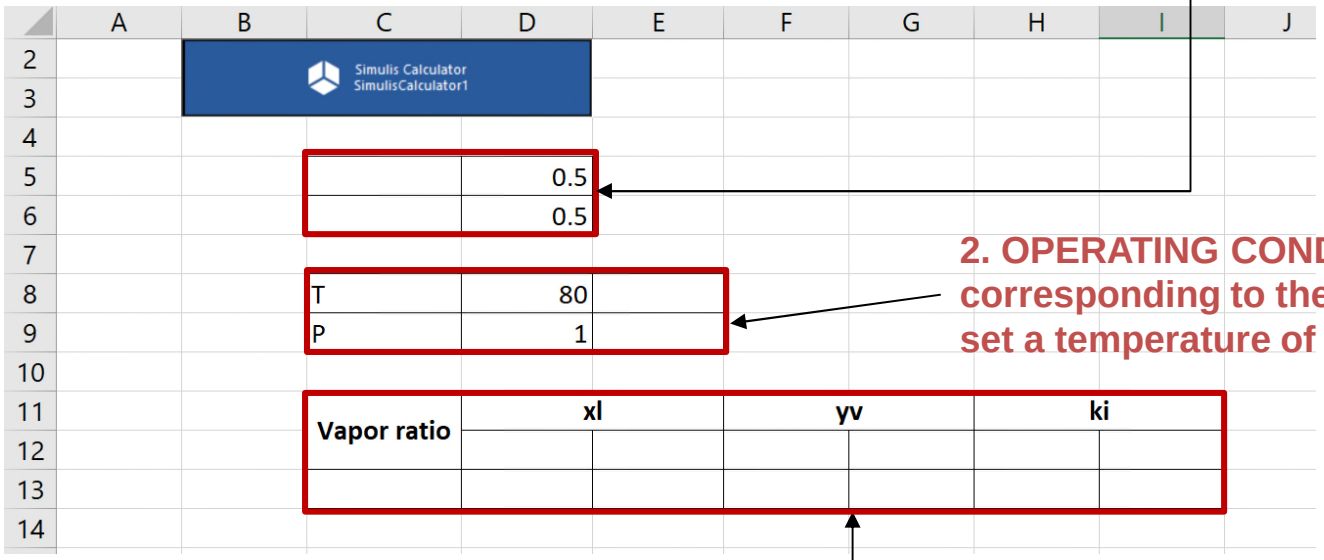
Both input and output units systems can be customized

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

Prepare your Excel spreadsheet by providing the input data and the table where the results will be displayed:

1. COMPOSITION: prepare the table corresponding to the input composition (in this example, set a composition of 50% mol Water and 50% mol Ethanol)



2. OPERATING CONDITIONS: Prepare the table corresponding to the input data (in this example, set a temperature of 80°C and a pressure of 1 bar)

The empty cells will be filled by Simulis Thermodynamics functions

3. RESULTS: Prepare the table corresponding to the results:

- **Vapor ratio: range of 1 cell**
- **Liquid composition (xl): range of 2 cells**
- **Vapor composition (yv): range of 2 cells**
- **Equilibrium constants (ki): range of 2 cells**

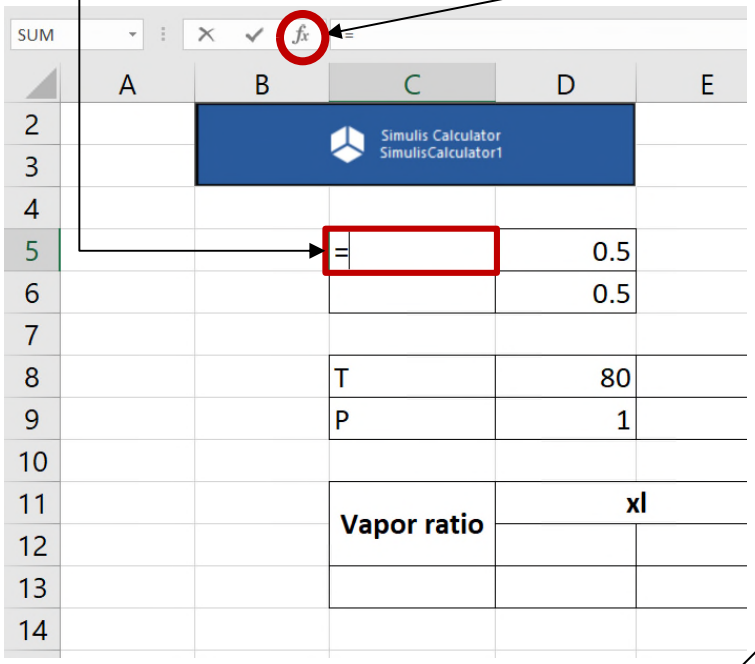
Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

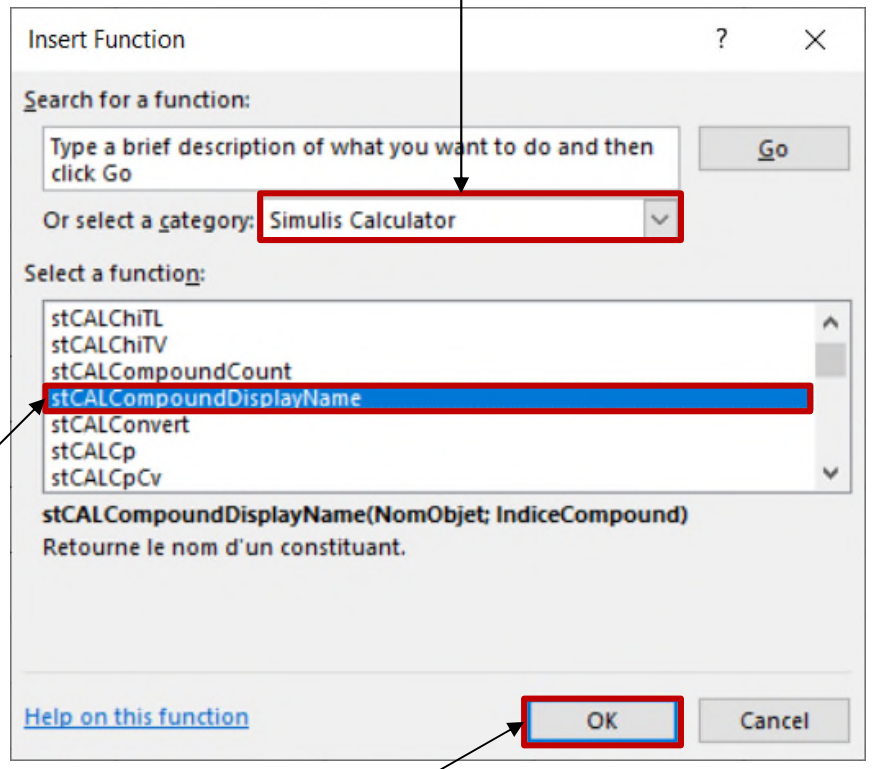
Use the Simulis function to display the name of the compounds in the spreadsheet :

1. Select the first cell of the input composition table

2. Click on "*fx*" to insert a function



3. Choose the "*Simulis Calculator*" set of functions

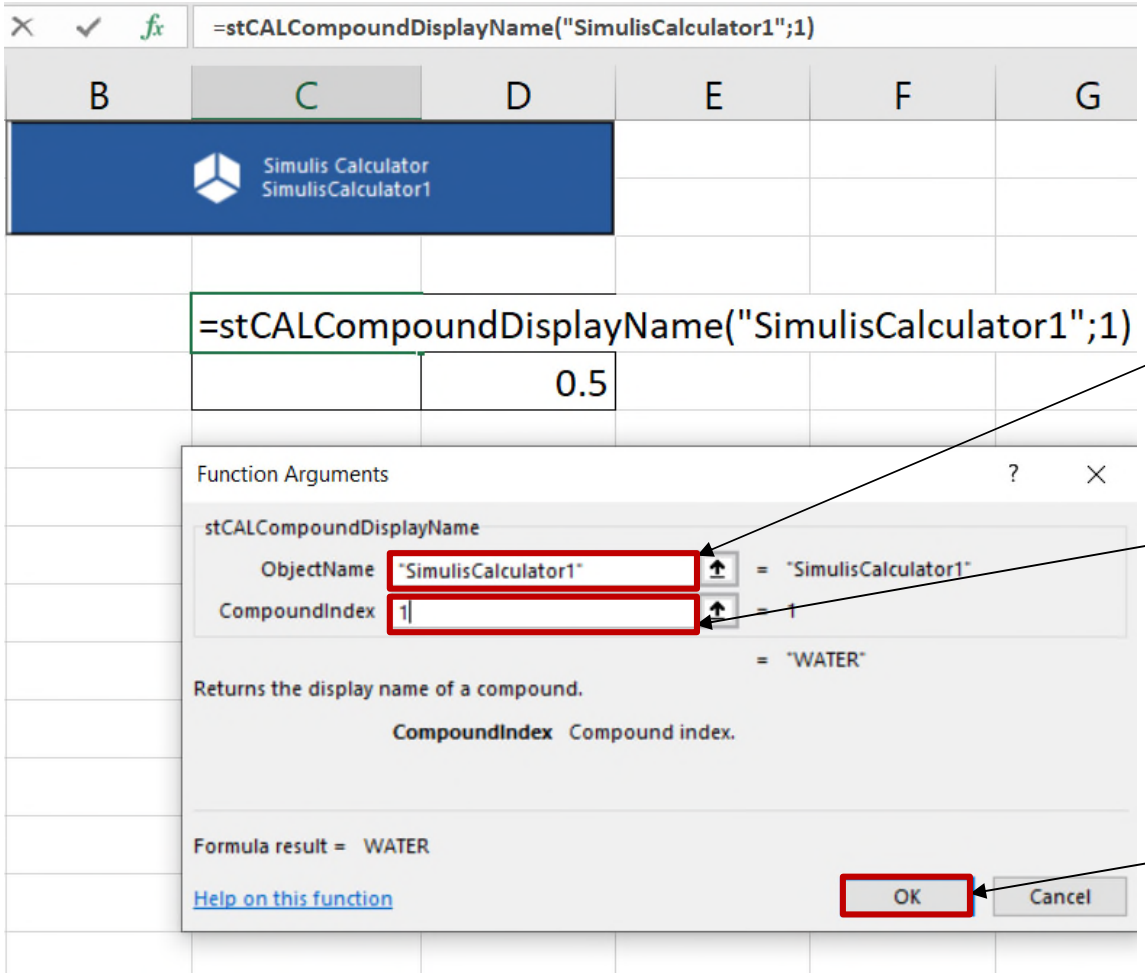


4. Select "*stCALCompoundDisplayName*"

5. Click on "*OK*" to confirm and enter the function arguments window

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)



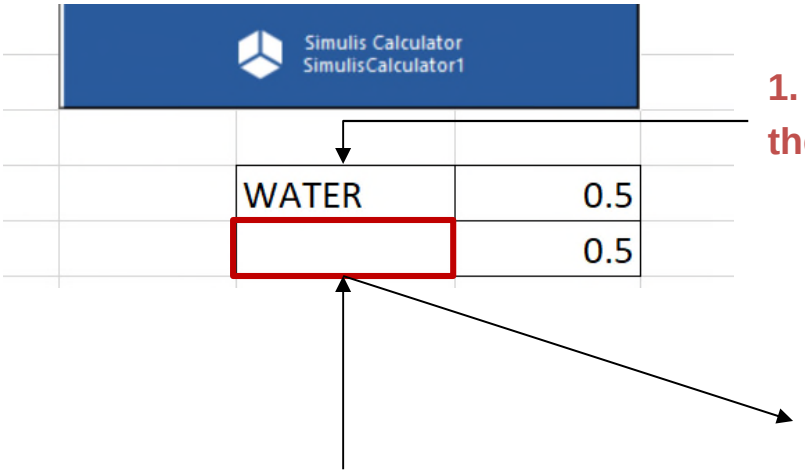
1. Enter the name of the Simulis Object that you want to use (in this example, "*SimulisCalculator1*")

2. Enter the compound index which is based on the list of compounds imported in the calculator (in this example, enter "*1*" corresponding to the first compound of the list)

3. Click on *"OK"* to confirm

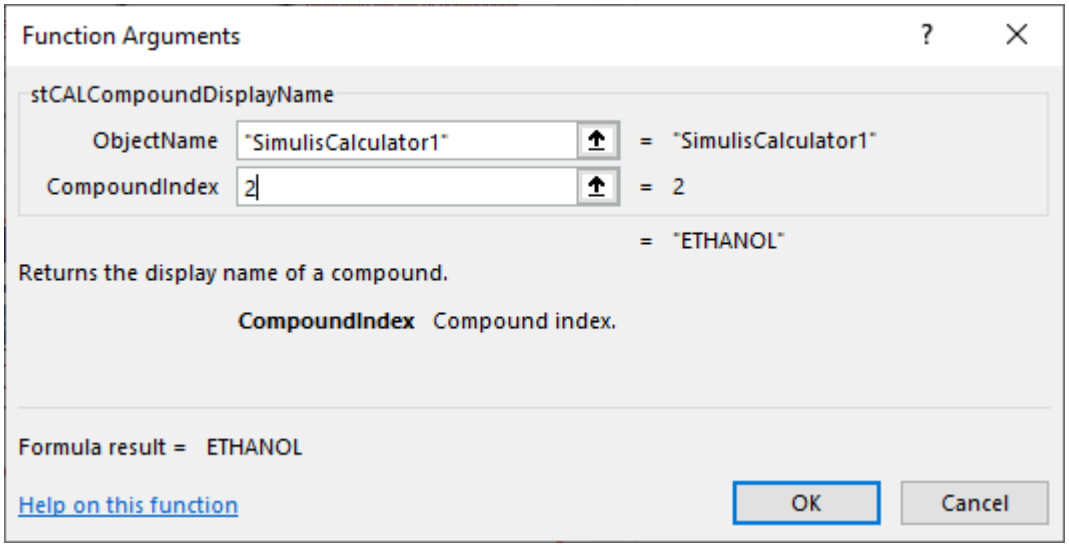
Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

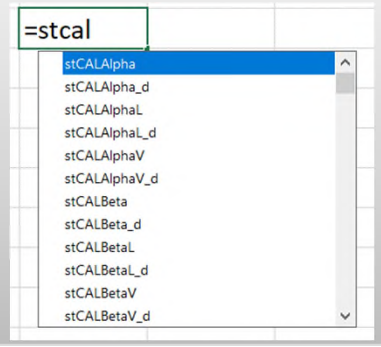


1. The name of the first compound (Water) is now displayed in the table

2. Repeat the operation for the second compound (Ethanol). In this case, the compound index is "*2*"



Instead of selecting "*fx*", you can directly enter "*=stcal*" in a cell to display the list of functions available in the *Simulis Calculator* category. Scroll down to identify the function you want to use, then double click on it and click on "*fx*" to open the function arguments window.



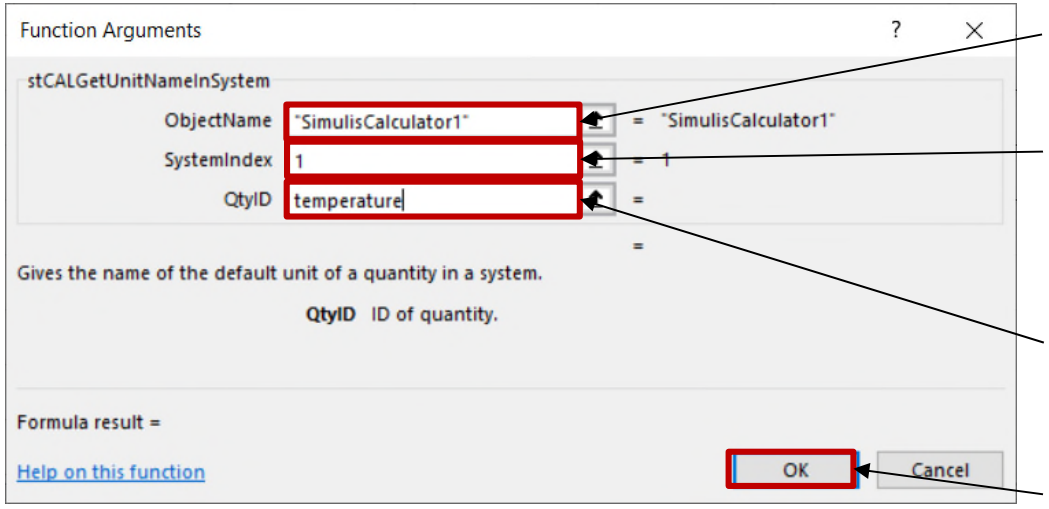
Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

Use the Simulis function to display the input units system for temperature and pressure :

	B	C	D	E	F	G	H	I	J	K
		Simulis Calculator SimulisCalculator1								
		WATER	0.5							
		ETHANOL	0.5							
		T	80	=stCALGetUnitNameInSystem("SimulisCalculator1";1;temperature)						
		P	1							

1. Select the function "*stCALGetUnitNameInSystem*"



2. Enter the name of the Simulis object (in this example, "*SimulisCalculator1*")

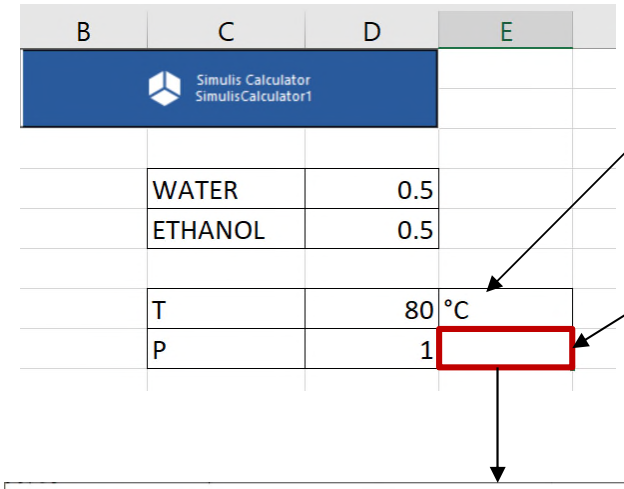
3. Enter the system index, *i.e.*, "*1*" for the input unit system or "*2*" for the output unit system (in this example, select "*1*")

4. Enter the quantity ID (in this example, "*temperature*")

5. Press "*OK*" to confirm

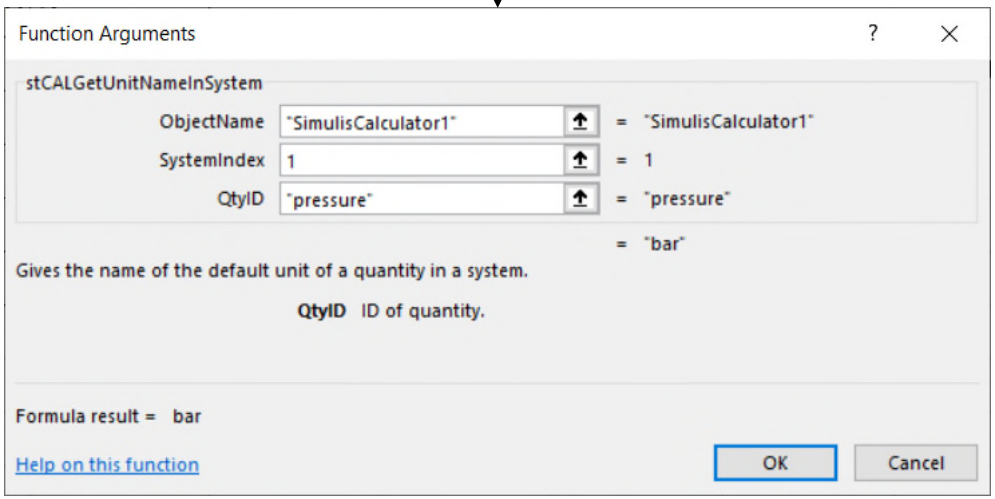
Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)



The input unit used for the temperature is now displayed

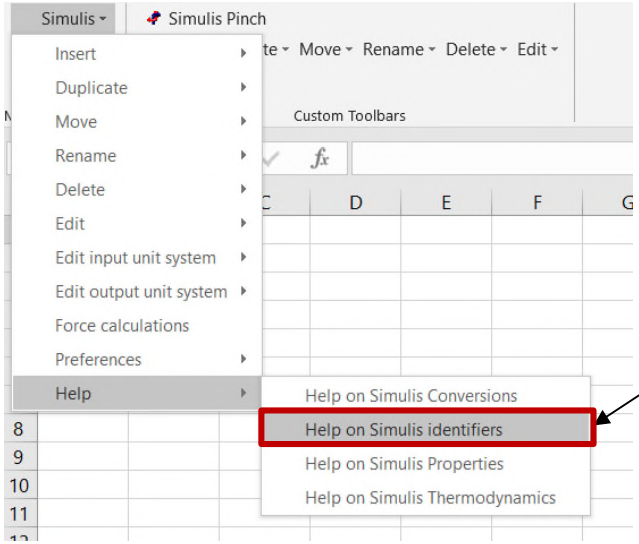
Repeat the operation to display the input unit used for the pressure. In this case, the quantity ID is "*pressure*"



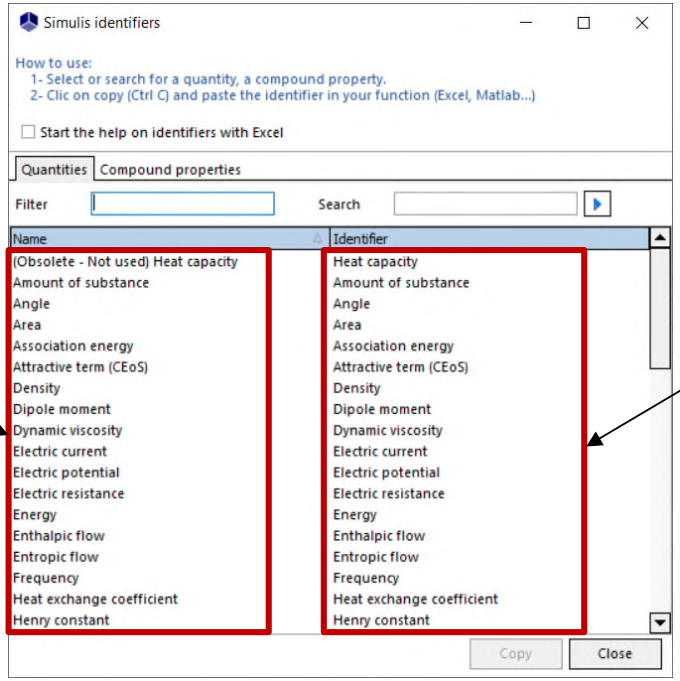
For a more flexible and efficient spreadsheet: it is recommended to enter the input arguments in the spreadsheet cells, and then select these cells from the function arguments window. Then, modifying input arguments in the cells automatically updates the results.

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)



In order to get the quantity ID, click on "*Help on Simulis Identifiers*", within the "*Help*" tab of "*Simulis*" menu



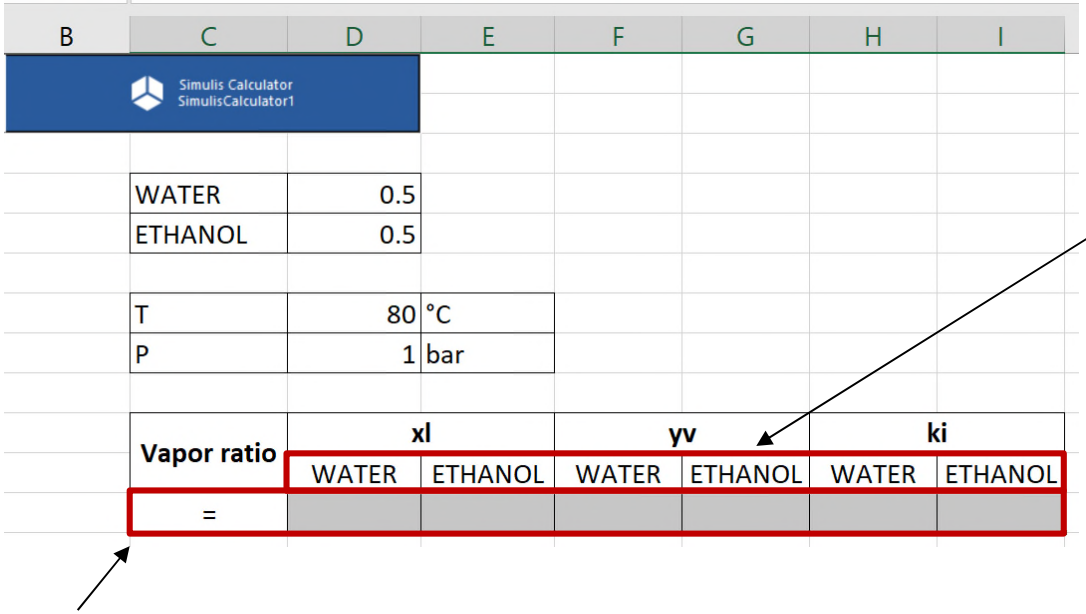
Quantity names

Quantity ID

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

Use the Simulis function to compute a vapor – liquid flash at given temperature and pressure



1. Copy and paste the function used previously to display the compounds name

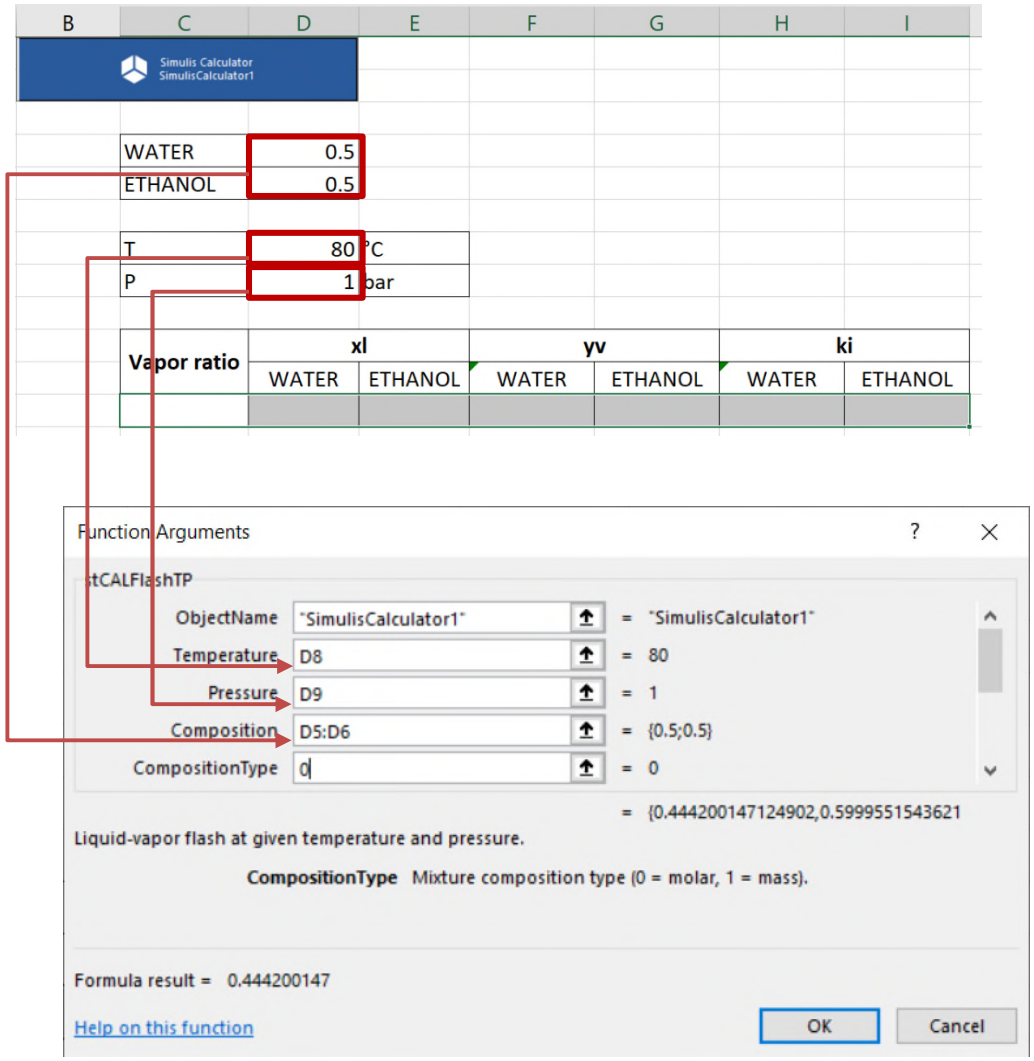
2. Select the range of cells corresponding to all the results that will be returned (in this example: vapor ratio, liquid composition, vapor composition and equilibrium constants)

3. Enter the name of the function: "*stCALFlashTP*" to open the function arguments window

Many Simulis functions return multiple results (corresponding to a vector). In this case, it is necessary to select a range of cells in Excel. The size of the range must be equivalent to the number of results to display.

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)



1. Enter the name of the Simulis Object (in this example, "*SimulisCalculator1*")

2. Select the cell with the input temperature

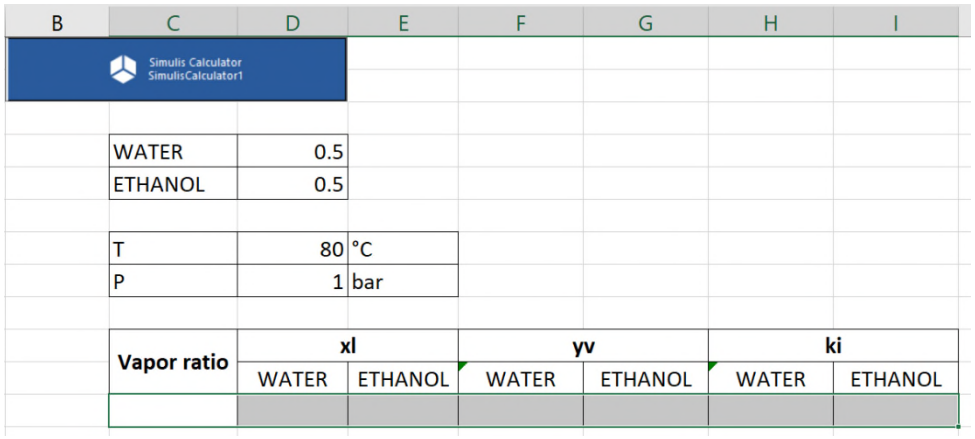
3. Select the cell with the input pressure

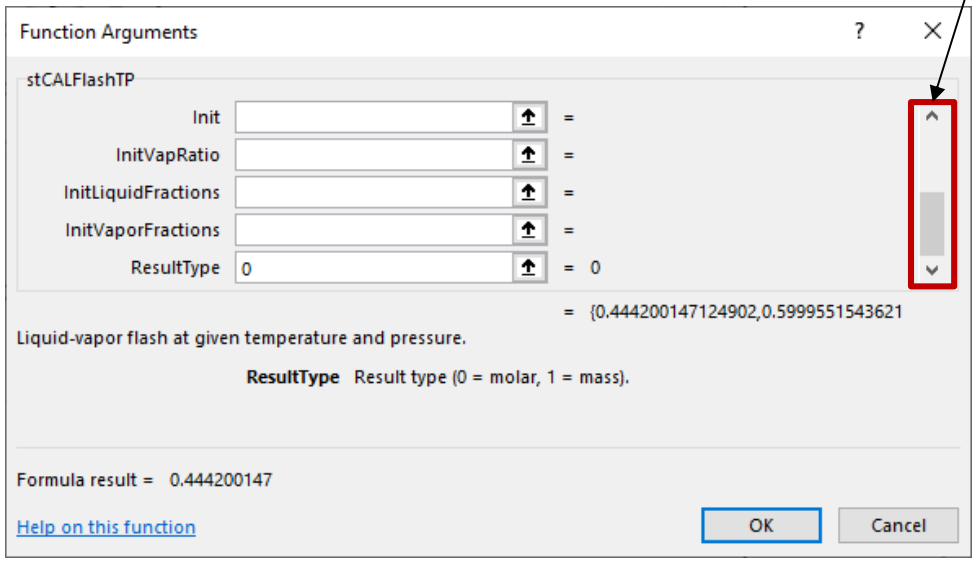
4. Select the range of cells with the input composition

5. Select the composition type (*i.e.*, "*0*" for molar or "*1*" for mass)

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)





6. Scroll down to access the other function arguments

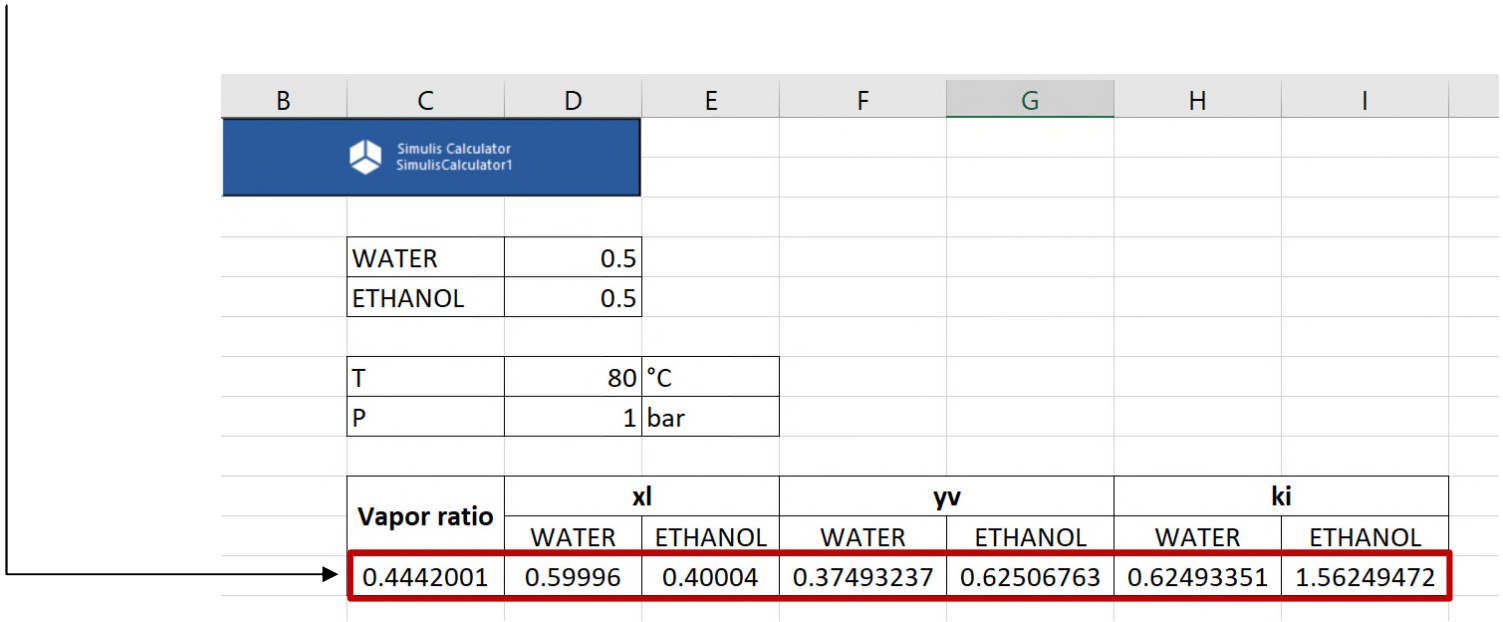
7. You have the possibility to provide initialization values. In this example, keep these arguments blank

8. Once you have provided all the function arguments, press simultaneously "*CTRL+SHIFT+ENTER*" to return a vector in Excel (pressing "*OK*" would only return the first result of the vector)

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

The vapor – liquid flash results are displayed in the spreadsheet



Simulis Calculator
SimulisCalculator1

WATER	0.5	
ETHANOL	0.5	

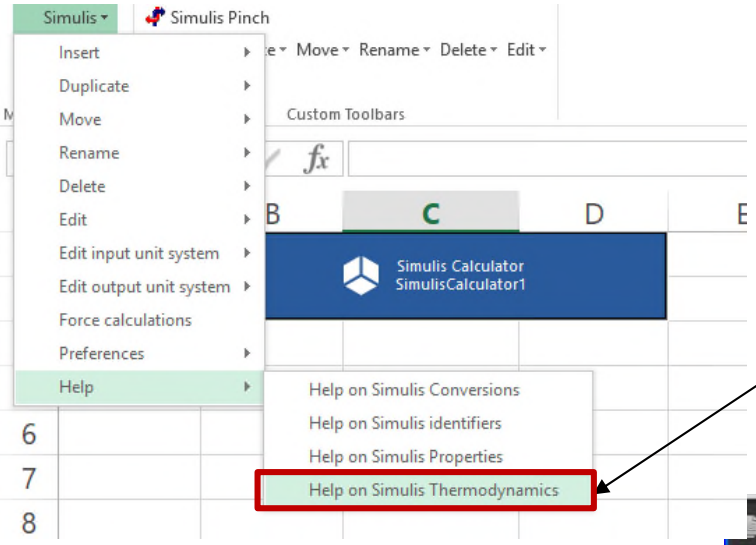
T	80	°C
P	1	bar

Vapor ratio	xl		yv		ki	
	WATER	ETHANOL	WATER	ETHANOL	WATER	ETHANOL
0.4442001	0.59996	0.40004	0.37493237	0.62506763	0.62493351	1.56249472

If you change the operating conditions (*i.e.*, composition, pressure or temperature), the results are automatically updated.

Step 5: Calculation of the TP flash in Excel

(This step requires to have Simulis Thermodynamics Excel Add-in)

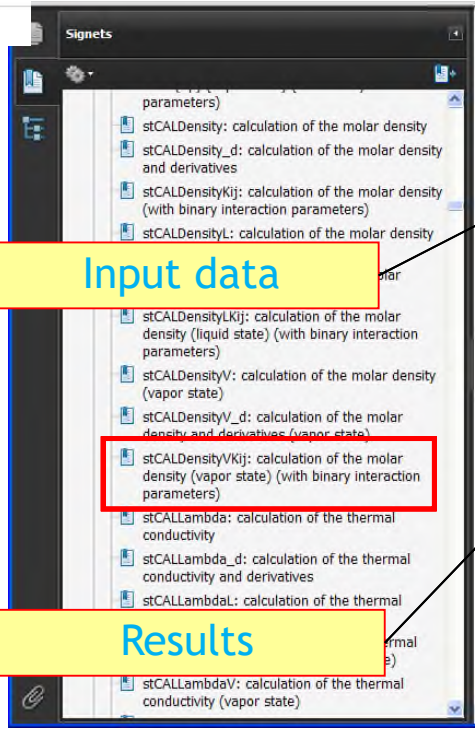


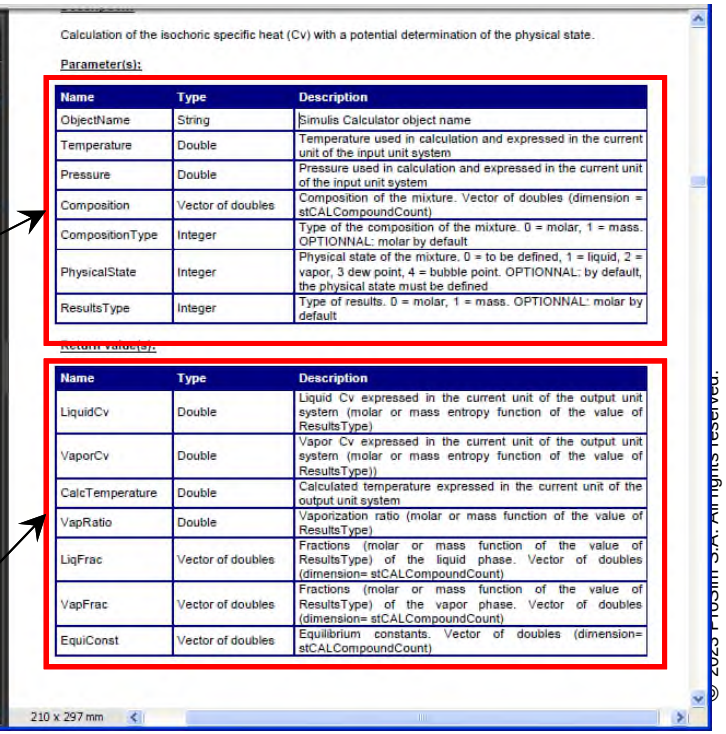
In order to know the input parameters and return values of any Simulis function, access the help file by selecting "*Help on Simulis Thermodynamics*", within the "*Help*" tab of the "*Simulis*" menu

For each function

Input data

Results





Calculation of the isochoric specific heat (Cv) with a potential determination of the physical state.

Parameter(s):

Name	Type	Description
ObjectName	String	Simulis Calculator object name
Temperature	Double	Temperature used in calculation and expressed in the current unit of the input unit system
Pressure	Double	Pressure used in calculation and expressed in the current unit of the input unit system
Composition	Vector of doubles	Composition of the mixture. Vector of doubles (dimension = stCALCompoundCount)
CompositionType	Integer	Type of the composition of the mixture. 0 = molar, 1 = mass. OPTIONNAL: molar by default
PhysicalState	Integer	Physical state of the mixture. 0 = to be defined, 1 = liquid, 2 = vapor, 3 dew point, 4 = bubble point. OPTIONNAL: by default, the physical state must be defined
ResultsType	Integer	Type of results. 0 = molar, 1 = mass. OPTIONNAL: molar by default

Return Value(s):

Name	Type	Description
LiquidCv	Double	Liquid Cv expressed in the current unit of the output unit system (molar or mass entropy function of the value of ResultsType)
VaporCv	Double	Vapor Cv expressed in the current unit of the output unit system (molar or mass entropy function of the value of ResultsType))
CalcTemperature	Double	Calculated temperature expressed in the current unit of the output unit system
VapRatio	Double	Vaporization ratio (molar or mass function of the value of ResultsType)
LiqFrac	Vector of doubles	Fractions (molar or mass function of the value of ResultsType) of the liquid phase. Vector of doubles (dimension= stCALCompoundCount)
VapFrac	Vector of doubles	Fractions (molar or mass function of the value of ResultsType) of the vapor phase. Vector of doubles (dimension= stCALCompoundCount)
EquiConst	Vector of doubles	Equilibrium constants. Vector of doubles (dimension= stCALCompoundCount)

ProSim

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