

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








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

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- **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:



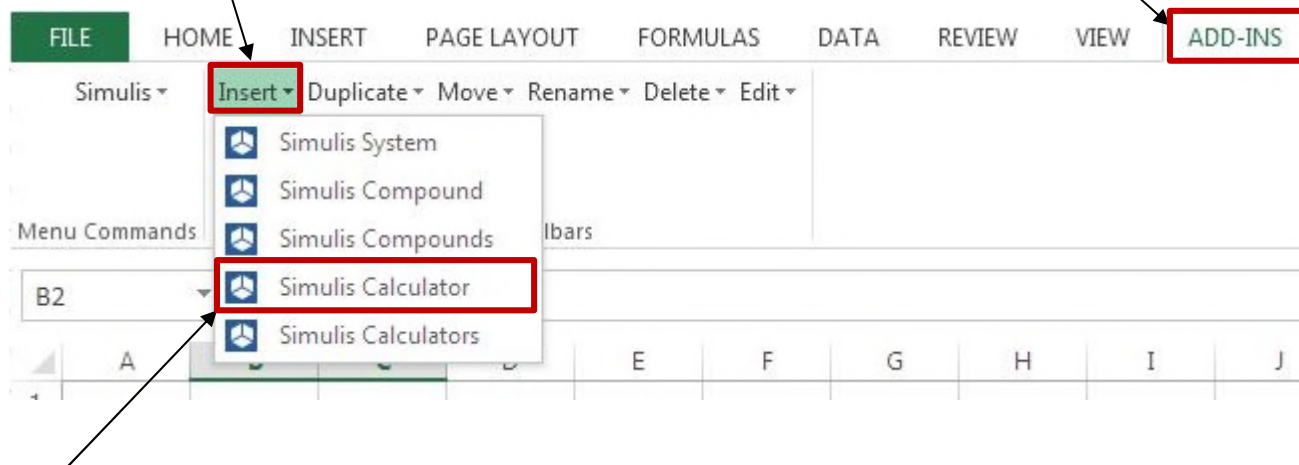
or



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

2. Click on the “*Insert*” menu

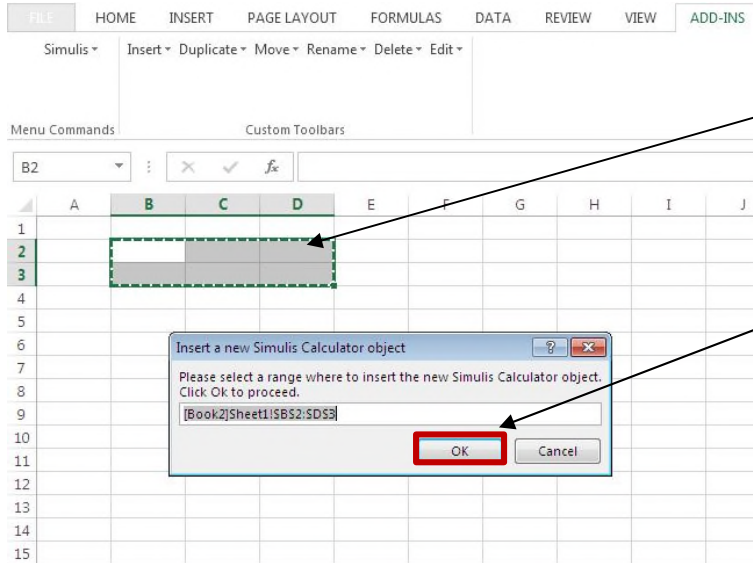
1. Select the “*Add-Ins*” tab



3. Select the “*Simulis Calculator*” object

Step 1: Accessing the thermodynamic calculator editor

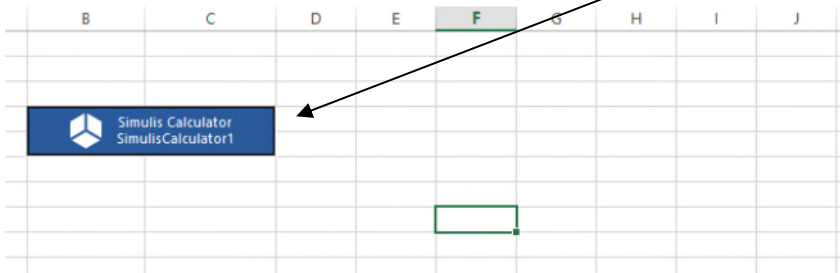
■ Case 2: If you are using Simulis Thermodynamics in Excel



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

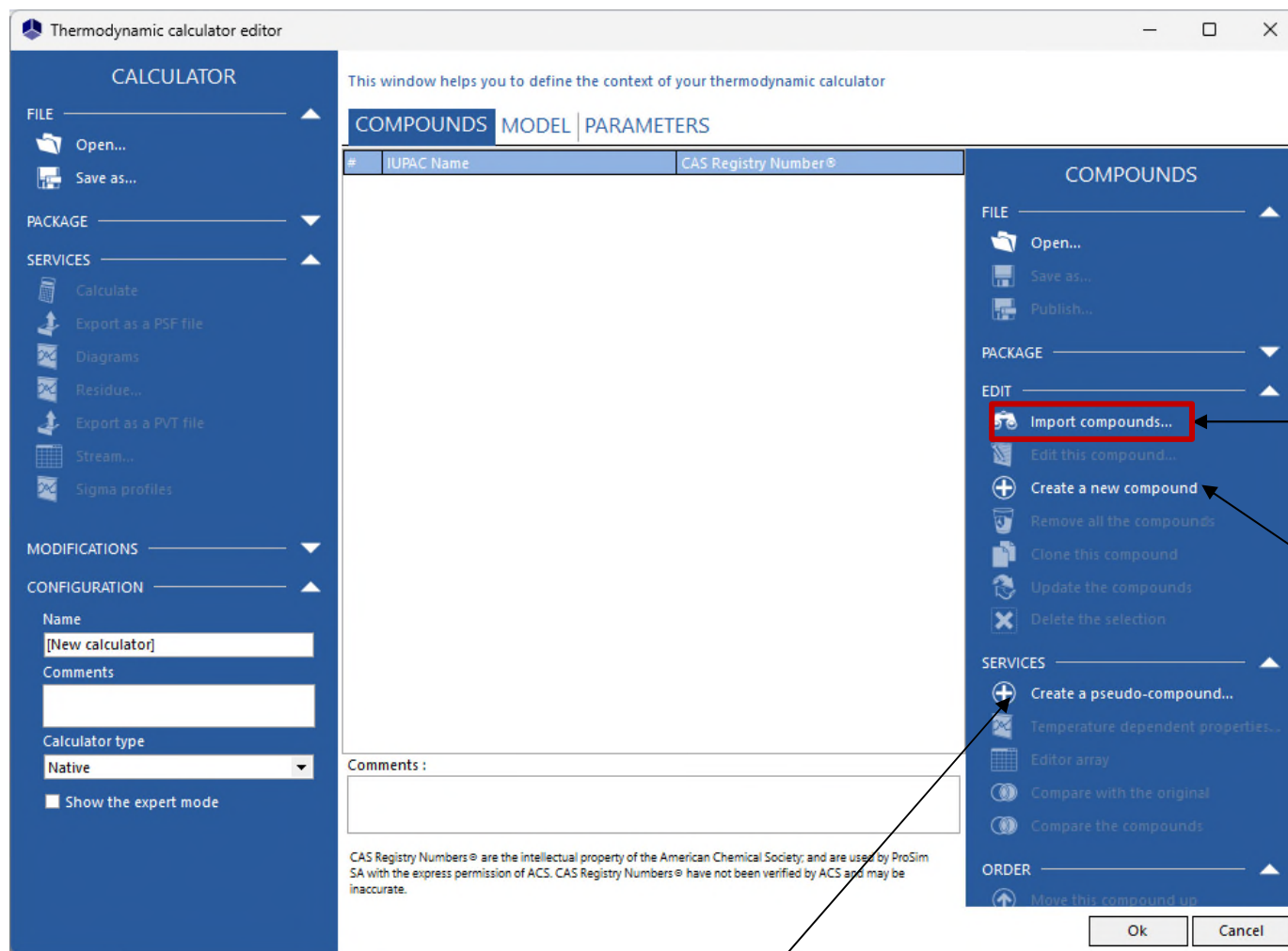
5. Click on “OK”

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*”



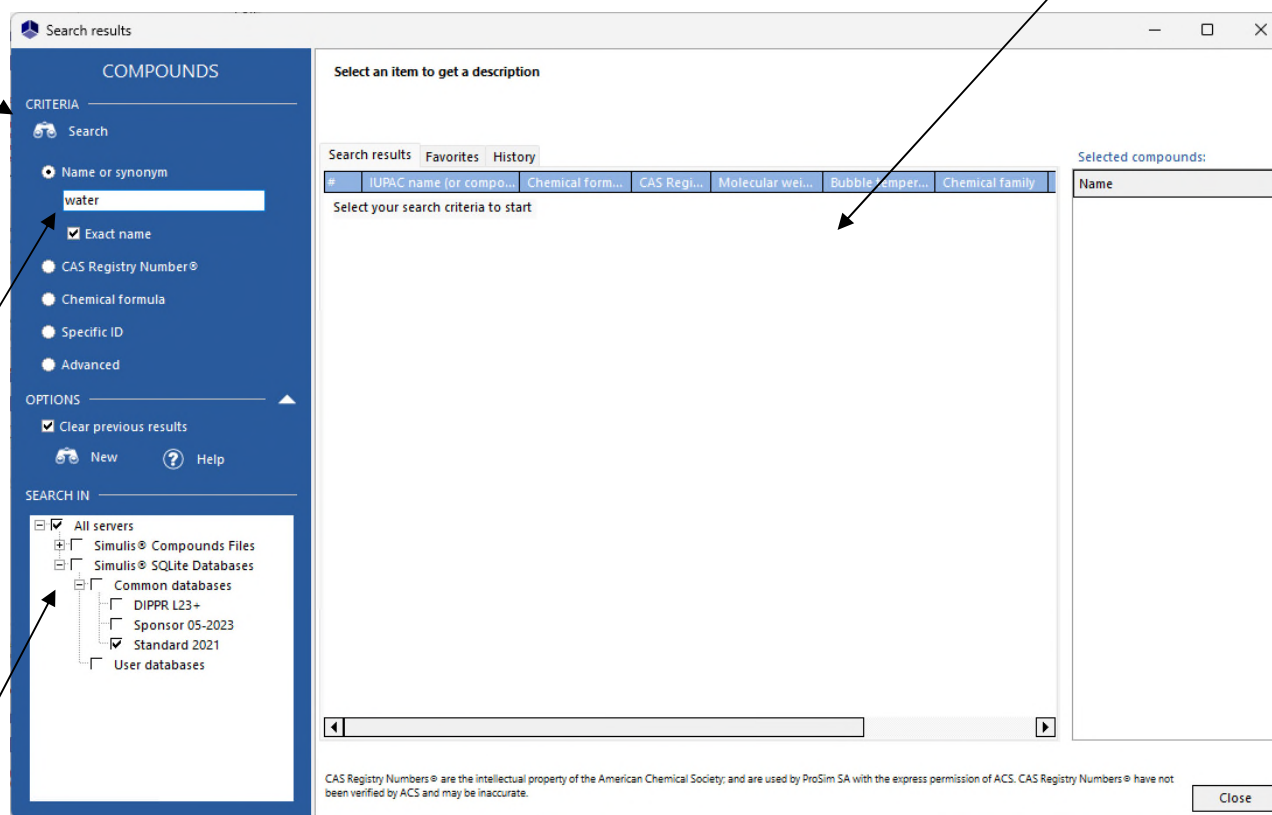
To create pseudo-compounds corresponding to a petroleum cut, please consult “*Getting Started with Simulis Thermodynamics, use case 5*”

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

The screenshot shows the 'Search results' window in ProSim. On the left is a sidebar with search criteria and options. The main area displays search results for 'ethanol'. A table lists compounds with columns for IUPAC name, chemical formula, CAS Registry Number, molecular weight, bubble temperature, and chemical family. The first row is 'ETHANOL' with formula C2H6O and CAS number 64-17-5. To the right of the table is a 'Selected compounds:' list containing 'WATER' and 'ETHANOL'. Arrows from the numbered instructions point to these elements: instruction 1 points to the 'ETHANOL' row in the table; instruction 2 points to the 'ETHANOL' entry in the 'Selected compounds' list; instruction 3 points to the 'Selected compounds' list area; and instruction 4 points to the 'Close' button at the bottom right.

COMPOUNDS

CRITERIA

Search

Name or synonym

ethanol

☒ Exact name

☐ CAS Registry Number®

☐ Chemical formula

☐ Specific ID

☐ Advanced

OPTIONS

☒ Clear previous results

New Help

SEARCH IN

☒ All servers

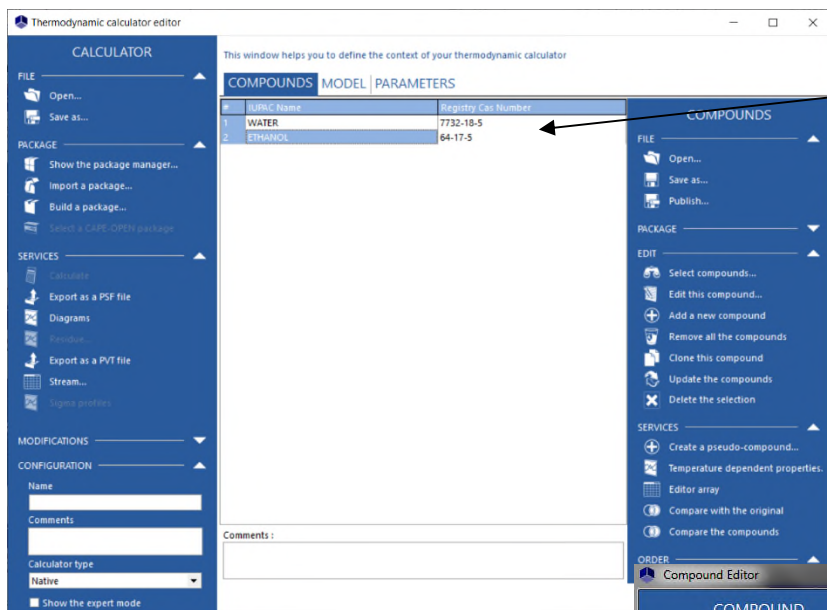
- ☐ Simulis® Compounds Files
- ☐ Simulis® SQLite Databases
 - ☐ Common databases
 - ☐ DIPPR L23+
 - ☐ Sponsor 05-2023
 - ☒ Standard 2021
 - ☐ User databases

3. The selected compounds are listed in this area

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

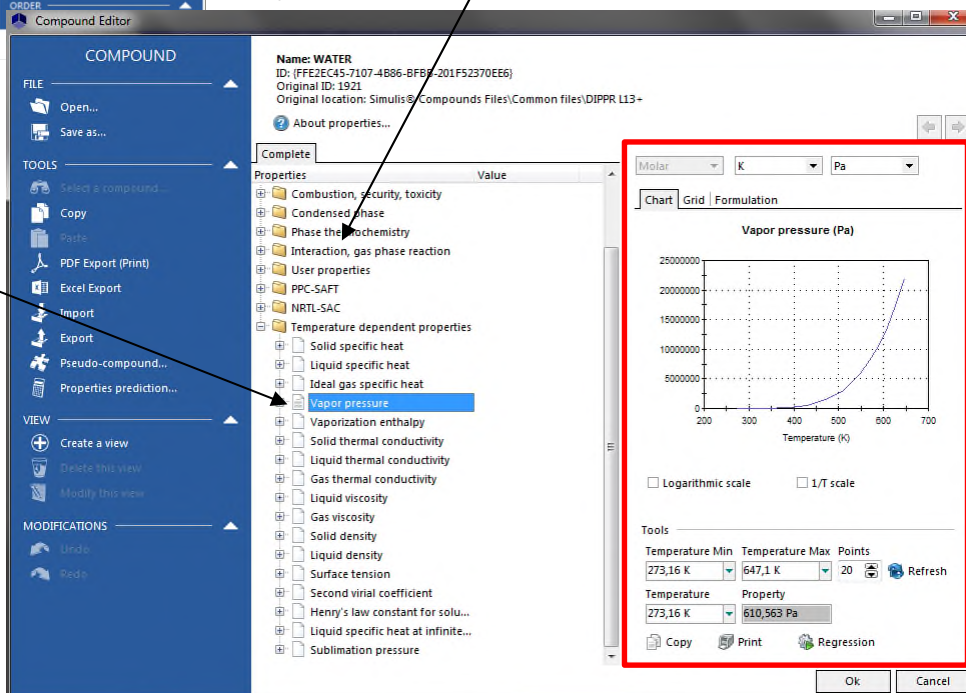
4. Click on "Close" to end the compounds selection process

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

Thermodynamic calculator editor

This window helps you to define the context of your thermodynamic calculator

COMPOUNDS **MODEL** BINARIES PARAMETERS

NAME: NRTL

CATEGORY: All the profiles

PROFILE: NRTL

APPROACH TYPE: From activity coefficients

EQUATION OF STATE: Perfect gas

ALPHA FUNCTION: Not defined

MIXING RULES: Not defined

ACTIVITY COEFFICIENT MODEL: NRTL

PURE LIQUID FUGACITY STANDARD STATE: Vapor pressure

LIQUID MOLAR VOLUME: Ideal mixture

TRANSPORT PROPERTIES: Classic methods

ENTHALPY CALCULATION: $H^*=0$, ideal gas, 25°C, 1 atm

USER-DEFINED THERMODYNAMIC MODEL: None

MODEL INDEX: 1

COMMENTS:

THERMODYNAMIC MODEL

DOCUMENTATION

- Thermodynamic assistant
- Thermodynamic help

ADDITIONAL PARAMETERS

MODEL INFORMATION

WATER-HYDROCARBON

PURE WATER

Ok Cancel

2. Select the thermodynamic profile (in this example, select “NRTL”)

Step 3: Selecting the thermodynamic model

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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

Thermodynamic calculator editor

Calculator

FILE

- Open...
- Save as...

PACKAGE

SERVICES

- Calculate
- Export as a PSF file
- Diagrams
- Residue...
- Export as a PVT file
- Stream...
- Sigma profiles

MODIFICATIONS

CONFIGURATION

Name

[New calculator]

Comments

Calculator type

Native

Show the expert mode

This window helps you to define the context of your thermodynamic calculator

COMPOUNDS | MODEL | **BINARIES** | PARAMETERS

These parameters correspond to the general values and are used if the user has not provided specific parameters (buttons to the right of each option in the thermodynamic profile)

Binaries view: ☒ Grid ☐ Matrix

Formulation : $g_{ij} - g_{jj} = C_{ij}0 + C_{ij}T*(T - 273.15)$, $a_{ij} = a_{ij}0 + a_{ij}T*(T - 273.15)$

Compound	Compound	Cij0	Cji0	aij0	CijT
WATER	ETHANOL	1616,81	-635,56	0,1448	2,0177

Not supplied Supplied Imported Estimated Error

Comments :

OK Cancel

BINARIES

ACTIONS

- Import binaries...
- Clear all binaries...
- Estimate binaries...
- Save the binaries...

OPTIONS

Unit

cal/mole

☐ parameters will be ignored

☒ parameters are automatically loaded

Step 3: Selecting the thermodynamic model

For the calculator that is already defined in a simulation, if parameters are missing, if the loading is not activated: Import binaries
Import binaries from a private database

Thermodynamic calculator editor

CALCULATOR

FILE

- Open...
- Save as...

PACKAGE

SERVICES

- Calculate
- Export as a PSF file
- Diagrams
- Residue...
- Export as a PVT file
- Stream...
- Sigma profiles

MODIFICATIONS

CONFIGURATION

Name

[New calculator]

Comments

Calculator type

Native

☐ Show the expert mode

This window helps you to define the context of your thermodynamic calculator

COMPOUNDS | MODEL | **BINARIES** | PARAMETERS

These parameters correspond to the general values and are used if the user has not provided specific parameters (buttons to the right of each option in the thermodynamic profile)

Binaries view: ☒ Grid ☐ Matrix

Formulation : $g_{ij} - g_{jj} = C_{ij0} + C_{ijT}(T - 273.15)$, $a_{ij} = a_{ij0} + a_{ijT}(T - 273.15)$

Compound	Compound	C_{ij0}	C_{ijT}	a_{ij0}	a_{ijT}
WATER	ETHANOL				

Not supplied Supplied Imported Estimated Error

Comments :

BINARIES

ACTIONS

- Import binaries...**
- Clear all binaries...
- Estimate binaries...
- Save the binaries...

OPTIONS

Unit

cal/mole

☐ parameters will be ignored

☒ parameters are automatically loaded

Ok Cancel

Automatic load is not activated

Step 3: Selecting the thermodynamic model

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2. Click on
“Search”

4. Select the binary interaction parameters to be
used and click on “OK”

Search of binaries

BINARIES

CRITERIA

Search by

☐ Name ☐ CAS number

Compound

[Display all]

Compound

[Display all]

OPTIONS

SEARCH IN

- ☒ All servers
 - ☒ Simulis Binaries Files
 - ☒ Common files
 - ☒ Standard
 - ☒ User files

This window helps you to select the binaries to take into account during thermodynamic calculations

Search results Updated binaries

Database	Compound	Compound	Cij0	Cij0	aij0	CijT	CijT
Standard	WATER	ETHANOL	1616.81	-635.56	0.1448	2.0177	0.9907

3. Results are shown here

Ok Cancel

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

Thermodynamic calculator editor

CALCULATOR

FILE

- Open...
- Save as...

PACKAGE

SERVICES

- Calculate
- Export as a PSF file
- Diagrams
- Residue...
- Export as a PVT file
- Stream...
- Sigma profiles

MODIFICATIONS

CONFIGURATION

Name

[New calculator]

Comments

Calculator type

Native

Show the expert mode

This window helps you to define the context of your thermodynamic calculator

COMPOUNDS | MODEL | **BINARIES** | PARAMETERS

These parameters correspond to the general values and are used if the user has not provided specific parameters (buttons to the right of each option in the thermodynamic profile)

Binaries view: ☒ Grid ☐ Matrix

Formulation : $g_{ij} - g_{jj} = C_{ij0} + C_{ijT}(T - 273.15)$, $a_{ij} = a_{ij0} + a_{ijT}(T - 273.15)$

Compound	Compound	Cij0	CijT	aij0	CijT
WATER	ETHANOL	1616,81	-635,56	0,1448	2,0177

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

Unit

cal/mole

☐ parameters will be ignored

☒ parameters are automatically loaded

Not supplied Supplied Imported Estimated Error

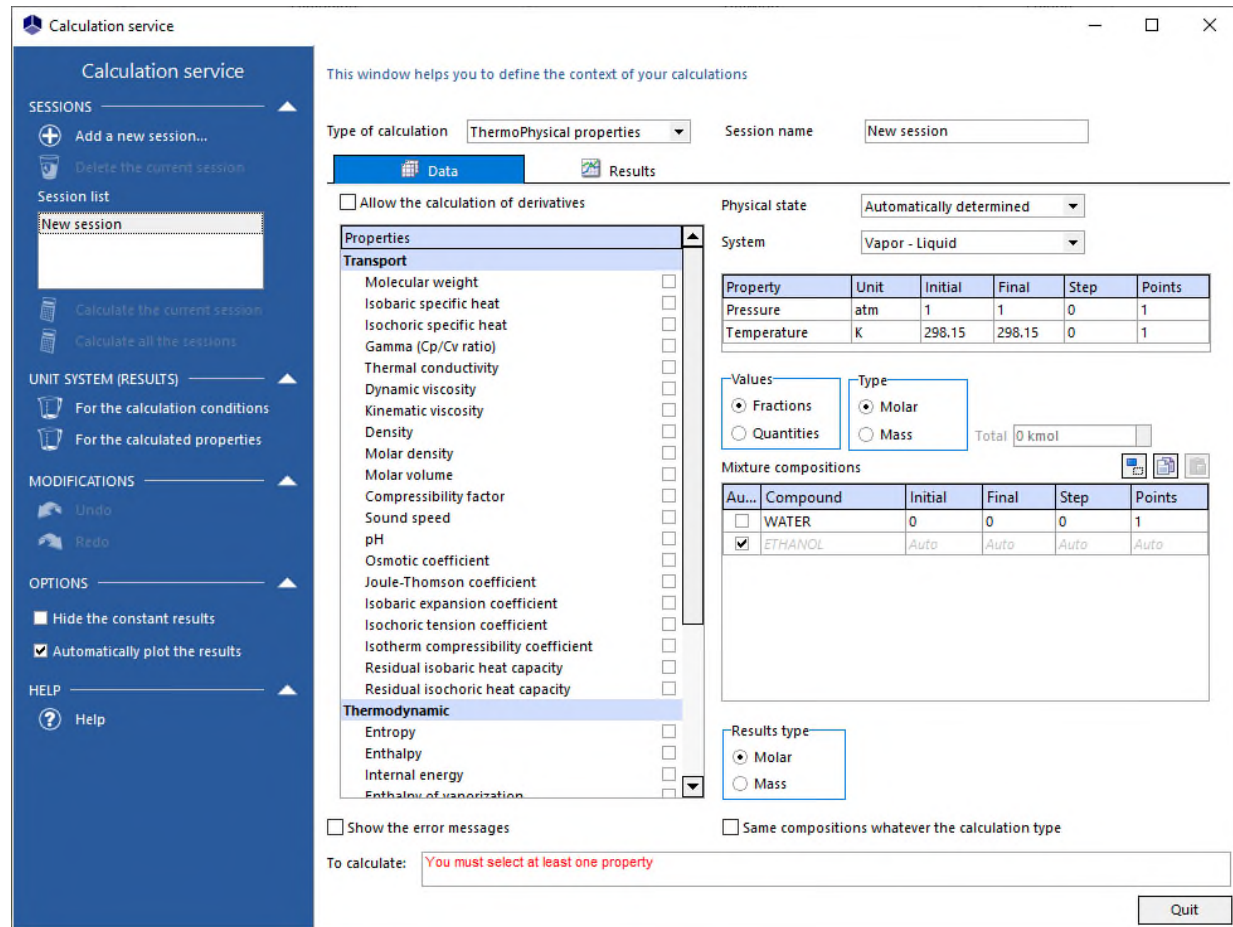
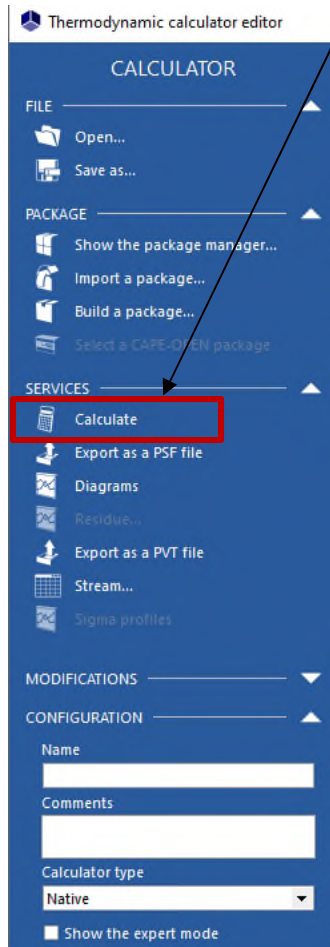
Comments :

Ok Cancel

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 choose 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*”)

Calculation service

This window helps you to define the context of your calculations

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

↶ Undo

↷ Redo

OPTIONS

■ Hide the constant results

☑ Automatically plot the results

HELP

🔍 Help

Type of calculation: Equilibria

Equilibria

Critical properties

Equilibria

K-values and surface tension

Phase envelope

Phase envelope deviation

ThermoPhysical properties

Reid Vapor Pressure

Exergy

Vapor - Liquid

Bubble and dew

Bubble and dew

wP - Flash at given

wT - Flash at given vaporization ratio and temperature

TP - Flash at given temperature and pressure

TV - Flash at given temperature and volume

PV - Flash at given pressure and volume

HT - Flash at given enthalpy and temperature

HP - Flash at given enthalpy and pressure

HV - Flash at given enthalpy and volume

HU - Flash at given enthalpy and energy

HS - Flash at given enthalpy and entropy

ST - Flash at given entropy and temperature

SP - Flash at given entropy and pressure

SV - Flash at given entropy and volume

SU - Flash at given entropy and energy

UT - Flash at given energy and temperature

UP - Flash at given energy and pressure

UV - Flash at given energy and volume

Henry constant

wH - Flash at given vaporization ratio and enthalpy

wS - Flash at given vaporization ratio and entropy

wU - Flash at given vaporization ratio and energy

wV - Flash at given vaporization ratio and volume

Liquid - Liquid

TP - Flash at given temperature and pressure

Vapor - Liquid - Liquid

Session name: New session

Property	Unit	Initial	Final	Step	Points
Temperature	K	298,15	298,15	0	1
Pressure	atm	1	1	0	1

Values

☑ Fractions

○ Quantities

Type

☑ Molar

○ Mass

Total: 0 kmol

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	WATER	0	0	0	1
<input checked="" type="checkbox"/>	ETHANOL	Auto	Auto	Auto	Auto

Results type

☑ Molar

○ Mass

Automatic initialization

Compound:

Show the error messages

Same compositions whatever the calculation type

To calculate:

Quit

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”

The screenshot shows the 'Calculation service' window. The 'Type of calculation' is set to 'Equilibria'. The 'Session name' is 'New session'. The 'Data' tab is active, showing a list of calculation types under 'Vapor - Liquid'. The 'TP - Flash at given temperature and pressure' option is selected. The 'Calculate the current session' button in the left sidebar is highlighted with a red box and an arrow. The 'Results' tab is also visible, showing a table of properties and mixture compositions.

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

- Undo
- Redo

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

Vapor - Liquid

- Bubble and dew temperatures
- Bubble and dew pressures
- wP - Flash at given vaporization ratio and pressure
- wT - Flash at given vaporization ratio and temperature
- TP - Flash at given temperature and pressure
- TV - Flash at given temperature and volume
- PV - Flash at given pressure and volume
- HT - Flash at given enthalpy and temperature
- HP - Flash at given enthalpy and pressure
- HV - Flash at given enthalpy and volume
- HU - Flash at given enthalpy and energy
- HS - Flash at given enthalpy and entropy
- ST - Flash at given entropy and temperature
- SP - Flash at given entropy and pressure
- SV - Flash at given entropy and volume
- SU - Flash at given entropy and energy
- UT - Flash at given energy and temperature
- UP - Flash at given energy and pressure
- UV - Flash at given energy and volume
- Henry constant
- wH - Flash at given vaporization ratio and enthalpy
- wS - Flash at given vaporization ratio and entropy
- wU - Flash at given vaporization ratio and energy
- wV - Flash at given vaporization ratio and volume

Liquid - Liquid

- TP - Flash at given temperature and pressure

Vapor - Liquid - Liquid

Property

Property	Unit	Initial	Final	Step	Points
Temperature	°C	80	80	0	1
Pressure	bar	1	1	0	1

Values

- Fractions
- Quantities

Type

- Molar
- Mass

Total: 0 kmol

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	WATER	0.5	0.5	0	1
<input checked="" type="checkbox"/>	ETHANOL	Auto	Auto	Auto	Auto

Results type

- Molar
- Mass

Automatic initialization

Compound

Show the error messages

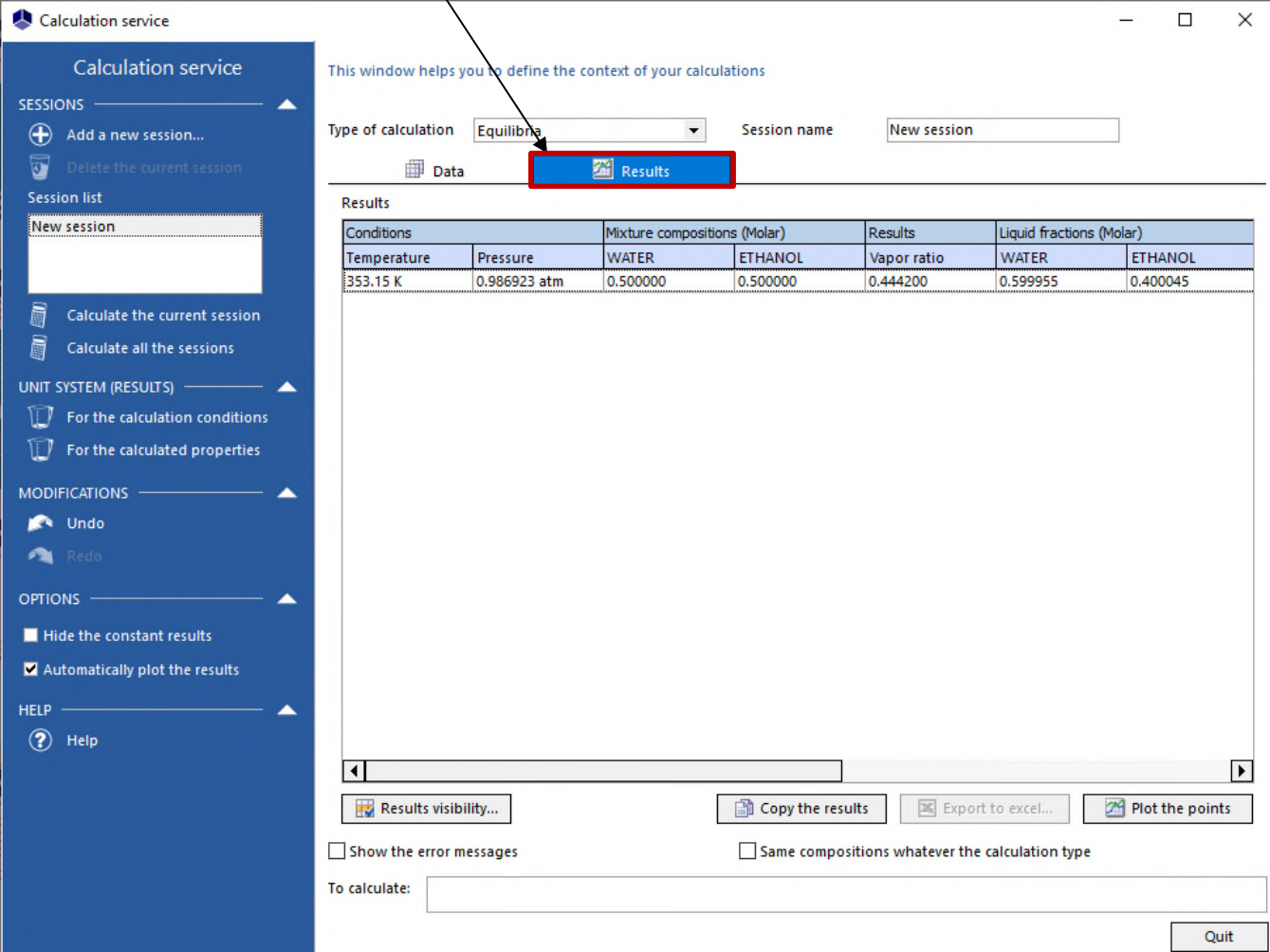
Same compositions whatever the calculation type

To calculate:

Quit

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

The results are displayed as a table in the “Results” tab



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

- Undo
- Redo

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: Equilibrium

Session name: New session

Data Results

Results

Conditions		Mixture compositions (Molar)		Results	Liquid fractions (Molar)	
Temperature	Pressure	WATER	ETHANOL	Vapor ratio	WATER	ETHANOL
353.15 K	0.986923 atm	0.500000	0.500000	0.444200	0.599955	0.400045

Results visibility...

Copy the results

Export to excel...

Plot the points

☐ Show the error messages

☐ Same compositions whatever the calculation type

To calculate:

Quit



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

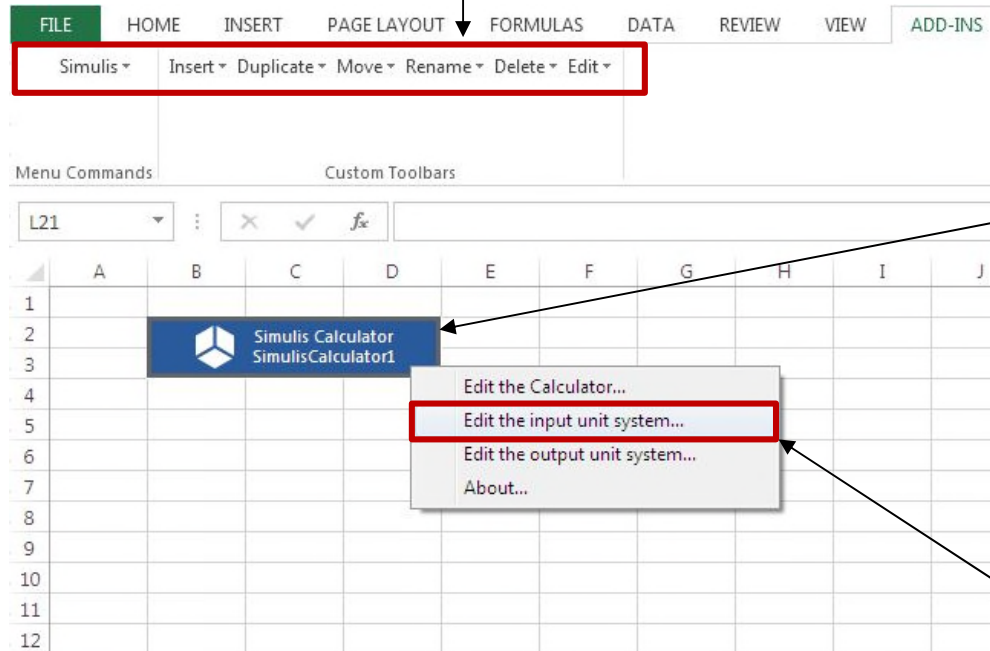
Step 5: Calculation of the TP flash in Excel

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(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**



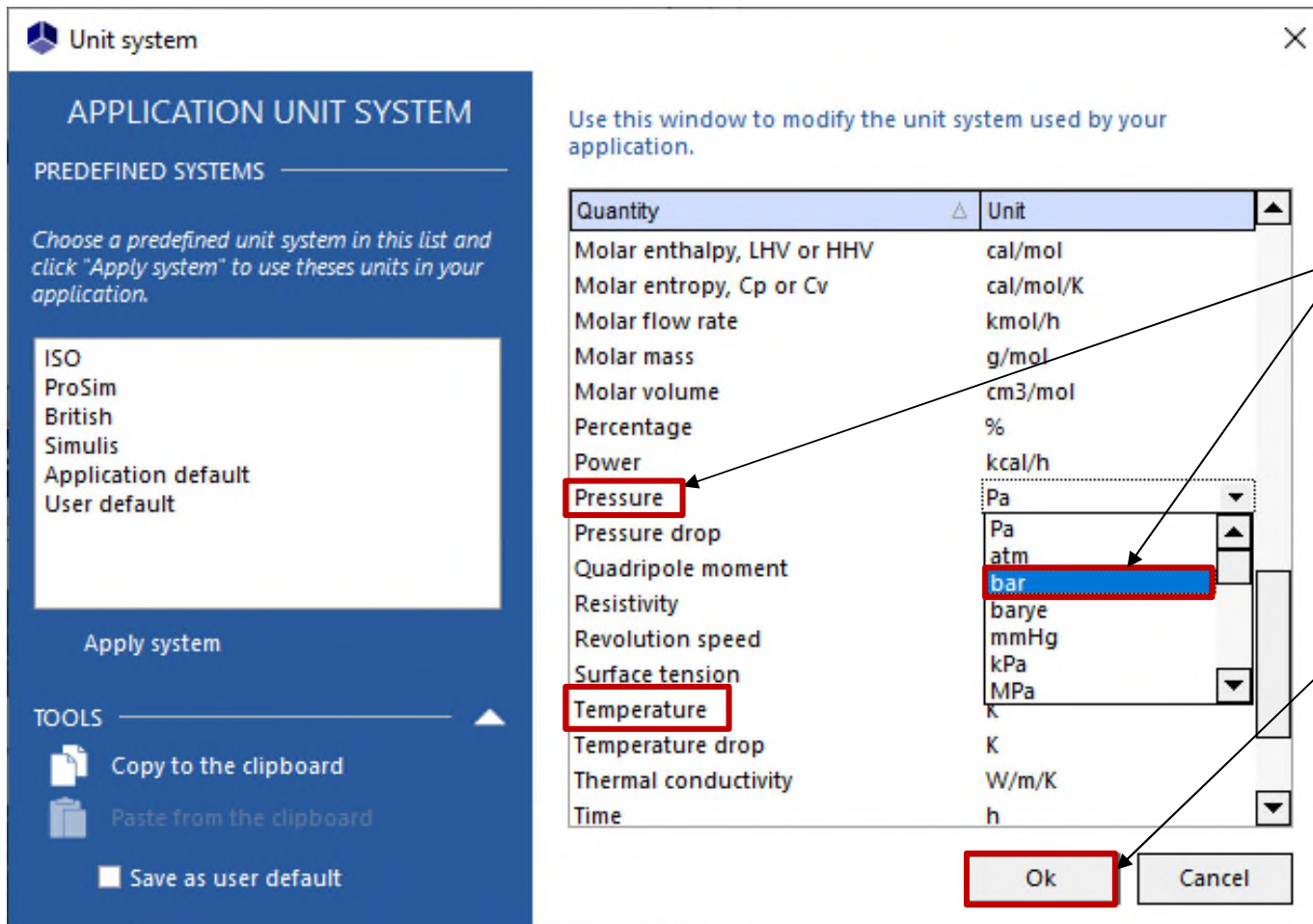
1. Right click on the *Simulis Calculator* object

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

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(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)

	A	B	C	D	E	F	G	H	I	J
2		 Simulis Calculator SimulisCalculator1								
3										
4										
5				0.5						
6				0.5						
7										
8			T	80						
9			P	1						
10										
11			Vapor ratio	xl		yv		ki		
12										
13										
14										

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

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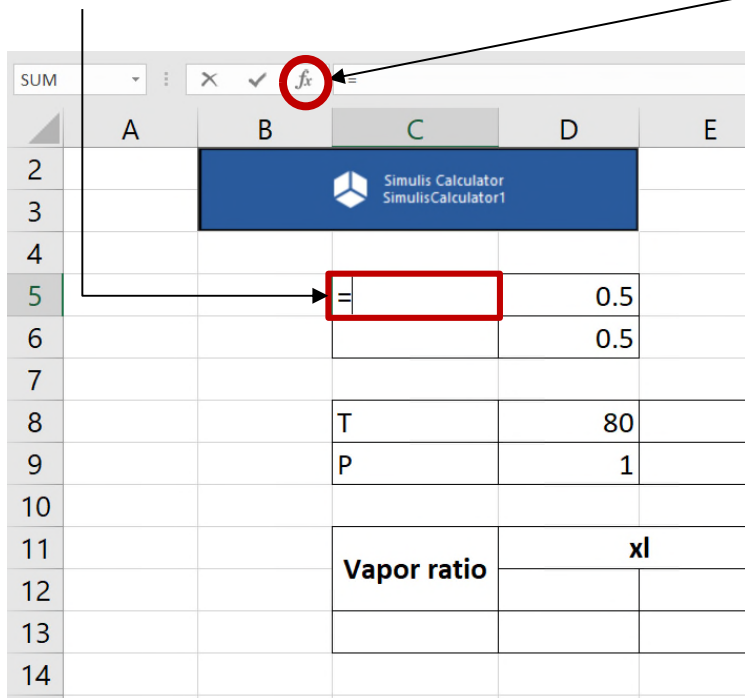
(This step requires to have Simulis Thermodynamics Excel Add-in)

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

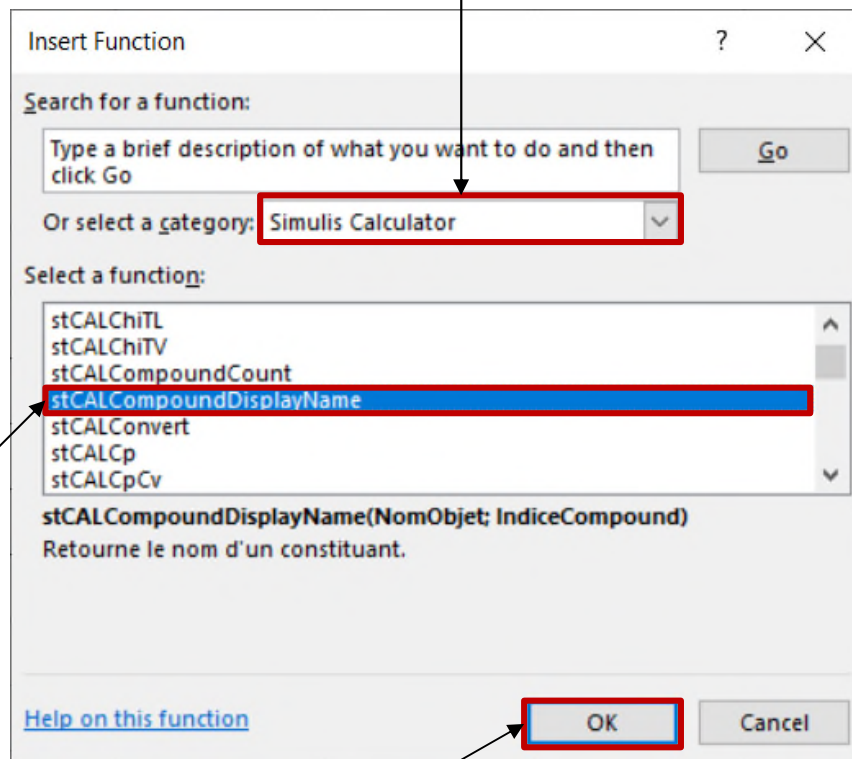
1. Select the first cell of the input composition table

2. Click on “fx” to insert a function

3. Choose the “*Simulis Calculator*” set of functions



	A	B	C	D	E
2					
3					
4					
5		=		0.5	
6				0.5	
7					
8		T		80	
9		P		1	
10					
11		Vapor ratio		xl	
12					
13					
14					



4. Select “*stCALCompoundDisplayName*”

5. Click on “OK” to confirm and enter the function arguments window

Step 5: Calculation of the TP flash in Excel

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

The screenshot shows an Excel spreadsheet with the Simulis Calculator add-in installed. The formula bar displays `=stCALCompoundDisplayName("SimulisCalculator1";1)`. The spreadsheet shows the result of the formula in cell D1, which is 0.5. The Function Arguments dialog box is open, showing the arguments for the `stCALCompoundDisplayName` function. The `ObjectName` is set to "SimulisCalculator1" and the `CompoundIndex` is set to 1. The dialog also shows the result of the formula, which is "WATER".

Function Arguments

`stCALCompoundDisplayName`

ObjectName: "SimulisCalculator1" = "SimulisCalculator1"

CompoundIndex: 1 = 1

Returns the display name of a compound.

CompoundIndex Compound index.

Formula result = WATER

[Help on this function](#)

OK Cancel

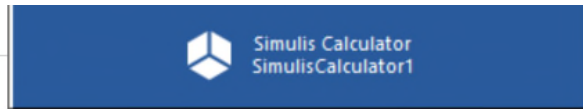
1. Enter the name of the Simulis Object that you want to use (in this example, "*SimulisCalculator1*")

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

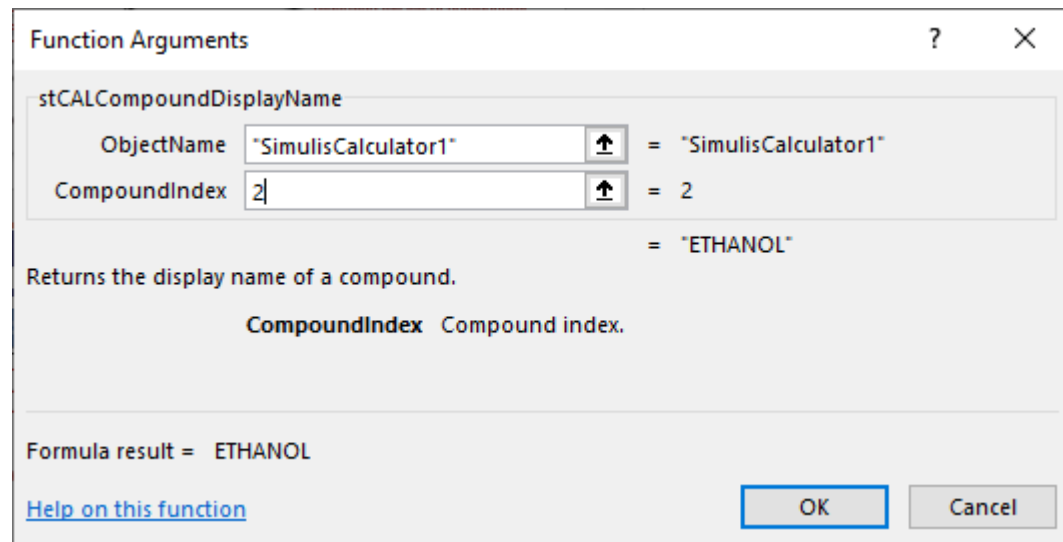
(This step requires to have Simulis Thermodynamics Excel Add-in)



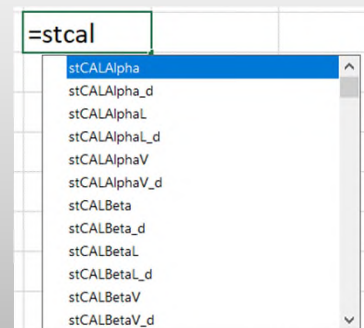
WATER	0.5
	0.5

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*”

Function Arguments

stCALGetUnitNameInSystem

ObjectName: = "SimulisCalculator1"

SystemIndex: = 1

QtyID: =

Gives the name of the default unit of a quantity in a system.

QtyID ID of quantity.

Formula result =

[Help on this function](#)

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)

B	C	D	E
 Simulis Calculator SimulisCalculator1			
	WATER	0.5	
	ETHANOL	0.5	
	T	80	°C
	P	1	

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"*

Function Arguments

stCALGetUnitNameInSystem

ObjectName "SimulisCalculator1" = "SimulisCalculator1"

SystemIndex 1 = 1

QtyID "pressure" = "pressure"

= "bar"

Gives the name of the default unit of a quantity in a system.

QtyID ID of quantity.

Formula result = bar

[Help on this function](#)

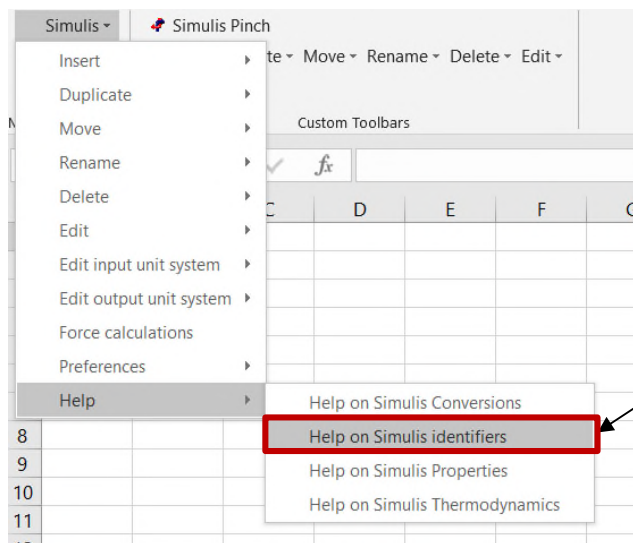
OK Cancel



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.

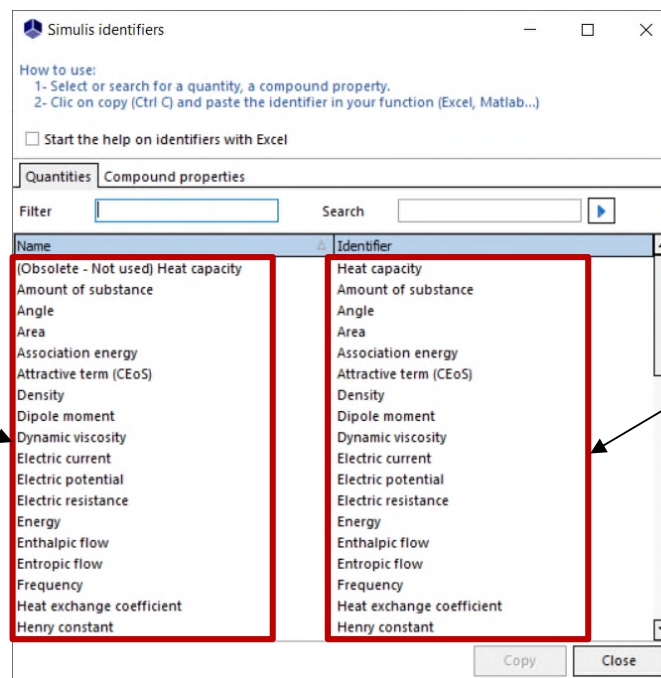
Step 5: Calculation of the TP flash in Excel

(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

B	C	D	E	F	G	H	I
 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
	=						

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)

B	C	D	E	F	G	H	I
	WATER	0.5					
	ETHANOL	0.5					
	T	80 °C					
	P	1 bar					
	Vapor ratio	xl	yv	ki			
		WATER	ETHANOL	WATER	ETHANOL	WATER	ETHANOL

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)

Function Arguments

stCALFlashTP

ObjectName: "SimulisCalculator1" = "SimulisCalculator1"

Temperature: D8 = 80

Pressure: D9 = 1

Composition: D5:D6 = {0.5;0.5}

CompositionType: 0 = 0

= {0.444200147124902,0.5999551543621}

Liquid-vapor flash at given temperature and pressure.

CompositionType Mixture composition type (0 = molar, 1 = mass).

Formula result = 0.444200147

[Help on this function](#)


OK Cancel

Step 5: Calculation of the TP flash in Excel

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

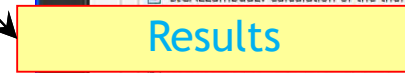
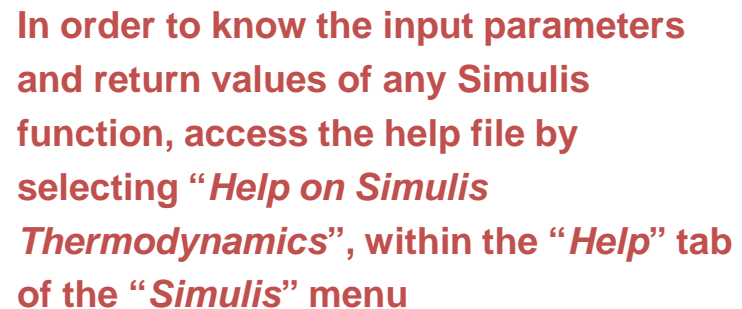
The vapor – liquid flash results are displayed in the spreadsheet

B	C	D	E	F	G	H	I
<div> Simulis Calculator SimulisCalculator1</div>							
	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.

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Input data

Results

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)



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