

# 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.**

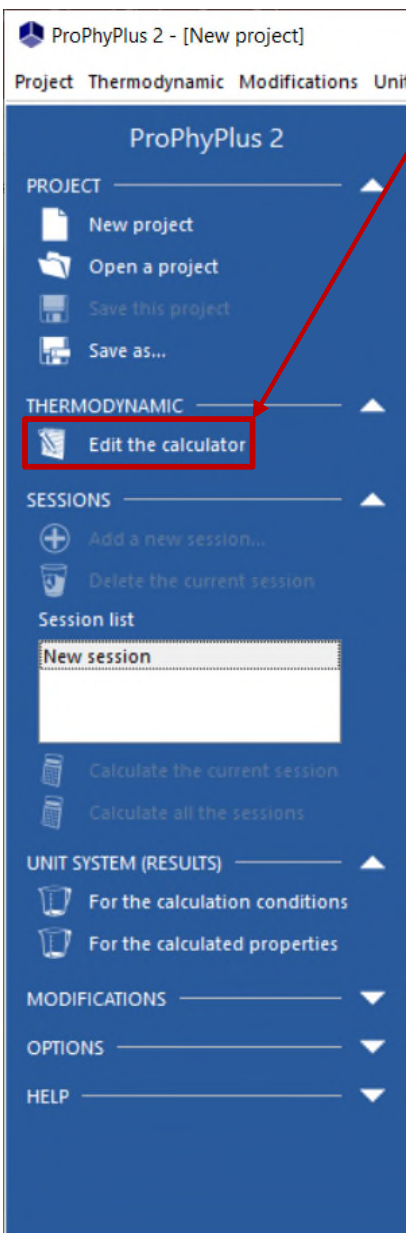
**The steps are the following:**

-  **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**

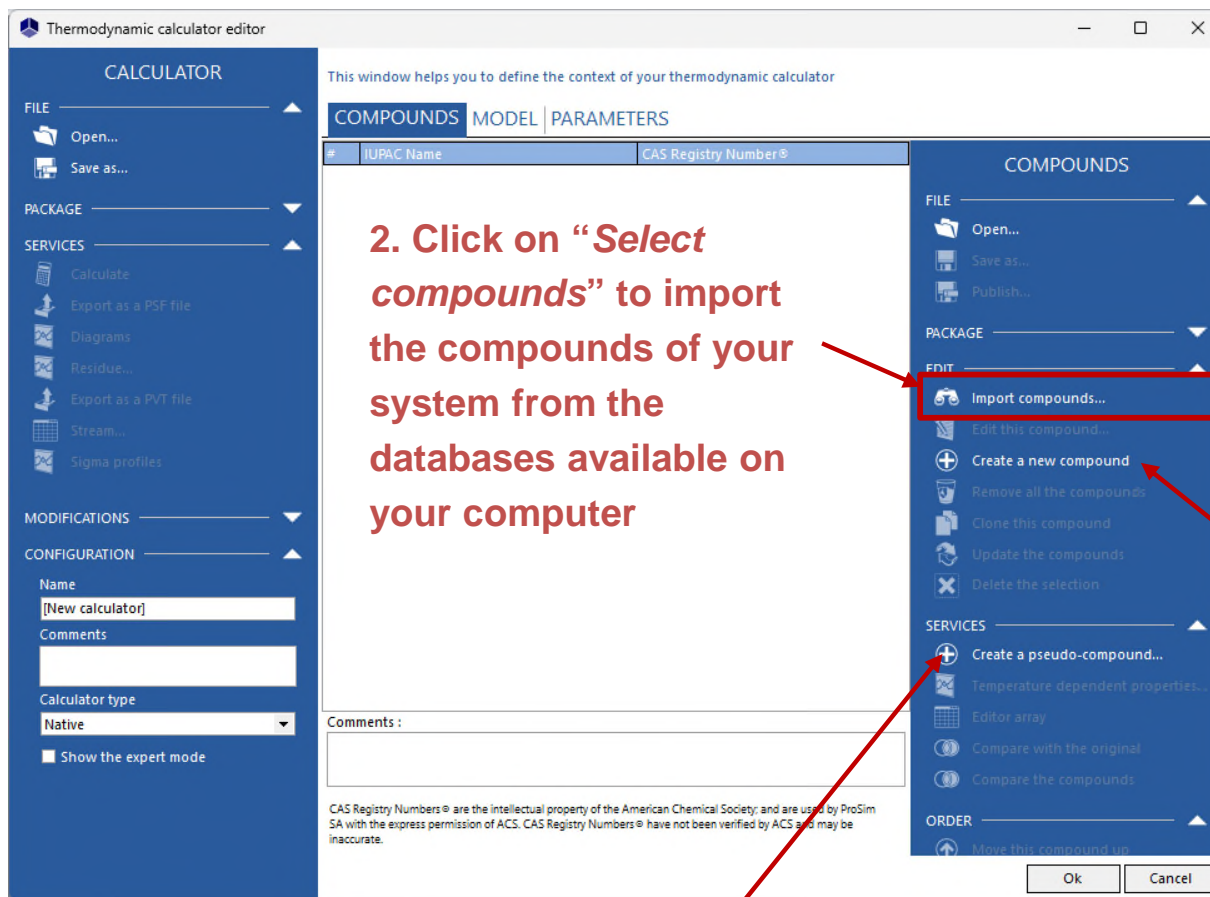


For additional tutorials, please consult « Getting started with Simulis Thermodynamics » documents.

# Step 1: select your compounds



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



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



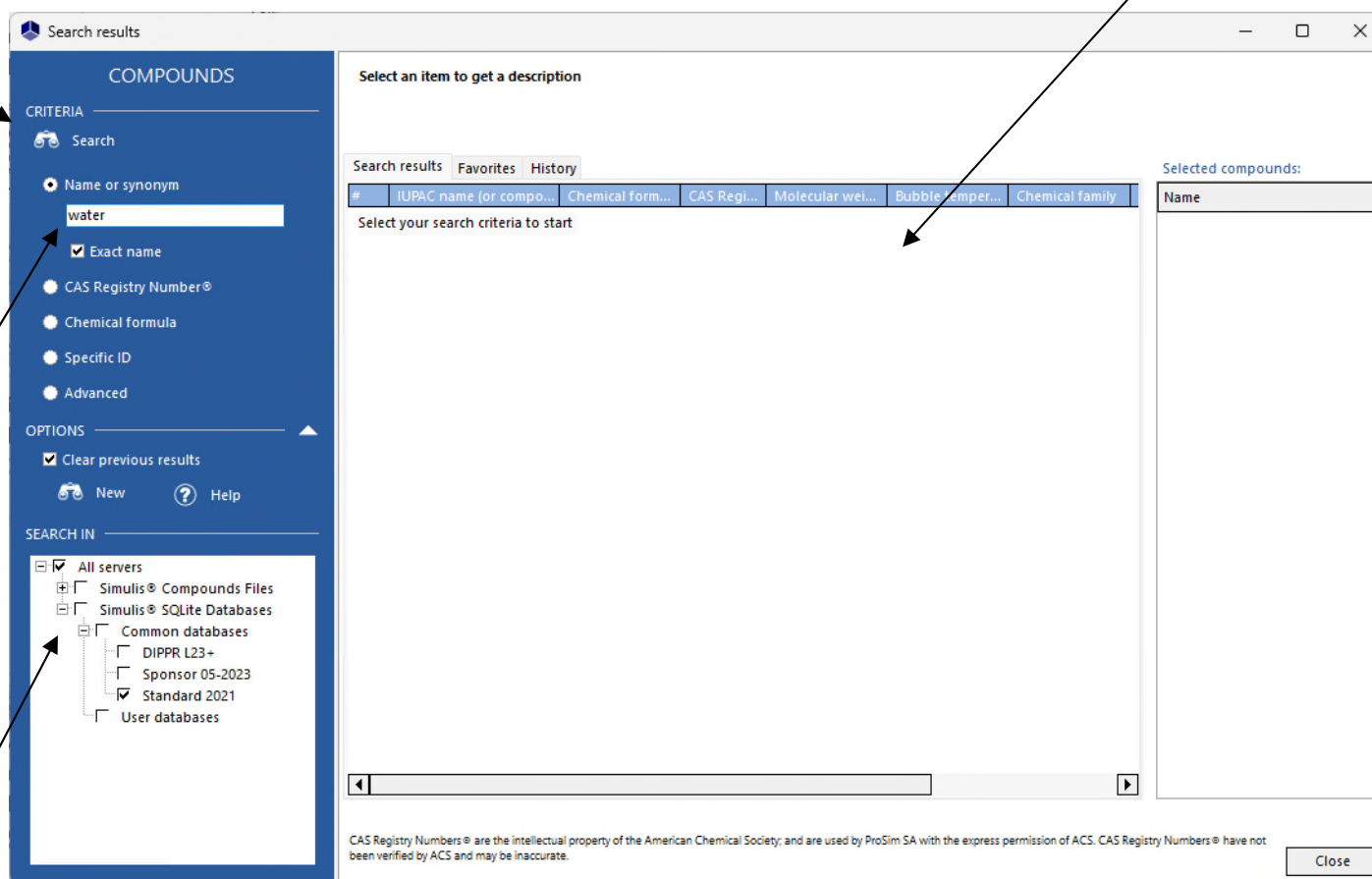
You can create pseudo-compounds corresponding to a petroleum cut, by clicking on ***“Create a pseudo-compound”***

# 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

**Search results**

**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

**Name: ETHANOL**

Location: Standard 2021 (Simulis® SQLite Databases\Common databases)

CAS Registry Number®: 64-17-5

Specific ID: {615B2F0C-4783-463E-B0E2-5DDC614CB4FA}

Search results Favorites History

#	IUPAC name (or compo...	Chemical form...	CAS Regi...	Molecular wei...	Bubble temper...	Chemical family
4	ETHANOL	C2H6O	64-17-5	46,0684	351,440	n-Alcohols

Selected compounds:

Name
WATER
ETHANOL

CAS Registry Numbers® are the intellectual property of the American Chemical Society; and are used by ProSim SA with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.

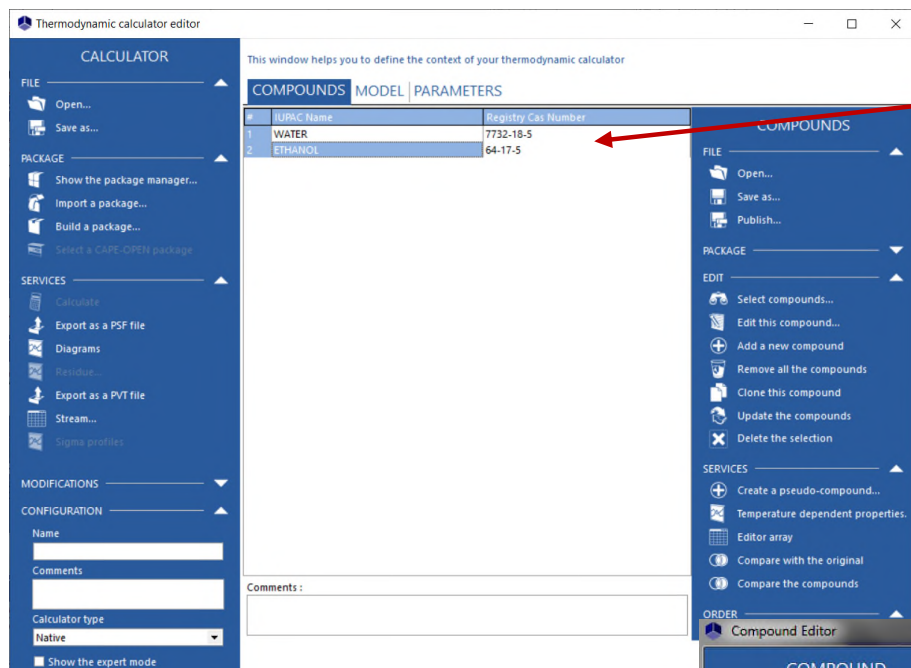
Close

3. The selected compounds are listed in this area

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

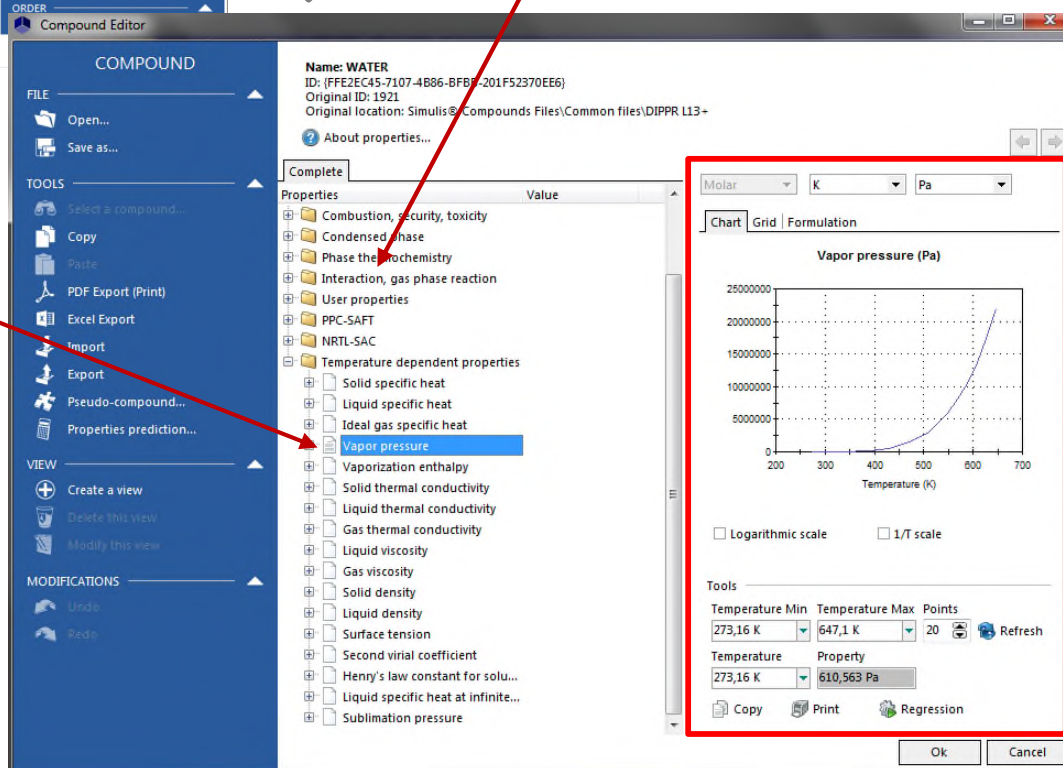
4. Click on "Close" to end the compounds selection process

# Step 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 display 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

Thermodynamic calculator editor

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

COMPOUNDS MODEL BINARIES PARAMETERS

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

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

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

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 :

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



# Step 2: select 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 :  $g_{ij} - g_{jj} = C_{ij}^0 + C_{ij}^1(T - 273.15)$ ,  $a_{ij} = a_{ij}^0 + a_{ij}^1(T - 273.15)$

Compound	Compound	$C_{ij}^0$	$C_{ij}^1$	$a_{ij}^0$	$C_{ij}^1$
WATER	ETHANOL				

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

Automatic load is not activated

# Step 2: select the thermodynamic model

2. Click on  
“Search”

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

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)

☒ Search

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

<input checked="" type="checkbox"/>	Database	Compound	Compound	Cij0	Cji0	aij0	CijT	CjiT
<input checked="" type="checkbox"/>	Standard	WATER	ETHANOL	1616.81	-635.56	0.1448	2.0177	0.9907

3. Results are shown here

Ok Cancel

# 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”

You can provide or replace the parameters from the database by selecting the cells of the table

Click on “OK” to validate your inputs and return to the main window

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

COMPOUNDS MODEL BINARIES PARAMETERS

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

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	$C_{ij}0$	$C_{ji}0$	$a_{ij}0$	$C_{ij}T$
WATER	ETHANOL	1616,81	-635,56	0,1448	2,0177

Unit

cal/mole

parameters will be ignored

parameters are automatically loaded

Not supplied Supplied Imported Estimated Error

Comments :

Ok Cancel



# Step 3: manage the unit system

Different unit systems can be used for the:

- calculation conditions
- calculated properties

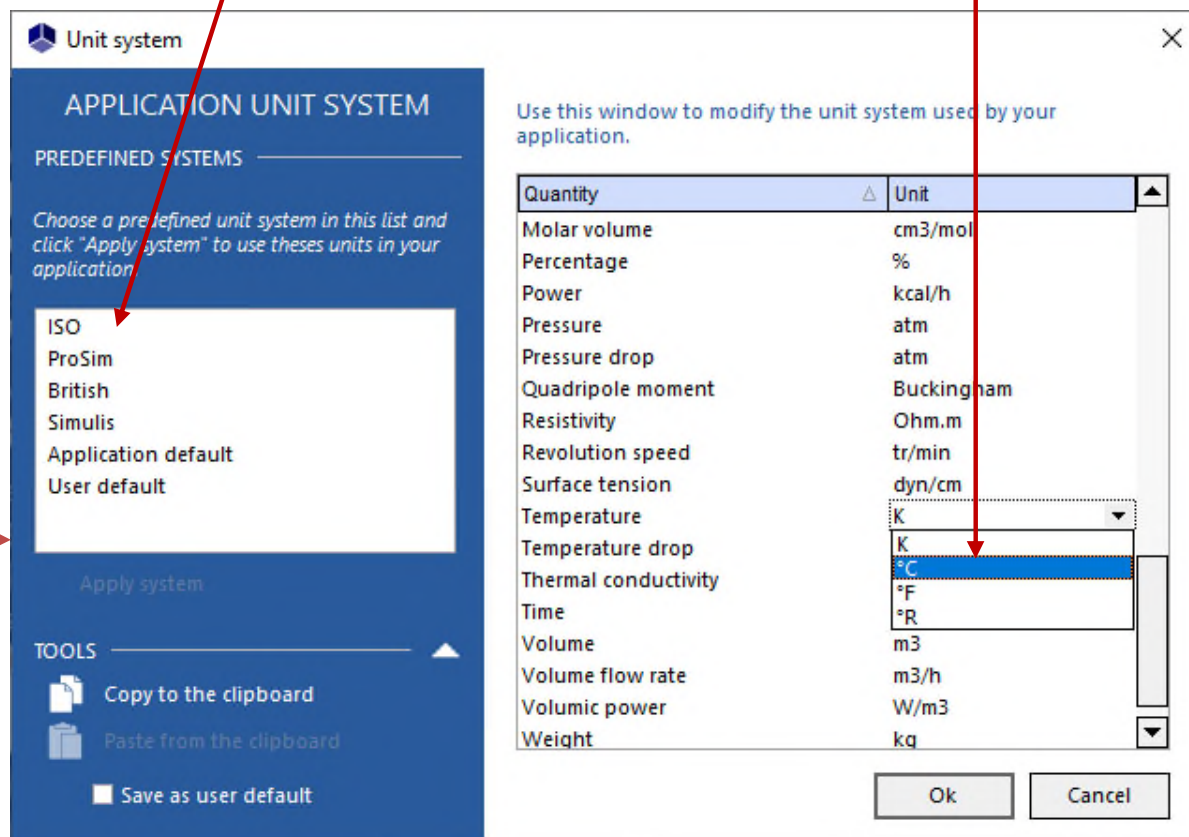
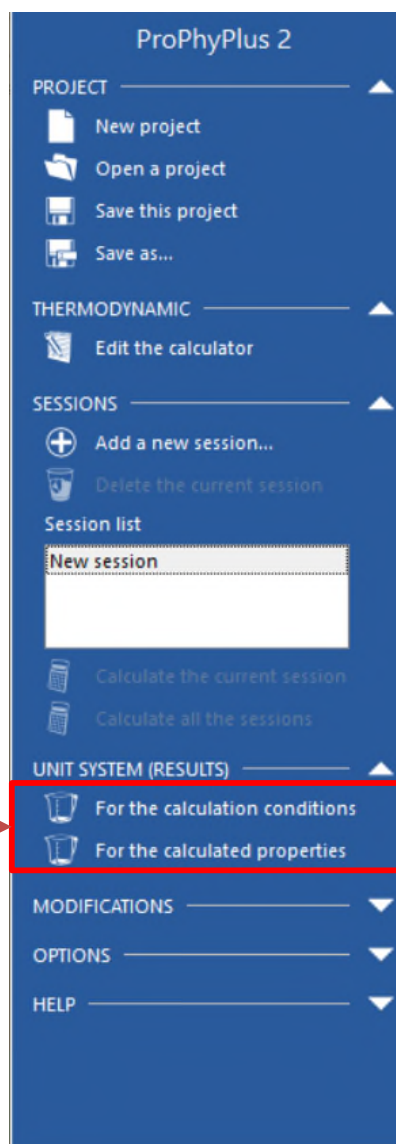


- Both input and output unit systems can be customized.
- You can choose different unit systems for the input and for the output

You can select predefined unit systems...

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

Click



# Step 4: define calculation conditions

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, “*Bubble and dew temperature*”)

ProPhyPlus 2 - [New project] (Modified)

Project Thermodynamic Modifications Unit systems Sessions Options Help

This window helps you to define the context of your calculations

Project

Type of calculation **Equilibria**

Session name

**Vapor - Liquid**

- Bubble and dew
- Bubble and dew
- wP - Flash at given pressure and volume
- 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

Values

☒ Fractions ☒ Molar

☐ Quantities ☐ Mass

Total

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:



# 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)

ProPhyPlus 2 - [New project] (Modified)

Project Thermodynamic Modifications Unit systems Sessions Options Help

This window helps you to define the context of your calculations

Project

Type of calculation  Session name

**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

Property Unit Initial Final Step Points

Pressure atm 1 1 0 1

Values: ☒ Fractions ☐ Quantities Type: ☒ Molar ☐ Mass Total 0 kmol

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input checked="" type="checkbox"/>	WATER	Auto	Auto	Auto	Auto
<input type="checkbox"/>	ETHANOL	0	1	0.01	101

Results type: ☒ Molar ☐ Mass ☐ Automatic initialization Compound

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

To calculate:

## 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

ProPhyPlus 2 - [New project] (Modified)

Project Thermodynamic Modifications Unit systems Sessions Options Help

This window helps you to define the context of your calculations

Project

Type of calculation  Session name

**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  
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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

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

Values: ☒ Fractions ☐ Quantities Type: ☒ Molar ☐ Mass Total

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input checked="" type="checkbox"/>	WATER	Auto	Auto	Auto	Auto
<input type="checkbox"/>	ETHANOL	0	1	0.01	101

Results type: ☒ Molar ☐ Mass ☐ Automatic initialization Compound

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

To calculate:

**ProPhyPlus 2**

PROJECT

- New project
- Open a project
- Save this project
- Save as...

THERMODYNAMIC

- Edit the calculator

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

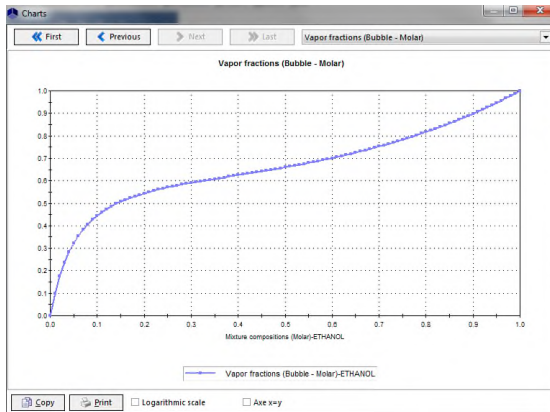
HELP

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

# Step 5: generate the results

Results are displayed in a table...

... and charts are automatically generated.



ProPhyPlus 2 - [New project] (Modified)

Project Thermodynamic Modifications Unit systems Sessions Options Help

Project: [New project] [Open a project] [Save this project] [Save as...]

Thermodynamic: [Edit the calculator]

Sessions: [Add a new session...] [Delete the current session]

Session list: [New session]

Unit system (Results): [For the calculation conditions] [For the calculated properties]

Options: [Hide the constant results] [Automatically plot the results]

Help

This window helps you to define the context of your calculations

Project: [New session]

Type of calculation: Equilibria Session name: New session

Data Results

Results

Conditions	Mixture compositions (Molar)		Results		Liquid fractions (Bubble - Molar)		Vapor fractions (Bubble - Molar)	
Pressure	WATER	ETHANOL	Bubble tempera...	Dew temperature	WATER	ETHANOL	WATER	ETHANOL
1 atm	1.00000	0.00000	373.168 K	373.168 K	1.00000	0.00000	1.00000	0.00000
1 atm	0.990000	1.00000E-002	370.512 K	372.911 K	0.990000	1.00000E-002	0.900086	9.99140E-00
1 atm	0.980000	2.00000E-002	368.347 K	372.652 K	0.980000	2.00000E-002	0.823935	0.176065
1 atm	0.970000	3.00000E-002	366.552 K	372.391 K	0.970000	3.00000E-002	0.764175	0.235825
1 atm	0.960000	4.00000E-002	365.045 K	372.128 K	0.960000	4.00000E-002	0.716168	0.283832
1 atm	0.950000	5.00000E-002	363.765 K	371.864 K	0.950000	5.00000E-002	0.676858	0.323142
1 atm	0.940000	6.00000E-002	362.668 K	371.597 K	0.940000	6.00000E-002	0.644149	0.355851
1 atm	0.930000	7.00000E-002	361.721 K	371.328 K	0.930000	7.00000E-002	0.616562	0.383438
1 atm	0.920000	8.00000E-002	360.898 K	371.058 K	0.920000	8.00000E-002	0.593021	0.406979
1 atm	0.910000	9.00000E-002	360.177 K	370.785 K	0.910000	9.00000E-002	0.572725	0.427275
1 atm	0.900000	0.100000	359.543 K	370.51 K	0.900000	0.100000	0.555067	0.444933
1 atm	0.890000	0.110000	358.982 K	370.233 K	0.890000	0.110000	0.539578	0.460422
1 atm	0.880000	0.120000	358.484 K	369.954 K	0.880000	0.120000	0.525892	0.474108
1 atm	0.870000	0.130000	358.04 K	369.672 K	0.870000	0.130000	0.513714	0.486286
1 atm	0.860000	0.140000	357.642 K	369.389 K	0.860000	0.140000	0.502810	0.497190
1 atm	0.850000	0.150000	357.284 K	369.103 K	0.850000	0.150000	0.492988	0.507012
1 atm	0.840000	0.160000	356.961 K	368.815 K	0.840000	0.160000	0.484090	0.515910
1 atm	0.830000	0.170000	356.668 K	368.524 K	0.830000	0.170000	0.475985	0.524015
1 atm	0.820000	0.180000	356.402 K	368.231 K	0.820000	0.180000	0.468564	0.531436
1 atm	0.810000	0.190000	356.158 K	367.936 K	0.810000	0.190000	0.461733	0.538267

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

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

To calculate: [ ]

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

ProPhyPlus 2 - [New project] (Modified)

Project Thermodynamic Modifications Unit systems Sessions Options Help

This window helps you to define the context of your calculations

Project

Type of calculation  Session name

**Data** Results

**Vapor - Liquid**

Bubble and dew temperatures  
Bubble and dew pressures  
wP - Flash at given vaporization ratio and pressure  
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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

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

Values  
☒ Fractions  
☐ Quantities  
 Type  
☒ Molar  
☐ Mass  
 Total

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input checked="" type="checkbox"/>	WATER	Auto	Auto	Auto	Auto
<input type="checkbox"/>	ETHANOL	0	1	0.01	101

Results type  
☒ Molar  
☐ Mass  
☐ Automatic initialization  
 Compound

☐ Show the error messages

To calculate:

☐ Same compositions whatever the calculation type



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# ProSim

Software & Services In Process Simulation

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