

Getting started with Simulis® Thermodynamics

Use Case 13: Estimating binary interaction parameters
from predictive models

Software & Services In Process Simulation

We guide You to efficiency



ProSim

Introduction

- Some thermodynamic models require binary interaction parameters (BIPs) to correctly predict fluid phase equilibria. Unfortunately these BIPs are not always available in the software database or in the literature. In such case two possibilities:
 1. Regression of the binary interaction parameters from experimental data:
Necessity for the user to create its own tools (e.g. in MS-Excel using Simulis® Thermodynamics Add-In)



Refer to “Getting Started with Simulis® Thermodynamics, use case 8: Fitting binary interaction parameters from experimental data in Excel”

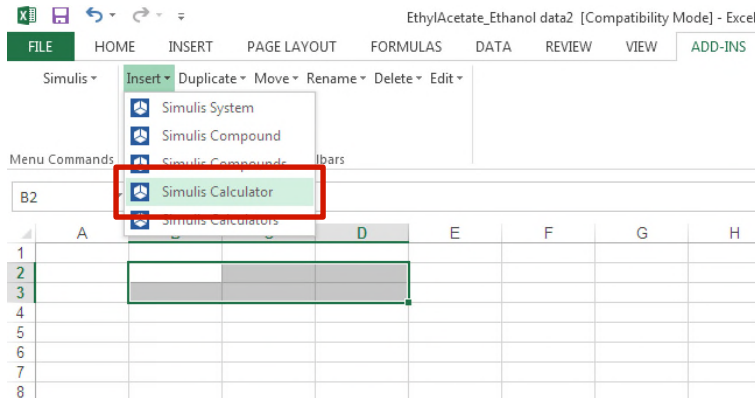
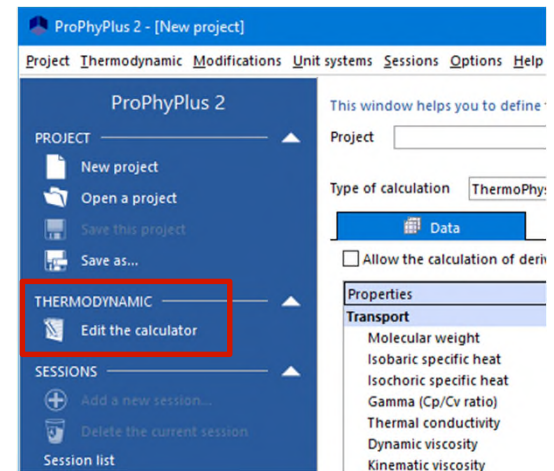
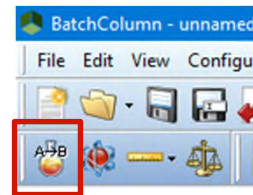
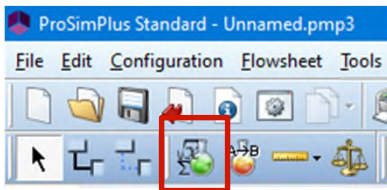
2. For Dechema-compatible Wilson, NRTL, NRTL ProSim, UNIQUAC and UNIQUAC ProSim models, it's possible to estimate the BIPs from one of the predictive models if their parameters are available (UNIFAC type group decompositions or COSMO-SAC-dsp files or NRTL-SAC parameters).



This document presents this second possibility to represent the vapor-liquid equilibria at atmospheric pressure of the quaternary system isopropanol, dichloromethane, tetrahydrofuran, methyl chloride

Step 1: Define the thermodynamics

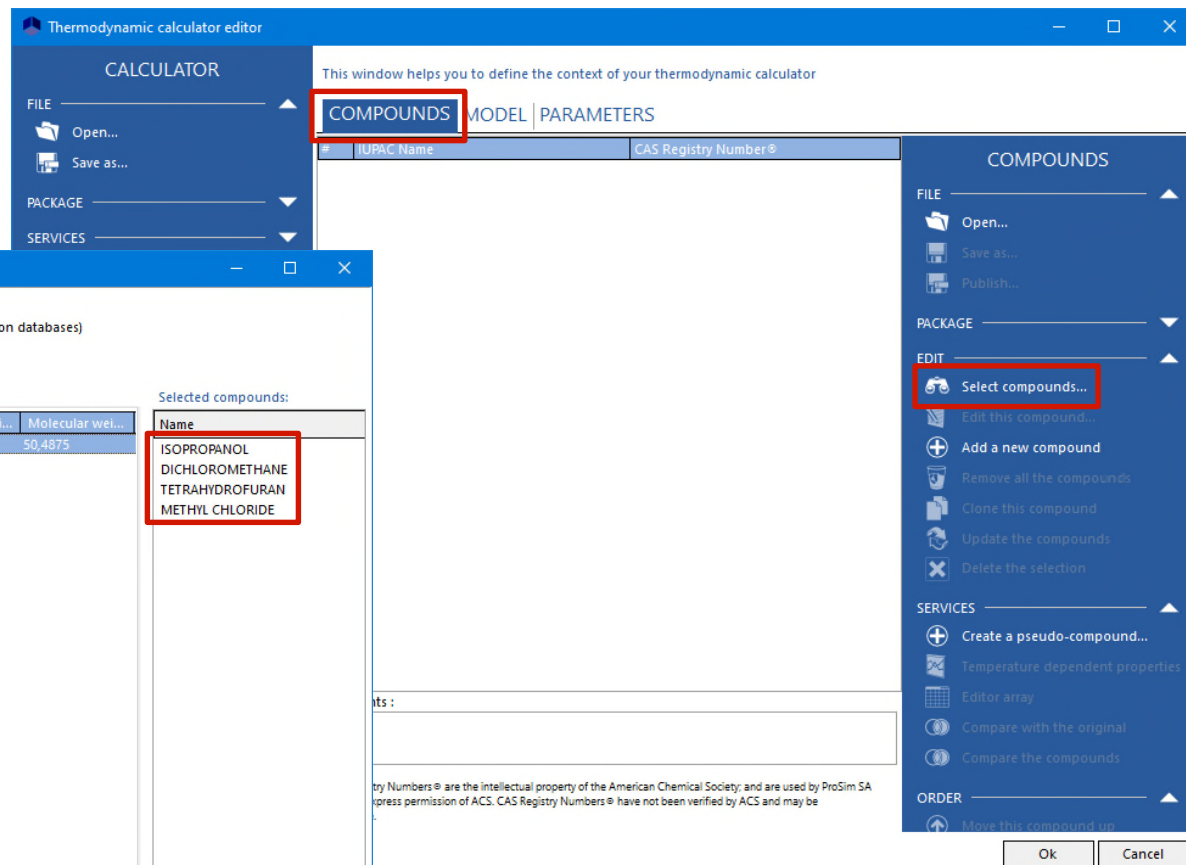
- Depending on your software add, edit or open a calculator



Refer to Getting Started “Use case 1” of your software for details about how to perform the operations of the Step 1 of this document

Step 1: Define the thermodynamics

- Select the compounds isopropanol, dichloromethane, tetrahydrofuran and methyl chloride from the latest compounds database



Step 1: Define the thermodynamics

- Select the NRTL thermodynamic profile
 - Note that the “binaries” tab appears only when the selected thermodynamic model requires BIPs and at least 2 compounds are present

Thermodynamic calculator editor

Calculator window tabs: COMPOUNDS | MODEL | PARAMETERS

#	IUPAC Name	CAS Registry Number®
1	ISOPROPANOL	67-63-0
2	DICHLOROMETHANE	75-09-2
3	TETRAHYDROFURAN	109-99-9
4	METHYL CHLORIDE	74-87-3

Thermodynamic calculator editor

Calculator window tabs: COMPOUNDS | MODEL | BINARIES | PARAMETERS

Model configuration:

- 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

Thermodynamic Model Configuration:

- Parameters
- Thermodynamic assistant
- Thermodynamic help
- Use a specific model for pure water
- Advanced:
 - Water-hydrocarbons model
 - Sol A: 6.25043
 - Sol B: 4.015,3
 - The liquid phase splitting is taken into account
 - Predictive model parameters...
 - True species model
 - Reactive model parameters...

Ok Cancel

Step 2: Choice of the predictive models

- Use the “Editor array” service to analyze which predictive models can be used

Thermodynamic calculator editor

Calculator

FILE

Open...

Save as...

PACKAGE

SERVICES

MODIFICATIONS

CONFIGURATION

Name

Comments

Calculator type

Native

Show the expert mode

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

COMPOUNDS MODEL PARAMETERS

#	IUPAC Name	CAS Registry Number®
1	ISOPROPANOL	67-63-0
2	DICHLOROMETHANE	75-09-2
3	TETRAHYDROFURAN	109-99-9
4	METHYL CHLORIDE	74-87-3

COMMENTS

Comments :

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.

COMPOUNDS

FILE

Open...

Save as...

Publish...

PACKAGE

EDIT

Select compounds...

Edit this compound...

Add a new compound

Remove all the compounds

Clone this compound

Update the compounds

Delete the selection

SERVICES

Create a pseudo-compound...

Temperature dependent properties

Editor array

Compare with the original

Compare the compounds

ORDER

Move this compound up

Ok Cancel

Step 2: Choice of the predictive models

Analyze of the available parameters

Properties	ISOPROPANOL	DICHLOROMETHANE	TETRAHYDROFURAN	METHYL CHLORIDE
Identification				
IUPAC name				
Specific name	ISOPROPANOL	DICHLOROMETHANE	TETRAHYDROFURAN	METHYL CHLORIDE
CAS Registry Number®	67-63-0	75-09-2	109-99-9	74-87-3
Chemical family	Other Aliphatic ...	C1/C2 Aliphatic Chlorides	Epoxydes	C1/C2 Aliphatic Chlorides
Chemical formulae	C3H8O	CH2Cl2	C4H8O	CH3Cl
Smiles	CC(O)C	ClCCl	C1COCC1	C[Cl]
Set identifier				
Intrinsic number (ProSim specific)	134	53	168	57
Synonyms	1-METHYLETHAN...	FREON 30	BUTYLENE OXIDE	ARTIC
Compound comments				
Cosmo file	Known	Known	Known	Known
Group contribution model				
Standard				
UNIFAC modified (Dortmund) 1993 chemical structure	[OH(s)] 1 [CH3] 2 ... [CH2CL2] 1		[c-CH2OCH] 1 [c-CH2] 2	<unknown>
UNIFAC original chemical structure	[OH] 1 [CH3] 2 [C... [CH2CL2] 1		[THF] 1 [CH2] 3	<unknown>
UNIFAC PSRK chemical structure	[OH] 1 [CH3] 2 [C... [CH2CL2] 1		[THF] 1 [CH2] 3	<unknown>
UNIFAC LLE chemical structure	[P2] 1 [CH2CL2] 1		[CH2] 3 [FCH2O] 1	<unknown>
UNIFAC modified (Dortmund) chemical structure	[OH (S)] 1 [CH3] 2... [CH2CL2] 1		[THF] 1 [CY-CH2] 2	<unknown>
UNIFAC modified (Larsen) chemical structure	[CH3] 2 [CH] 1 [O... [CH2CL2] 1		[FCH2O] 1 [CH2] 3	<unknown>
PPR 78 chemical structure	<unknown>	<unknown>	<unknown>	<unknown>
UNIFAC VTPR chemical structure	[OH (S)] 1 [CH3] 2... [CH2CL2] 1		[THF] 1 [CY-CH2] 2	[CH3Cl] 1
UNIFAC UMRPRU chemical structure	[OH] 1 [CH3] 2 [C... [CH2CL2] 1		[THF] 1 [CH2] 3	<unknown>
NRTL PR chemical structure	<unknown>	<unknown>	<unknown>	<unknown>
GC-PPC-SAFT chemical structure	[OHb](2, 0) 1 [CH... <unknown>		[-O-](3, 0) 1 [CH2c](1, 0) 4	<unknown>
UNIFAC modified (NIST) chemical structure	[OH (S)] 1 [CH3] 2... [CH2CL2] 1		[THF] 1 [CY-CH2] 2	<unknown>
User				
Atomic				
Phase change				
Combustion, security, toxicity				
Condensed phase				
Phase thermochemistry				
Interaction, gas phase reaction				
User properties				
PPC-SAFT				
NRTL-SAC				
Number of hydrophobic segments type (X)	0,332	0,459	0,235	<unknown>
Number of hydrophilic segments type (Z)	0,636	0,038	0	<unknown>
Number of polar segments type (Y-)	0	0	0,04	<unknown>
Number of polar segments type (Y+)	0	0,427	0,32	<unknown>

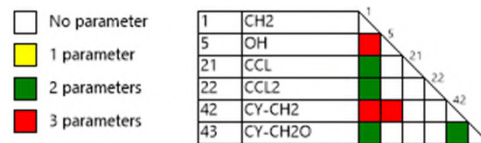
COSMO-SAC-dsp model can be used for all binaries

Only UNIFAC VTPR can be used for all binaries.
All the other UNIFACs models can be used for all binaries except the ones with methyl chloride.

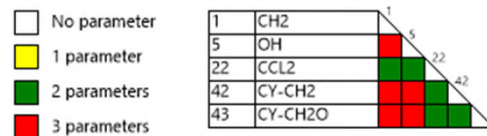
NRTL-SAC can be used for all binaries except the ones with methyl chloride

Step 2: Choice of the predictive models

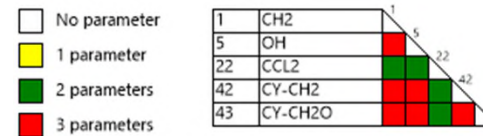
- NTRL-SAC is more particularly adapted for the solubility of organic solids in solvents, which is not the scope in this example. Thus, other models will be selected.
- UNIFAC VTPR will not be used because some interaction between groups are missing:



UNIFAC modified (Dortmund) or UNIFAC modified (NIST) can be used to predict binary sub-systems of the ternary isopropanol - dichloromethane - tetrahydrofuran system because interactions between groups are known:



UNIFAC modified (Dortmund)



UNIFAC modified (NIST)

- However, COSMO-SAC-dsp must be used to predict the binaries involving the methyl chloride.

Step 2: Choice of the predictive models

- It's reported that the behavior of the following binaries is zeotropic
 - Isopropanol - Dichloromethane
 - Isopropanol - Tetrahydrofuran
 - Dichloromethane - Tetrahydrofuran

Gmehling J., Menke J., Krafczyk J., Fischer K., "Azeotropic Data", 2nd edition, Wiley-VCH (2004)

- The UNIFAC modified (Dortmund) model predicts a zeotropic behavior for two of the three binaries: Isopropanol - Dichloromethane and Dichloromethane - Tetrahydrofuran. But it predicts an azeotrope behavior for the Isopropanol - Tetrahydrofuran. Thus, it cannot be used for that binary.
- The UNIFAC modified (NIST) model predicts a zeotropic behavior for the two binaries with isopropanol but an azeotropic behavior for the binary Dichloromethane - Tetrahydrofuran. This, it cannot be used for that binary.



If no experimental data is available, it's interesting to compare the predictions done by the different usable predictive models to verify if they are coherent with each other. Refer to "Getting started with ProPhyPlus[®], use case 1: Main features overview » to plot a vapor-liquid equilibrium curve.

Step 2: Choice of the predictive models

- To sum up the models used to predict the BIPs
 - All binaries with methyl chloride: COSMO-SAC-dsp
 - Isopropanol - Dichloromethane: UNIFAC modified (Dortmund)
 - Isopropanol - Tetrahydrofuran: UNIFAC modified (NIST)
 - Dichloromethane - Tetrahydrofuran: UNIFAC modified (Dortmund)

Step 3: Prediction of the BIPs

- Go to “Binaries” tab and click on “Binaries estimation...”

Thermodynamic calculator editor

Calculator

FILE

Open...

Save as...

PACKAGE

SERVICES

MODIFICATIONS

CONFIGURATION

Name

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

Compound	Compound	Cij0	Cji0	aij0	CijT
ISOPROPANOL	DICHLOROMETHANE				
ISOPROPANOL	TETRAHYDROFUR				
ISOPROPANOL	METHYL CHLORIDE				
DICHLOROMETHANE	TETRAHYDROFUR				
DICHLOROMETHANE	METHYL CHLORIDE				
TETRAHYDROFUR	METHYL CHLORIDE				

Not supplied Supplied Imported Estimated

Comments :

BINARIES

ACTIONS

Import binaries...

Clear all binaries...

Binaries estimation...

Save the binaries...

OPTIONS

Unit

cal/mole

parameters will be ignored

Ok Cancel

Step 3: Prediction of the BIPs

■ Prediction of the 1st set of BIPs

5. Generate

1. Select the predictive model
UNIFAC modified (Dortmund)

2. a_{ij}^0 is generally set to 0.3 for vapor-liquid equilibria (current case) and to 0.2 for liquid phase splitting case

Binary interaction parameters (BIP) estimation

This window allows you to estimate the binary interaction parameters from a predictive model.

DATA Binaries

Identification model: UNIFAC modified (Dortmund)

a_{ij}^0 : 0,3

Warnings: 10

Estimate the infinite dilution activity coefficients at:

☒ The bubble temperature of each compounds at the pressure: 101325 Pa

☐ Fixed temperatures

Temperature 1: 293,15 K

Temperature 2: 298,15 K

BIP to calculate	ISOPROPANOL	DICHLOROMETHANE	TETRAHYDROFURAN	METHYL CHLORIDE
ISOPROPANOL		<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
DICHLOROMETHANE			<input checked="" type="checkbox"/>	<input type="checkbox"/>
TETRAHYDROFURAN				<input type="checkbox"/>
METHYL CHLORIDE				

☒ Select all

Ok Cancel

3. If the process is roughly isobaric, specify the corresponding pressure (current case). If the process works at two pressures (or more), specify the working temperatures at these two pressures (or the two extremes)

4. Select the binaries to estimate. In grey, the ones that cannot be estimated using the selected predictive model

Step 3: Prediction of the BIPs

- Prediction of the 1st set of BIPs
 - Visualization of the predicted BIPs

Click to continue and predict the 2nd set of BIPs

Binary interaction parameters (BIP) estimation

BINARY ESTIMATION PARAMETERS

ACTIONS

- Generate
- Save the binaries

This window allows you to estimate the binary interaction parameters from a predictive model.

Data **Binaries**

Compound	Compound	Cij0	Cji0	aij0	CijT	CjiT	aijT
ISOPROPANOL	DICHLOROMETHANE	-429,916	1880	0,3	2,21423	-9,33757	0
ISOPROPANOL	TETRAHYDROFUR	0	0	0	0	0	0
ISOPROPANOL	METHYL CHLORIDE	0	0	0	0	0	0
DICHLOROMETHANE	TETRAHYDROFUR	-685,591	573,552	0,3	-2,26141	1,94737	0
DICHLOROMETHANE	METHYL CHLORIDE	0	0	0	0	0	0
TETRAHYDROFUR	METHYL CHLORIDE	0	0	0	0	0	0

Ok Cancel

Step 3: Prediction of the BIPs

■ Prediction of the 2nd set of BIPs

5. Generate

1. Select the predictive model
UNIFAC modified (NIST)

2. a_{ij}^0 set to 0.3

Binary interaction parameters (BIP) estimation

Binary Estimation Parameters

ACTIONS

Generate

Save the binaries

This window allows you to estimate the binary interaction parameters from a predictive model.

Data Binaries

Identification model UNIFAC modified (NIST)

a_{ij}^0 0,3

Warnings 10

Estimate the infinite dilution activity coefficients at:

☒ The bubble temperature of each compounds at:
the pressure 101325 Pa

☐ Fixed temperatures

Temperature 1 293,15 K

Temperature 2 298,15 K

BIP to calculate	ISOPROPANOL	DICHLOROMETHANE	TETRAHYDROFURAN	METHYL CHLORIDE
ISOPROPANOL		<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
DICHLOROMETHANE			<input type="checkbox"/>	<input type="checkbox"/>
TETRAHYDROFURAN				<input type="checkbox"/>
METHYL CHLORIDE				

☒ Select all

Ok Cancel

3. Estimation at atmospheric pressure

4. Select the binaries to be estimated

Step 3: Prediction of the BIPs

- Prediction of the 2nd set of BIPs
 - Visualization of the predicted BIPs

Click to continue and predict the 3rd set of BIPs

Binary interaction parameters (BIP) estimation

BINARY ESTIMATION PARAMETERS

ACTIONS

- Generate
- Save the binaries

This window allows you to estimate the binary interaction parameters from a predictive model.

Data Binaries

Compound	Compound	Cij0	Cji0	aij0	CijT	CjiT	aijT
ISOPROPANOL	DICHLOROMETHANE	420,916	1880	0,3	2,31432	0,33757	0
ISOPROPANOL	TETRAHYDROFUR	666,054	-84,6405	0,3	-4,96081	2,25479	0
ISOPROPANOL	METHYL CHLORIDE	0	0	0	0	0	0
DICHLOROMETHANE	TETRAHYDROFUR	-685,591	573,552	0,3	-2,26141	1,94737	0
DICHLOROMETHANE	METHYL CHLORIDE	0	0	0	0	0	0
TETRAHYDROFUR	METHYL CHLORIDE	0	0	0	0	0	0

Ok Cancel

Step 3: Prediction of the BIPs

■ Prediction of the 3rd set of BIPs

5. Generate

1. Select the predictive model
COSMO-SAP-dsp

2. a_{ij}^0 set to 0.3

Binary interaction parameters (BIP) estimation

This window allows you to estimate the binary interaction parameters from a predictive model.

BINARY ESTIMATION PARAMETERS

ACTIONS

Generate

Save the binaries

Data Binaries

Identification model: COSMO-SAC-dsp

a_{ij}^0 : 0,3

Warnings: 10

Estimate the infinite dilution activity coefficients at:

☒ The bubble temperature of each compounds at the pressure: 101325 Pa

☐ Fixed temperatures

Temperature 1: 293,15 K

Temperature 2: 298,15 K

BIP to calculate	ISOPROPANOL	DICHLOROMETHANE	TETRAHYDROFURAN	METHYL CHLORIDE
ISOPROPANOL		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
DICHLOROMETHANE			<input type="checkbox"/>	<input checked="" type="checkbox"/>
TETRAHYDROFURAN				<input checked="" type="checkbox"/>
METHYL CHLORIDE				

☒ Select all

Ok Cancel

3. Estimation at atmospheric pressure

4. Select the binary to be estimated

Step 3: Prediction of the BIPs

- Prediction of the 3rd set of BIPs
 - Visualization of the predicted BIPs

Binary interaction parameters (BIP) estimation

BINARY ESTIMATION PARAMETERS

ACTIONS

- Generate
- Save the binaries

This window allows you to estimate the binary interaction parameters from a predictive model.

Data Binaries

Compound	Compound	Cij0	Cji0	aij0	CijT	CjiT	aijT
ISOPROPANOL	DICHLOROMETHANE	429,816	1880	0,3	2,21423	0,33757	0
ISOPROPANOL	TETRAHYDROFUR	666,054	-84,6405	0,3	-4,96081	2,25479	0
ISOPROPANOL	METHYL CHLORIDE	-299,995	1974,79	0,3	-2,00594	-0,218641	0
DICHLOROMETHANE	TETRAHYDROFUR	-685,591	573,552	0,3	-2,26141	1,94737	0
DICHLOROMETHANE	METHYL CHLORIDE	-331,795	256,504	0,3	-1,20235	2,29365	0
TETRAHYDROFUR	METHYL CHLORIDE	-5,58433	-169,151	0,3	-2,59393	3,09703	0

Ok Cancel

Click to validate

Step 3: Prediction of the BIPs

- The model is ready to use

Thermodynamic calculator editor

CALCULATOR

FILE

Open...

Save as...

PACKAGE

SERVICES

MODIFICATIONS

CONFIGURATION

Name

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 : $g_{ij} - g_{ij}^0 = C_{ij}^0 + C_{ij}^1(T - 273.15)$, $a_{ij} = a_{ij}^0 + a_{ij}^1(T - 273.15)$

Compound	Compound	C_{ij}^0	C_{ij}^1	a_{ij}^0	C_{ij}^T	a_{ij}^T	
ISOPROPANOL	DICHLOROMETHANE	-429,9163092	1879,9956505	0,3	2,2142341885	-9,337568368	0
ISOPROPANOL	TETRAHYDROFURAN	666,05388238	-84,64048228	0,3	-4,960814644	2,2547891770	0
ISOPROPANOL	METHYL CHLORIDE	-299,9953334	1974,7938063	0,3	-2,005937041	-0,218641268	0
DICHLOROMETH	TETRAHYDROFURAN	-685,5905644	573,55211238	0,3	-2,261412793	1,9473662408	0
DICHLOROMETH	METHYL CHLORIDE	-331,7953045	256,50426794	0,3	-1,202354559	2,2936540960	0
TETRAHYDROFU	METHYL CHLORIDE	-5,584329769	-169,1513138	0,3	-2,593929905	3,0970325231	0

Not supplied Supplied Imported Estimated

Comments :

BINARIES

ACTIONS

Import binaries...

Clear all binaries...

Binaries estimation...

Save the binaries...

OPTIONS

Unit

cal/mole

parameters will be ignored

Ok Cancel



It's interesting to verify that the model with the predicted BIPs gives for each binary the same behavior as the predictive model used for them. Refer to "Getting started with ProPhyPlus®, use case 1: Main features overview » to plot a vapor-liquid equilibrium curve.

Step 3: Prediction of the BIPs

- It's possible to visualize the BIPs in form of a matrix instead of a grid.
 - Place the mouse on a binary or click on it to see its BIP values

Thermodynamic calculator editor

CALCULATOR

FILE — Open... Save as...

PACKAGE —

SERVICES —

MODIFICATIONS —

CONFIGURATION —

Name

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 : $g_{ij} - g_{jj} = C_{ij}0 + C_{ji}T(1 - 273.15)$, $a_{ij} = a_{ij}0 + a_{ij}T(T - 273.15)$

Zoom: 100 %

☐ Not supplied
☒ Supplied
☐ Imported
☐ Estimated

1	ISOPROPANOL	1				
2	DICHLOROMET		2			
3	TETRAHYDROF			3		
4	METHYL CHLO				4	

Binary values

Compound	Compound	Cij0	Cji0	aij0	CijT	CjiT	aijT
ISOPROPANOL	METHYL CHLORIDE	-299,9953334	1974,7938063	0,3	-2,005937041	-0,218641268	0

Not supplied Supplied Imported Estimated

Ok Cancel

Binary	Cij0	Cji0	aij0	CijT	CjiT	aijT
ISOPROPANOL METHYL CHLORIDE	-299,995	1974,79	0,300000	-2,00594	-0,218641	0,000000

Comments :

Ok Cancel

BINARIES

ACTIONS —

Import binaries...
Clear all binaries...
Binaries estimation...
Save the binaries...

OPTIONS —

Step 4: Save the binaries

- It's possible to save the binaries in your own BIPs database to reuse them in another project. Several users databases can be created and managed.

Thermodynamic calculator editor

CALCULATOR

FILE — Open... Save as...

PACKAGE —

SERVICES —

MODIFICATIONS —

CONFIGURATION —

Name

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 : $g_{ij} - g_{ij}^0 = C_{ij}^0 + C_{ij}^1(T - 273.15)$, $a_{ij} = a_{ij}^0 + a_{ij}^1(T - 273.15)$

Compound	Compound	C_{ij}^0	C_{ij}^1	a_{ij}^0	C_{ij}^1
ISOPROPANOL	DICHLOROMETHANE	-429,9163092	1879,9956505	0,3	2,214234
ISOPROPANOL	TETRAHYDROFURAN	666,05388238	-84,64048228	0,3	-4,960814
ISOPROPANOL	METHYL CHLORIDE	-299,9953334	1974,7938063	0,3	-2,005937
DICHLOROMETHANE	TETRAHYDROFURAN	-685,5905644	573,55211238	0,3	-2,261412
DICHLOROMETHANE	METHYL CHLORIDE	-331,7953045	256,50426794	0,3	-1,202354
TETRAHYDROFURAN	METHYL CHLORIDE	-5,584329769	-169,1513138	0,3	-2,593929

Not supplied Supplied Imported Estimated

Comments :

BINARIES

ACTIONS —

Import binaries...

Clear all binaries...

Binaries estimation...

Save the binaries...

OPTIONS —

Unit

cal/mole

parameters will be ignored

1. "Save the binaries..."



Users databases are stored in:
C:\Users\XXX[current user]\Roaming\Prosim\Stardust\Binaries\Databases

Step 4: Save the binaries

2. Enter a name to create a new user database or select an existing user database.

In the case of an existing user database you can:

- * Add the selected binaries to the user database
- * Replace the values of the user database by the ones selected

Export of binaries

Enter the name of the database or select an existing

My_Private_Database

Select the binaries to save

	Compound	Compound	Cij0	Cji0	aij0	CijT	CjiT
<input checked="" type="checkbox"/>	SOPROPANOL	DICHLOROMETHANE	-429,916	1880	0,3	2,21423	-9,33757
<input checked="" type="checkbox"/>	SOPROPANOL	TETRAHYDROFURAN	666,054	-84,6405	0,3	-4,96081	2,25479
<input checked="" type="checkbox"/>	SOPROPANOL	METHYL CHLORIDE	-299,995	1974,79	0,3	-2,00594	-0,218641
<input checked="" type="checkbox"/>	DICHLOROMETHANE	TETRAHYDROFURAN	-685,591	573,552	0,3	-2,26141	1,94737
<input checked="" type="checkbox"/>	DICHLOROMETHANE	METHYL CHLORIDE	-331,795	256,504	0,3	-1,20235	2,29365
<input checked="" type="checkbox"/>	TETRAHYDROFURAN	METHYL CHLORIDE	-5,58433	-169,151	0,3	-2,59393	3,09703

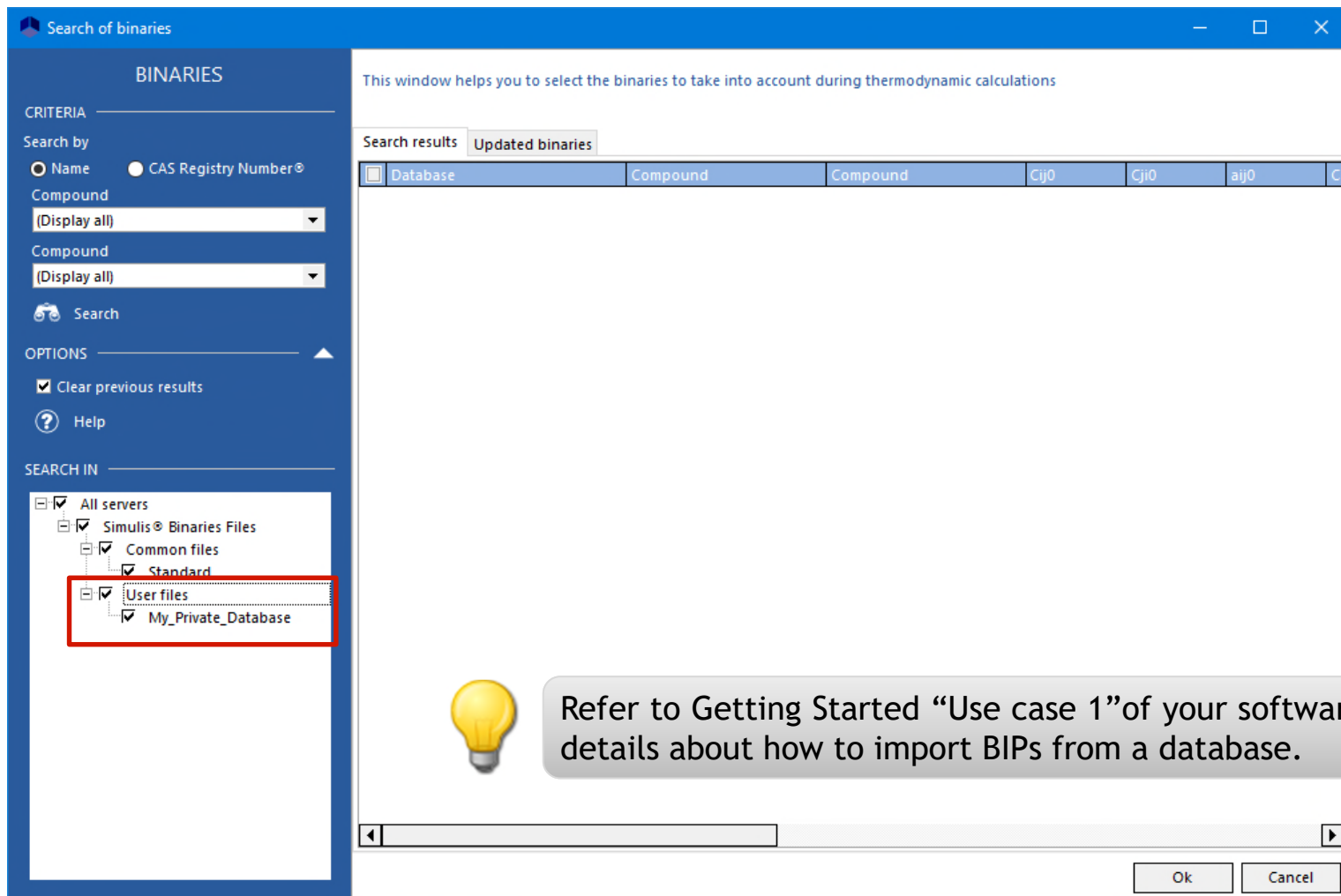
Ok Cancel

3. Select the binaries to be saved

4. "Ok" to validate

Step 4: Save the binaries

- To perform a search in your private database, select it in the “Search of binaries” window



**ProSim SA**

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

☎: +33 (0) 5 62 88 24 30



Software & Services In Process Simulation

www.prosim.net
info@prosim.net

**ProSim, Inc.**

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

☎: +1 215 600 3759