

Getting started with Simulis® Thermodynamics

Use Case 14: Definition and properties calculation of a
polymer/solvent mixture

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ProSim

Introduction

A polymer is not considered as a classic component because:




- **Its properties depend on the length of its chain (represented by the number and the weight average molar mass),**
- **Its properties depend on the considered repeat units (segments),**
- **All properties of classical component are not defined for a polymer (no critical point, no saturation pressure...),**
- **Predictive methods available for property calculations of classical components are not adapted.**

Moreover, high molar mass value of polymers leads to particular behaviors of mixtures containing this type of component. As an example, the vapor phase of this type of mixture at vapor-liquid equilibria will never contain polymer.

Consequently, the treatment of polymer/solvent mixtures requires a specific approach in Simulis Thermodynamics. This document presents in details the different steps to follow in order to perform calculation concerning this type of mixture.

Introduction

The following steps are described in this document:

-  Step 1: Add a new polymer component
(Which data are required? How to supply them?)
-  Step 2: Calculation of pure polymer properties
(Which properties can be calculated? How to calculate them?)
-  Step 3: Calculation of polymer/solvent mixture properties
(Which thermodynamic model to use? How to calculate these properties?)

The example presented in this document is based on the following mixture:

Acetone / poly(Styrene5%molar-Butadiene95%molar) with a weight average molar mass of 300 kg/mol and a number average molar mass of 40 kg/mol

Before studying this chapter, it is recommended to consult:

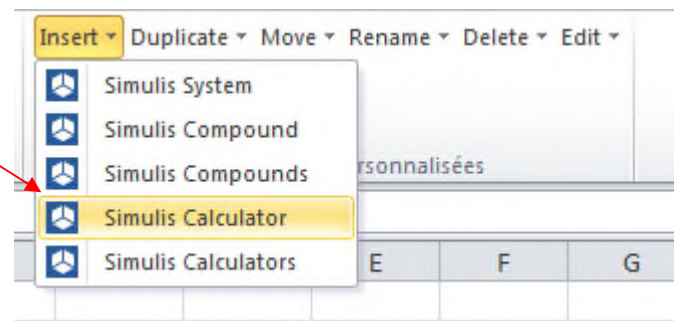
- « Getting Started with Simulis Thermodynamics: Use Case 1 » that explains the method to select components and configure a thermodynamic profile,
- « Getting Started with Simulis Thermodynamics: Use Case 4 » that explains the method to calculate thermodynamic properties of pure components and mixtures in Simulis Thermodynamics.

Step 1: Add a new polymer component

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- If you are using Simulis Thermodynamics in Excel:

Create the calculator object in a spreadsheet



- If you are using Simulis Thermodynamics within another ProSim environment (ProSimPlus, BatchReactor, BatchColumn etc...):

Click on the thermodynamic icon to open the calculator editor:

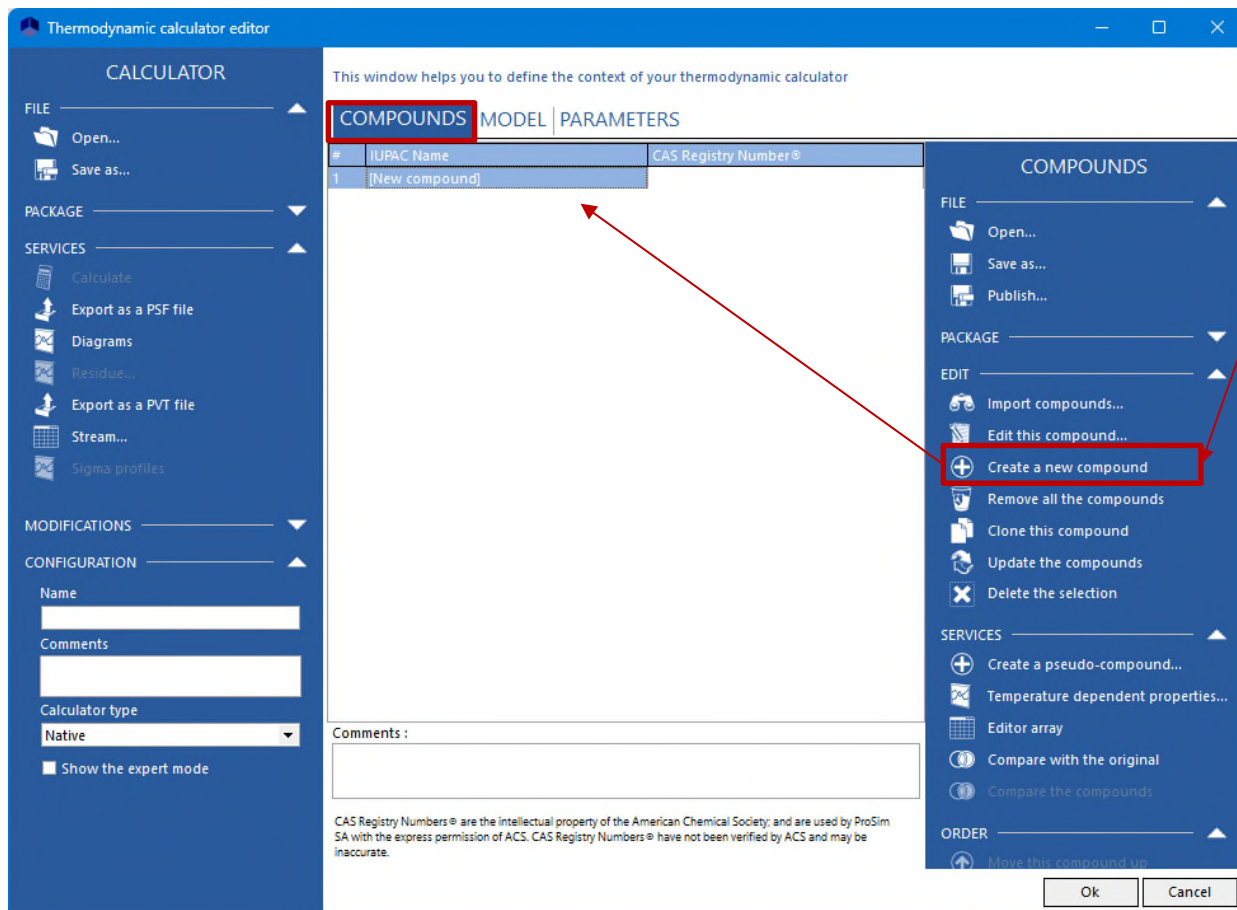


or



Simulis Thermodynamics is a « software component » that you can integrate into different applications: ProSim software, Excel, Matlab, your own software, etc...

Step 1: Add a new polymer component



1. In « COMPOUNDS » tab:
Click on « Create a new compound »



For more details about the creation of a new compound,
please consult:
« *Getting started with Simulis Thermodynamics, use case 9* »

Step 1: Add a new polymer component

The screenshot shows two windows from the ProSim software. The top window is the 'Thermodynamic calculator editor' with a 'COMPOUNDS' tab. It contains a table with columns 'IUPAC Name' and 'CAS Registry Number'. The first row is labeled '1' and contains the text '[New compound]'. A red arrow points from this entry to the 'Compound Editor' window below. The 'Compound Editor' window shows the 'Identification' properties for a compound named 'SBR'. The 'Specific name' field is highlighted with a red box and contains the text 'SBR'. The 'IUPAC name' field is also highlighted with a red box. The 'Properties' list on the left includes 'IUPAC name', 'Specific name', 'CAS Registry Number', 'Chemical family', 'Chemical formulae', 'Smiles', 'Set identifier', 'Intrinsic number (ProSim spec... 0', 'Synonyms', 'Compound comments', 'Cosmo file', 'Group contribution models', 'Atomic', 'Phase change', 'Combustion, security, toxicity', 'Condensed phase', 'Phase thermochemistry', 'Interaction, gas phase reaction', 'User properties', 'PPC-SAFT', 'NRTL-SAC', 'CPA', 'Polymers-Segments', and 'Sanchez-Lacombe'.

Thermodynamic calculator editor

COMPOUNDS MODEL PARAMETERS

#	IUPAC Name	CAS Registry Number
1	[New compound]	

Compound Editor

Name: SBR
ID: [28B4F506-F03D-4E17-A31B-899D1E6E7728]
Original ID:
Original location: \\

Complete

Properties	Value
Identification	
IUPAC name	
Specific name	SBR
CAS Registry Number	<unknown>
Chemical family	<unknown>
Chemical formulae	<unknown>
Smiles	
Set identifier	
Intrinsic number (ProSim spec... 0	
Synonyms	
Compound comments	
Cosmo file	<unknown>
Group contribution models	
Atomic	
Phase change	
Combustion, security, toxicity	
Condensed phase	
Phase thermochemistry	
Interaction, gas phase reaction	
User properties	
PPC-SAFT	
NRTL-SAC	
CPA	
Polymers-Segments	
Sanchez-Lacombe	

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.

2. Double-click or right-click on the [New compound] added in order to define the polymer

3. In the « identification » folder, give a name to the polymer (« SBR » in this example for Styrene-Butadiene-Rubber)

Step 1: Add a new polymer component

In order to:

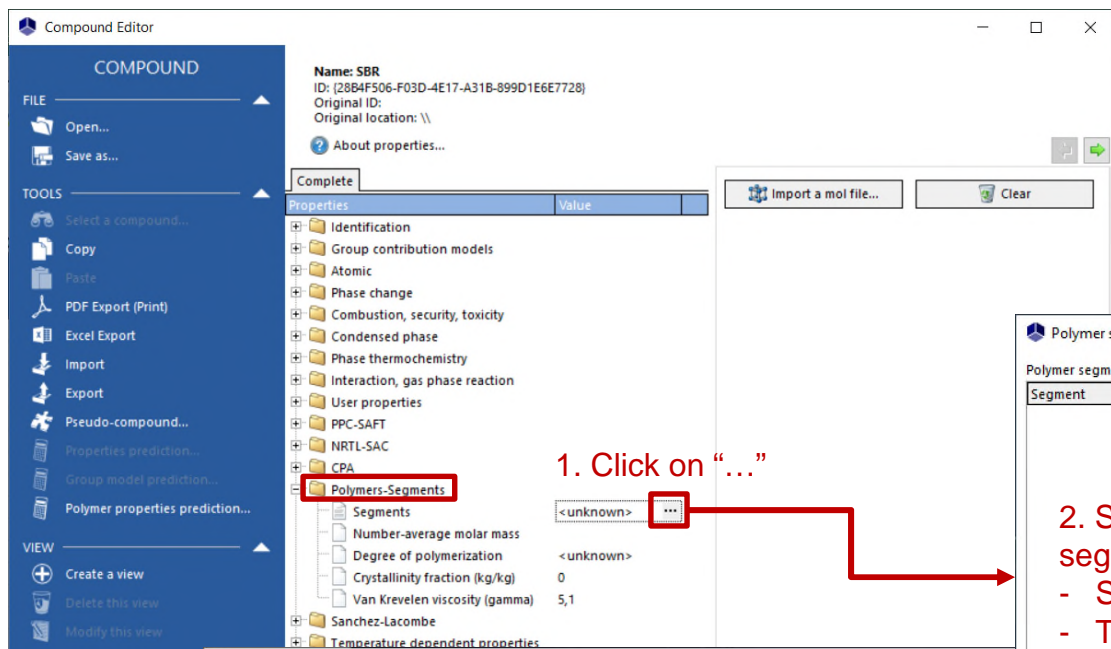
- Predict pure polymer properties,
- Perform calculations of thermodynamic or transport properties of mixtures containing polymers,

the following data must be filled in:

- Segments and segment molar fractions of the polymer,
- The number average molar mass of the polymer (M_n),
- The weight average molar mass of the polymer (M_w).

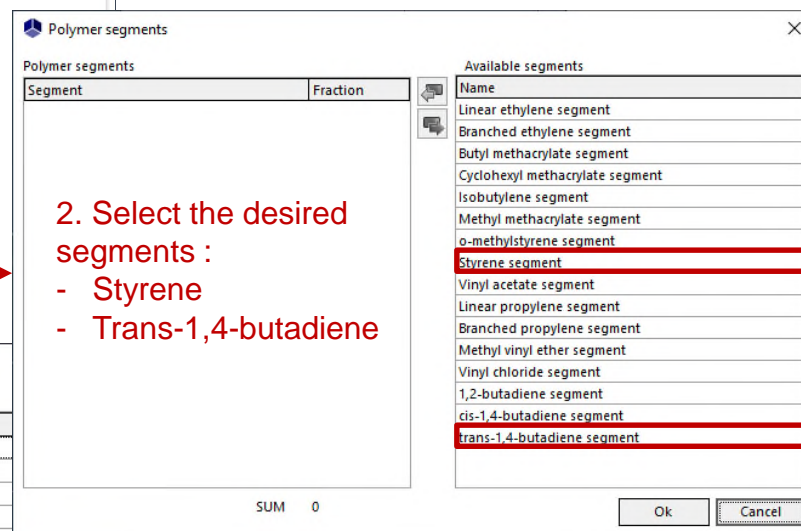
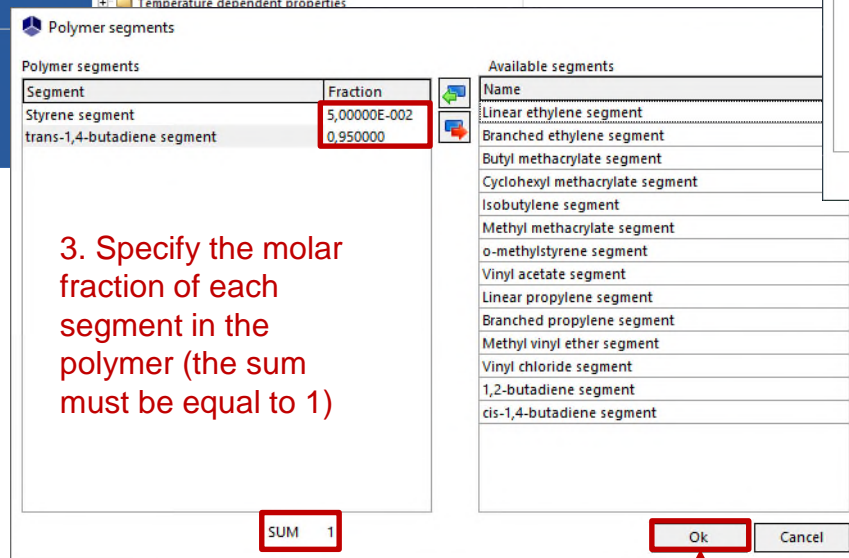
The following slides explain how to supply these data for the new “SBR” polymer component

Step 1: Add a polymer component



In the « Polymers-Segments » folder:

I. Specify segments contained in the polymer



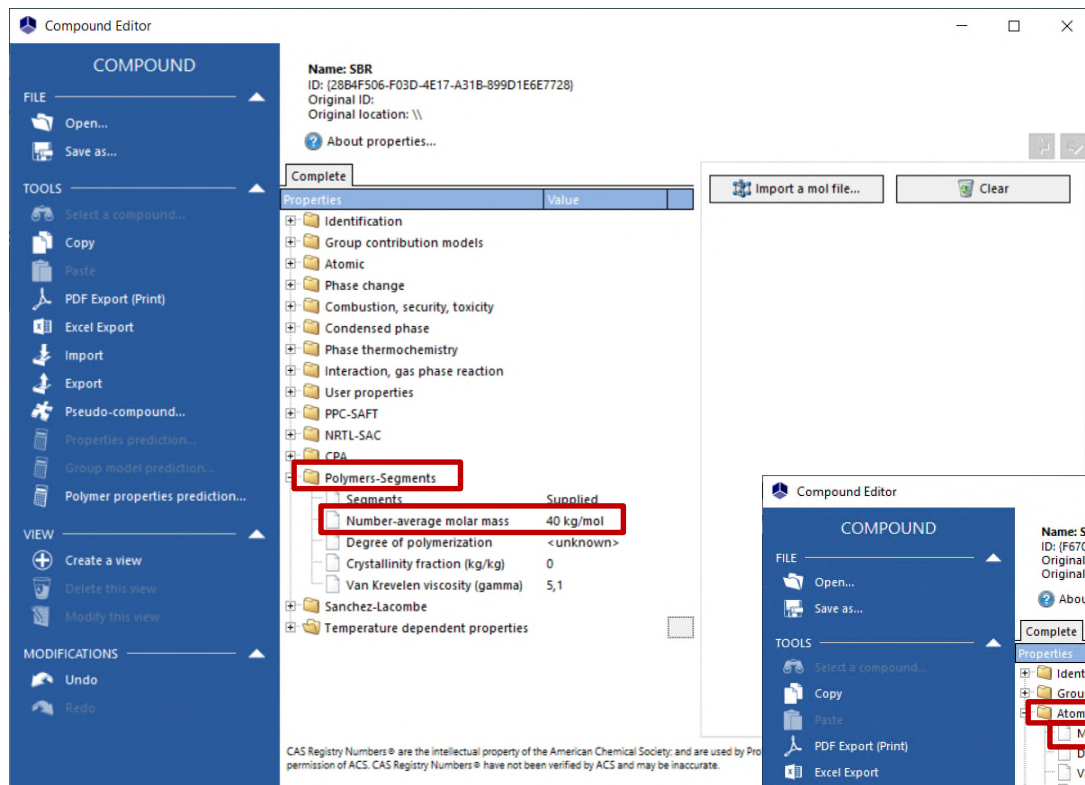
1. Click on "..."

2. Select the desired segments :
- Styrene
- Trans-1,4-butadiene

3. Specify the molar fraction of each segment in the polymer (the sum must be equal to 1)

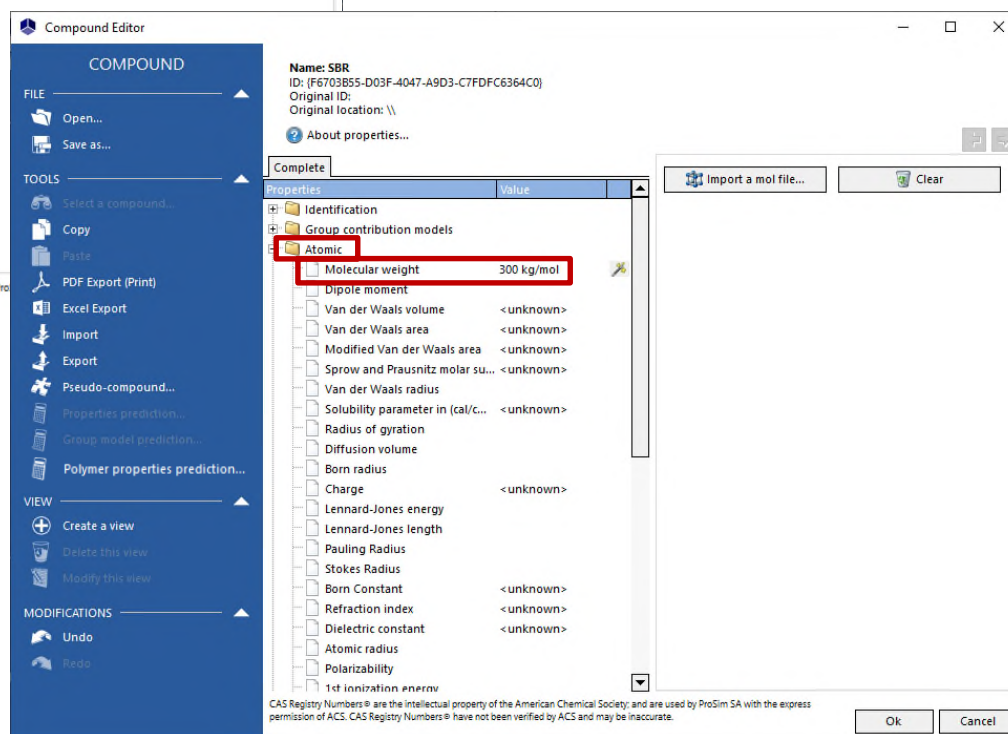
4. Click on "OK"

Step 1: Add a polymer component



In the « Polymers-Segments » folder:

II. Specify the number average molar mass of the polymer



In the « Atomic » folder:

III. Specify the weight average molar mass of the polymer

Step 2: Calculation of pure polymer properties

The temperature-independent properties and the correlations of temperature-dependent properties of a pure polymer can be:

- Directly provided by the user
- Or predicted from data supplied at step 1

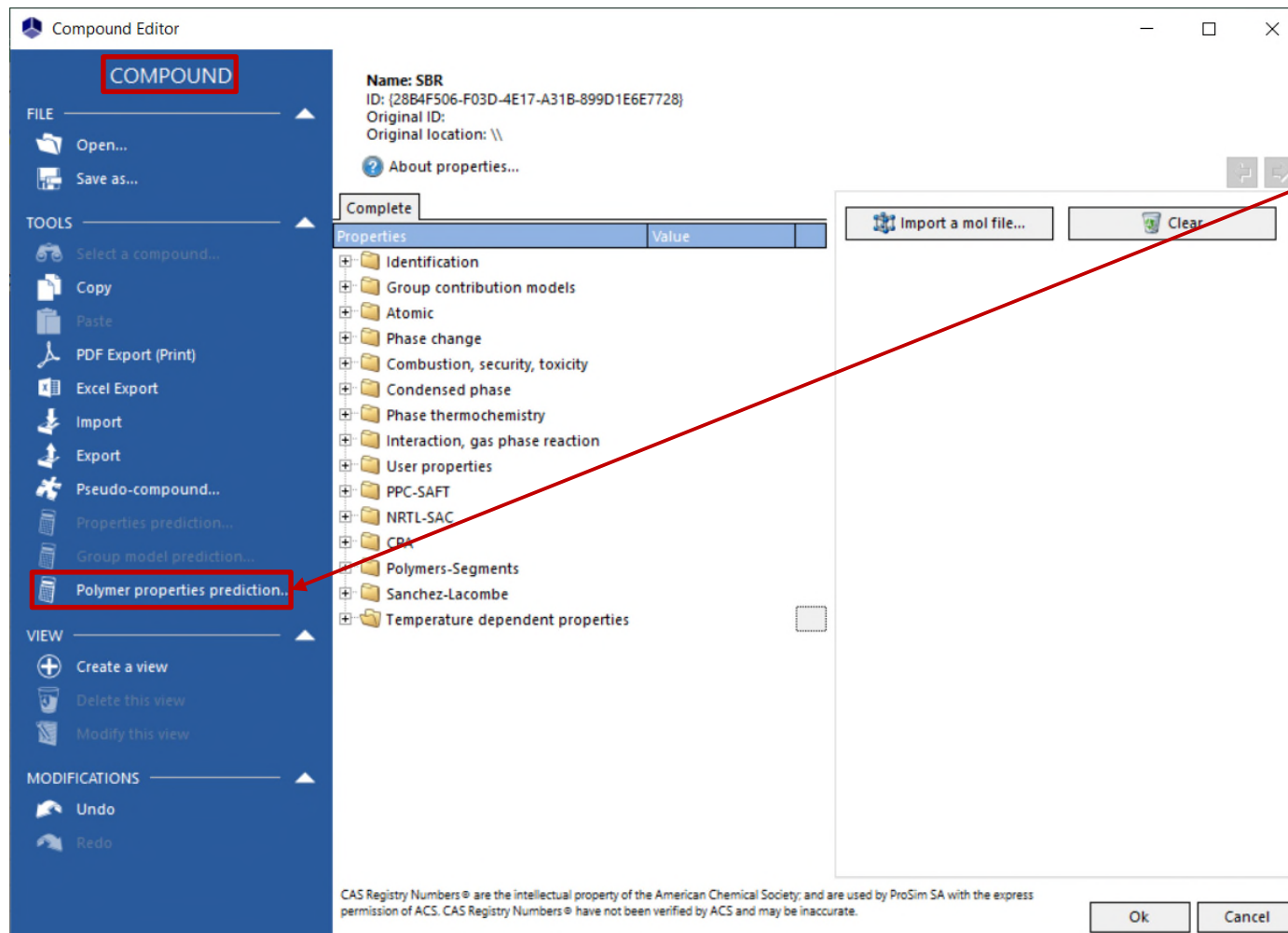
Temperature-independent properties used for a polymer are:

- The glass-transition temperature (« Phase change » folder)
- The melting temperature (« Phase change » folder)
- The van der Waals volume (« Atomic » folder)
- The ideal gas enthalpy and Gibbs energy of formation at 25°C (« Phase thermochemistry » folder)
- The vaporization and fusion enthalpies (« Phase change » folder)
- The parachor (« Condensed phase » folder)
- The degree of polymerization (« Polymers-Segments » folder)
- The *hypothetical* critical temperature (« Phase change » folder)
- The *hypothetical* critical pressure (« Phase change » folder)
- The *hypothetical* boiling temperature (« Phase change » folder)
- The *hypothetical* acentric factor (« Phase change » folder)

For temperature-dependent properties, correlations called « Polymers », specific to polymers are available for calculation of:

- Vapor pressure (fixed to avoid polymer in vapor phase)
- The ideal gas specific heat
- The liquid specific heat
- The solid specific heat
- The liquid density
- The solid density
- The liquid viscosity
- The liquid thermal conductivity
- The solid thermal conductivity
- The surface tension

Step 2: Calculation of pure polymer properties



In order to predict pure polymer properties:

- On the “COMPOUND” tab, click on “Polymer properties prediction...”



The predictions of the properties of a pure polymer can only be made correctly if step 1 has been carried out previously

Step 2: Calculation of pure polymer properties

2. Select the properties you want to predict

Polymers properties prediction

Use a prediction system to calculate the properties of a compound.

☐ Expand all

Property	Current value	Overwrite	Predicted value
<input checked="" type="checkbox"/> Constant properties		<input checked="" type="checkbox"/> Select all	
Degree of polymerization	706,714	<input checked="" type="checkbox"/>	706,714
Critical temperature	1143,80 K	<input checked="" type="checkbox"/>	1143,80 K
Critical pressure	8,31019 atm	<input checked="" type="checkbox"/>	8,31019 atm
Acentric factor	17,4487	<input checked="" type="checkbox"/>	17,4487
Van der Waals volume	3,88400E-005	<input checked="" type="checkbox"/>	3,88400E-005
Ideal gas enthalpy of formation at 25°C	6,64794 kcal/mol	<input checked="" type="checkbox"/>	6,64794 kcal/mol
Ideal gas Gibbs energy of formation at 25°C	20821,6 kcal/mol	<input checked="" type="checkbox"/>	20821,6 kcal/mol
Enthalpy of vaporization (boiling point)	5,90433 kcal/mol	<input checked="" type="checkbox"/>	5,90433 kcal/mol
Enthalpy of fusion (melting point)	1,82242 kcal/mol	<input checked="" type="checkbox"/>	1,82242 kcal/mol
Parachor	150,295	<input checked="" type="checkbox"/>	150,295
Glass-transition temperature	206,829 K	<input checked="" type="checkbox"/>	206,829 K
Normal melting point	424,306 K	<input checked="" type="checkbox"/>	424,306 K
Normal boiling point	1013,40 K	<input checked="" type="checkbox"/>	1013,40 K
T* parameter	618,067 K	<input checked="" type="checkbox"/>	618,067 K
P* parameter	4489,43 bar	<input checked="" type="checkbox"/>	4489,43 bar
rho* parameter	2716,03 kg/m3	<input checked="" type="checkbox"/>	2716,03 kg/m3
r parameter	1286,62	<input checked="" type="checkbox"/>	1286,62
epsilon* parameter	5138,88 J/mol	<input checked="" type="checkbox"/>	5138,88 J/mol
v* parameter	1,14466E-005 m3/m	<input checked="" type="checkbox"/>	1,14466E-005 m3/mol
c volume translation parameter	0,00000 cm3/g	<input checked="" type="checkbox"/>	0,00000 cm3/g
Number of segments (m)	5899,10	<input checked="" type="checkbox"/>	5899,10
Segment diameter (sigma)	3,83944 angstrom	<input checked="" type="checkbox"/>	3,83944 angstrom
Interaction energy between segments (eps/k)	311,309 K	<input checked="" type="checkbox"/>	311,309 K
<input checked="" type="checkbox"/> Temperature dependent properties			
+ Vapor pressure		<input checked="" type="checkbox"/>	
+ Ideal gas specific heat		<input checked="" type="checkbox"/>	
+ Liquid specific heat		<input checked="" type="checkbox"/>	
+ Solid specific heat		<input checked="" type="checkbox"/>	
+ Liquid density		<input checked="" type="checkbox"/>	
+ Solid density		<input checked="" type="checkbox"/>	
+ Liquid viscosity		<input checked="" type="checkbox"/>	
+ Liquid thermal conductivity		<input checked="" type="checkbox"/>	
+ Solid thermal conductivity		<input checked="" type="checkbox"/>	
+ Surface tension		<input checked="" type="checkbox"/>	

Note that it is also possible to predict values of Sanchez-Lacombe and GC-PPC-SAFT equations of state pure polymer parameters

3. Use

Step 2: Calculation of pure polymer properties

Compound Editor

COMPOUND

FILE

- Open...
- Save as...

TOOLS

- Select a compound...
- Copy
- Paste
- PDF Export (Print)
- Excel Export
- Import
- Export
- Pseudo-compound...
- Properties prediction...
- Group model prediction...
- Polymer properties prediction...

VIEW

- Create a view
- Delete this view
- Modify this view

MODIFICATIONS

- Undo
- Redo

Name: SBR
ID: (AD67EA88-8257-4024-A8E9-D1F33259C1D8)
Original ID:
Original location: \\

Complete

Properties

Properties	Value
Phase change	
Normal melting point	424,30646643109...
Normal boiling point	
Enthalpy of fusion (melting p...	1,8224187380497...
Triple point temperature	
Triple point pressure	
Physical state at 25°C	<unknown>
Physical state in aqueous sol...	<unknown>
Diffusion coefficient	
Enthalpy of vaporization (boil...	5,9043260038240...
Octanol-Water partition coeff...	<unknown>
soil sorption coefficient (Koc...	
Liquid vapor calculation type	<unknown>
Acentric factor	<unknown>
Modified acentric factor	<unknown>
Critical temperature	
Critical pressure	
Critical volume	
Critical compressibility factor	<unknown>
Critical density	
Heat of sublimation at the tri...	
Glass-transition temperature	206,8288692579...

Combustion, security, toxicity

Condensed phase

Phase thermochimistry

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The predicted properties can be viewed in the different folders of "COMPOUND" tab

Compound Editor

COMPOUND

FILE

- Open...
- Save as...

TOOLS

- Select a compound...
- Copy
- Paste
- PDF Export (Print)
- Excel Export
- Import
- Export
- Pseudo-compound...
- Properties prediction...
- Group model prediction...
- Polymer properties prediction...

VIEW

- Create a view
- Delete this view
- Modify this view

MODIFICATIONS

- Undo
- Redo

Name: SBR
ID: (F0DDFA29-EB3A-48AB-BFEF-046E2BA0782E)
Original ID:
Original location: \\

Complete

Properties

Properties	Value
User properties	
PPC-SAFT	
NRTL-SAC	
CPA	
Polymers-Segments	
Sanchez-Lacombe	
Temperature dependent properties	
Solid specific heat	
Liquid specific heat	
Ideal gas specific heat	
Vapor pressure	
Vaporization enthalpy	
Solid thermal conductivity	
Liquid thermal conductivity	
Correlation	Polymers
TMin	206,8288692579...
TMax	1000 K
Coef A	0,15819422598003
Gas thermal conductivity	
Liquid viscosity	
Gas viscosity	
Solid density	
Liquid density	
Surface tension	
Second virial coefficient	

Molar K W/m/K

Chart Grid Formulation

Liquid thermal conductivity (W/m/K)

Logarithmic scale 1/T scale

Tools

Temperature Min Temperature Max Points

206,82886925 1000 K 20 Refresh

Temperature Property

206,82886925 0,173489 W/m/K

Copy Print Regression

OK Cancel

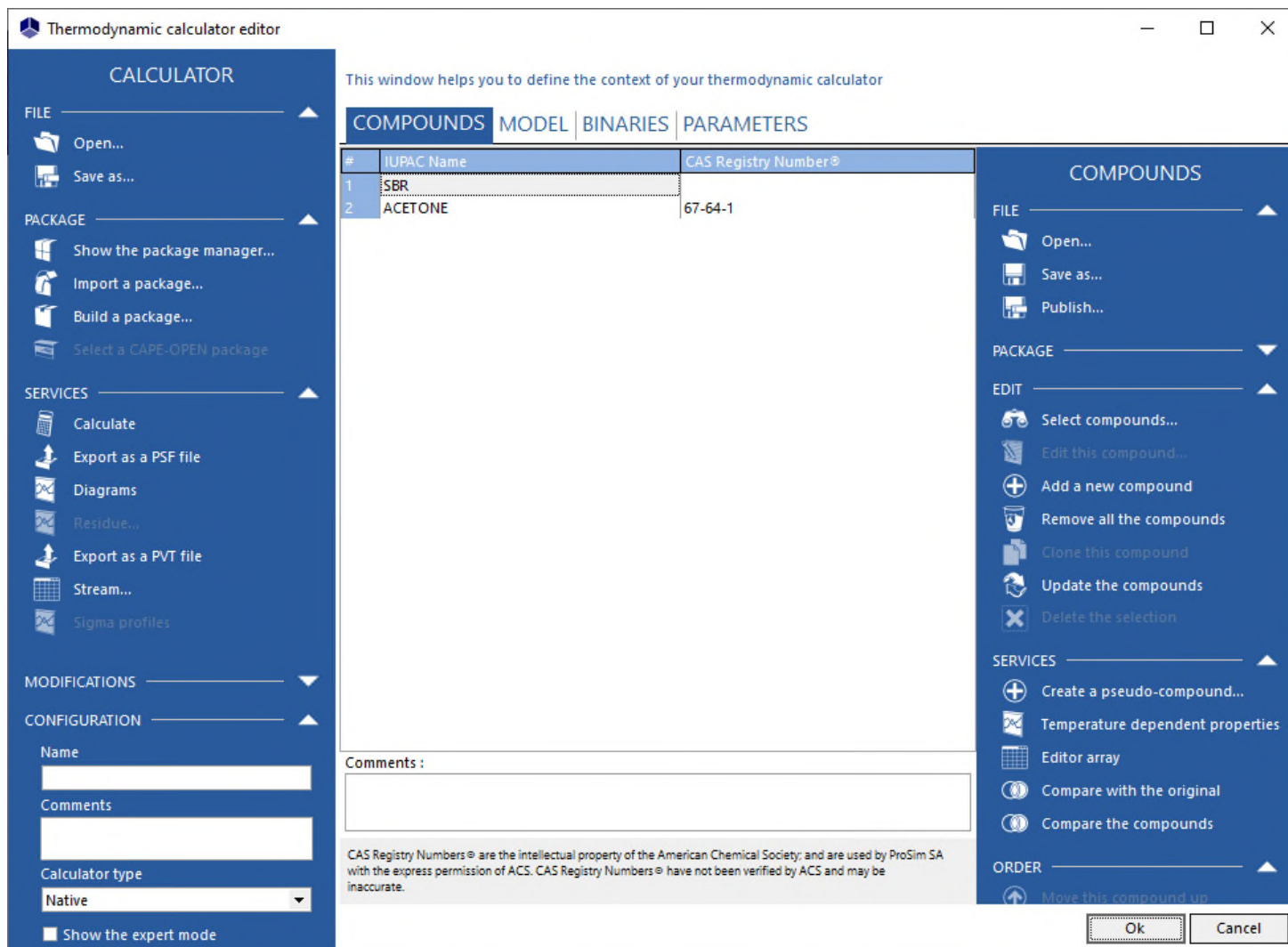
CAS Registry Numbers® are the intellectual property of the American Chemical Society, and are used by ProSim SA with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.

For more details about the component properties, please consult:
« *Getting started with Simulis Thermodynamics, use case 4* »

Step 3: Calculation of polymer/solvent mixture properties

Add the solvent component (acetone in this example)

(For a detailed description of this step, please consult: « Getting started with Simulis Thermodynamics: use case 1 »)



Step 3: Calculation of polymer/solvent mixture properties

In the “MODEL” tab:

1. Select a thermodynamic model well suited to mixtures containing polymers
2. Select a set of methods for transport properties calculation which is adapted to mixtures containing polymers

Thermodynamic calculator editor

FILE — Open... Save as...

PACKAGE — Show the package manager... Import a package... Build a package... Select a CAPE-OPEN package

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

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

Name Sanchez-Lacombe

Category All the profiles

Profile Sanchez-Lacombe

Approach type Using Equation of state

Equation of state Sanchez-Lacombe

Alpha function Not defined

Mixing rules Not defined

Activity coefficient model Not defined

Pure liquid fugacity standard state Standard

Liquid molar volume Equation d'état

Transport properties Polymers

Enthalpy calculation $H^*=0$, ideal gas, 25°C, 1 atm

User-defined thermodynamic model None

Model index 1

Comments :

THERMODYNAMIC MODEL

CONFIGURATION — Parameters Thermodynamic assistant Thermodynamic help Use a specific model for pure water Advanced

Ok Cancel

The recommended thermodynamic models for this type of mixtures are:

- The Sanchez-Lacombe equation of state (considered in this example)
- The GC-PPC-SAFT equation of state
- The UNIFAC-FV activity coefficients model
- The Flory-Huggins activity coefficients model

The «Polymers » set of properties is well suited to calculation of transport properties of this type of mixture

Step 3: Calculation of polymer/solvent mixture properties

In the “BINARIES” tab:

- Add the binary interaction parameter of the equation of state by providing a value to the Akij coefficient (Akij = 0.035)

Thermodynamic calculator editor

Calculator

FILE

- Open...
- Save as...

PACKAGE

- Show the package manager...
- Import a package...
- Build a package...
- Select a CAPE-OPEN package

SERVICES

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

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 : $K_{ij} = A_{Kij} + B_{Kij} \cdot 298.15/T + C_{Kij} \cdot \ln(T/298.15) + D_{Kij} \cdot T/298.15 + E_{Kij} \cdot (T/298.15)^2$, L_{ij}

Compound	Compound	AKij	BKij	CKij	DKij	EKij	ALij	BLij	CLij	DLij	ELij
SBR	ACETONE	0.035	0	0	0	0	0	0	0	0	0

Not supplied Supplied Imported Estimated

Comments :

BINARIES

ACTIONS

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

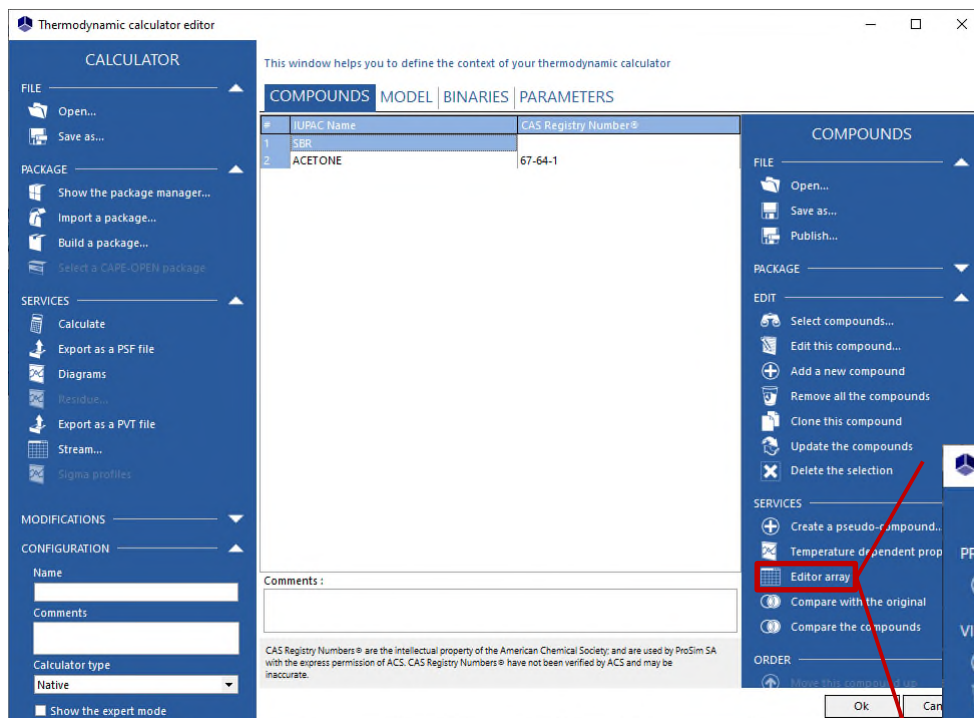
OPTIONS

Unit

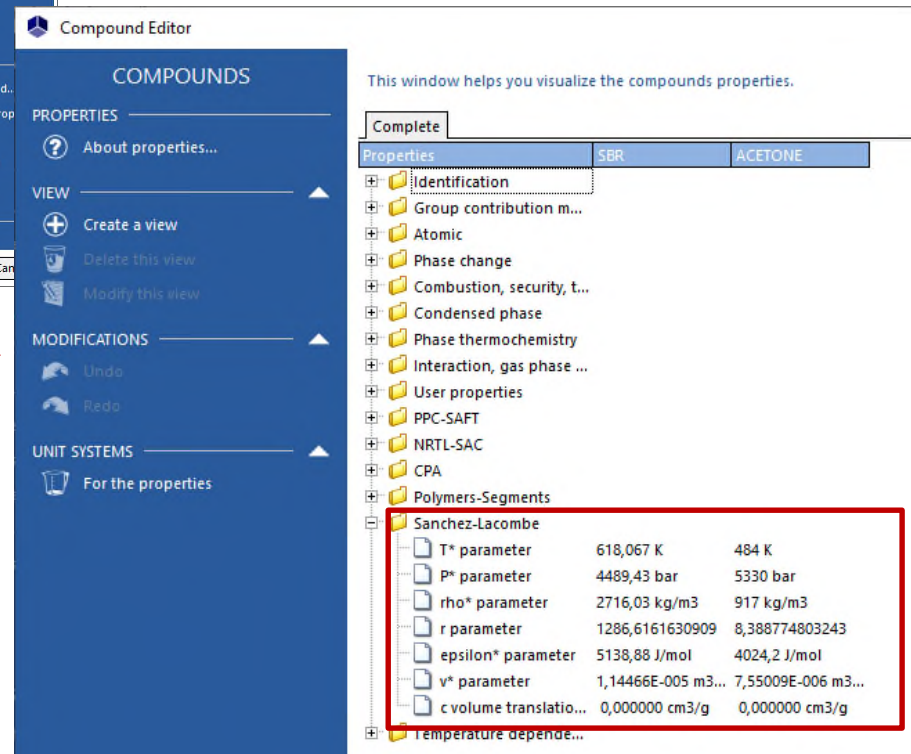
parameters will be ignored

Ok Cancel

Step 3: Calculation of polymer/solvent mixture properties



Before using a thermodynamic model (Sanchez-Lacombe equation of state in this case), the user must be sure that all the required parameters are available for all components



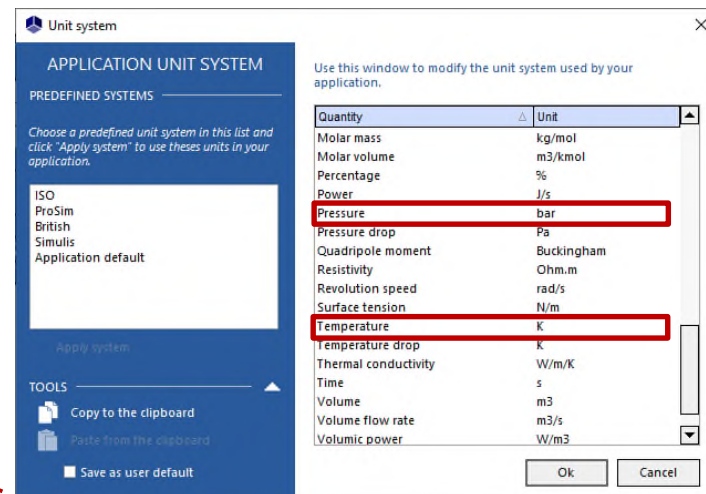
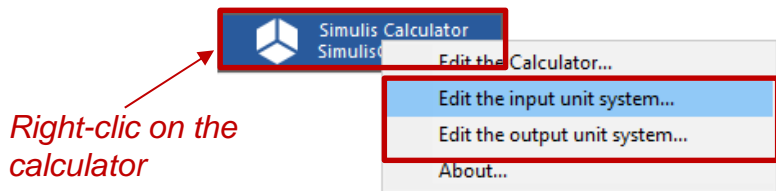
If one of these parameters is not available:

- For a polymer component, the « polymer prediction » method presented on step 2 can be employed
- For a solvent component, these parameters are implicitly estimated from other data during the calculation of a property. *(For more details about these estimation methods, please consult the Sanchez-Lacombe paragraph of the thermodynamic models manual, available from the « MODEL » tab of the calculator)*

Step 3: Calculation of polymer/solvent mixture properties

In the excel sheet of your calculator:

1. Select the « bar » unit for the pressure and the « K » unit for the temperature for the input and output unit systems



For more details about the modification of unit systems, please consult:

« Getting started with Simulis Thermodynamics, use case 1 »

2. Display the name of the components and the selected units

		input	output
		1	2
Index comp	Name compound		
1	SBR	K	K
2	=stCALCompoundDisplayName(\$C\$5;B9)	bar	=stCAL.GetUnitNameInSystem(;\$G\$7;\$E9)

Notes :

- The index of the polymer is 1, the index of the solvent is 2
- In this example, the weight fraction is employed. As the polymer is a heavy molecule, its weight fraction is high even if its molar fraction is very low

3. Provide the experimental data (bubble pressure data in this example)

EXP	
Liquid Equilibria of Copolymer + Solvent and Homopolymer + Solvent Binaries: New Experimental Data and Their Correlation", J. Chem. Eng.	
T / K	323,15
w2 / kg/kg	P Bubble / bar
0,003	0,137
0,023	0,265
0,04	0,363
0,056	0,415
0,067	0,453
0,072	0,465
0,067	0,472
0,066	0,473
0,078	0,511
0,079	0,523
0,08	0,533
0,091	0,552
0,115	0,596
0,11	0,597
0,12	0,613

Step 3: Calculation of polymer/solvent mixture properties

4. Perform a TP-Flash calculation with the Sanchez-Lacombe equation of state (calculation of the vapor ratio, the liquid and vapor phases compositions at fixed temperature, pressure and global composition)

4.1. Preparation of the calculation in the Excel sheet: Create the following table

TP flash calculation						
w1 / kg/kg	w2 / kg/kg					
0,8	0,2					
P / bar	T / K	tvap	w1	w2	y1	y2
0,01	323,15					
0,02	323,15					
0,03	323,15					
0,04	323,15					
0,05	323,15					
0,1	323,15					
0,15	323,15					
0,2	323,15					
0,25	323,15					
0,3	323,15					
0,35	323,15					
0,4	323,15					
0,45	323,15					
0,5	323,15					
0,55	323,15					
0,6	323,15					
0,65	323,15					
0,7	323,15					

Provide the global weight composition of the mixture, the temperature and the pression for the calculation

Define a table area dedicated to the calculated values

Step 3: Calculation of polymer/solvent mixture properties

4. Perform a TP-Flash calculation with the Sanchez-Lacombe equation of state (calculation of the vapor ratio, the liquid and vapor phases compositions at fixed temperature, pressure and global composition)

4.2. Add the calculation function

TP flash calculation						
w1 / kg/kg	w2 / kg/kg					
0,8	0,2					
P / bar	T / K	twap	w1	w2	y1	y2
0,01	323,15					
0,02	323,15					
0,03	323,15					
0,04	323,15					
0,05	323,15					
0,1	323,15					
0,15	323,15					
0,2	323,15					
0,25	323,15					
0,3	323,15					
0,35	323,15					
0,4	323,15					
0,45	323,15					
0,5	323,15					
0,55	323,15					
0,6	323,15					
0,65	323,15					
0,7	323,15					

1. Select the first line of the table and click on the excel button dedicated to the insertion of a function



Insert Function

Search for a function:

Type a brief description of what you want to do and then click Go

Go

Or select a category: Simulis Calculator

Select a function:

- stCALFlashST
- stCALFlashSTKij
- stCALFlashSU
- stCALFlashSUKij
- stCALFlashSV
- stCALFlashSVKij
- stCALFlashTP**

stCALFlashTP(ObjectName; Temperature; Pressure; Composition;...)
Liquid-vapor flash at given temperature and pressure.

[Help on this function](#)

OK Cancel

2. In "Insert Function" window, select "Simulis Calculator"

3. In the list of functions, select "stCALFlashTP"

Step 3: Calculation of polymer/solvent mixture properties

21

4. Perform a TP-Flash calculation with the Sanchez-Lacombe equation of state (calculation of the vapor ratio, the liquid and vapor phases compositions at fixed temperature, pressure and global composition)

4.2. Add the calculation function

4. Provide the function arguments

Function Arguments

stCALFlashTP

ObjectName	\$C\$6	= SimulisCalculator1*
Temperature	F16	= 523,15
Pressure	E16	= 0,01
Composition	\$E\$14:\$F\$14	= (0,8\0,2)
CompositionType	1	= 1
Init	FALSE	= FALSE
InitVapRatio		=
InitLiquidFractions		=
InitVaporFractions		=
ResultType	1	= 1

Liquid-vapor flash at given temperature and pressure.

ResultType Result type (0 = molar, 1 = mass).

Formula result = 0,199284983

[Help on this function](#) OK Cancel

Provide the name of the calculator

Provide the temperature for the TP Flash calculation

Provide the pressure for the TP Flash calculation

Provide the global composition of the mixture for the TP Flash

Provide the type of the input composition (1 = weight composition)

Provide if initial values must be taken into account (here FALSE)

Provide the type of the output composition

5. Validate the matrix function with Ctrl+Shift+Enter

Some arguments must be set by adding « \$ » in order to extend the function in the table (see next slide)

Step 3: Calculation of polymer/solvent mixture properties

4. Perform a TP-Flash calculation with the Sanchez-Lacombe equation of state (calculation of the vapor ratio, the liquid and vapor phases compositions at fixed temperature, pressure and global composition)

4.2. Add the calculation function

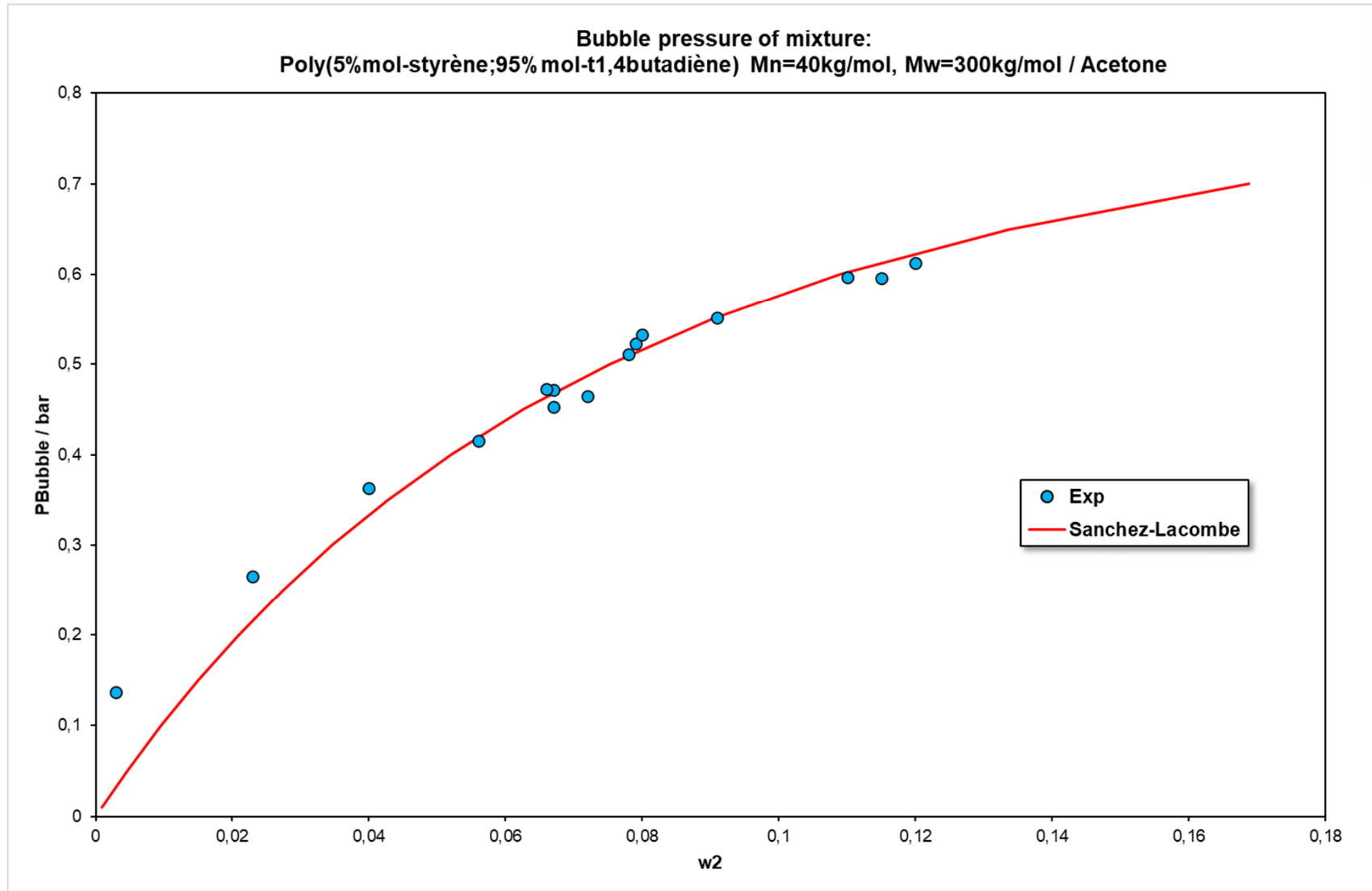
TP flash calculation						
w1 / kg/kg	w2 / kg/kg					
0,8	0,2					
P / bar	T / K	twap	w1	w2	y1	y2
0,01	323,15	0,199285	0,999107	0,000893	0	1
0,02	323,15					
0,03	323,15					
0,04	323,15					
0,05	323,15					
0,1	323,15					
0,15	323,15					
0,2	323,15					
0,25	323,15					
0,3	323,15					
0,35	323,15					
0,4	323,15					
0,45	323,15					
0,5	323,15					
0,55	323,15					
0,6	323,15					
0,65	323,15					
0,7	323,15					

6. Extend the calculation vertically over the whole table

TP flash calculation						
w1 / kg/kg	w2 / kg/kg					
0,8	0,2					
P / bar	T / K	twap	w1	w2	y1	y2
0,01	323,15	0,199285	0,999107	0,000893	0	1
0,02	323,15	0,198558	0,998201	0,001799	0	1
0,03	323,15	0,197819	0,997281	0,002719	0	1
0,04	323,15	0,197067	0,996346	0,003654	0	1
0,05	323,15	0,196301	0,995398	0,004602	0	1
0,1	323,15	0,192263	0,990422	0,009578	0	1
0,15	323,15	0,187827	0,985012	0,014988	0	1
0,2	323,15	0,18292	0,979096	0,020904	0	1
0,25	323,15	0,177443	0,972577	0,027423	0	1
0,3	323,15	0,171272	0,965335	0,034665	0	1
0,35	323,15	0,164236	0,957208	0,042792	0	1
0,4	323,15	0,156097	0,947976	0,052024	0	1
0,45	323,15	0,146512	0,93733	0,06267	0	1
0,5	323,15	0,134958	0,924817	0,075183	0	1
0,55	323,15	0,120625	0,909737	0,090263	0	1
0,6	323,15	0,102046	0,890925	0,109075	0	1
0,65	323,15	0,076462	0,866247	0,133753	0	1
0,7	323,15	0,037399	0,831133	0,168867	0	1

Step 3: Calculation of polymer/solvent mixture properties

The results obtained are plotted on the following graph



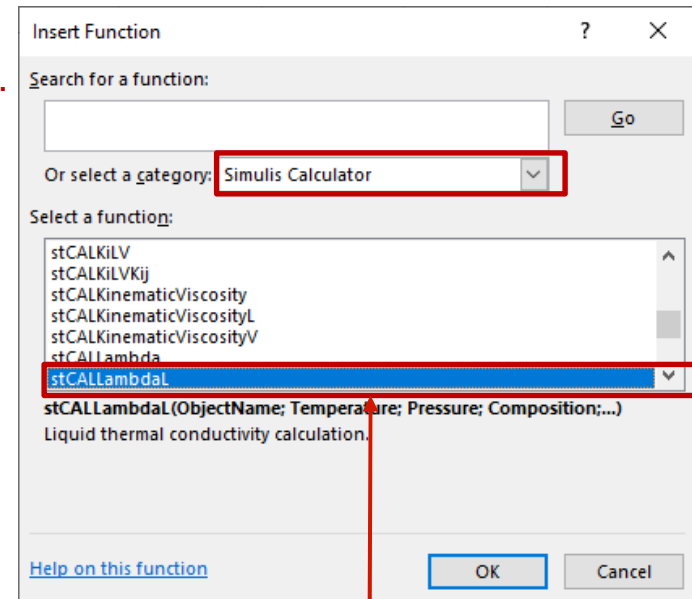
Step 3: Calculation of polymer/solvent mixture properties

Calculation of transport properties can also be performed.
An example of liquid thermal conductivity calculation is presented here.

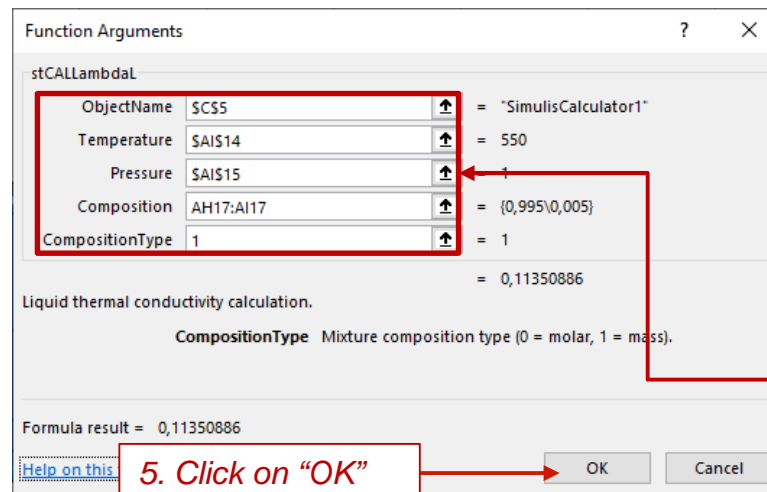
1. Create the following table

T / K	550	
P / bar	1	
w1 / kg/kg	w2 / kg/kg	λ_L / W/m/K
0,995	0,005	
0,99	0,01	
0,985	0,015	
0,98	0,02	
0,975	0,025	
0,97	0,03	
0,965	0,035	
0,96	0,04	
0,955	0,045	
0,95	0,05	
0,945	0,055	
0,94	0,06	
0,935	0,065	
0,93	0,07	
0,925	0,075	
0,92	0,08	
0,915	0,085	
0,91	0,09	
0,905	0,095	
0,9	0,1	
0,895	0,105	
0,89	0,11	
0,885	0,115	
0,88	0,12	

2. Select the first line of this table and click on the excel button dedicated to the insertion of a function



3. In the "Simulis Calculator" category, select the function "stCALLambdaL"



5. Click on "OK"

4. Provide the arguments of the function :

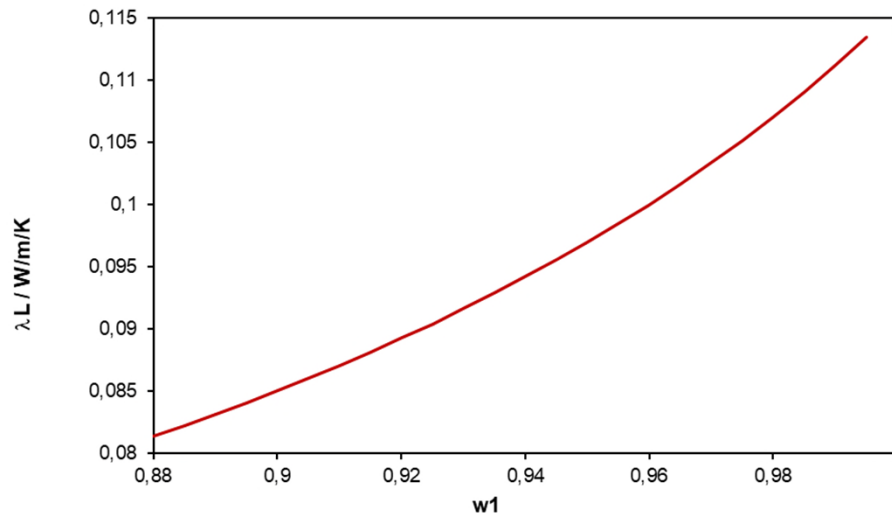
- The name of the calculator
- The temperature
- The pressure
- The composition of the mixture
- The type of the composition

Step 3: Calculation of polymer/solvent mixture properties

T / K	550	
P / bar	1	
w1 / kg/kg	w2 / kg/kg	λ_L / W/m/K
0,995	0,005	0,11350886
0,99	0,01	
0,985	0,015	
0,98	0,02	
0,975	0,025	
0,97	0,03	
0,965	0,035	
0,96	0,04	
0,955	0,045	
0,95	0,05	
0,945	0,055	
0,94	0,06	
0,935	0,065	
0,93	0,07	
0,925	0,075	
0,92	0,08	
0,915	0,085	
0,91	0,09	
0,905	0,095	
0,9	0,1	
0,895	0,105	
0,89	0,11	
0,885	0,115	
0,88	0,12	

6. Extend vertically the calculation in all the table

T / K	550	
P / bar	1	
w1 / kg/kg	w2 / kg/kg	λ_L / W/m/K
0,995	0,005	0,11350886
0,99	0,01	0,11124356
0,985	0,015	0,10910869
0,98	0,02	0,10709219
0,975	0,025	0,10518352
0,97	0,03	0,10337339
0,965	0,035	0,10165361
0,96	0,04	0,10001691
0,955	0,045	0,0984568
0,95	0,05	0,09696748
0,945	0,055	0,09554377
0,94	0,06	0,09418099
0,935	0,065	0,0928749
0,93	0,07	0,09162168
0,925	0,075	0,09041787
0,92	0,08	0,08926029
0,915	0,085	0,08814606
0,91	0,09	0,08707255
0,905	0,095	0,08603732
0,9	0,1	0,08503816
0,895	0,105	0,08407302
0,89	0,11	0,08314002
0,885	0,115	0,0822374
0,88	0,12	0,08136356



Step 3: Calculation of polymer/solvent mixture properties

Thermodynamic calculator editor

FILE

- Open...
- Save as...

PACKAGE

- Show the package manager...
- Import a package...
- Build a package...
- Select a CAPE-OPEN package

SERVICES

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

MODIFICATIONS

CONFIGURATION

Name

Comments

Calculator type

Native

Show the expert mode

COMPOUNDS MODEL BINARIES PARAMETERS

#	IUPAC Name	CAS Registry Number
1	SBR	
2	ACETONE	67-64-1

COMPOUNDS

FILE

- Open...
- Save as...
- Publish...

PACKAGE

Calculation service

SESSIONS

- Add a new session...
- Delete the current session

Session list

- New session

Calculate the current session

Calculate all the sessions

For the calculation conditions

For the calculated properties

UNIT SYSTEM (RESULTS)

MODIFICATIONS

OPTIONS

- Hide the constant results
- Automatically plot the results

HELP

This window helps you to define the context of your calculations

Type of calculation: ThermoPhysical properties

Session name: New session

Physical state: Liquid

System:

Property	Unit	Initial	Final	Step	Points
Pressure	bar	1	1	0	1
Temperature	K	550	550	0	1

Values

Type

- Fractions
- Quantities
- Molar
- Mass

Total: 0 kg

Mixture compositions

Au...	Compound	Initial	Final	Step	Points
<input type="checkbox"/>	SBR	0,995	0,88	-0,005	24
<input checked="" type="checkbox"/>	ACETONE	Auto	Auto	Auto	Auto

Results type

- Molar
- Mass

Same compositions whatever the calculation type

Properties

Transport

- Molecular weight
- Isobaric specific heat
- Isochoric specific heat
- Gamma (Cp/Cv ratio)
- Thermal conductivity**
- Dynamic viscosity
- Kinematic viscosity
- Density
- Molar density
- Molar volume
- Compressibility factor
- Sound speed
- pH
- Osmotic coefficient
- Joule-Thomson coefficient
- Isobaric expansion coefficient
- Isochoric tension coefficient
- Isotherm compressibility coefficient
- Residual isobaric heat capacity
- Residual isochoric heat capacity

Dynamic

Thermal conductivity

Thermal conductivity (W/mK)

Thermal conductivity-Liquid (MIXK)

Copy Print Logarithmic scale Key Axis

Quit

When all the required information are provided, click on "Calculate the current session"

These calculations can be directly performed in the calculator editor. For more details about the property calculations, please consult « *Getting started with Simulis Thermodynamics, use case 4* »



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