

What's New in *ChemSep*[™] 8.2

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The following features were added:

- Automatic loading of thermodynamic model parameters while loading components / changing models thereby simplifying the setting up a new simulation or CAPE-OPEN Property Package (COPP)
- A new property diagram option that can show any physical property as function of temperature, pressure, or composition
- Expander and compressor operations (as well as other flash types that include entropy)
- Use of multiple condensers / reboilers for Dividing Wall Columns (DWC)
- Calculation of Total Annualized Cost on flowsheet level

Automated Loading of Model Parameters

To facilitate a quicker setup of a new simulation, we added the automated loading of Binary Interaction Parameters (BIPs) for activity coefficient models, Equations of State, and Group Contribution methods. It is activated by default in the new version 8v2 but can optionally be switched off with the check box in the Components panel under Tools & Interface Settings:

Components Write as text in sep-file Check PCD date+time				
Default ID	Name	•		
Synonyms	c:\program files\cher	😂 Browse		
Auto-loading BIPs for thermodynamics				

Settings are loaded from the configuration file chemsep.cnf that each user has in the C:\users\user.name\Application Data\ChemSep folder. When we now load Water, Ethanol, and Acetone as components and select DECHEMA as K-value model, a switch in activity coefficient model automatically reloads the respective BIPs for these components from the appropriate libraries. Selection of Wilson activity model gives for the binary interaction parameters:

Select Thermodynamic	: Model parameters (when re	(quirea)				
Wilson						
Units J/mol	BIP estimation	BIP T est. (0	C) 76.8500	T dependence	None	•
Reset	i•i	A-ii	A-ji			
	Water - Ethanol	3997.60	1599.54			
🗁 Load	Water - Acetone	5880.57	1839.45			
	Ethanol - Acetone	1052.51	843.613			
Save						
Auto-Load						

A switch to the UNIQUAC automatically reloads the BIPs:

Select Thermodynamic	Model parameters (when re	quired)				
Units J/mol	BIP estimation	BIP T est. (0	C) 76.85	00 T dependence	None	
Reset	i-i	A-ii	A-ji			
	Water - Ethanol	459.691	727.183			
🗁 Load	Water - Acetone	-461.842	2923.77			
	Ethanol - Acetone	394.307	413.180			
Save						
Auto-Load						

And a switch to NRTL reloads the parameters once more:

Select Thermodynamic	Model parameters (when re	quired)					
Units J/mol	BIP estimation	BIP T est. (0	() 76.8	500 T deper	ndence	None	•
Reset	i-i	A-ij	A-ji	a-ij			
	Water - Ethanol	5195.44	-242.505	0.293700			
🕞 Load	Water - Acetone	5543.70	3406.38	0.566300			
	Ethanol - Acetone	1819.30	151.865	0.298700			
Save							
Auto-Load							

Similarly, selecting Modified UNIFAC loads the Group Interaction Parameters:

Select Thermodynamic Model parameters (when required)							
Modified UNIFAC (D)	Modified UNIFAC (D) GIPs						
		'					
	i-i	A-ij	A-ji	B-ij	B-ji	C-ij	C-ji
	H20 - CH2	-17.2530	1391.30	0.838900	-3.61560	9.0210E-04	0.00114400
	H20 - OH	1460.00	-801.900	-8.67300	3.82400	0.0164100	-7.514E-03
	H20 - CH2CO	190.500	770.600	-3.66900	-0.587300	0.00883800	-3.252E-03
	CH2-OH	2777.00	1606.00	-4.67400	-4.74600	0.00155100	9.1810E-04
	CH2 - CH2CO	433.600	199.000	0.147300	-0.870900	0.000000	0.000000
	OH - CH2CO	-250.000	653.300	2.85700	-1.41200	-6.022E-03	9.5400E-04

(note that the GIPs are always loaded automatically irrespective of the checkbox)

Binary Property Diagrams

To validate the modeling of physical properties we added the ability to generate a physical property diagram which allow a quick model comparison with available experimental data. One or two properties can be compared in one go. For example, plotting both the liquid density and viscosity for the Acetone/Ethanol system as function of composition is simple:



Clicking the property selection box for property A or B shows the list of available physical and thermodynamic properties that can be displayed: Vapor or liquid molar mass, density, viscosity, thermal conductivity, and heat capacity or the surface tension. Thermodynamic properties such as K-values, activity coefficients, fugacity coefficients, vapor pressures, Henry coefficient, volumes, enthalpies, and entropies also can be plotted. The plot can be done at constant {T,p} over a specified composition range, or at constant composition over a

specifed temperature or pressure range. Alternatively, the properties can be computed at VLE conditions at a fixed p or T. Note that to get the liquid densities accurate for this system, we need to select the component density to predicted from the pure component T correlation model and the Mixture model to Amagat's law:

Liquid density:		
Pure component	T correlation	•
Mixture	Amagat"s law	•

0.000

The data points shown in the diagram come from the literature. The data were entered in the comments panel of the sep-file as follows:

I.-C.Wei, R.L. Rowley, J.Chem.Eng.Data, 29(3), 332-335, 1984 # 1 Acetone 2 Ethanol T=298.15K P=101.325kPa # X Lig.Density xΔ 0.0000 785.2 0.1163 785.6 0.2030 785.7 0.3396 785.6 0.4016 785.8 0.5058 785.5 0.5437 785.5 0.7084 785.2 0.8097 784.9 1.0000 784.4 # J. B. Irving, "Viscosity of binary liquid mixtures, a survey of mixture equations", # NEL Report 630, National Eng Lab, East Kilbride, UK, 1977. # X Liq.Viscosity xВ 1.000 0.349 0.900 0.362 0.383 0.800 0.700 0.412 0.600 0.455 0.500 0.504 0.579 0.400 0.300 0.671 0.200 0.792 0.100 0.950 1.180

This facilities easy import using the file button on the "data" panel. Note that there are two sets, one for property A which is the liquid density (in blue, using the left axis). This is indicated by the keyword "xA". The data for the second property B is liquid viscosity (in red, using right axis) and starts with the keyword "xB" (indicated there will be pairs of mole fractions and viscosities). Data sets are separated by " \sim ".

After selecting the right order of the components and the temperature and pressure, values are computed and plotted by clicking the [Calculate] button. Adjustment to the axis were made on the "settings" panel. The color and property of the lines and symbols can be selected on that panel as well. When done, the diagram can be copied to be pasted in a text or presentation.

Expander & Compressors

The range of flash operations available in ChemSep has been extended to now include expanders and compressors as to be able to make use of ChemSep to perform flash calculations for the isentropic type of operations in flowsheets. These type of unit operations typically operate in the single (gas) phase regions and so do not separate phases. However, since ChemSep flash calculations always report two-phases, we need both a vapor and a liquid product stream:



For example we can now compute the resulting temperature and physical properties for a 50-50mol% gas mixture of Acetone-Ethanol of 100 C that is compressed with a 75% isentropic efficiency from 1.1 to 2.0 bar:

Stream	Feed1	Тор	Bottom
Pressure (bar) Vapour fraction (-) Temperature (C) Enthalpy (kJ/kmol) Entropy (J/kmol/K)	1.1 1.0 100.0 5706 21854	2.0 1.0 131.0 8329 23511	2.0 0.0 131.0 0.0 -40440
Total molar flow (mol/s) Total mass flow (kg/s) Vapour std.vol.flow (NCMD)	1000.0 52.1 1.94e+6	1000.0 0.0 52.1 1.94e+6	0.0
Mole flows (mol/s) Acetone Ethanol	500.0 500.0	500.0 500.0	0.0 0.0
Vapour: Mole weight (kg/kmol) Density (kg/m3) Std.density (kg/m3) Viscosity (cP) Heat capacity (J/kmol/K) Thermal cond. (J/s/m/K)	52.07 1.846 2.198 0.01026 82163 0.02020	52.07 3.1 2.1981 0.01109 87116 0.02351	

DWCs with extra Condensers and Reboilers

Extractive distillation processes can be simplified when the extractive column is combined with the solvent recovery into one column shell by using a dividing wall. Frequently this provides also significant economic benefits. An example of such an operation looks like this:



Note that in COCO flowsheets the wall and stage configurations are visualized on the column icons e.g. as seen below for various DWC arrangement for the separation of the ternary DiMethylEther / Water / Methanol mixture:



where the Methanol is recycled to the reactor inlet. Each extra condenser and extra reboiler gives the column an extra product stream and set of specifications.

Calculation of Total Annualized Cost

The *Rating* panel in ChemSep includes improved cost calculation accounting for different levels of heating and/or cooling. That is, the different steam levels for reboilers and refrigerants for the condenser. The key parameters to computes the Total Annualized Cost (TAC) are calculated based on the uptime, cost index, general fuel price and materials of construction, all of which can defined as shown below:

Tables Graphs	McCabe-Thiele Ratin	ng			
Quick column rating					
Reference	ChemSep CO Unit O	Insert Aut	0		Vendor tools
Default internals	Sieve 2ft	Remove As De	sign		Сору
Default system factor	1 System factors	C	- 1	- 1	
	O Noton	Section	2	<u> </u>	50
Deafult fraction of flood	0.75 O Specified	Start stage	4	5 40	50
		End stage	4 Ciaura 20	47 Ciaura 20	07 Circus 20
Defends affection and	Efficiencies	Custon (astar	Sleve∠rt 1	sieve zit	
Derault erriclency	L 🖲 Duss-Taylor 🗌	Sustem ractor	0.75	0.75	0.75
Default height liq. feed (m)	0.8 C Traditional	Mothed alone equilibrium li	0.75 Phonol	0.75 Dimothul oort	0.75 Mothanol
	Maldistribution	Efficiency estimated	0.29	0.62	n 52
Liq. Maldistribution (%)	5 © Klemas	HETS estimated (m)	1.529	1 154	1 154
May #/bad	35 O Lockett	FPL /Maldistribution	1	1.134	1
Max.#/Deu		Area fraction	1	1	1
Rebailer real times (s)	10 Product 180	Flow parameter	, 0.016	N 106	0 147
Nebolier res. (imes (s)		Canacitu factor (m/s)	0.073	0.069	0.06
Show details		Diameter section (m)	1 14	13	1 41
		Design stage	2	49	59
		Height section (m)	4.8	52.2	11.4
		Emptu (m3)	0	0	0
		Diameter (m)	1 41	-	<u> </u>
		Height (m)	69.98		
Simple column costing					
ACCP (1 August)	32 Co	Du Shell TIC (k\$)	4	26	
ACCK (Tryear)		Internals TIC (k	:\$) 1(08	
Uptime (hrs/year)	Л6	Condenser TIC	(k\$) 2	35	
Materiale 1	Carbon Steel	 Reboiler TIC (k 	\$) 32	27	
	100	AC OPEX (k\$/	ur) 19	5	
M&S Index (\$)	100	MPS OPEX (ks	5/yr) 72	20	
Evel price (\$/GJ)	2.5 (1.6bl oil = 6.1.6.0	Total Annual C	ost (k\$/yr) 1	101	
ruerprice (\$700)	(1 DD 1 OI = 0.1 OJ)				

The resulting TAC can now also can used in the Parametric Studies to plot the cost as function of the reflux ratio, or any operating parameters e.g. the column pressure, or the column configuration e.g. the number of stages.

The TAC can also be selected as a CAPE-OPEN parameter and exported to a flowsheet. To do this select the CAPE-OPEN panel and assign the TAC as output parameter:



After which the TAC becomes visible as CAPE-OPEN parameter:

😣 Unit oper	ration ED1:
Name Status Edit Balance	Ports Info
Parameter	Value Unit 🔺
RelativePerturbationTemperature	0.001 K
RelativePerturbationPressure	0.001 Pa
PerturbationComposition	0.001
OutletFlash	Auto
UseOnlyKValuesAndEnthalpyFromCOSE	No
RestartDataAvailable	Yes
OmitStageFromPortName	No
WilsonEstimate	No
LogPropertyCalls	No
EnergyPorts	No
Allowed temperature difference	12 K
Total Annual Cost	1101
Temperature profile	[337.75, 337.75, 337 K
Pressure profile	[101325, 101325, 102 Pa
Vapour Flow profile	[40.4092, 68.6956, 68 mol / s 🛛 🔍 🚽
•	
Edit	

Now we can add an additional (information) port which we assign to the TAC:

6	S Un	it operation	ED1:	
	Name Status Edit Bala	ance Ports	Info	
	Port Direc	ti Type	Connected to:	
	Feed2(split)_stage50 INLE Feed1_stage5 INLE TopProduct OUTL BottomProduct OUTL Parameter Total Annual Cost OUTL	T material T material LET material LET information	Feed1 Solvent1 MeDH1 BED1 TAC ED1 (parameter TACed)	
	Port operations	ŧ		

On the flowsheet we add an information stream and hook it up to the TAC port. In that manner we can add all the TAC's for the various pieces of equipment in a flowsheet and compute an overall TAC, see the example for the Extractive Distillation of the azeotropic DMC/Methanol mixtures on our web site: <u>http://chemsep.org/downloads/data/MeOH-DMC_ChERD127p189.fsd</u>



Note that we computed the TAC values for the heat exchangers by using subflowsheets as to maintain readability.

Fitting multiple VLE data sets

When VLE data is entered in multiple sets on the comments section and separated with \sim , then these multiple data sets can also be automatically imported on the data panel of the binary phase diagram. The keywords c1= and c2= followed by the CAS numbers of the respective compounds enables the simultaneous fitting of systems with different components:

ref=ChERD127p189 c1=616-38-6 c2=119-36-8 title=DMC + Methyl salicylate Txy@p=101.3kPa 494.3 0 0 463.3 0.043 0.522 0.06 0.62 455.7 448.6 0.077 0.693 441.9 0.096 0.753 438.7 0.106 0.778 433.3 0.125 0.816 420.2 0.183 0.888 412.1 0.231 0.921 406.3 0.273 0.94 402.0 0.309 0.952 395.4 0.374 0.967 390.4 0.433 0.976 0.547 0.986 382.7 375.0 0.696 0.994 373.9 0.72 0.994 371.4 0.77 0.996 368.9 0.828 0.997 366.8 0.886 0.998 365.4 0.934 0.999 363.1 1 1 ref=ChERD127p189 c1=67-56-1 c2=119-36-8 title=MeOH + Methyl salicylate Txy@p=101.3kPa 494.3 0 0 427.5 0.024 0.832 402.2 0.052 0.925 391.3 0.072 0.947 375.3 0.128 0.978 371.1 0.156 0.98 365.5 0.204 0.987 361.1 0.264 0.99 357.5 0.336 0.992 355.2 0.396 0.994 352.2 0.472 0.995 351.4 0.496 0.996 350.2 0.532 0.996 0.58 348.7 0.997 346.5 0.656 0.998 345.1 0.708 0.998 342.6 0.8 0.998 342.2 0.816 0.998 0.999 339.6 0.92 338.7 0.952 0.999 337.8 1 1

Note that the keywords Txy and pxy indicate the type of VLE data. They are followed by the conditions at which the data were measured; e.g. Txy@p=101.3kPa states that the measurements were obtained at a constant pressure of one atmosphere. For measurements at equal pressure we use, for example, pxy@T=30C to indicate data measured at 30 degrees Celcius. Note that the units of measure are optional and in the above data the default temperature units was set to Kelvin. To enable the selection of a data-set we need to assign a title. It is possible to enter dozens of data-sets, which facilitates the fitting of group interaction parameters. Optional keywords are "ref=" and "url=" that in the future will be used to enable linking to original sources and documentation.

After all the data sets were entered and imported, each individual data sets can be selected for plotting by using the data pull down menu on the data panel:

8	Binary Phase Diagram
1: DMC 💌	Plot Settings Data Fitting
2: Ethyl benzoate Include all Type Txy VLE Pressure (N/m2)	DP Rectangle Image: Color Colored-Filled BP Dot Image: Color Colored-Filled Data Loaded 15 data sets. Select data set Phenol/DMC; Txy@p=101.3kPa, ; 616-38-6 DMC; 108-95-2 PhOH; 111; 136 c1=67- Methanol-Phenol; Txy@p=101.3kPa, ; 67-56-1 Methanol; 108-95-2 Phenol; 136; 161
101300 Number of points 51	c2=616DMC+MIBK; Txy@p=93.32kPa, ; 616-38-6 DMC; 108-10-1 MIBK; 161; 185 Txy; MeOH+MIBK; Txy@p=93.32kPa, ; 67-56-1 MeOH; 108-10-1 MIBK; 185; 211 p=100.1DMC+Ethyl benzoate; Txy@p=101.3kPa, ; 616-38-6 DMC; 93-89-0 Ethyl benzoate; 21 p=100.1MeOH+Ethyl benzoate; Txy@p=101.3kPa, ; 616-38-6 DMC; 119-36-8 Methyl benzoate p=100.1DMC+Methyl salicylate; Txy@p=101.3kPa, ; 616-38-6 DMC; 119-36-8 Methyl salicylate p=100.1MeOH+Methyl salicylate; Txy@p=101.3kPa, ; 67-56-1 Methanol; 119-36-8 Methyl salicylate p=100.17kPa, T=342.1, x=0.312, y=0.640; p=100.17kPa, T=344.1, x=0.352, y=0.674; p=100.17kPa, T=338.0, x=0.622, y=0.761; p=100.17kPa, T=337.4, x=0.735, y=0.808;
Calculate Redo axis Copy data	p=100.17kPa, T=337.0, x=0.829, y=0.855; p=100.17kPa, T=336.9, x=0.858, y=0.871; p=100.17kPa, T=336.9, x=0.893, y=0.890; p=100.17kPa, T=336.9, x=0.910, y=0.900; p=100.17kPa, T=337.0, x=0.917, y=0.907; p=100.17kPa, T=337.1, x=0.943, y=0.920; p=100.17kPa, T=337.2, x=0.965, y=0.949;
Copy plot	p=100.17kPa, T=337.3, x=0.982, y=0.972; p=100.17kPa, T=337.5, x=1.000, y=1.000; ~; c1=67-56-1 MeOH;
Clear	c2=616-38-6 DMC; Tx; T=336.61, x=0.0; T=326.03, x=0.1001; T=320.55, x=0.2003;

After the selection of the data the VLE can be computed and plotted by pressing the Calculate button:



Clicking the right mouse button enables changing the graph settings directly without having to switch to the settings panel. We can plot Txy or pxy for multiple conditions but only for one system of compounds. However, it is possible to export a plot to file and to then import it again over plot with a different system. For this we need to ensure the T or p ranges are set to cover the same range so as to ensure that the axes properly align.

Miscellaneous Updates

Version 8.2 includes many small improvements such as:

- PPR78 equation of state
- Improved prediction methods for petroleum fractions
- Bug fixes in the automated assignment of key compounds for the McCabe-Thiele diagrams
- Bug fixes in the parametric study
- Bug fixes liquid Cp & viscosity errors for supercritical compounds
- Bug fixes for handling Group Contribution Methods

Availability

As always, *ChemSep* Lite is available free from <u>http://chemsep.com</u>.