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al al a CETONE Heat of formation [k/hg] Meal ges Cp. C(1) [k)/hg Keil
2305,2993 0,5823
A HEXANE
R(AD) VLXE Project Sheet1 (+)
VIXEBLEND

VLXE Blend: Standard System

No other product offers such a full range of models and calculations options.



Welcome to VLXE Blend: Standard System



In the VLXE world a standard system is a system without a polymer. A wide range of systems are supported including associating and polar systems.

A complete set of calculations are included and they can be linked, like all Excel functions, to simulate unit operations.

The associating module lets the user view the bonding fraction and, if needed, define a custom scheme. This allows full flexibility when dealing with associating molecules.

The Kij fitting allows the user to quickly fit Kij to data, and PC-SAFT parameters can be fitted to pure component data with ease.

Due to the unique nature of VLXE Blend, the handling of VLE and LLE is robust and simple. In relevant calculations the user simply has to ask for either an LLE, VLE or Auto type of system. This allows for a robust handling of systems, be they either LLE or VLE.



Advantages & Models

VLXE Blend offers a broad variety of computations for:

Calculations:	Applications:
Flash Calculations	 Multi-phase flash, VLE, LLE and VLLE Full range of flash calculations (Pressure/Temperature, Pressure/Enthalpy, Pressure/Entropy + more). No limit to the number of phases.
Link Flash	• Flash calculations can be linked in an Excel sheet to create a flow sheet.
Critical Point	• Allows the calculation of critical points found in a mixture, no matter the type of mixture.
Cloud Point	VLE and LLE
Phase Diagram	• Trace lines, critical point, spinodal curves, based on a given feed.
Txy/Pxy Curves	 These functions let the user perform Txy and Pxy calculations, respectively, for a given binary system.
Fit Parameters	Both pure components and Kijs.

Thermodynamic Models

All phase equilibria calculations performed in VLXE Blend are based on the use of Equations of State (EOS). Six EOS are included in VLXE Blend. We recommend the use of PC-SAFT.

Depending on the EOS, a different number of mixing rules are included.

Equation of States	 PC-SAFT Peng/Robinsen Soave/Redlick/Kwong Sanchez/Lacombe (Orignal) Sanchez/Lacombe (Ideal Gas Limit) CPA
Models For Ideal Gas Heat Capacity	DIPPR ExpressionPolynomial Expression

Creating a new project

Setting up a new project is simple, made easy by the database and wizards provided. It is only a few mouse clicks away.

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Solvent / Polymer	Status DB Index Name	2 Sneet Version Number of solvents Number of polymers Equation of state 3 14 2 0 PC-SAFT
4 Sanchez/Lacombe	4 V Short Name Formula + 1 New 472 ACETONE Back Back	4
6 Modified Sanchez/Lacombe	6 9 n-HEXANE C6H14	6 1 ACETONE 472
7 Polymer blend PC-SAFT	7	7 2 n-HEXANE 9
g coPolymer blend CPA		9 Solvent Index Name Heat of formation [kJ/kg] Ideal gas Cp: C(1) [kJ/(kg Ke]
1 Ideal Gas Cp Expression (Standard)	1	10 1 ACETONE -3713,897967 0,9821
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	18	READY

Select the Components

Generate Project Sheet

Define the System

Cloud Point

Cloud points are implemented so the user can handle both VLE and LLE. The function also includes an auto function. Output can be given either as an Excel range or in just one row. The latter makes it easy to perform calculations over a wide range.

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9		Acetone [Massfraction]	0.5	0.5	0.5	0.562769119				7		0,9) 0,	1 20	0 T,D(1),H(1	i) All	C(In,Mass	IVLE	178,020	8 0,5541	4 -143,839 (
10		n-hexane [Massfraction]	0,5	0,5	0,5	0,437230881				8		0,9) 0,	1 25	5 T,D(1),H(1	i) All	C(In,Mass	IVLE	191,819	0,52850)1 -101,831 (
11										9		0,9) 0,	1 30	0 T,D(1),H(1	i) All	C(In,Mass	IVLE	203,729	0,50348	81 -63,5496 (
12		Phase Fraction [Mole]			1	0				10		0,9) 0,	1 3	5 T,D(1),H(1	i) All	C(In,Mass	IVLE	214,274	2 0,47828	3 -27,6305 0
13		Phase Fraction [Weight]			1	0	1		_	11		0,9) 0	1 40	0 T D(1) H(1	l'All	C(In Mass	IVIF	223 77	4 0 45214	7 6,933397 0
14		Compressibility [-]	0,036095	0,036095	0,036095226	0,838358588			- 8	12		0,9)		Dro		Entholm			413	5 41,07316 0
15		Density [g/cm^3]	0,561177	0,561177	0,561176634	0,023584539	1		- 1	13					Pres	ssure vs	. Enunalpy	,			
16		Molar Volume [cm^3/mol]	123,6524	123,6524	123,6524042	2871,988011				14			100								
1/		Enthalpy [kJ/Kg]	-151,562	-151,562	-151,561542	163,6931147			-	15									_		
10		Cn [k //(Kokin kg)]	-0,40031	-0,40031	-0,400309055	1 07501057			- 1	16			0					-			
20		Cy [k I/(Kelvin kg)]	1 986809	1 986809	1 986809334	1 7/2610659			- 11	17			-100	-	10	20		4	0	50	
21		.ITCoeffient [Kelvin/Bar]	1,500005	0.006898	0.006897822	1 429255861			_	18											
22		Velocity of Sound [m/s]		610 1338	610 1337773	198 160109			_	19			-200								
23		MolecularWeight [g/mol]	69,39084	69,39084	69,39083992	67,7345131				20			-300	/							
24		ThermalConductivity [W/(m Kelvin)]		0,099658	0,099657901	0,02470328				21			500	1							
25		Viscosity [centiPoise]		N/A	N/A	N/A				22			-400	/							
26		Surface Tension [N/m]	N/A							00				-							
														1							

Cloud Point Calculation as fixed output

Cloud Point Calculation as a function range output ()

Phase Diagram

Obtaining the phase diagram for a system gives a very good overview of its behavior. VLXE Blend comes with a range of options including the auto function shown below. Note how the critical point is included in the output.

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17		12:	172,										
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19		14:	192,3		05 -								
20		15:	200,8		05							-	_
21		10:	208,5	_	00				1			-	_
22		17.	215,	-50	C	0 50	100	150	200	250		-	

Flash Calculation

The flash calculation for a standard system is the same as for polymer systems, making it very robust no matter the system. It can therefore handle heavy components without any problems for all types of systems, VLE, LLE, VLLE or VLLLE.

X∄	🖯 🍤 👌 👘 🕞	- -							Ac	×I .	5.00	x* 🖾 🖾	÷							Acet	tone + nHex
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E13		f_x {	[=Flash_TP((B3:C3; D3;	E3; F3; G3;	; H3; I3)}					A B	С	D	E	F	G	Н	I	J	К	L
	A B	С	D	F	F	G	н			2	Acetone	n-hexane (Temperatu	Pressure [Ir	nitial Kii	IndexI	IndexJ	Output	Compo	nen Units	Kii [-]
1										3	3,85E-02	0,9615	40,02	0,4719	0		0	1 Kij	All	C(In,Molefr	0,017262
2	Acetone [Massfrac	n-hexane	[Temperati	Pressure [FlashType	e Output	Compone	en Units		4	5,40E-02	0,946	40,02	0,5017	0		0	1 Kij	All	C(In,Molefi	0,015563
3	0.5	0.6	140	10	2	Fixed 2D	All	C(In Mass		5	7,82E-02	0,9218	40,02	0,5391	0		0	1 Kij	All	C(In,Molefr	0,012886
4	Property	System	Feed	Phase 1	Phase 2			0(,		6	1,22E-01	0,8776	40,02	0,5891	0		0	1 Kij	All	C(In,Molefi	0,009112
5	Pressure [Bar]	10)	Time: 87 [1					7	1,42E-0 1 92E-0	0,8583	40,02	0,6079	0		0	1 KIJ 1 Kij		C(In,IVIOIefi C(In Molefi	0,008412
6	Temperature [Cels	i 140)							9	1,95E-0	0.8								In Molefr	0.005322
7										10	2,37E-0	0,76		Ac	etone n	nolefra	ction vs.	Kij		In,Molefr	0,003952
8	Components									11	2,47E-0	0,75	0,02							In,Molefi	0,003697
9	Acetone (Massfra	c 0.5	5 0.5	0.40745	0.505962	2				12	2,53E-0	0,74 ₀	018							In,Molefr	0,003434
10	n-hexane (Massfra	N 0.5	5 0.5	0.59255	0.494038	3				13	2,96E-0	0,70	016							In,Molefr	0,002549
11										14	3,14E-0 3,50E-0	0.65	014							In Molefi	0,001062
12	Phase Fraction [M	le -		0,058342	0,941658	3				16	3.86E-0	0.61 0	012							In.Molefr	0.001138
13	Phase Fraction (W	1		0,060524	0,939476	6				17	4,13E-0	0,58	0.01							In,Molefr	0,001308
14	Compressibility [-]	0,787359	0,8331	0,038082	0,833781	1				18	4,37E-0	0,56	008	N						In,Molefr	0,001234
15	Density [g/cm^3]	0,025656	6 0,024247	0,550286	0,024171	1				19	4,95E-0	0,50	006	\backslash						In,Molefr	0,001473
16	Molar Volume [cm	2704,687	2861,816	130,8161	2864,156	5				20	5,55E-01	0,4	004							In,Molefi	0,00139
17	Enthalpy [kJ/Kg]	150,4802	2 168,7983	-129,684	168,5294	1				21	6,15E-0	0,30 0	002							in,ivioleti In Molefr	0.002935
18	Entropy [kJ/(Kg K	0,266016	6 0,310345	-0,39833	0,308815	5				23	8.76E-0	0.1	002			-				In.Molefr	0.000856
19	Cp [kJ/(Kelvin kg)]	2,06084	2,016433	2,807008	2,012769)				24	9,26E-0	0,07	0.00E+00	2.00E-01	4.00E-01	6.00E-01	L 8.00F-0	01 1.00F+	00 1.20F	+00 In,Molefr	0,001505
20	Cv [kJ/(Kelvin kg)]	1,794961	1,783529	2,027275	1,779994	1				25	9,40E-0	0,05		-,		-, 01	-			_ In,Molefr	0,001029
21	JTCoeffient [Kelvin	1	1,425262	0,008982	1,424083	3				26	9,65E-01	0,0355	40,02	0,6147	0		0	1 Kij	All	C(In,Molefr	0,000986

Flash Calculation (Acetone+ n-Hexane)

Bubble Kij fit (Acetone+ n-Hexane)

The bubble Kij function is very efficient when it comes to matching the Kij to data. It will simply get the Kij that matches each point. The user can then plot the Kij vs. temperature and observe the trend. In the example below note how one of the datapoints looks like an outline, plus note how it will be very difficult to match this system to a simple temperature dependendent Kij.

Acetone + nHexane.xlsx

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Txy/Pxy Calculations for Association Components

The associating term is very powerful in VLXE Blend. The user can enter custom defined schemes and view the bonding fraction as part of the output. Below is an example with Methane + Methanol, where the associating term is used. Note how VLXE Blend allows the user to obtain both the LLE and VLE line.

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	Α	В	С	D	E	F	G	Н	I	J	K	L	М	N	-
															- 11
!		Pressure	e [LineTyp	e Output	Compone	e Units			Pressur	e [LineType	Output	Compone	units		-81
			1 LLE		All	C(In,Mass				1 VLE		All	C(In,Mass		
_		Number	r: X: METH	IAIY: METH	AlTemperat	Pressure:	K(Mixture		Number	r: X: METHA	Y: METHA	Temperat	Pressure:	K(Mixture	-
			[Massfr	ad Macetra	d Colciuch	Dorl	r 1			Macefron	Mossfrac	[Celsius]	[Bar]	[-]	-11
		1:	0,0057			VLE	and LL	E lines			1000	80,5198	1,0000	104,2259	- 11
_		2:	0,0096	90 -							831	80,1770	1,0000	103,9022	-
		3:	0,0130								1010	79,1371	1,0000	102,7781	-
		4:	0,0176	80							855	78,0794	1,0000	101,4048	-
		5: 6.	0,0210	70 -							1080	77,0028	1,0000	99,75418	-
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7		12:	0.0515	e 20 -	/					T(D	1280	69.2319	1.0000	79.03438	
3		13:	0,0560	E 10							w) .915	68,1720	1,0000	74,8768	
)		14:	0,0606	10 -				\backslash			245	66,8685	1,0000	69,30619	
)		15:	0,0652	00 +							469	65,5283	1,0000	63,06275	
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2		17:	0,0747	-20							874	62,7283	1,0000	48,46982	
3		18:	0,0795			METHANOL	[Massfracti	on]			211	61,2653	1,0000	40,15556	
4		19:	0.0893	70 0.31541	5 53.1574	1.0000	10.74742		17.	0.012205	0.279757	59,7615	1.0000	31.28552	

Txy/Pxy Calculations

Pxy Calculations for Polar Components

VLXE Blend has the polar term implemented in PC-SAFT. It allows modelling of polar components. Note in the example the close match to the data:





"With references like Chevron, ConocoPhillips, Dow Chemicals, ExxonMobil, Merck, Nova Chemicals, Sasol, Statoil and world leading universities VLXE has become a preferred supplier for the industry."

Dr. Torben Laursen, CEO & Founder



Solutions worldwide...

...for Chevron, ConocoPhillips, Dow Chemicals, Exxon-Mobil, Merck, Nova Chemicals, Sasol, Statoil and many others.



VLXE ApS Nordre Frihavnsgade 13A, 2, tv 2100 Copenhagen Ø Denmark

If you are interested and would like more information, please contact us:

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