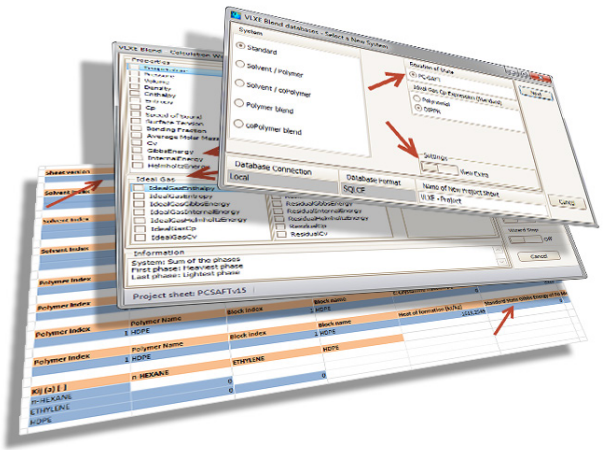
VLXE
ADVANCED PVT SIMPLIFIED



VLXE | BLEND® Version 8.0

What's new?

Version 8 is the 2015 major release of VLXE Blend. The focus of this release is user experience where the user interface inside Excel is further simplified.

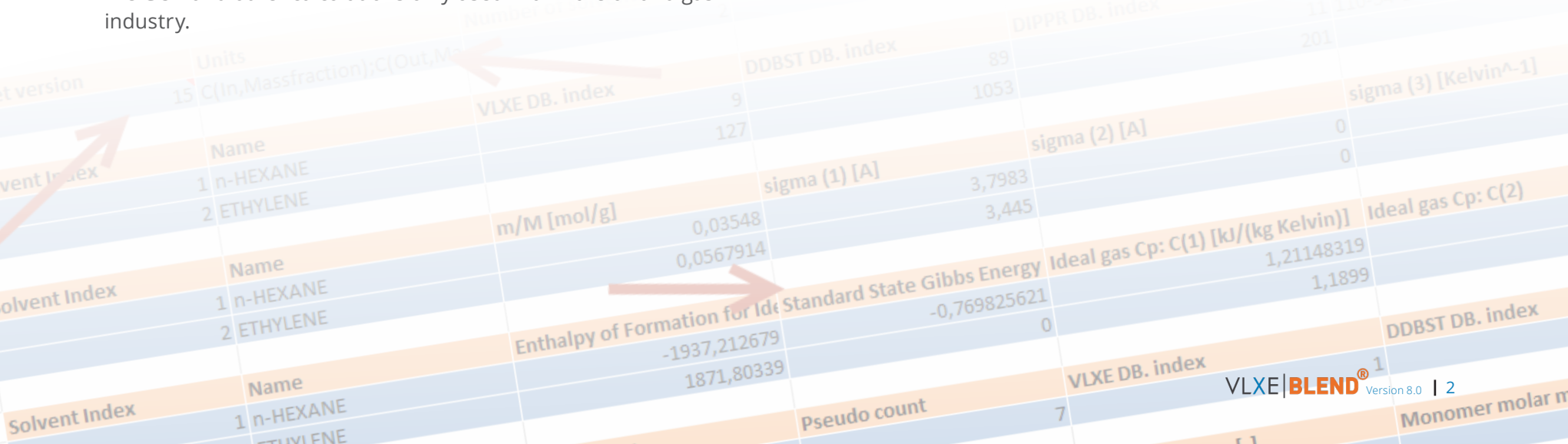
Introduction

Version 8 is the 2015 major release of VLXE Blend. The focus of this release is user experience where the user interface inside Excel is further simplified. Arguments to Excel functions that are often the same in many calculations either can now be store in a central location or omitted from the calculation.

The oil and gas module have been removed due to VLXE now focusing entirely on the polymer and chemical industry. Researchers in the oil and gas industry can still take advantage of VLXE Blend. However, they no longer have direct access to common calculations like GOR and other calculations only used within the oil and gas industry.

More properties can now be obtained from VLXE Blend including internal energy and Helmholtz energy. The user can also obtain both residual and ideal property values. A new function "PropertyOfMixing" has been added that lets the user calculate a complete range of mixing properties.

The speed have been improved on average with about 10% and for phase envelope with an average of 20%.



Breaking changes

Excess enthalpy function removed

The function: “ExcessEnthalpy” has been removed and replaced by the general function:
“PropertyOfMixing”.

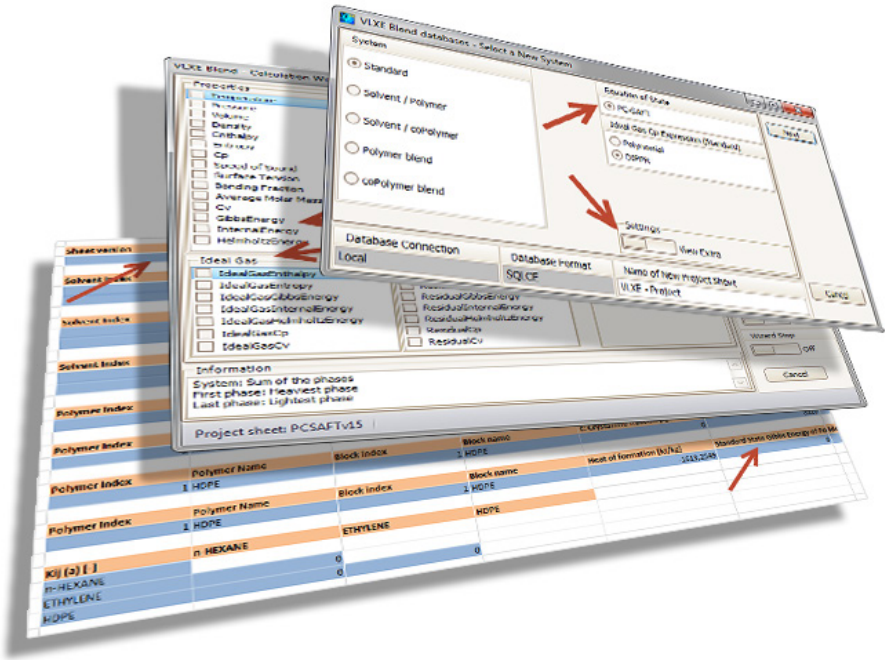
The new function let the user calculate a complete range of mixing properties including Excess Enthalpy.

Chemical potential now complete

The chemical potential is now complete and include the full ideal gas term. This means that the user can sum the product of mole-numbers times the chemialpotential and obtain the Gibbs Energy. Units of chemical potential is now “J/mole”.

Oil and gas removed

This module has been in VLXE Blend for some years but has not been used much. It include only calculations unique to the oil and gas industry and is therefore removed.



Improvements

Project sheet

Version 15 of the project is new. It now has a new color scheme that is more in line with the two other colors used in VLXE Blend.

Removed items

It has been updated so unused parameters are removed and one new introduced. The removed parameters are: “Association Kappa” and “Association Epsilon” These two matrix’s allowed the user to overwrite the internal calculation of the same matrix. It found very little use and has been removed. The use of the two matrix’s were controlled with the “Association Matrix” input that has also been removed.

Added items

New parameter is: “Standard State Gibbs Energy”. It is taken from DIPPR and is used to calculate the complete entropy including the entropy of formation.

Units are now stored in the project sheet in cell: “C3”. This allows the user to store units used in a central location and avoid using the “Units” argument to all function calls.

Sheet version	Units	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas Cp
15	C(In,Massfraction);C(Out,M	2	1	PC-SAFT	DIPPR

Solvent Index	Name	VLXE DB. index	DDBST DB. index	DIPPR DB. index	CAS Number
1	n-HEXANE	9	89	11	110-54-3
2	ETHYLENE	127	1053	201	

Solvent Index	Name	m/M [mol/g]	sigma (1) [A]	sigma (2) [A]	sigma (3) [Kelvin^-1]
1	n-HEXANE	0,03548	3,7983	0	0
2	ETHYLENE	0,0567914	3,445	0	0

Solvent Index	Name	Enthalpy of Formation for Id	Standard State Gibbs Energy	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
1	n-HEXANE	-1937,212679	-0,769825621	1,21148319	4,088175553
2	ETHYLENE	1871,80339	0	1,1899	3,3789

Polymer Index	Name	Block count	Pseudo count	VLXE DB. index	DDBST DB. index
1	HDPE	1	7	1	4

Polymer Index	Polymer Name	Block index	Block name	Monomer name [-]	Monomer molar mass [g/mol]
1	HDPE	1	HDPE	Ethylene	28,054

Polymer Index	Polymer Name	Block index	Block name	c: Crystalline fraction [-]	Enthalpy of melting (Hu) [J/mol]
1	HDPE	1	HDPE	0	8220

Polymer Index	Polymer Name	Block index	Block name	Heat of formation [kJ/kg]	Standard State Gibbs Energy of Fo
1	HDPE	1	HDPE	-1613,2549	0

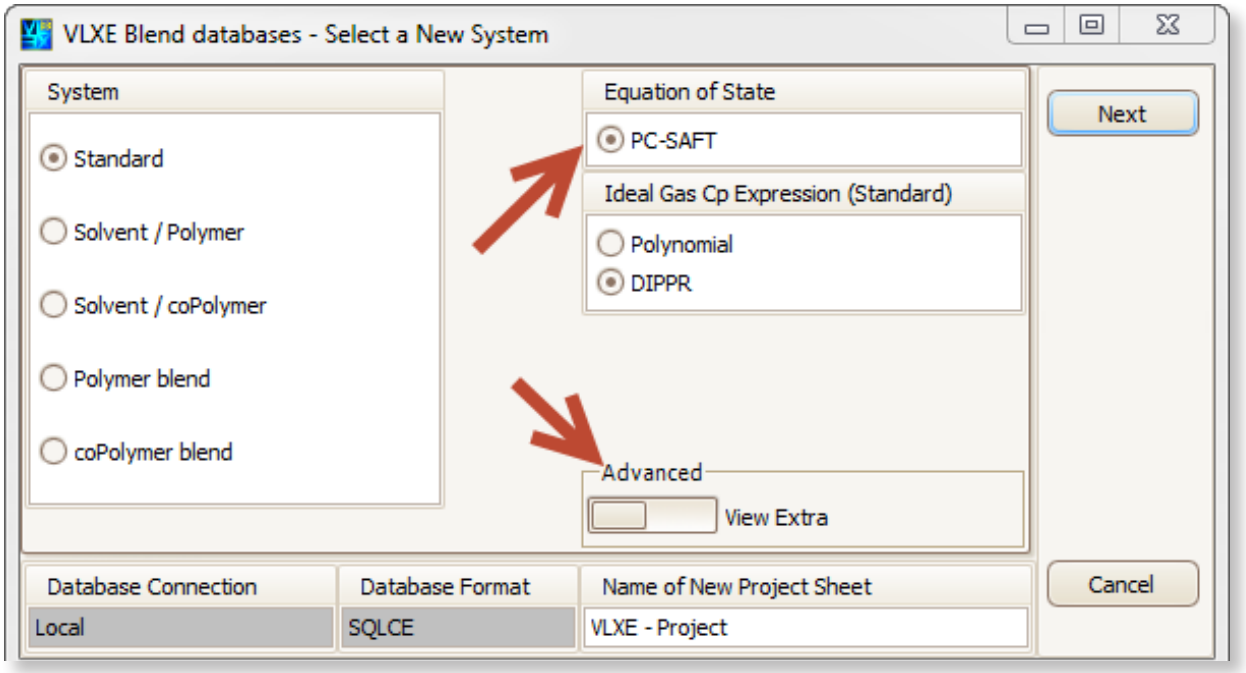
Kij (a) [-]	n-HEXANE	ETHYLENE	HDPE
n-HEXANE			
ETHYLENE	0		
HDPE	0	0	

Units are now stored in the project sheet in cell: “C3”. This allows the user to store units used in a central location + avoid using the “Units” argument to all function calls.

Wizards

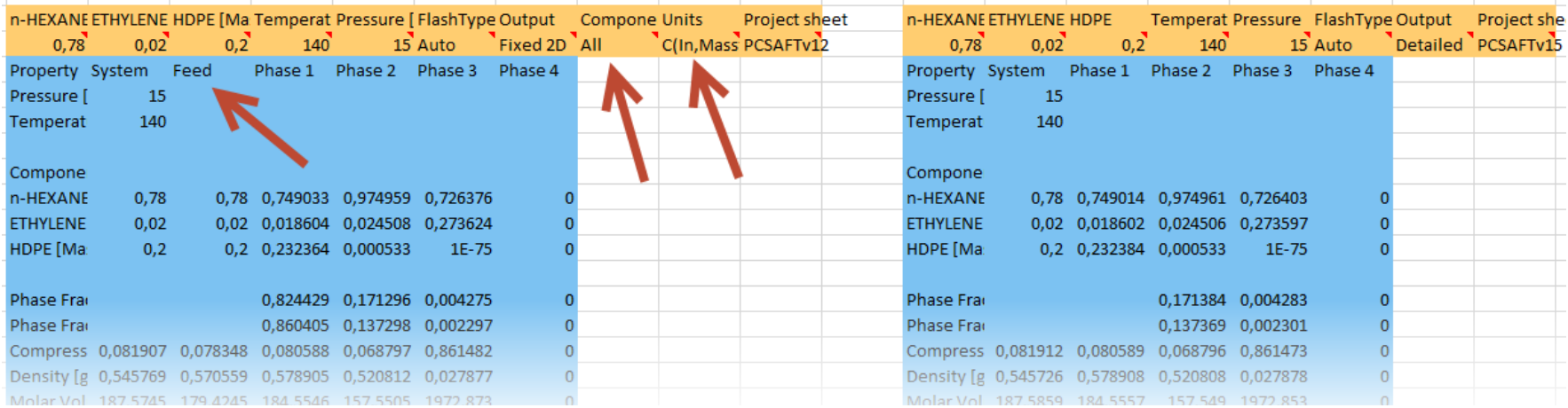
New mixture

PC-SAFT is now default for all new mixtures. Other equations of state still there but are hidden behind an “Advanced” setting.



Functions

Arguments



n-HEXANE	ETHYLENE	HDPE [Ma	Temperat	Pressure [	FlashType	Output	Compone	Units	Project sheet
0,78	0,02	0,2	140	15	Auto	Fixed 2D	All	C(In,Mass	PCSAFTv12

Property	System	Feed	Phase 1	Phase 2	Phase 3	Phase 4
Pressure [	15					
Temperat	140					
Compone						
n-HEXANE	0,78	0,78	0,749033	0,974959	0,726376	0
ETHYLENE	0,02	0,02	0,018604	0,024508	0,273624	0
HDPE [Ma	0,2	0,2	0,232364	0,000533	1E-75	0
Phase Frac			0,824429	0,171296	0,004275	0
Phase Frac			0,860405	0,137298	0,002297	0
Compress	0,081907	0,078348	0,080588	0,068797	0,861482	0
Density [g	0,545769	0,570559	0,578905	0,520812	0,027877	0
Molar Vol	187,5745	179,4245	184,5546	157,5505	1972,873	0

n-HEXANE	ETHYLENE	HDPE	Temperat	Pressure	FlashType	Output	Project she
0,78	0,02	0,2	140	15	Auto	Detailed	PCSAFTv15

Property	System	Phase 1	Phase 2	Phase 3	Phase 4
Pressure [	15				
Temperat	140				
Compone					
n-HEXANE	0,78	0,749014	0,974961	0,726403	0
ETHYLENE	0,02	0,018602	0,024506	0,273597	0
HDPE [Ma	0,2	0,232384	0,000533	1E-75	0
Phase Frac			0,171384	0,004283	0
Phase Frac			0,137369	0,002301	0
Compress	0,081912	0,080589	0,068796	0,861473	0
Density [g	0,545726	0,578908	0,520808	0,027878	0
Molar Vol	187,5859	184,5557	157,549	1972,853	0

Units

"Units" argument is now optional. Starting with project sheet 15 units are included in the project sheet. The user can therefore omit the "Units" argument. If needed it can still be used.

Components

The "Components" arguments is now optional. Default value is taken to be "All".

Output

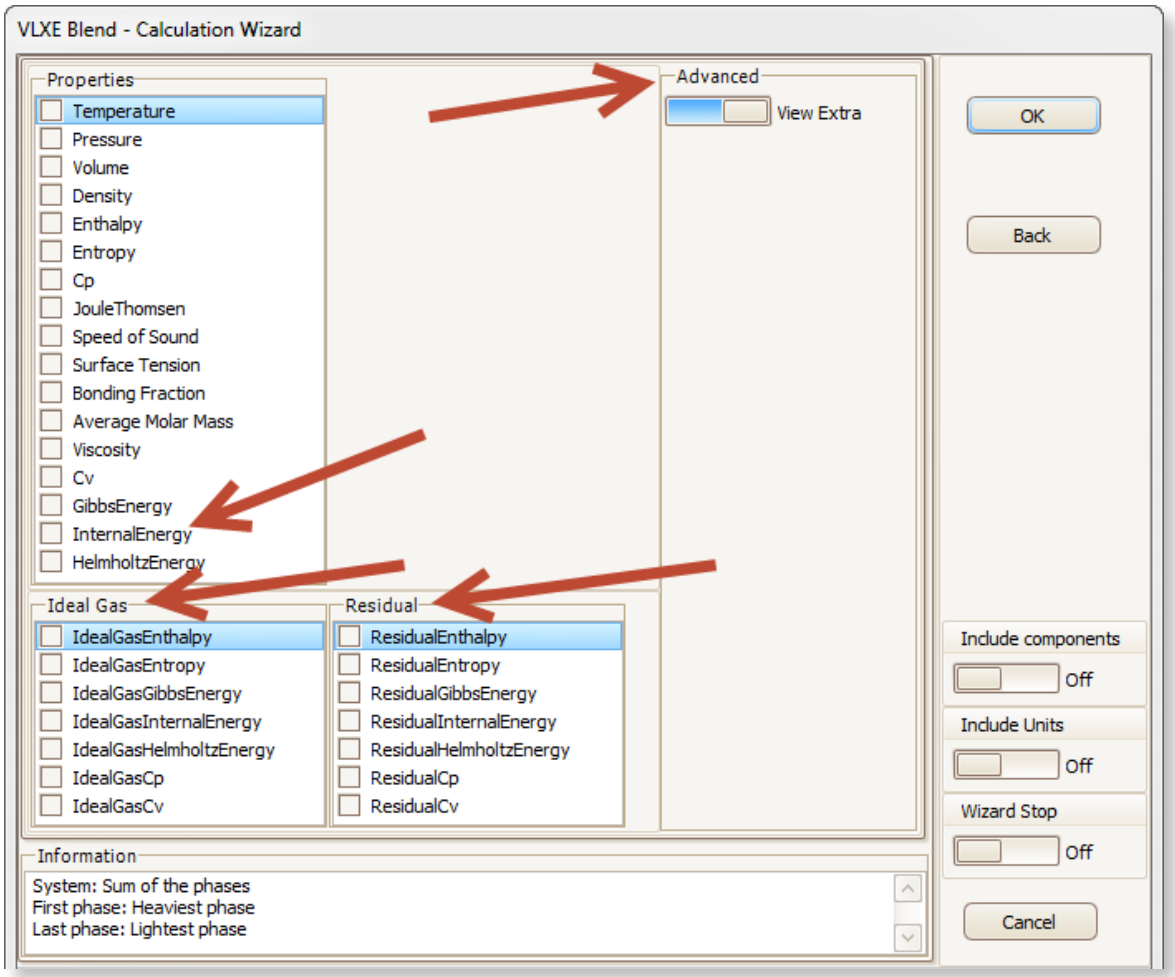
New output format: "Detailed". In the previous versions of VLXE Blend the user could chose a fixed output format: "Fixed 2D".
It would always include the feed and system phase. Often this information is not wanted and when using the new fixed format output: "Detailed" it is not included. This makes the output smaller. Bubble and dew point calculations no longer include the "System" and "feed" phase. It was always the same as the starting phase and can therefore be removed.

Properties

Changes

More properties can now be obtained:
Internal energy and Helmholtz energy.
A full range of residual end ideal properties can also now be obtained

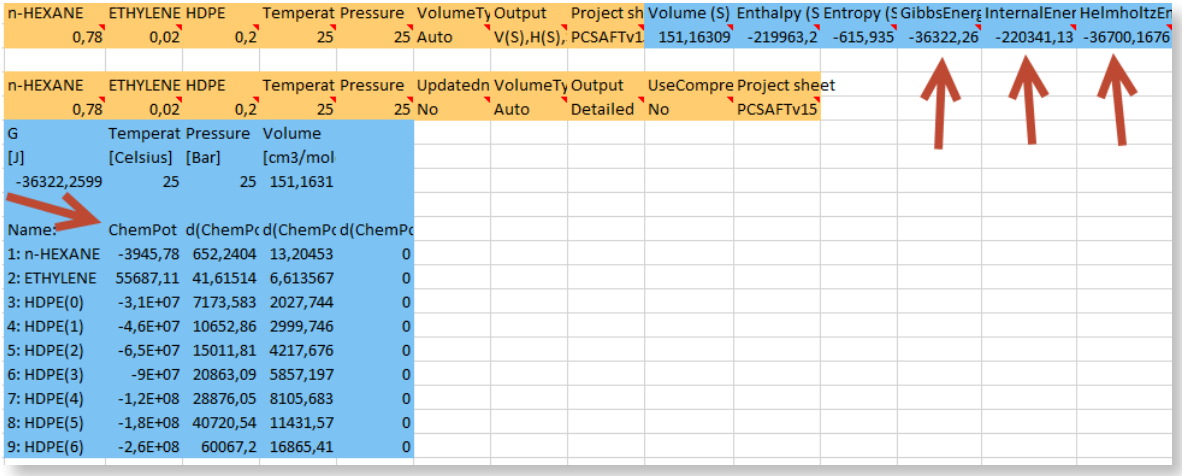
A new button: “Advanced” has been added. It allows the user to show/hide new extra residual and ideal gas properties as seen here.



New Properties

Changes

VLXE Blend now gives the user access to more properties. This includes Gibbs Enerby, Helmholtz Energy and Internal Energy.
In addition the chemcial potential has been changes to they match the property values. This means that the full ideal gas term is included and that the sum of molenumbers times the chemical potential at fixed temperature and pressure will give the Gibbs Energy.



n-HEXANE	ETHYLENE	HDPE	Temperat	Pressure	VolumeTy	Output	Project sh	Volume (S)	Enthalpy (S	Entropy (S	GibbsEnerg	InternalEner	HelmholtzEr
0,78	0,02	0,2	25	25	Auto	V(S),H(S),	PCSAFTv1	151,16309	-219963,2	-615,935	-36322,26	-220341,13	-36700,1676

n-HEXANE	ETHYLENE	HDPE	Temperat	Pressure	Updatedn	VolumeTy	Output	UseCompre	Project sheet
0,78	0,02	0,2	25	25	No	Auto	Detailed	No	PCSAFTv15

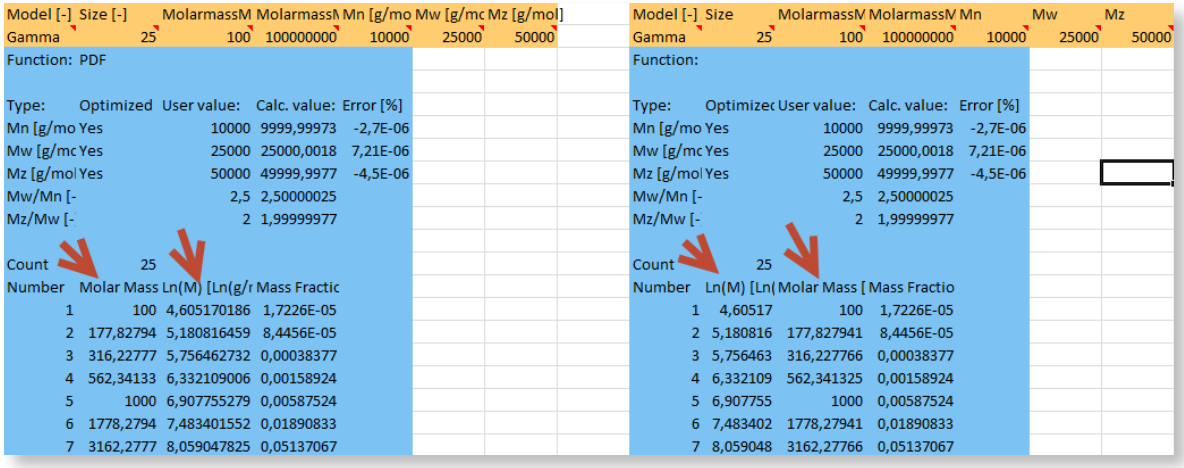
G	Temperat	Pressure	Volume
[J]	[Celsius]	[Bar]	[cm3/mol
-36322,2599	25	25	151,1631

Name:	ChemPot	d(ChemPc	d(ChemPc	d(ChemPc
1: n-HEXANE	-3945,78	652,2404	13,20453	0
2: ETHYLENE	55687,11	41,61514	6,613567	0
3: HDPE(0)	-3,1E+07	7173,583	2027,744	0
4: HDPE(1)	-4,6E+07	10652,86	2999,746	0
5: HDPE(2)	-6,5E+07	15011,81	4217,676	0
6: HDPE(3)	-9E+07	20863,09	5857,197	0
7: HDPE(4)	-1,2E+08	28876,05	8105,683	0
8: HDPE(5)	-1,8E+08	40720,54	11431,57	0
9: HDPE(6)	-2,6E+08	60067,2	16865,41	0

Distribution

Changes

All VLXE Blend PVT calculation functions has a argument that lets the give a distribution. This is used for example when linking flash calculations. The output from the “Distribution” calculation did not follow the format used by this argument. This has now been changes. This was done by reversing the two first output columns.



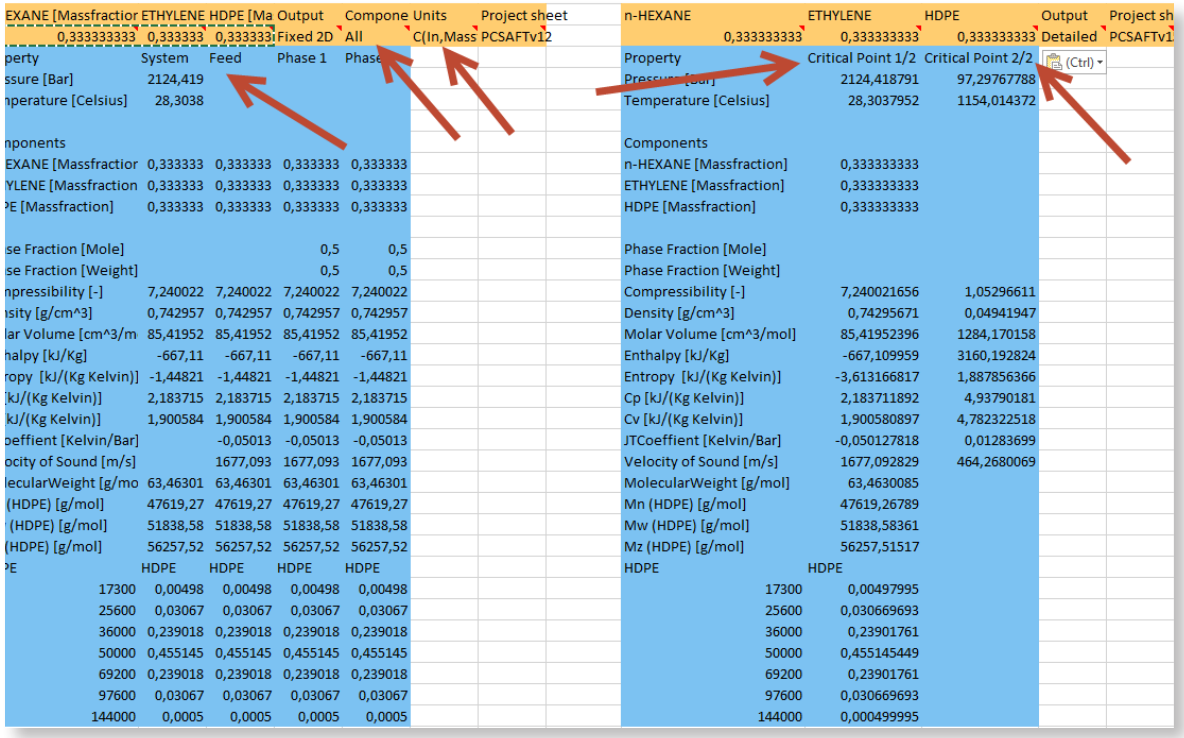
Model [-]	Size [-]	MolarmassM	MolarmassN	Mn [g/mo	Mw [g/mc	Mz [g/mol]
Gamma	25	100	100000000	10000	25000	50000
Function:	PDF					
Type:	Optimized	User value:		Calc. value:	Error [%]	
Mn [g/mo	Yes	10000		9999,99973	-2,7E-06	
Mw [g/mc	Yes	25000		25000,0018	7,21E-06	
Mz [g/mol	Yes	50000		49999,9977	-4,5E-06	
Mw/Mn [-		2,5		2,50000025		
Mz/Mw [-		2		1,99999977		
Count	25					
Number	Molar Mass	Ln(M)	[Ln(g/r	Mass Fractic		
1	100	4,605170186		1,7226E-05		
2	177,82794	5,180816459		8,4456E-05		
3	316,22777	5,756462732		0,00038377		
4	562,34133	6,332109006		0,00158924		
5	1000	6,907755279		0,00587524		
6	1778,2794	7,483401552		0,01890833		
7	3162,2777	8,059047825		0,05137067		

Model [-]	Size	MolarmassM	MolarmassN	Mn	Mw	Mz
Gamma	25	100	100000000	10000	25000	50000
Function:						
Type:	Optimizec	User value:		Calc. value:	Error [%]	
Mn [g/mo	Yes	10000		9999,99973	-2,7E-06	
Mw [g/mc	Yes	25000		25000,0018	7,21E-06	
Mz [g/mol	Yes	50000		49999,9977	-4,5E-06	
Mw/Mn [-		2,5		2,50000025		
Mz/Mw [-		2		1,99999977		
Count	25					
Number	Ln(M)	[Ln(	Molar Mass [	Mass Fractio		
1	4,60517		100	1,7226E-05		
2	5,180816		177,827941	8,4456E-05		
3	5,756463		316,227766	0,00038377		
4	6,332109		562,341325	0,00158924		
5	6,907755		1000	0,00587524		
6	7,483402		1778,27941	0,01890833		
7	8,059048		3162,27766	0,05137067		

Critical Point

Changes

The putput format used for a critical point calculation was not optimal. It would give information for a range of phases even that they are equal at the critical point. Plus it did not take into account the precens of several critical point at given conditions.
The new format gives one phase information for each critical point found as seen on the right side.



EXANE [Massfractior	ETHYLENE	HDPE [Ma	Output	Compone	Units	Project sheet
0,333333333	0,333333	0,333333	Fixed 2D	All	C(In,Mass	PCSAFTv12
perty	System	Feed	Phase 1	Phase		
ssure [Bar]	2124,419					
nperature [Celsius]	28,3038					
nponents						
EXANE [Massfractior	0,333333	0,333333	0,333333	0,333333		
YLENE [Massfraction	0,333333	0,333333	0,333333	0,333333		
E [Massfraction]	0,333333	0,333333	0,333333	0,333333		
se Fraction [Mole]			0,5	0,5		
se Fraction [Weight]			0,5	0,5		
npressibility [-]	7,240022	7,240022	7,240022	7,240022		
sity [g/cm^3]	0,742957	0,742957	0,742957	0,742957		
ar Volume [cm^3/m	85,41952	85,41952	85,41952	85,41952		
halpy [kJ/Kg]	-667,11	-667,11	-667,11	-667,11		
ropy [kJ/(Kg Kelvin)]	-1,44821	-1,44821	-1,44821	-1,44821		
kJ/(Kg Kelvin)]	2,183715	2,183715	2,183715	2,183715		
kJ/(Kg Kelvin)]	1,900584	1,900584	1,900584	1,900584		
oeffient [Kelvin/Bar]		-0,05013	-0,05013	-0,05013		
ocity of Sound [m/s]		1677,093	1677,093	1677,093		
lecularWeight [g/mo	63,46301	63,46301	63,46301	63,46301		
(HDPE) [g/mol]	47619,27	47619,27	47619,27	47619,27		
(HDPE) [g/mol]	51838,58	51838,58	51838,58	51838,58		
(HDPE) [g/mol]	56257,52	56257,52	56257,52	56257,52		
E	HDPE	HDPE	HDPE	HDPE		
17300	0,00498	0,00498	0,00498	0,00498		
25600	0,03067	0,03067	0,03067	0,03067		
36000	0,239018	0,239018	0,239018	0,239018		
50000	0,455145	0,455145	0,455145	0,455145		
69200	0,239018	0,239018	0,239018	0,239018		
97600	0,03067	0,03067	0,03067	0,03067		
144000	0,0005	0,0005	0,0005	0,0005		

n-HEXANE	ETHYLENE	HDPE	Output	Project sh
0,333333333	0,333333333	0,333333333	Detailed	PCSAFTv1
Property	Critical Point 1/2	Critical Point 2/2	(Ctrl)	
Pressure [Bar]	2124,418791	97,29767788		
Temperature [Celsius]	28,3037952	1154,014372		
Components				
n-HEXANE [Massfraction]	0,333333333			
ETHYLENE [Massfraction]	0,333333333			
HDPE [Massfraction]	0,333333333			
Phase Fraction [Mole]				
Phase Fraction [Weight]				
Compressibility [-]	7,240021656	1,05296611		
Density [g/cm^3]	0,74295671	0,04941947		
Molar Volume [cm^3/mol]	85,41952396	1284,170158		
Enthalpy [kJ/Kg]	-667,109959	3160,192824		
Entropy [kJ/(Kg Kelvin)]	-3,613166817	1,887856366		
Cp [kJ/(Kg Kelvin)]	2,183711892	4,93790181		
Cv [kJ/(Kg Kelvin)]	1,900580897	4,782322518		
JTCoeffient [Kelvin/Bar]	-0,050127818	0,01283699		
Velocity of Sound [m/s]	1677,092829	464,2680069		
MolecularWeight [g/mol]	63,4630085			
Mn (HDPE) [g/mol]	47619,26789			
Mw (HDPE) [g/mol]	51838,58361			
Mz (HDPE) [g/mol]	56257,51517			
HDPE	HDPE			
17300	0,00497995			
25600	0,030669693			
36000	0,23901761			
50000	0,455145449			
69200	0,23901761			
97600	0,030669693			
144000	0,000499995			

"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 industri."

Dr. Torben Laursen, CEO & Founder

Solutions worldwide...

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

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

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

Cell phone	+45 31 41 01 19
e-mail	tl@vlxe.com
Homepage	www.vlxe.com
Skype:	vlxe.Inc

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ADVANCED PVT SIMPLIFIED