VLXE
ADVANCED PVT SIMPLIFIED

VLXE|BLEND®

VLXE Blend: Standard System

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

VLXE
ADVANCED PVT SIMPLIFIED

VLXE|BLEND®

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 uniqe 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.

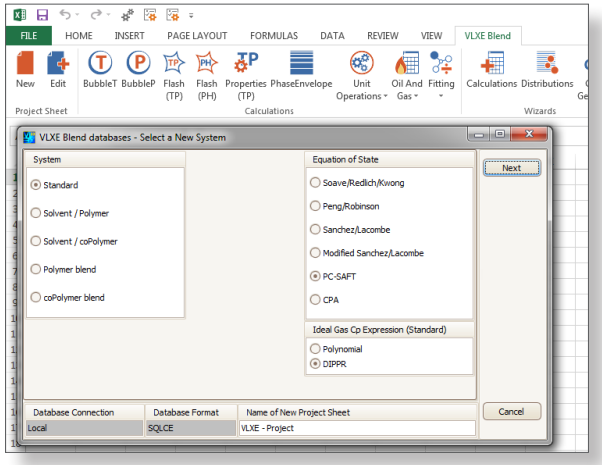
Depending on the EOS, a different number of mixing rules are included.

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 Expression • Polynomial Expression

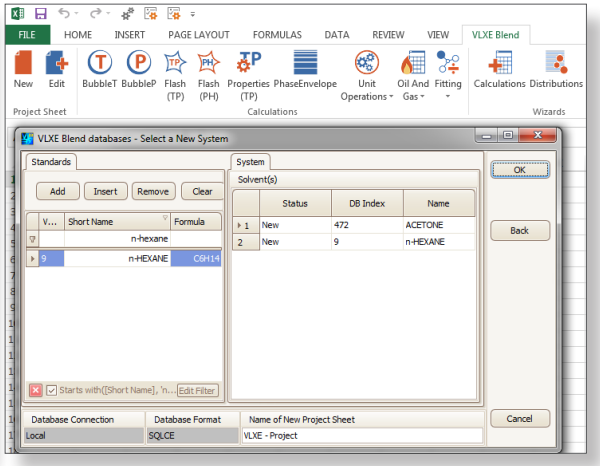
VLXE Examples:

Creating a new project

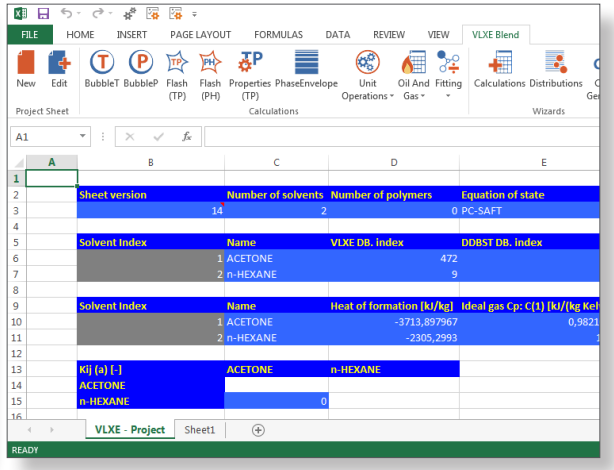
Setting up a new project is simple, made easy by the database and wizards provided. It is only a few mouse clicks away.



Select the Components



Generate Project Sheet

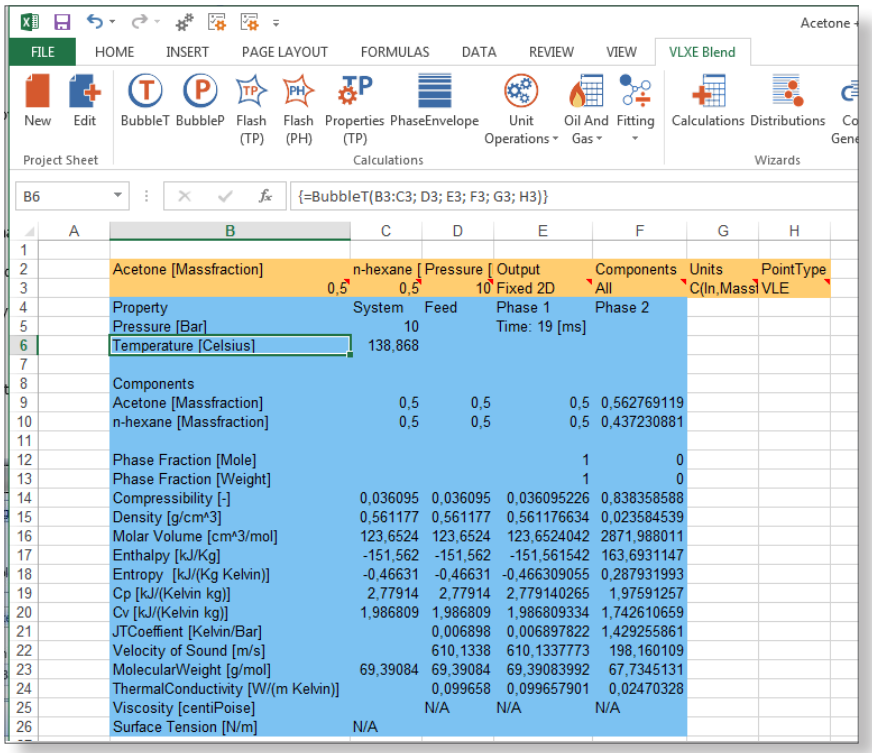


Define the System

VLXE Examples:

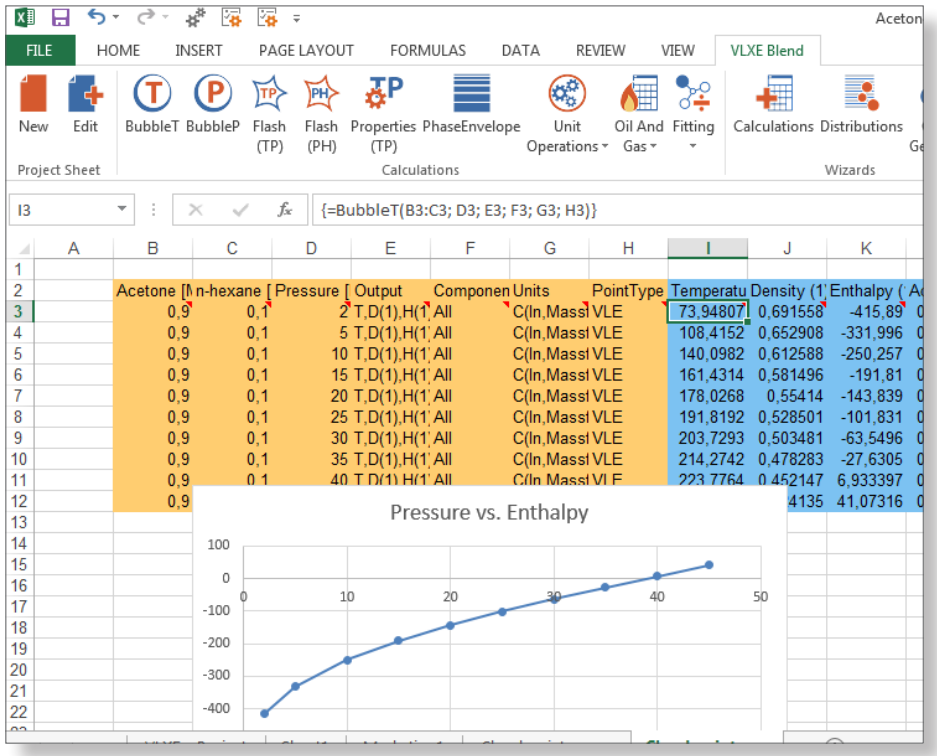
Cloud Point

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.



	Acetone [Massfraction]	n-hexane [	Pressure [	Output	Components	Units	PointType
	0,5	0,5	10	Fixed 2D	All	C(ln,Mass	VLE
	Property	System	Feed	Phase 1	Phase 2		
	Pressure [Bar]	10		Time: 19 [ms]			
	Temperature [Celsius]	138,868					
	Components						
	Acetone [Massfraction]	0,5	0,5	0,5	0,562769119		
	n-hexane [Massfraction]	0,5	0,5	0,5	0,437230881		
	Phase Fraction [Mole]			1	0		
	Phase Fraction [Weight]			1	0		
	Compressibility [-]	0,036095	0,036095	0,036095226	0,838358588		
	Density [g/cm^3]	0,561177	0,561177	0,561176634	0,023584539		
	Molar Volume [cm^3/mol]	123,6524	123,6524	123,6524042	2871,988011		
	Enthalpy [kJ/Kg]	-151,562	-151,562	-151,561542	163,6931147		
	Entropy [kJ/(Kg Kelvin)]	-0,46631	-0,46631	-0,466309055	0,287931993		
	Cp [kJ/(Kelvin kg)]	2,77914	2,77914	2,779140265	1,97591257		
	Cv [kJ/(Kelvin kg)]	1,986809	1,986809	1,986809334	1,742610659		
	JTCoeffient [Kelvin/Bar]		0,006898	0,006897822	1,429255861		
	Velocity of Sound [m/s]		610,1338	610,1337773	198,160109		
	MolecularWeight [g/mol]	69,39084	69,39084	69,39083992	67,7345131		
	ThermalConductivity [W/(m Kelvin)]		0,099658	0,099657901	0,02470328		
	Viscosity [centiPoise]		N/A	N/A	N/A		
	Surface Tension [N/m]	N/A					

Cloud Point
Calculation as fixed output

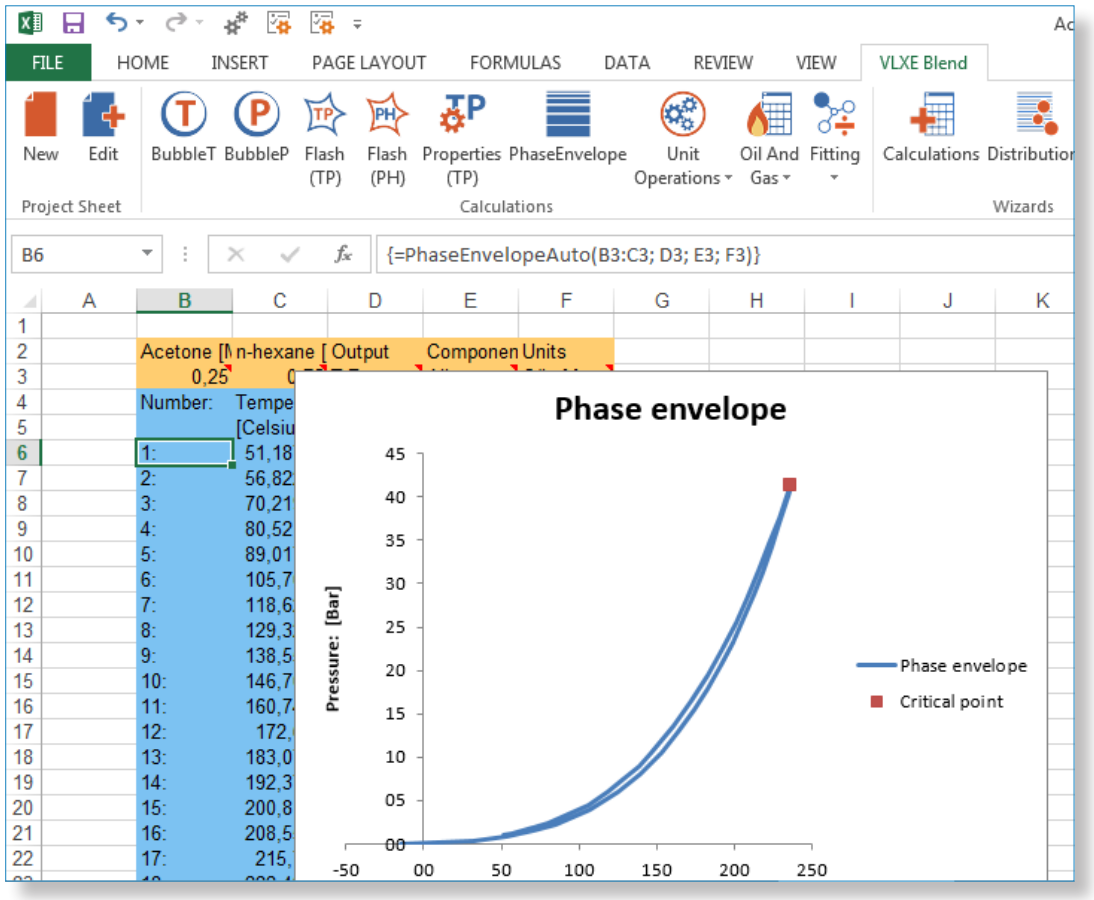


	Acetone [M	n-hexane [	Pressure [	Output	Componen	Units	PointType	Temperatu	Density (1'	Enthalpy (	A
	0,9	0,1	2	T,D(1),H(1'	All	C(ln,Mass	VLE	73,94807	0,691558	-415,89	0
	0,9	0,1	5	T,D(1),H(1'	All	C(ln,Mass	VLE	108,4152	0,652908	-331,996	0
	0,9	0,1	10	T,D(1),H(1'	All	C(ln,Mass	VLE	140,0982	0,612588	-250,257	0
	0,9	0,1	15	T,D(1),H(1'	All	C(ln,Mass	VLE	161,4314	0,581496	-191,81	0
	0,9	0,1	20	T,D(1),H(1'	All	C(ln,Mass	VLE	178,0268	0,55414	-143,839	0
	0,9	0,1	25	T,D(1),H(1'	All	C(ln,Mass	VLE	191,8192	0,528501	-101,831	0
	0,9	0,1	30	T,D(1),H(1'	All	C(ln,Mass	VLE	203,7293	0,503481	-63,5496	0
	0,9	0,1	35	T,D(1),H(1'	All	C(ln,Mass	VLE	214,2742	0,478283	-27,6305	0
	0,9	0,1	40	T,D(1),H(1'	All	C(ln,Mass	VLE	223,7764	0,452147	6,933397	0
	0,9								4135	41,07316	0

Cloud Point
Calculation as a function range output ()

Phase Diagram

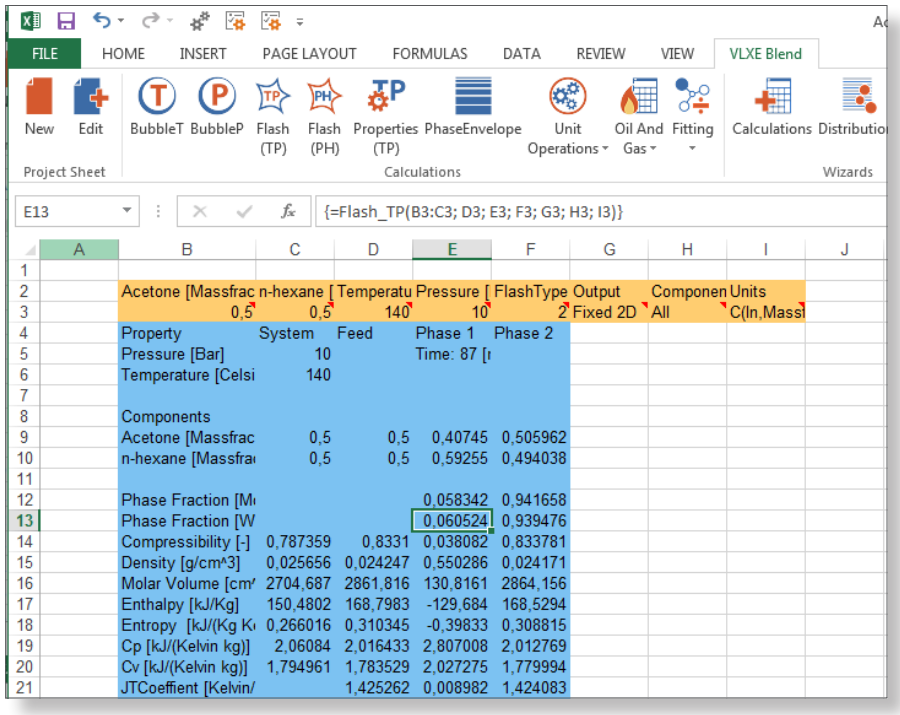
Obtaining the phase diagram for a system gives a very good overview of its behavior. VLXE Blend comes with a range of options including the auto function shown below. Note how the critical point is included in the output.



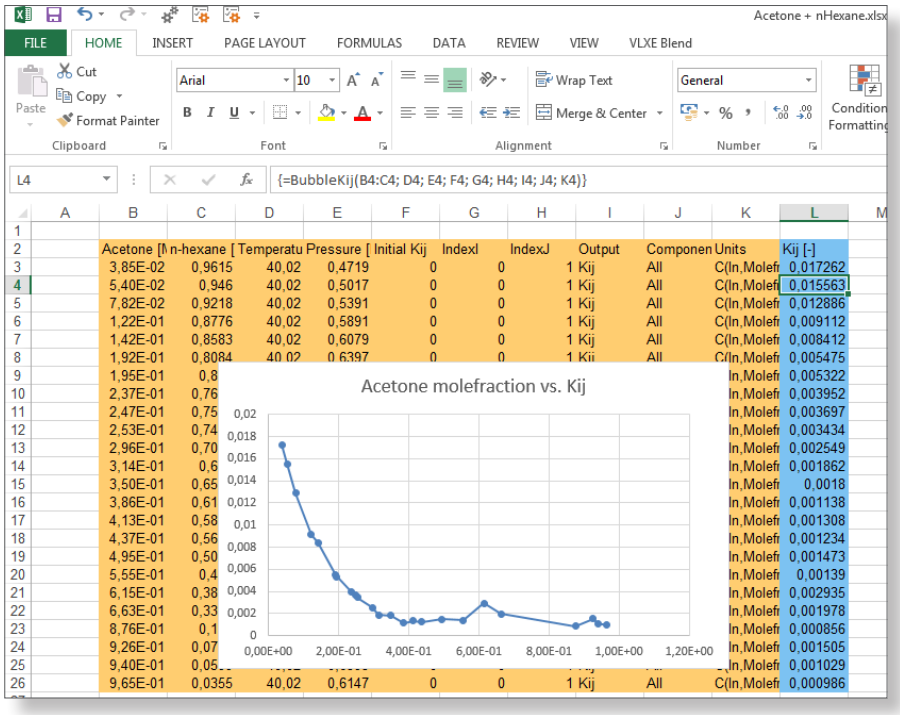
Phase envelope (Acetone+ n-Hexane)

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.



Flash Calculation (Acetone+ n-Hexane)

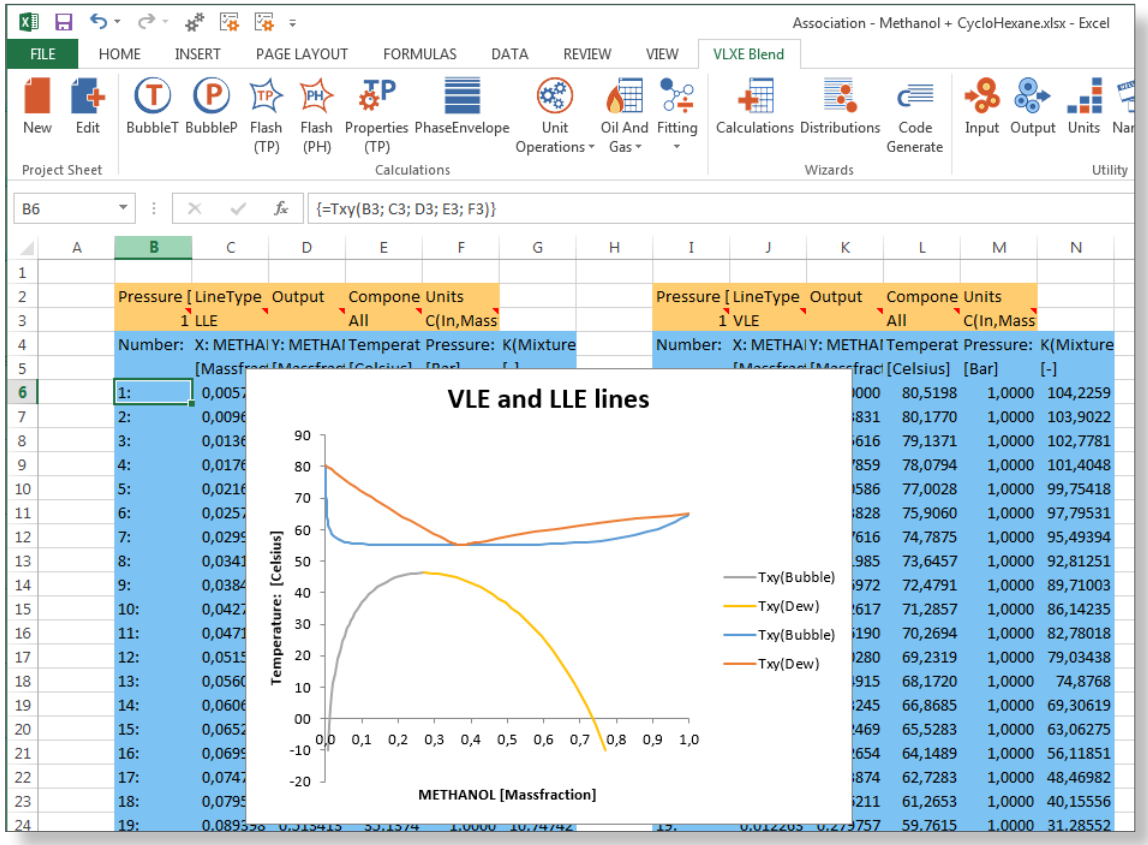


Bubble Kij fit (Acetone+ n-Hexane)

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.

Txy/Pxy Calculations for Association Components

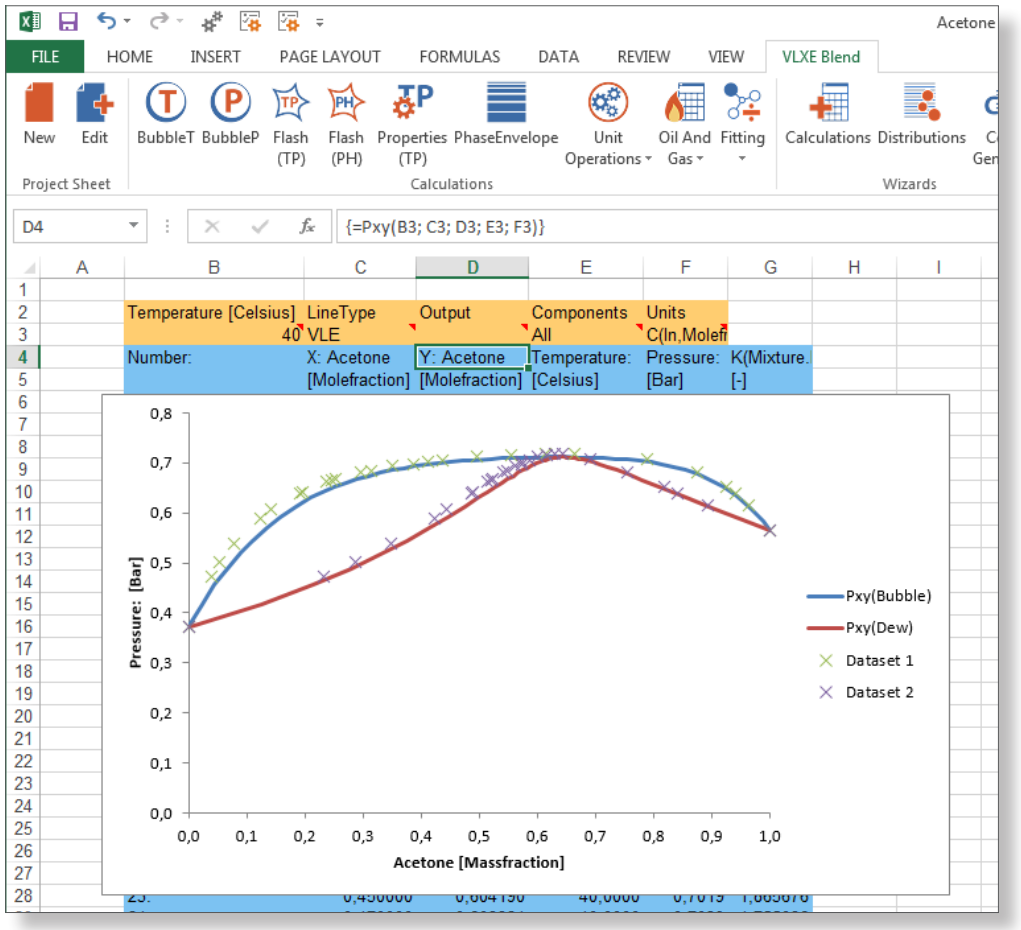
The associating term is very powerful in VLXE Blend. The user can enter custom defined schemes and view the bonding fraction as part of the output. Below is an example with Methane + Methanol, where the associating term is used. Note how VLXE Blend allows the user to obtain both the LLE and VLE line.



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:



Pxy Calculations for Polar System

"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:

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

VLXE
ADVANCED PVT SIMPLIFIED