VLXE
ADVANCED PVT SIMPLIFIED

VLXE Blend: Polymers

VLXE Blend is unique when it comes to PVT calculations for polymer systems.

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

VLXE|BLEND®

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Welcome to VLXE Blend: Polymers

Highlights are:

Robust LLE and VLLE calculations
Support for polydisperse polymers
Support for blends.
Supports copolymers
Include PC-SAFT and copolymer PC-SAFT, both with polar and association term
Include parameter fitting routine
Has been in production since 2003 and it continues to expand.

Advantages & Models

Calculations:	Applications:
Flash Calculations	• Multi-phase flash calculation, 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 spreadsheet sheet to create a flow sheet.
Critical Point	• Calculate the 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.
SLE	• These functions perform SLE polymer massfractions and SLE temperature.
Fit Parameters	• Both pure components and kij's.
Properties	• Properties like density, Enthalpy etc. are avaiable for both pure polymer and systems with polymers.
Process simulator	• Links to common process simulators through Excel.

Thermodynamic Models

All phase equilibria calculations performed in VLXE Blend are based on the use of equations of state (EOS). Four EOS are included that can handle polymers.

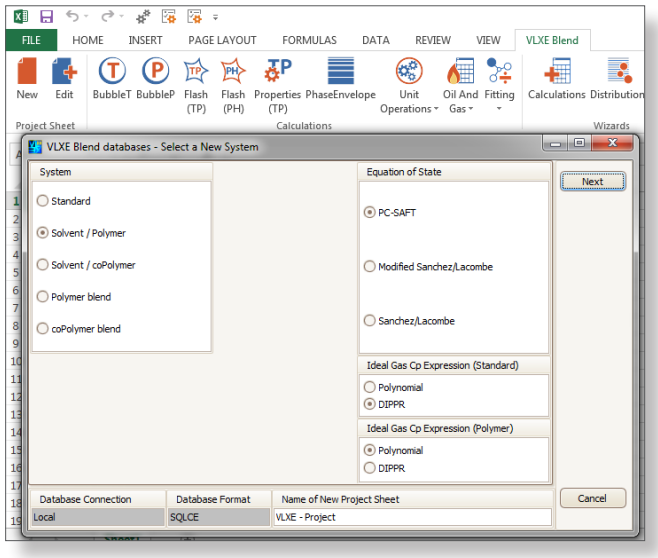
The main equations are PC-SAFT and copolymer PC-SAFT.

Equation of States	• PC-SAFT • Copolymer PC-SAFT • Sanchez/Lacombe (Orignal) • Sanchez/Lacombe (Ideal Gas Limit)
Models For Ideal Gas Heat Capacity	• DIPPR Expression • Polynomial Expression

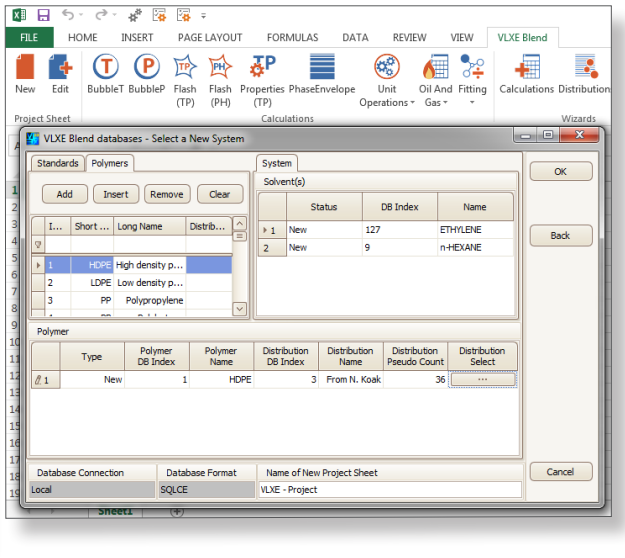
Polymer systems made simple

In VLXE Blend polymer systems are as simple to handle as any other system.

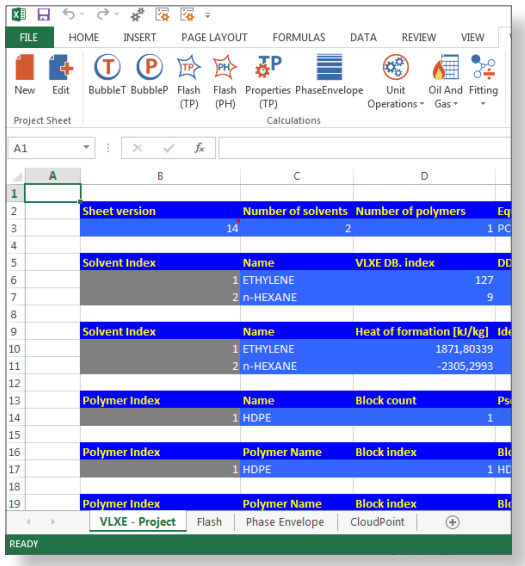
Handling any system is as simple as if it were a binary alkane system.



Define the System



Select the Components

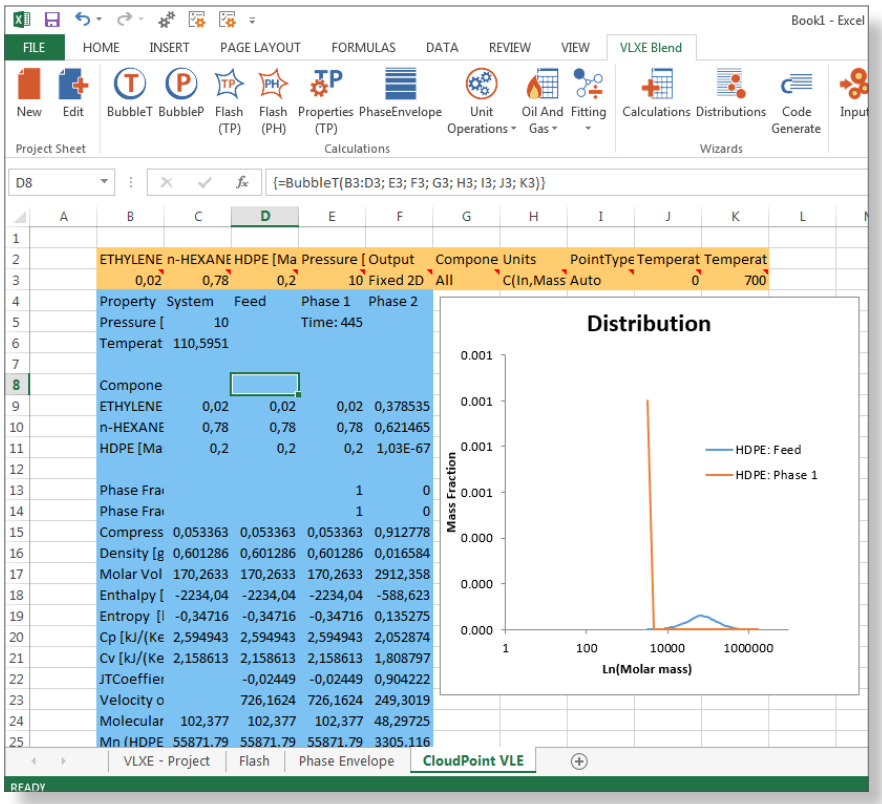


Generate project sheet

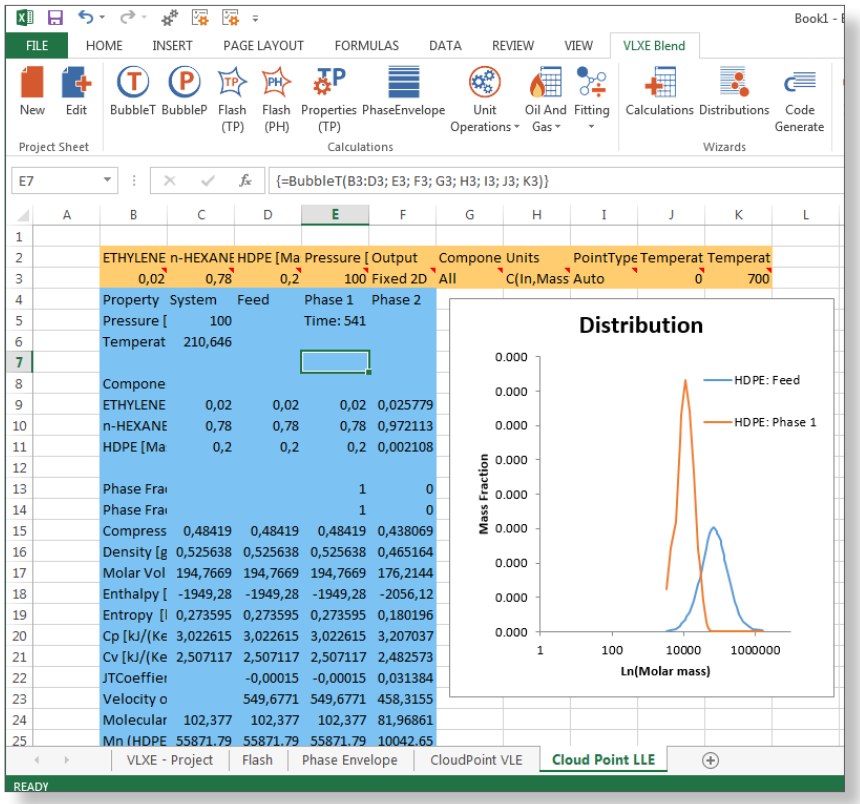
Cloud Point

VLXE Blend comes with a robust cloud point routine for polymers.

It can handle both LLE and VLE as shown below. The only extra user input required, when compared to a simple alkane system, is the temperature or pressure range for the solution. In the example below note how the distribution changees between VLE and LLE.



Cloud point | VLE

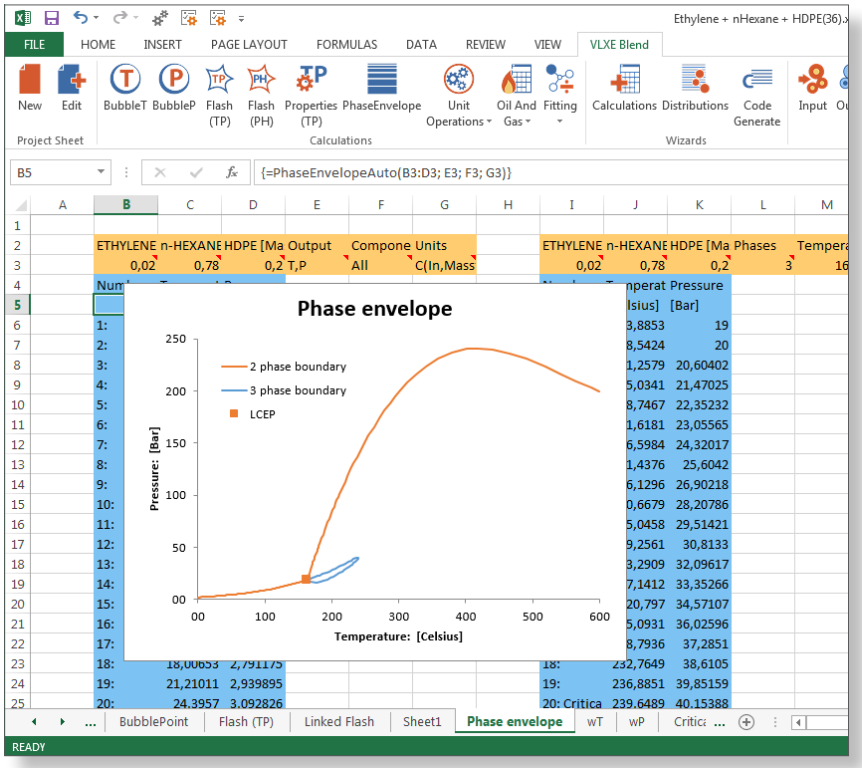


Cloud point | LLE

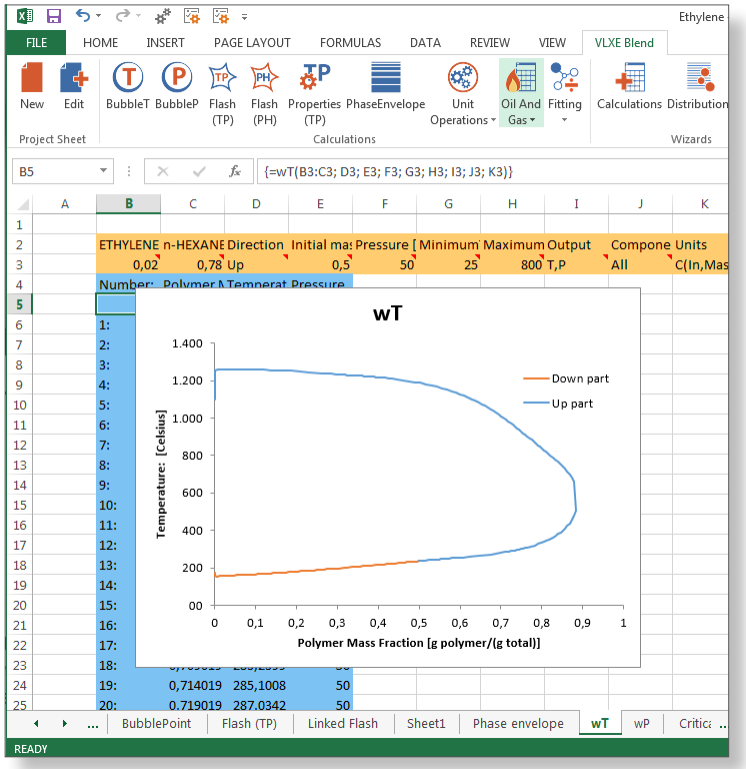
Phase Diagram

Knowing the entire phase diagram for a system allows an optimal process design. VLXE Blend allows the calculation of the entire phase diagram, not only in the temperature, pressure space but also in both the polymer fraction, temperature/pressure space.

The example below illustrates a complete phase diagram. Note the 3 phase area on the right and note the complete curve on the right which is calculated for a fixed pressure. Also note how the 2 curves, when put together, gives a 3D phase diagram.



Polymer Mass Fraction versus Temperature (wT)

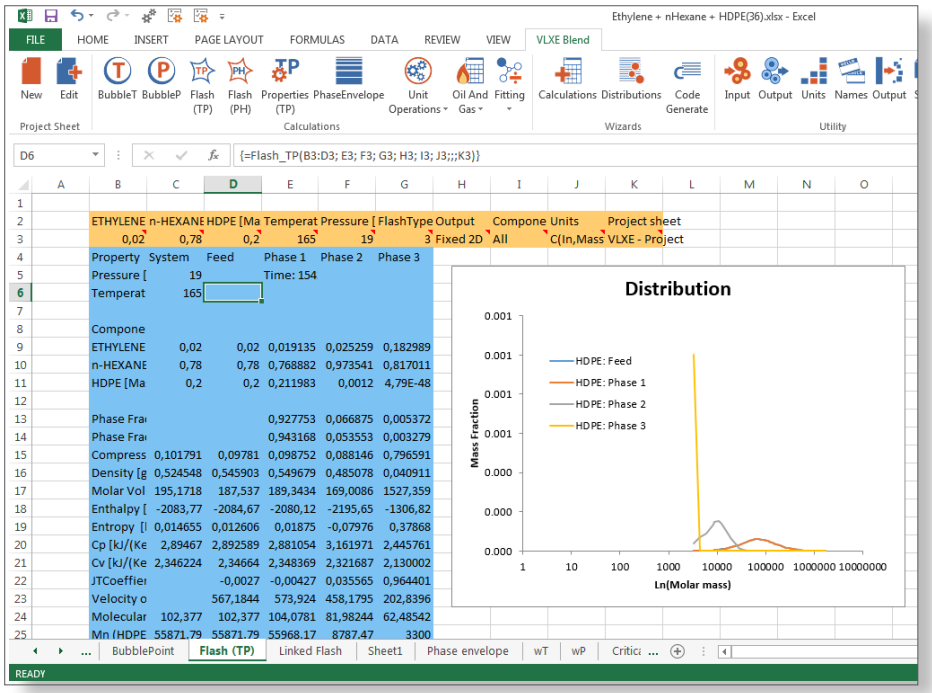


Phase envelope

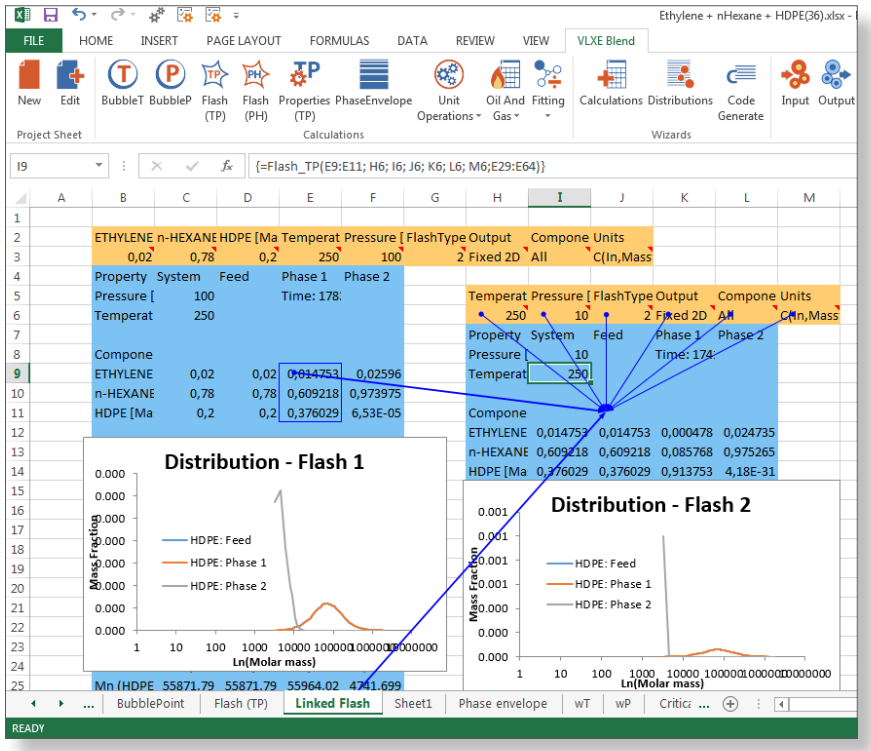
Flash Calculation

VLXE Blend comes with the best polymer flash calculator in the world. It gives you access to robust VLE, LLE, VLLE and VLLLE flash calculations. No extra input is required when compared to a simple alkane system.

In the examples below a 3 phase flash calculation is shown plus how 2 flashes are linked to simulate a separation unit. Note how the pseu-do-components are distributed between the phases in the two-process step.



Flash Calculation

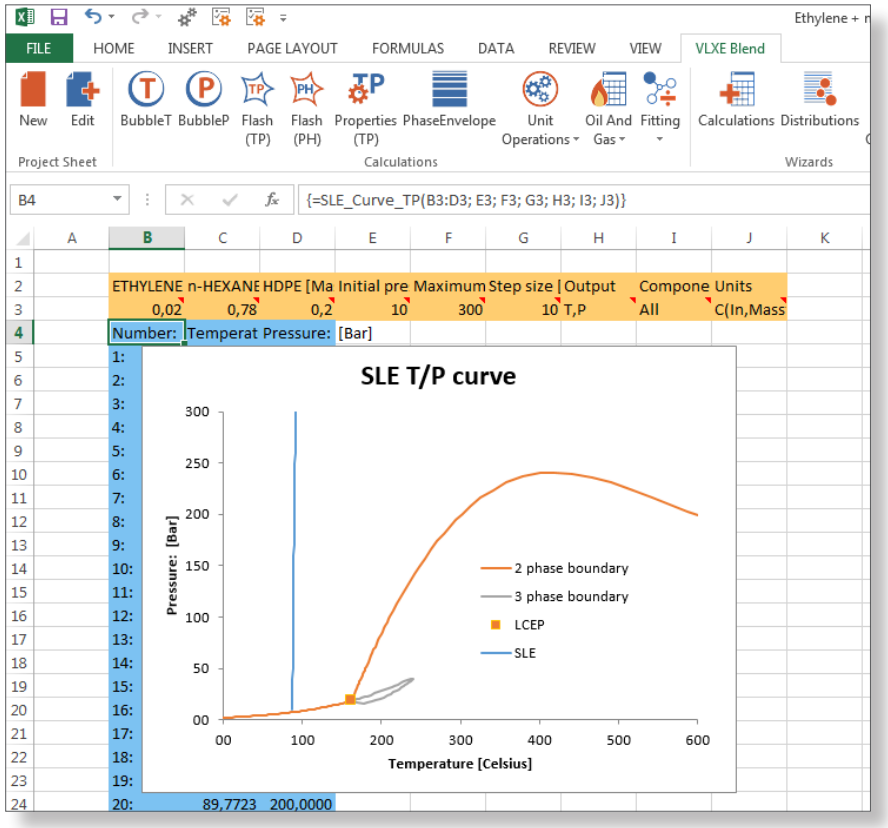


How to link Flash Calculation to create flow sheet

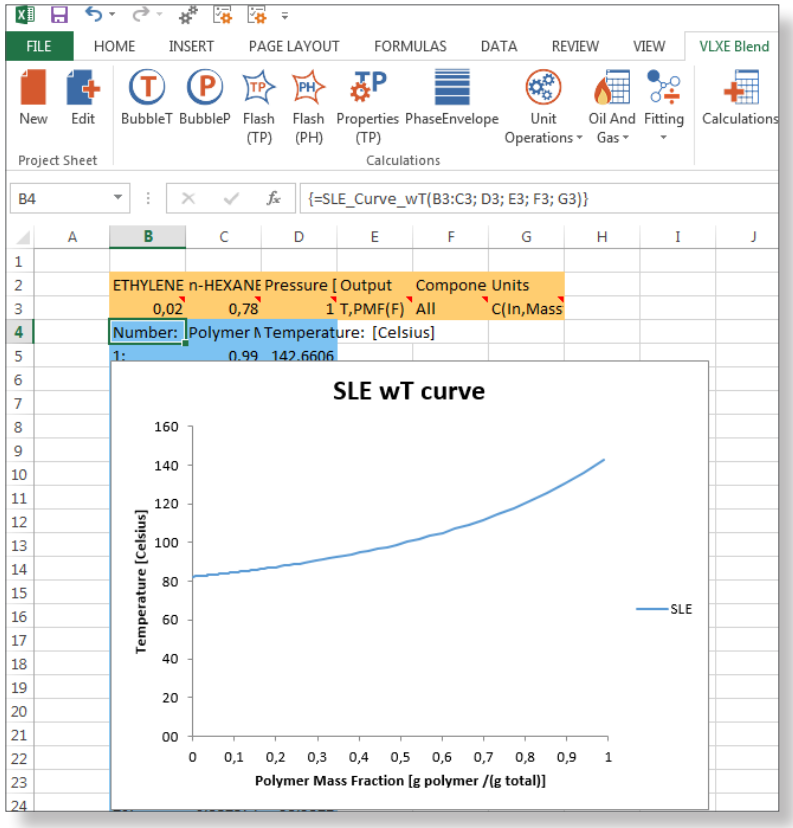
SLE

SLE calculations are often performed to avoid a solid phase in the wrong place. VLXE Blend provides a range of SLE calculations.

In the example below the SLE line is added to the phase diagram. On the right the SLE line is traced against polymer massfraction at a fixed pressure.



SLE T/P Curve

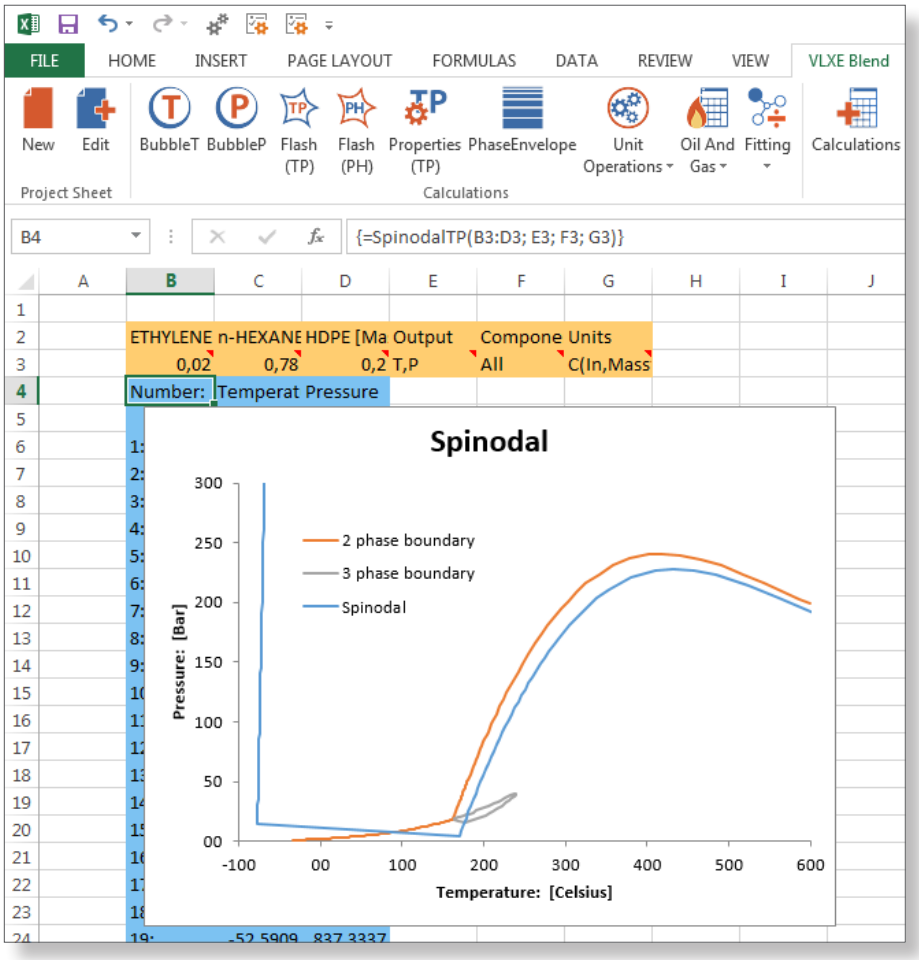


Effect of polymer massfraction on SLE temperature

Spinodal & Critical Point

These two calculations are directly avaiable in VLXE Blend.

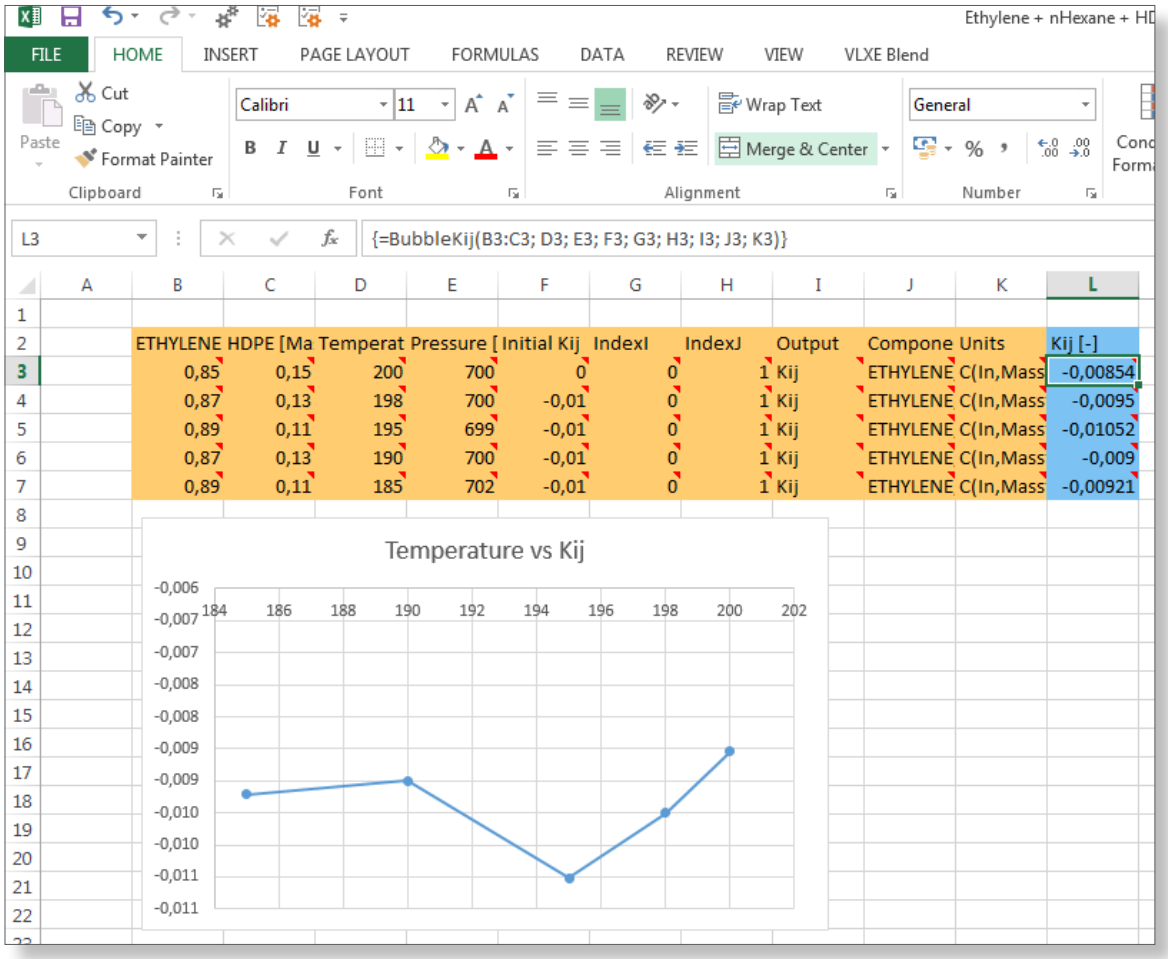
Both are of interest when planning or optimizing separation steps.



Kij fitting

A full fitting range is included in VLXE Blend. The most commonly used is BubbleKij.

It allows the user to solve for the Kij at each datapoint, yielding a precise picture of how the model performs, plus which Kij value will give the best fit. It is a fast and robust method to fit your data.

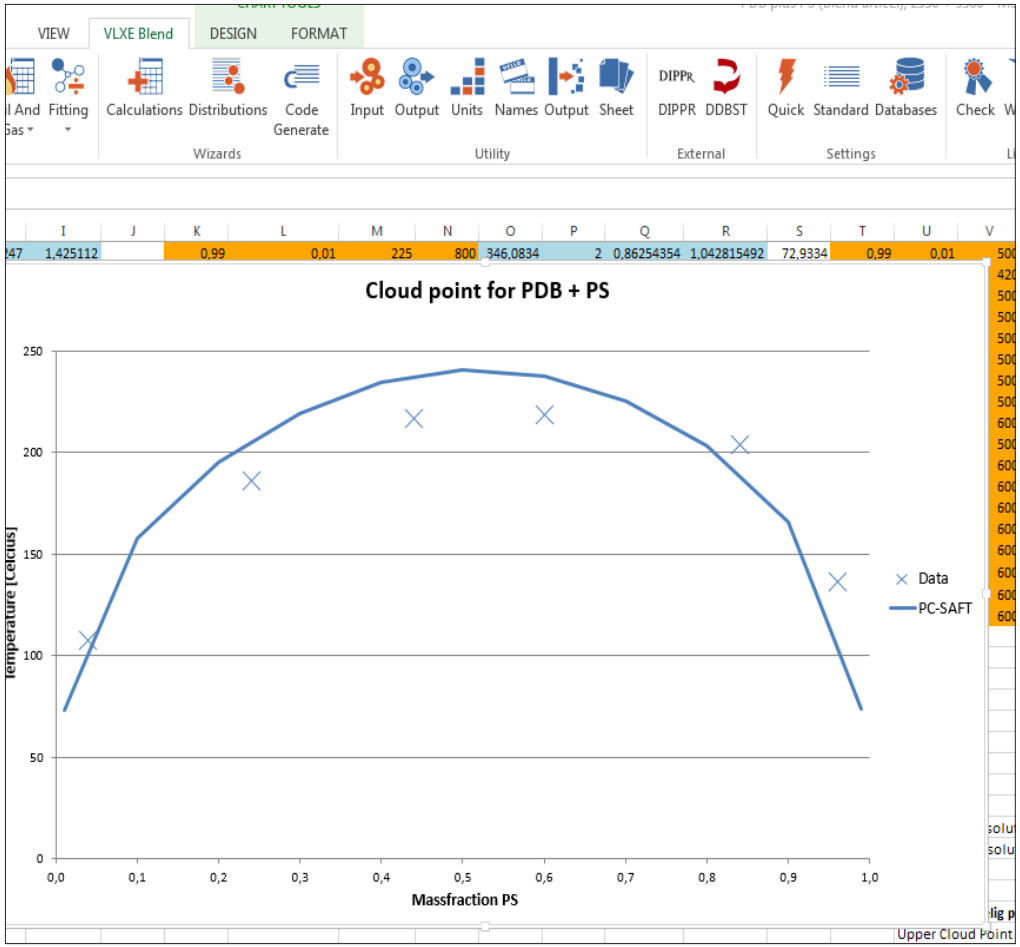


ETHYLENE	HDPE [Ma	Temperat	Pressure [	Initial Kij	IndexI	IndexJ	Output	Compone	Units	Kij [-]
0,85	0,15	200	700	0	0	1	Kij	ETHYLENE	C(In,Mass	-0,00854
0,87	0,13	198	700	-0,01	0	1	Kij	ETHYLENE	C(In,Mass	-0,0095
0,89	0,11	195	699	-0,01	0	1	Kij	ETHYLENE	C(In,Mass	-0,01052
0,87	0,13	190	700	-0,01	0	1	Kij	ETHYLENE	C(In,Mass	-0,009
0,89	0,11	185	702	-0,01	0	1	Kij	ETHYLENE	C(In,Mass	-0,00921

Blends

Blends are not simple to handle, but are, nonetheless, available in VLXE Blend.

Nothing special is required to perform all your calculations on blends. In the example shown the cloud point from PC-SAFT is compared to data for PDB + PS.



"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 others.

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