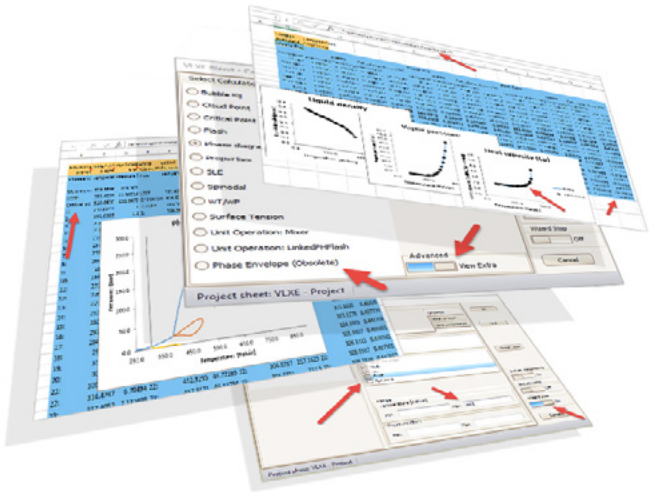
VLXE
ADVANCED PVT SIMPLIFIED



VLXE | BLEND® Version 9.0

What's new?

Version 9 is the 2016 major release of VLXE Blend.
User experience has been further improved and new phase diagram calculation has been added.

Introduction

Version 9 is the 2016 major release of VLXE Blend. The focus is further improvement of the user experience. This has partly been achieved by the addition of phase diagram calculations that collects a number of seperatly calculations into one call. In addition to this the temperature/pressure flash can now include a solid phase for polymer systems.

A new database format has been introduced. This was done to prepare for version 10 that will see a number of improvements in the way the databases are used. Users are now better warned when model parameters needed are missing. The “Stop” option has been improved so the user is shown a telling message when it is used.

The speed of the flash has been improved by a 15% on average. Using the new phase diagram option uses far less memory compared to the old phase curve routines it replaces.

Breaking change

Excel 2007

Excel 2007 is not official supported by this version. This is due to the release of Office 2016 that is supported by this version.

Properties calculated at fixed Temperature and Volume

The properties are calculated as the sum of the residual and ideal part. The sum is unchanged but the residual and ideal part obtained with fixed Volume and Temperature in version 8 was not correct. They were calculated at fixed temperature and pressure internal and that is not correct due to the “nRT” term. This term is due to the change in variable from fixed Temperature/Pressure to fixed Temperature/Volume.

Support for SQL Server and SQL compact database format

This year VLXE introduce the use of the SQLite database format. All future upgrades will only be made for this database format. Users of the other 2 formats: SQL Server and SQL Compact can still use their databases but they cannot edit them. This move is done to prepare for future upgrades to the database usage.

Component argument

The user can give a list of components to be included in the calculation using the “Component” argument. The separator used was “,”. Not a good selection since many components has a “,” in their name. Therefore “;” is not used as separator. So all calls using this argument with a list of component names has to be updated in order to work with version 9 and forward.

New database format

Support for SQL Server and SQL compact database format will expire

This year VLXE introduce the use of the SQLite database format. All future upgrades will only be made for this database format. Users of the other two formats: SQL Server and SQL Compact can still use their databases but they cannot edit them. This move is done to prepare for future upgrades to the database usage.
Users are strongly encouraged to move to SQLite from this version

Selected improvements

Ribbon change

The API Group icon has been moved to the right. This was done to make room for the new Phase diagram icon.

Stop message

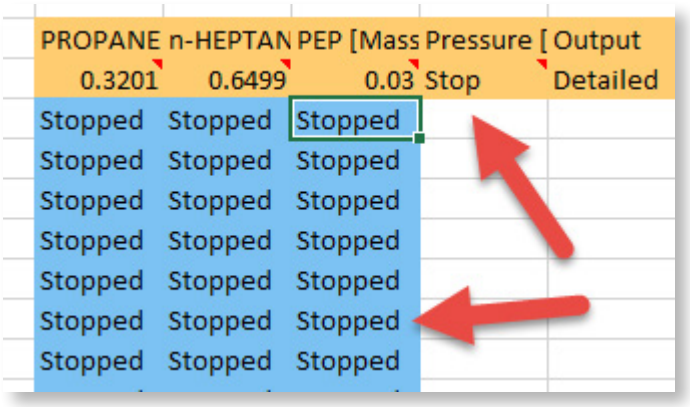
Better stop message implemented. In version 8 a stop method was added. It would write “Stop” in one of the arguments giving the user the option to change argument values before a calculation created by the wizard was run. However it would show an ugly error message in the output area. Now “User stopped” is shown in the output area.

Missing PC-SAFT parameters

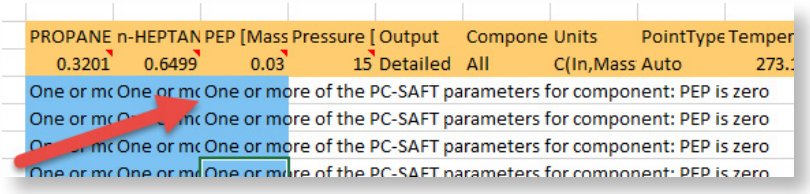
Even that PC-SAFT does not use critical values there are used to get initial guess for some calculations like cloud points. Version 8 and before would not tell the user that they are needed. Now a nice message is shown if they are needed and not given in the project sheet.

SLE temperature/pressure curve

In version 8 and before the curve would not detect entering the 2 phase area. In version 9 it does. However use of this function is discouraged since it is made obsolete by the new phase diagram functions.



Warning when parameters needed to perform the calculation is missing from the project sheet



SLE temperature/pressure curve

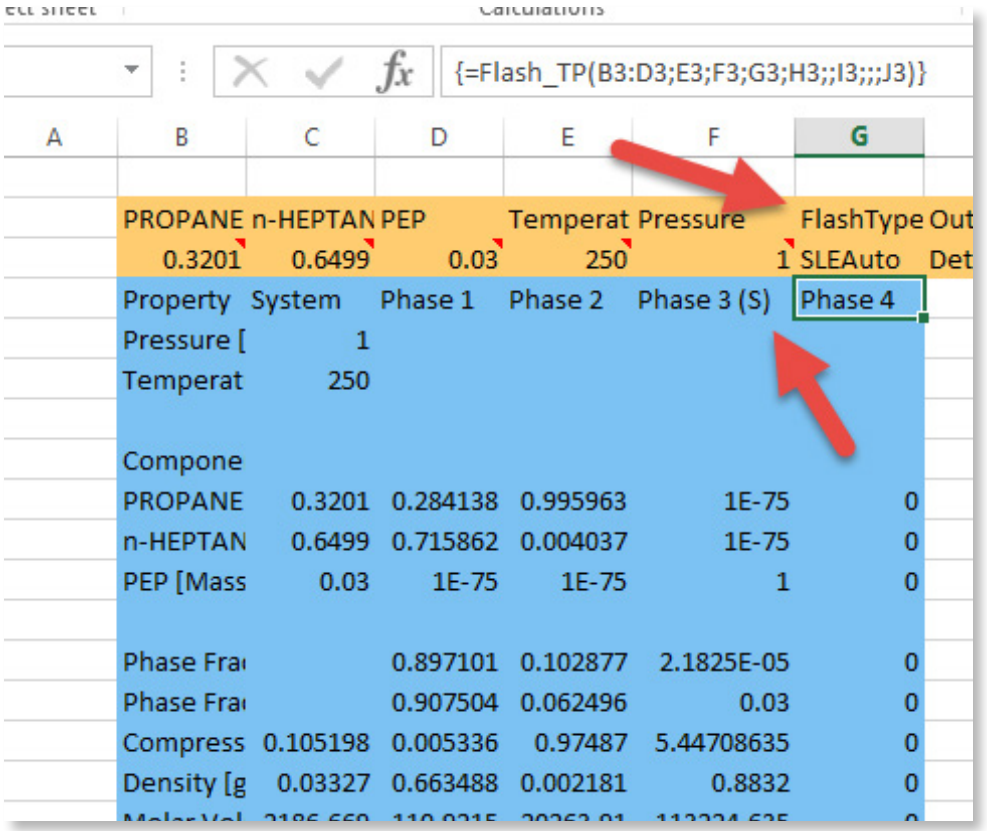
SLE flash.

The temperature/Pressure flash can now take a solid phase into account.

It is activated by adding “SLE” before the “FlashType” argument.

Limitations:

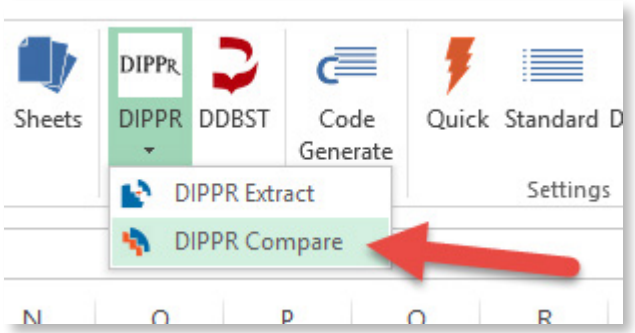
- Only supported in the Temperature/Pressure option
- It will only look for one solid phase
- Solid phase is assumed to be made of only one polymer.



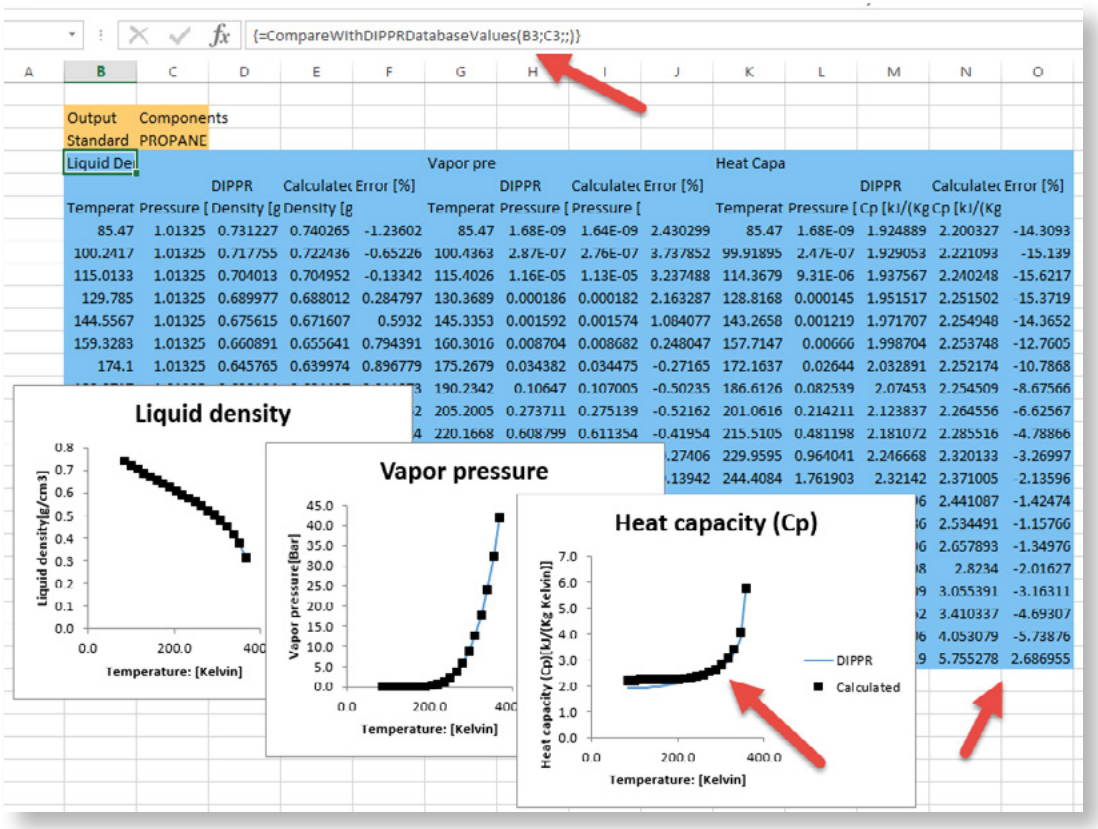
DIPPR compare

Often a user wants to check how PC-SAFT match data for a pure component. In version 8 and below this took a bit of work. But now a new function: “DipprCompare” is included that will compare to 3 data types in one calculation.

It is started using the new menu button:

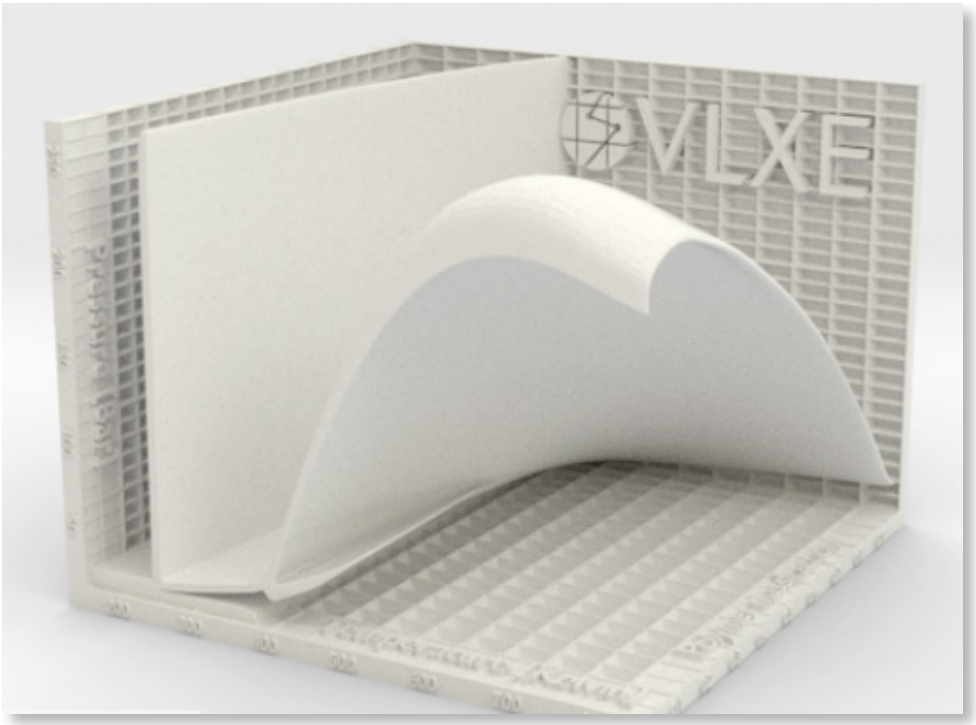


The wizard will create the result as seen here below:



3D printed phase diagrams

Understanding phase diagrams can be a real challenge, therefore I am excited to introduce the 3D printed phase diagram.
This will allow a user to get full understanding of the selected system.
Currently a print with n-Hexane + Ethylene + HDPE is avaiable.



The phase diagrams is complete with these boundaries:

- Phase envelope
- VLLE
- SLE
- Spinodal
- SLVE (New)

This print can be bougth here: http://shop.vlxe.com/3d-print
More options are planned and please contact VLXE it you need a system printed.

Note that the new phase diagram option in VLXE will allow you to calculate the 3 “slices” that can be made of the shown phase diagram.

New phase diagram option

VLXE has always offered the user to calculate complicated phase diagrams. But it was some work for the user since independent calculations like phase envelope, VLLE and SLE calculations had to be performed and then combined.

This has been much improved by introducing 3 new phase diagram calculations that will replace all the old functions. Note that the old are still included but are hidden under “Advanced”.

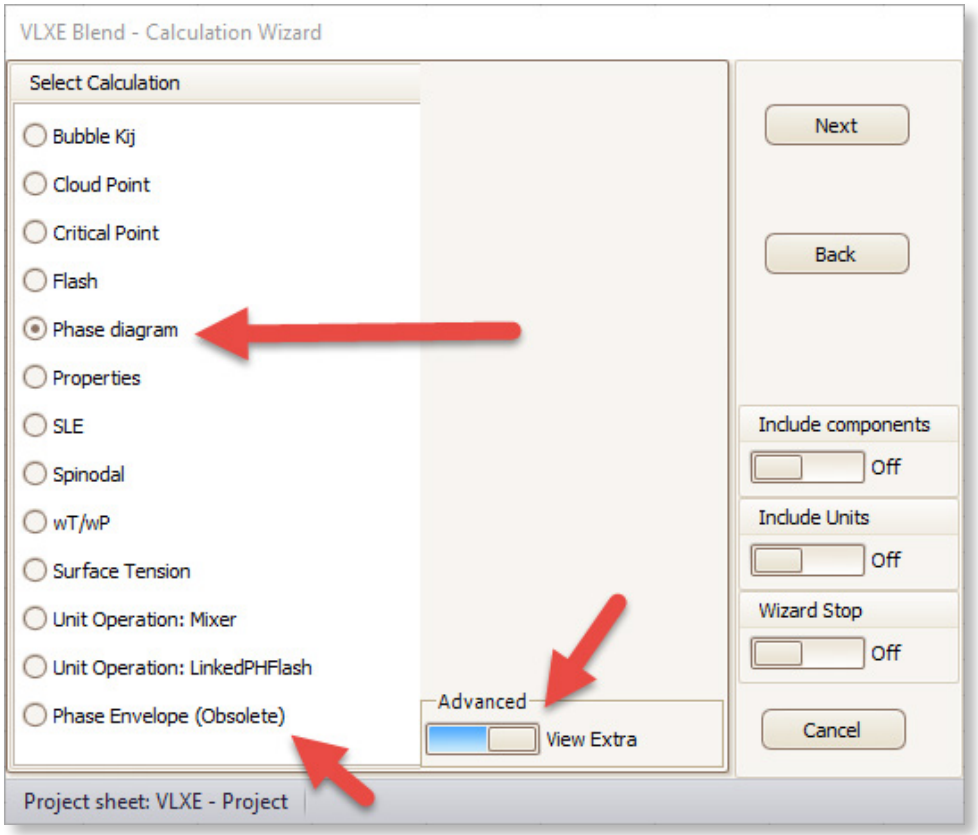
Users are encouraged to only use the new phase diagram from now on. The old options will only be improved in special cases.

The 3 new functions are:

- PhasediagramStandard
- PhasediagramFixedPressure
- PhasediagramFixedTemperature

Phase boundaries included are:

- Phase envelope
- VLLE
- SLE
- Spinodal
- SLVE (New)

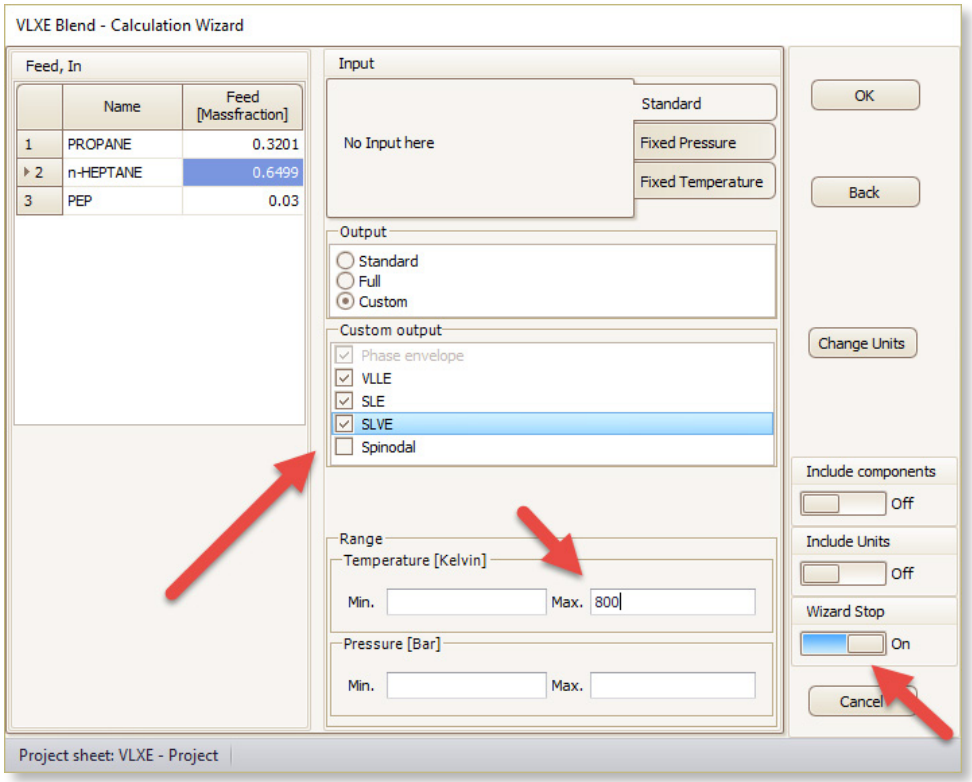


Phase diagram input

This will allow the user to map the diagram that best match the given problem.

The wizard lets the user setup the desired variation.

Note how the stop options is selected by default.

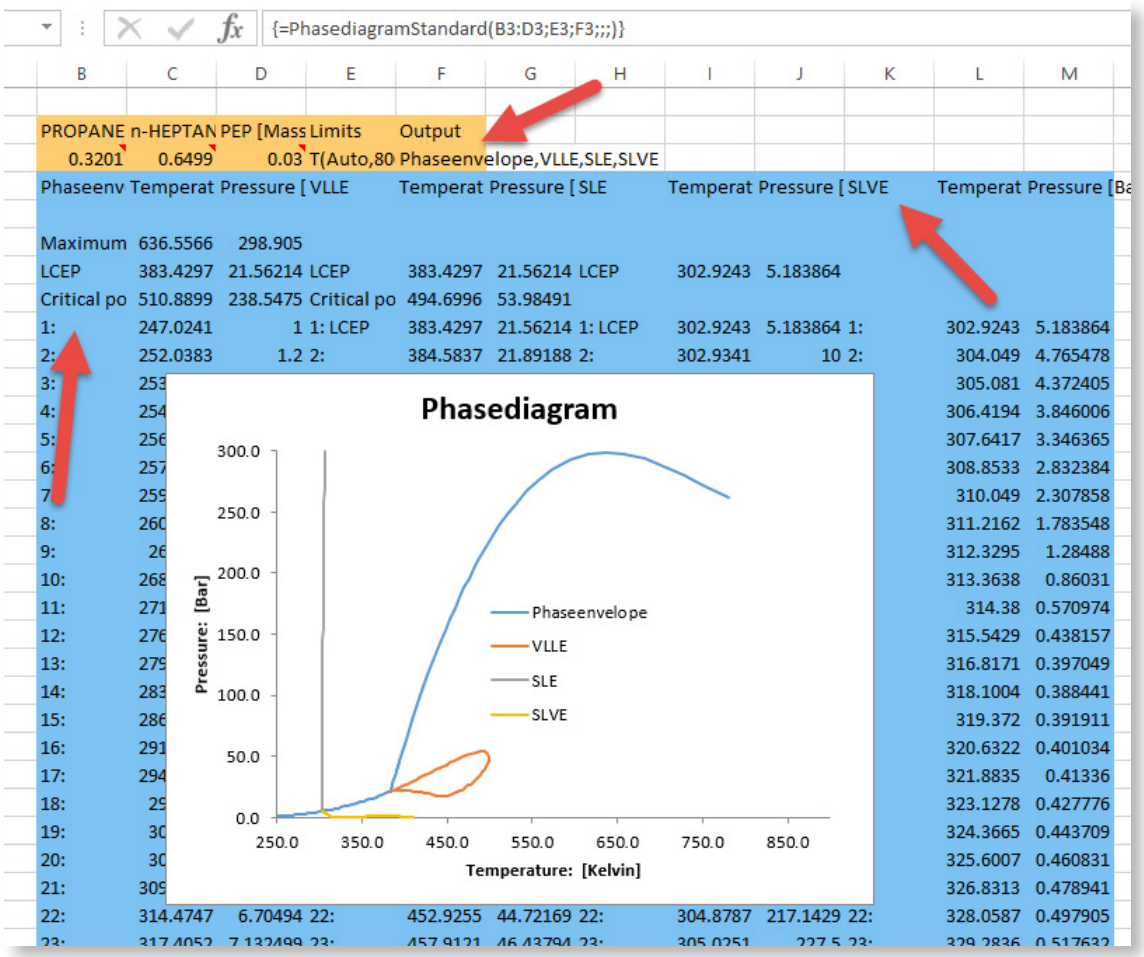


Phase diagram Standard (continued)

This phase diagram is standard where the polymer massfraction is fixed. This options is therefore used for systems with no polymer.

Note how the output is arranged. The extrema are listed on the top plus the name of the curves are given in the first output row.

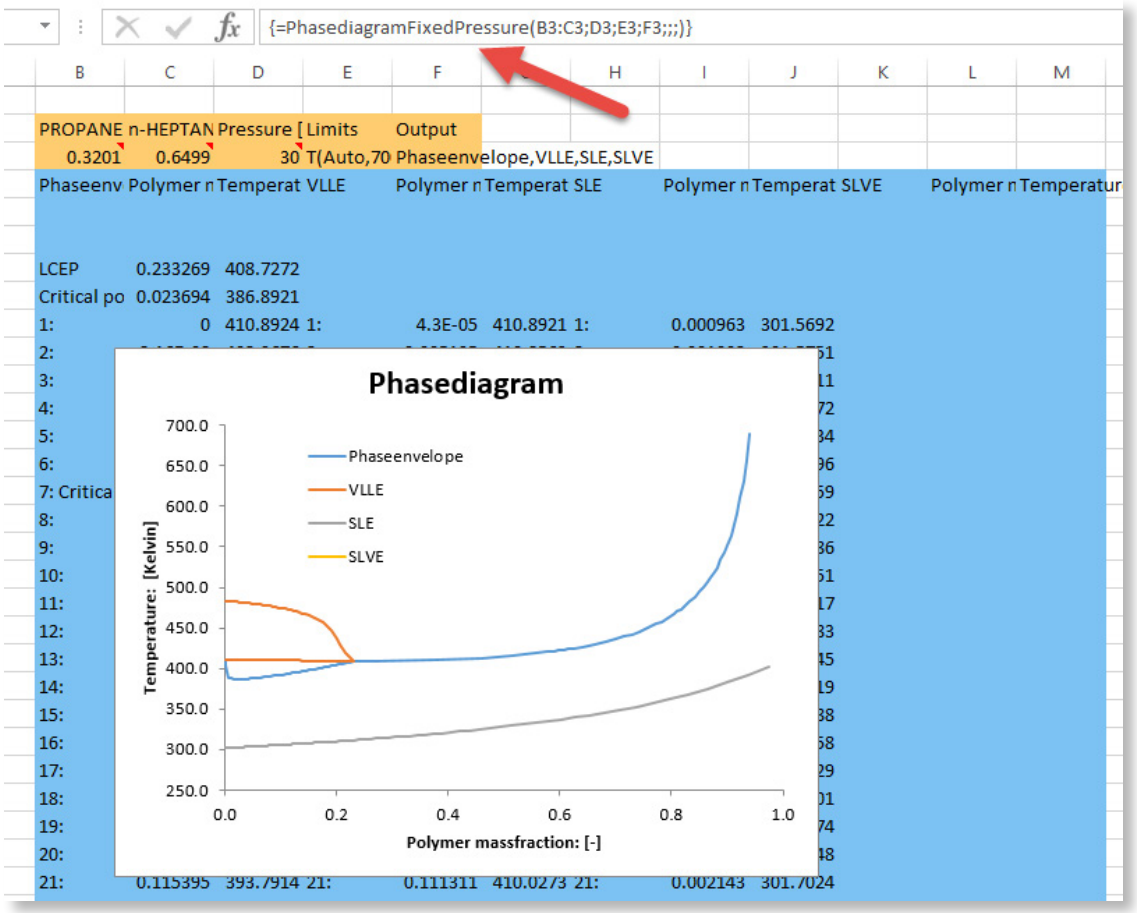
Note how this is one of the three possible way to “slice” the 3D phase diagram.



Phase diagram fixed pressure (continued)

At fixed pressure the temperature and polymer massfraction is traced.

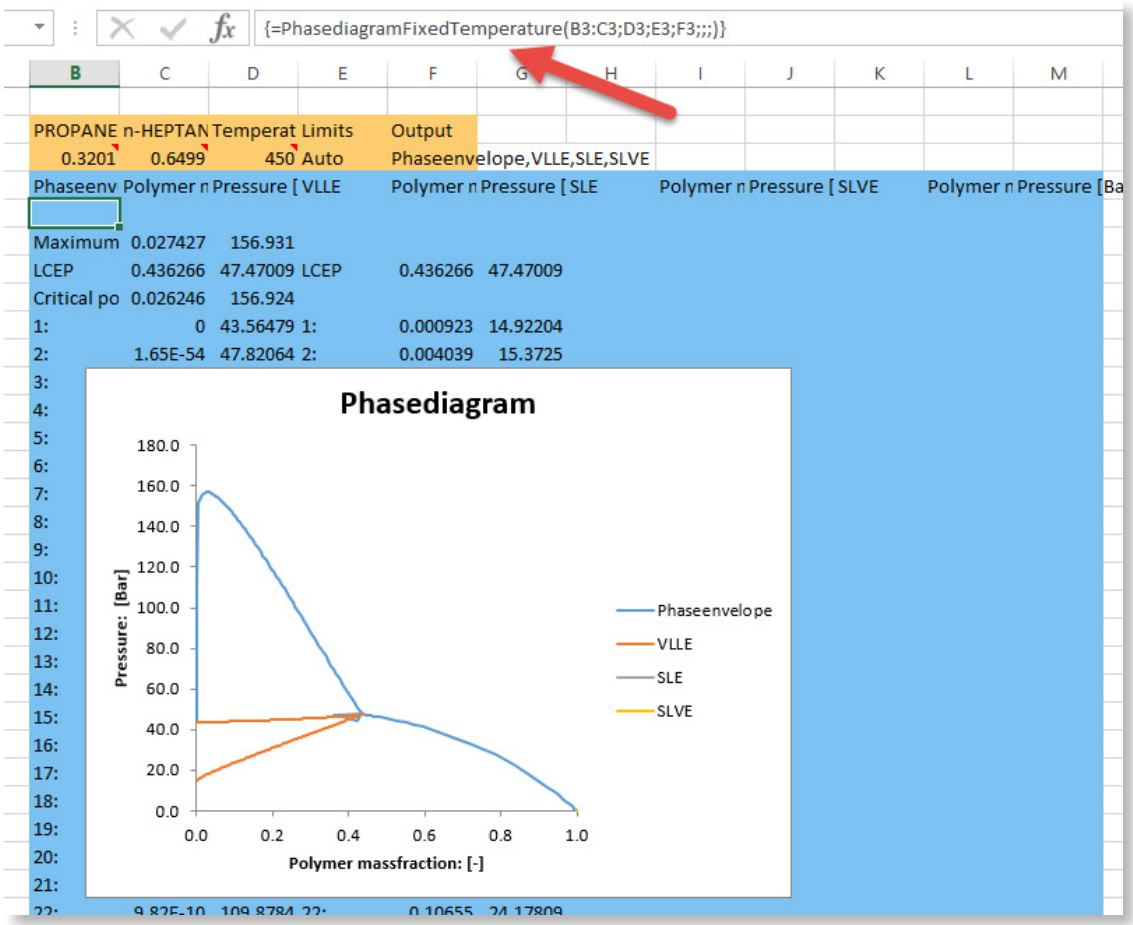
Note how this is one of the three possible way to “slice” the 3D phase diagram.



Phase diagram (continued)

At fixed temperature the pressure and polymer massfraction is traced.

Note how this is one of the three possible way to “slice” the 3D phase diagram.



Speed

The flash has been rewriting in order to improve speed. Depending on the system the flash is now between 15 and 50% faster.
Note that if flash speed is very important for you, the VLXE API is the best option. Using the API will result in a factor 2 speed improvement compared to running the flash from within Excel. Please contact VLXE for more information

Database

New database format supported.
In order to better support coming upgrades to the database in VLXE a new database format is now in use.
The selected on is SQLite. Excising users are encouraged to switch to the new format. There is no automatic migration included since it would be very time consuming to implement. Customers does not have to make the switch but the coming upgrades in version 10 will only be supported on this new format.

DIPPR
The DIPPR 801 file included with the install package has been upgraded to the 2016 version

License

The license software has been upgraded and a new license needed in order to use version 9. The license customers has for version 8 will not work with version 9.

"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.

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