Thermodynamic Software





20,21

How to get started!

A complete guide to the VLXE Software

Version 2. August 2014



www.vlxe.com

Thermodynamic Software

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General information about the VLXE software

VLXE Software

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Written in Denmark, June 2014



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1) Introduction

1.1 What can VLXE Blend Do?

VLXE Blend is a thermodynamic software package that is integrated into Excel. It provides a full range of PVT calculations inside Excel for a wide range of systems. The main focus is polymer and solvent systems, but it is also used for other systems with heavy components such as asphaltene systems. Customers looking to use PC-SAFT including associating and polar terms will similarly be fully covered by VLXE Blend. The VLXE API is not covered by this document.

1.2 How is this Documentation Organized?

A practical approach has been taken and two different set of sections are presented. First section (chapter 2) deals with the basic introduction to the software with simple examples. This includes calculation of cloud point and phase envelope both with binary components as well as more then two components. The chapters that follow each cover a feature of VLXE Blend.

1.3 Where to Start

If you are new user of VLXE Blend, you are advised to work through the entire second chapter. After that, pick and choose from the later chapters that are relevant for your needs.

1.4 Where to Find Additional Help

A help file is installed together with VLXE Blend. You can access it by selecting Support/Help under the VLXE Blend ribbon from inside Excel. The support webpage is also a great source of information: http://www.vlxe.com/support

All VLXE customers are encouraged to contact VLXE for support. Your questions are always welcome!

1.5 How to Proceed

Let's get started with the first section. Chapter 2 will show how to calculate cloud point and phase envelope for a simple mixture containing Methane and n-Hexane. Later examples are given with a mixture containing a few more components: methane, n-Hexane, n-octane and n-nonane. By working through this exercise, you will gain familiarity with the basic features of the package. Also you can get more practice by working on some advanced features of the software by following the examples given in the second section.

Some users may wish to jump right in and skip some (or all) of this tutorial. At any time whenever you are comfortable using the program, feel free to leave the tutorial and begin working on your own simulations.





2) Quick Overview

2

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1													
2		Pressure	[LineType	Output	Compone	Units			Pressu	re [LineType	Output	Compone	Units
3		1	LLE		All	C(In,Mass				1 VLE		All	C(In,Mass
4		A Louis Is a m	V. MACTUA	W METHAT	Temperat	Pressure:	K(Mixture		Numbe	er: X: METH	X: METHA	Temperat	Pressure:
5		Plot	of result	ssfract	[Celsius]	[Bar]	[-]			[Maria		101.1	(n)
6			, , , , , , , , , , , , , , , , , , ,	70911	-10,0655	1,0000	580,4028		1:	o	Functior	n input	0000
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8					Title					0,000154	0,015616	79,1371	1,0000
9				•						0,000283	0,027859	78,0794	1,0000
10		90]								0,000424	0,040586	77,0028	1,0000
11		80								0,000581	0,053828	75,9060	1,0000
12		70 -								0,000759	0,067616	74,7875	1,0000
13		60										6457	1,0000
14		[sn]								Func	tion outp	ut 4791	1,0000
15		S 50 -	_						hblo)	0,001471	0,1126	71,2857	1,0000
16		<u> </u>						TXy(DU	ibble)	0,001742	0,126190	70,2694	1,0000
17		5 30 -	/		\mathbf{i}			Txy(De	ew)	0,002060	0,140280	69,2319	1,0000
18		era	/					Txy(Bu	ibble)	0,002442	0,154915	68,1720	1,0000
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21						<u> </u>				0,004790	0,212654	64,1489	1,0000
22	Pro	ect shee	et used	0,3 0,4	0,5 0,6	0,7 0,8 0	0,9 1,0			0,006259	0,233874	62,7283	1,0000
23		12020.100					-			0,008505	0,256211	61,2653	1,0000
24		-20		METHANOL	Marcfreet	ionl				0,012263	0,279757	59,7615	1,0000
25			/	METHANOL	Lividssiract					0,016445	0,296173	58,7400	1,0000
	•	VLXE	- Project	Sheet1	(+)								
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VLXE Blend integrates into Excel. The picture below highlights its 5 main features.

Ribbon:

Provides easy access to all features in VLXE Blend.

Function:

VLXE Blend performs all calculations using extra Excel functions. They all work just like any other Excel function.

Function input:

Values given as input to the VLXE Blend Excel functions.

Function output:

Calculation results. They may be given in one or more cells.

Project sheet:

Is called before each calculation and holds all model and parameter information.



2.1 VLXE Blend in 10 seconds

- It integrates into Excel.
- It expands the standard functions found in Excel with the addition of thermodynamic functions.
- The VLXE Blend functions are like any other Excel function.
- All constant parameters used in a calculation are stored in the VLXE project sheet.
- Constants are taken from the VLXE Blend database and DIPPR database.
- Project sheets are created using a wizard.
- Calculations can be created by hand or using the wizard.
- All systems and calculations are handled the same way.
- Output is given either as a row or an area.
- The calculation engine can be used with in-house software using the API.

2.1.1 VLXE Blend basic rules

VLXE Blend covers a complete range of PVT calculations for a wide range of systems. But if you remember a few VLXE rules, you will find it very easy to use VLXE Blend, no matter how complex your system.

All calculations are used in the same way no-matter the type of system. Example: a flash calculation for an nhexane/Butane mixture is just as easy as for Ethylene/HDPE, even with 100 pseudo components.

The wizards included will make it easy to create a new calculation. However, since the VLXE Blend Excel functions work just like the built-in ones, you can also skip the wizards and create them yourself.

The VLXE database included can easily be edited using the tool provided. You can find it inside Excel, in the VLXE Ribbon under Support.

VLXE Blend supports the use of 2 databases. Personal and company wide. This allows a company to build an in-house parameter database that is available to all VLXE Blend users, while at the same time each user can have a private version.

2.1.2 Settings

VLXE Blend requires you to set a few settings. They are set to default values when the software is installed. But can be changed at any time.

Three wizards are included to make it easy to work with the settings, these are:

- Quick.
- Standard
- Databases

You find shortcuts to all 3 on the VLXE Blend ribbon, under settings.





The "Quick" menu lets you quickly view and change the license and database settings. It also allows you to export and import settings, if needed.

License Information Select Install Type Server Settings StandAlone Server Name lenovow 520 Port Number OS53 Database Information Location of DIPPR File Cancel C:\Install\Databases\DIPPR\Lite\Dippr801.mdb Select Active Connectionstring Select Database Format Select Active Connectionstring SQL CE O Local SQL Server (Advanced option) Company Wide SQL CE - Connection String Citylsers\Torben Laursen\AppData\Local\VLXE\Databases\SQLCE\VLXE_Standard_SQLCE_v40.sdf Export To XML Import From XML	🛂 VLXE Blend - User Settings			×				
Select Install Type Server Settings OK StandAlone Enovow520 Cancel O Network 5053 Cancel Database Information Cancel Location of DIPPR File C: (Install/Databases \DIPPR \Lite \Dippr801.mdb Select Database Format Select Active Connectionstring Image: SQL CE Image: Company Wide SQL CE - Connection String Company Wide C: (Jusers\Torben Laursen \AppData \Local \ULXE\Databases \SQLCE \VLXE_Standard_SQLCE_v40.sdf Export To XML Import From XML Import From XML	License Information							
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Port Number Cancel 5053 5053 Database Information Location of DIPPR File C: \Install\Databases\DIPPR\Lite\Dippr801.mdb Cencel Select Database Format Select Active Connectionstring Select Database Format Select Active Connectionstring SQL CE Iccal SQL Server (Advanced option) Company Wide SQL CE - Connection String C:\Users\Torben Laursen\AppData\Local\VLXE\Databases\SQLCE\VLXE_Standard_SQLCE_v40.sdf Export To XML Import From XML	StandAlone	lenovow520						
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Location of DIPPR File C: \Install\Databases\DIPPR \Lite\Dippr801.mdb Select Database Format Select Active Connectionstring Select Database Format Select Active Connectionstring Copy to ClipBoard Copy to ClipBoard Export To XML Import From XML	Database Information							
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Select Database Format Select Active Connectionstring Image: Sol_CE Image: Local Image: Sol_CE Image: Local Image: Sol_CE Image: Copy to ClipBoard Sol_CE - Connection String Image: C:\Users\Torben Laursen\AppData\Local\ULXE\Databases\SQLCE\VLXE_Standard_SQLCE_v40.sdf Export To XML Import From XML	C: \Install \Databases \DIPPR \Lite \Dippr80)1.mdb						
SQL CE Local Copy to ClipBoard SQL Server (Advanced option) Company Wide Copy to ClipBoard SQL CE - Connection String C:\Users\Torben Laursen\AppData\Local\VLXE\Databases\SQLCE\VLXE_Standard_SQLCE_v40.sdf Export To XML Import From XML Copy to ClipBoard Copy to ClipBoard	Select Database Format	Select Active Connectionstring						
O SQL Server (Advanced option) Company Wide SQL CE - Connection String C:\Users\Torben Laursen\AppData\Local\VLXE\Databases\SQLCE\VLXE_Standard_SQLCE_v40.sdf Export To XML Import From XML	⊙ SQL CE	Local		Copy to ClipBoard				
SQL CE - Connection String C:\Users\Torben Laursen\AppData\Local\VLXE\Databases\SQLCE\VLXE_Standard_SQLCE_v40.sdf Export To XML Import From XML	O SQL Server (Advanced option)	🔘 Company Wide						
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Export To XML	C: \Users \Torben Laursen \AppData \Loca	VLXE\Databases\SQLCE\VLXE_Standard_	SQLCE_v40.sdf					
Import From XML	E E							
				Import From XML				



2.1.3 Standard settings

2

In VLXE Blend each calculation has its own unit set. This is done using a unit argument for each calculation. However, a user will often work with the same set of units, and VLXE Blend allows the user to define a standard set of units that are used by the wizards each time a new calculation is created.

You set the default unit settings on the VLXE Blend ribbon under "Settings".

Click on the "Standard" icon to open the settings. In the menu you can set the default in- and out-put units.

VLXE Blend - Settings	
Units Charts	
Input	Output
Temperature	Temperature
Celsius	Celsius
Pressure	Pressure
Bar	Bar
Composition	Composition
Massfraction	Massfraction
Enthalpy	Enthalpy
kJ/Kg	kJ/Kg
Entropy	Entropy
kJ/(Kg Kelvin)	kJ/(Kg Kelvin)
Information	
The units that are selected here are used as default setting	ngs for new projects
Cancel	QK



2

2.2 How does the databases work?

In order to run a calculation a project sheet stating the model and parameters must be provided. When creating a new project sheet the parameters are taken from the VLXE database. Once the project sheet is created any change to the database has no effect on the project sheet.

	Α	В	С	D	E	F
1						
2		Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas Cp
3		14	2	0	PC-SAFT	DIPPR
4						
5		Solvent Index	Name	VLXE DB. index	DDBST DB. index	Туре
6			METHANOL	513	110	0
7		2	CYCLOHEXANE	101	50	1
8						
9		Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
10			METHANOL	-6271,171524	1,225022517	2,743286438
11		2	CYCLOHEXANE	-1465,075592	0,513311156	4,438002706
12						
13		Kij (a) [-]	METHANOL	CYCLOHEXANE		
14		METHANOL				
15		CYCLOHEXANE	0,051			
16						
17		Kij (b) [Kelvin^-1]	METHANOL	CYCLOHEXANE		
18		METHANOL				
19		CYCLOHEXANE	0			
20						
21	•	Association, Kappa [-]	METHANOL	CYCLOHEXANE		
22		METHANOL	0,035176			
23		CYCLOHEXANE	0	0		
24						
25	-	ociation, Epsilon [Kelvin]	METHANOL	CYCLOHEXANE		
4	Þ	VLXE - Project Sheet1	(+)			: •
READ	Y 🛅					

2.3 How to get properties from DIPPR using just a few clicks

VLXE Blend makes it very easy to obtain temperature dependent properties from DIPPR. Simply use the DIPPR wizard to make the calculation including a plot created inside Excel.

To open the wizard select "DIPPR" on the VLXE Blend ribbon.

🤧 象 📑 📹 😽 🖤	DIPPR	🕴 📰 🍃	1 1
Input Output Units Names Output Sheet	DIPPR DDBST	Quick Standard Databases	Check Wizard Locking
Utility	External	Settings	License

In the DIPPR wizard that opens up first select componet and then property. The select "OK". Here we will use the liquid density for cycloHexane as example.



2

Once created, the temperature can be changed to obtain a value for the liquid density at the desired value.

VLXE - Select Component From the DIPPR Data	base	
Select Component	Selected Component	
Index Short Name	CYCLOHEXANE	ОК
	Include chart in whard output	
► 137 CYCLOHEXANE C6H12 84.2	Select Property	
	🔘 Solid Density	
	Liguid Density	
	O Vapor Pressure of Solid (Sublimation Pressure)	
	O Vapor Pressure of Liquid	
	O Heat of Vaporization	
	O Heat Capacity of Solid	
	O Heat Capacity of Liquid	
	O Heat Capacity of Ideal Gas	
	O Second Virial Coefficient	
	O Viscosity of Liquid	
	O Viscosity of Vapor	
	 Thermal Conductivity of Solid 	
	O Thermal Conductivity of Liquid	
	 Thermal Conductivity of Vapor 	
	O Surface Tension	Cancel
Starts with([Short Name], 'cyclohEdit Filter		





2.3.1. VLXE Project Sheet

The project sheet holds all model information. It is called before each calculation and can be edited at any time. There is no difference between a project sheet and any other Excel sheet. Note that the sheet can be given any name.

VLXE Blend supports multi-project sheets. A function argument can be used to tell each calculation which project sheet to use.

Do not place any extra information in the project sheet. It may corrupt its reading.

	Α	В	С	D	E	F
1						
2		Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas Cp
3		14	2	0	PC-SAFT	DIPPR
4						
5		Solvent Index	Name	VLXE DB. index	DDBST DB. index	Туре
6		1	METHANOL	513	110	0
7		2	CYCLOHEXANE	101	50	1
8						
9		Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
10		1	METHANOL	-6271,171524	1,225022517	2,743286438
11		2	CYCLOHEXANE	-1465,075592	0,513311156	4,438002706
12						
13		Кіј (а) [-]	METHANOL	CYCLOHEXANE		
14		METHANOL				
15		CYCLOHEXANE	0,051			
16						
17		Kij (b) [Kelvin^-1]	METHANOL	CYCLOHEXANE		
18		METHANOL				
19		CYCLOHEXANE	0			
20						
21		Association, Kappa [-]	METHANOL	CYCLOHEXANE		
22		METHANOL	0,035176	0		
23		CYCLOHEXANE	0	0		
24		N				
25		ociation, Epsilon (Kelvin)	METHANOL	CYCLOHEXANE		
-	-	VLXE - Project Sheet1	÷			: •
READY	1					

2.3.2 How do the calculations work?

VLXE Blend performs a calculation using extra Excel functions. These functions work just like any other function in Excel.

Each calculation needs 2 sets of input:

- System information: Model, parameters etc.
- User information: Temperature, pressure, feed etc.

When a calculation is run, the project sheet is read. Then the arguments to the function are read and the calculation is performed.



| Page 12 |

2.4 New from database

2

This opens a wizard that helps the user define a new project sheet.

The parameters are taken from the database and can be edited at any time. Subsequent changes to the database have no effect on the project sheet. A project sheet can be created by hand, but it is far easier to use the wizard.

¥∎ FIL	В 5° Е Но И		P	PAGE		for JP	MULAS	DATA	REVI	EW	► }	VLXE Blend	Book1 - E
New Pro	Edit Edit System Stand Solve Solve Polym coPol	BubbleT Blend data lard nt / Polyme nt / coPolyme wer blend ymer blend	BubbleP Ibases - S r mer	Flash (TP) elect a N	Flash Pi (PH)	roperties (TP) m	PhaseEn	Equation Control Equati	Unit perations of State /Redlich/Kw Robinson ez/Lacombe ed Sanchez FT	Oil And Gas + yong /Lacombe	Fitting *	Calculations	Distributions
11 12 13 14 15 16 17	Databas Local	e Connecti	on	Databa SQLServ	se Format er	a VLXE	me of Nev E - Project	Polyna DIPPR	heet			Cance	

2.5 Standard Wizards

Thermodynamic calculations may require a large range of input and output values, to aid the user a number of wizards are provided. A full wizard covering all calculations can be opened plus the most commonly used calculations are placed directly on the VLXE Blend Ribbon (select the components to include) and output properties.

FIL	E H	DME I	NSERT	PAGE	LAYOUT	f for	MULAS	DATA	REVI	EW N	/IEW	VLXE Blend	DEVELOPE	R
1	í +		P	TP	PH	₽				6	\$₽	-		c
New	/ Edit	BubbleT	BubbleP	Flash	Flash	Properties	PhaseEnvelo	ope	Unit	Oil And	Fitting	Calculations	Distributions	Code
				(TP)	(PH)	(TP)		Ope	erations *	Gas 🔻	-			Generat
Proj	ect Sheet					💧 Calcul	ations						Wizards	
												/		
B2		- -	X	/ 3	s T									
· .														
	Α	В	C		D	E	F	0	G	Н		J	K	L
1														
2														
-			-											
5														



| Page 13 |

2.6 Common function arguments

A few arguments are used in all the VLXE Blend functions. They provide you with full flexibility.

They are:

Output - Lets you select the desired output from a calculation.

Components - You can select all or part of the components in the project sheet.

Units - Defines the units used in this calculation.

Distribution - Lets you override the polymer distribution given in the project sheet.

BlockMass fraction - Used for coPolymer only. Lets you override the blockmass fraction given in the project sheet. **AdvVLXE** - used internally by VLXE.

AdvUser - Provided for the users' convience. Can be used, for example, to trigger the function to recalculate, if the content of the referenced cell is changed.

2.7 Input and Output Color Scheme

In order to keep the Excel sheet organized, VLXE Blend uses a color scheme. Orange color represents input to the calculation and blue color represents output.

If a calculation is created using the wizard, the colorscheme is applied automatically. If you create a calculation by hand or change a existing one, the colors can be set using the buttons provided in the VLXE Blend ribbon.

	Association - N	/lethanol + C	CycloHexane	e.xlsx - Excel						
EW	VLXE Blend ┥	Control II	IN .							
\$₽	-		c	-& &	•			DIPPR	2 🕴	
Fitting *	Calculations E	Distributions	Code Generate	Input Outp	out Units	Names Out	put Sheet	DIPPR DD	BST Quid	k Standar
		Wizards			Uti	lity		External		Settir
I	J	К		М	N	0	Р	Q	R	S
	METHANC	CYCLOHEX	emperat	t Pressure [F ashType	Output	Compone	Units		
	0,5	0,5	25	i 10	2	Fixed 2D	All	C(In,Mass		
	Property	System	Feed	Phase 1	Plase 2					
	Pressure [10		Time: 4404						
	Temperat	25								
	Compone									
	METHANC	0,5	0,5	0,60366	0,047607	·				
	CYCLOHEX	0,5	0,5	0,39634	0,952393					
	Phase Fra	1		0,88923	0,11077	·				



3) Basic Features

3

3.1 How to Create a New Project

1. Open Excel, select "New" on the VLXE Blend ribbon.

2. In the window that opens select "System" on the left side and "Model" on the right side. In the lower right side you can change the name of the project sheet, if so desired. Note also how database information is given on the lower left side

🚺 🗄 ५- २	* 🗟 *	🙀 ÷						Book1 - I
FILE HOME	IN JERT	PAGE LAYOUT	FORMULAS	DATA	REVIEW	V	VLXE Blend	DEVELOPE
New Edit Bub	bleT BubbleP	ilash Flash (TP) (PH)	Properties PhaseEnv (TP)	relope U Opera	کی ک	And Fitting	Calculations	Distributions
Project Sheet			Calculations					Wizards
VLXE Blend datab	oases - Select a l	New System						
System				Equation	of State			
💿 Standard 🔫				O Soave	/Redlich/Kwor	ng		
O Solvent / Polymer	•			O Peng/F	Robinson		7	-
O Solvent / coPolymo	er			O Sanche	ez/Lacombe ed Sanchez/La	acombe		-
O Polymer blend			\rightarrow	PC-SAI	FT ,			
C coPolymer blend				O CPA				-
				Ideal Gas	s Cp Expressio	on (Standard)		
				Polyno DTDDD	omial			H
Database Connection	n Datab	ase Format	Name of New Proje	ct Sheet			Ca	incel
Local	SQLSer	ver	VLXE - Project					
C		-		1				

3. Click "Next" and add solvents from the data bank to define the system.

I		VLXE E	llend databases - S	elect a	New System						
	St	tandard	s				Syste	m		7	
	(-			Class		Solve	ent(s)			
		Add		emove	Clear			Status	DB Index	Name	
		VL	Short Name	Ŷ	Formula	님	▶ 1	New	1	METHANE	Back
	8			n-he		=	2	New	9	n-HEXANE	
	٠	9	n-ł	HEXANE	C6H14						
		14	n-HEPTANE C7H16								
		61	n-HEXAD	C16H34							
		62	n-HEPTAD	ECANE	C17H36						
		67	n-HENEIC	OSANE	C21H44						
	72 n-HEXACOSANE C26H54										
ſ	Database Connection Database Format							f New Project Shee	t		Cancel
	Local SQLServer							oject			



| Page 15 |

4. Click "OK". A new project sheet is now created.

Note how the model and parameters are included in the sheet. The sheet can be changed at any time, if needed.

	A	В	С	D	E	F	
1							
2		Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas Cp	Poly
3		14	2	0	PC-SAFT	DIPPR	Poly
4							
5		Solvent Index	Name	VLXE DB. index	DDBST DB. index	Туре	Tc [K
6			METHANE		1051		
7		2	n-HEXANE	9	89	1	
8							
9		Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)	Ideal
10			METHANE	-4645,172872	2,075616832	4,982589952	
11		2	n-HEXANE	-2305,2993	1,2115	4,0882	
12							
13		Kij (a) [-]	METHANE	n-HEXANE			
14		METHANE					
15		n-HEXANE	0				
16							
17		Kij (b) [Kelvin^-1]	METHANE	n-HEXANE			
18		METHANE					
19		n-HEXANE	0				
20							
21		Association, Kappa [-]	METHANE	n-HEXANE			
22		METHANE					
23		n-HEXANE	0	0			
24		N					
25		Ass. iation, Epsilon [Kelvin]	METHANE	n-HEXANE			
	€	VLXE - Project Sheet1	+			E 4	



3.2 Edit the Default Settings

The default settings in VLXE Blend include unit settings. Each calculation has its own set of units, but the settings here are used as default values when creating a new calculation.

To change the default settings follow these steps:

1. On the VLXE Blend ribbon, select "Standard Settings" click "Settings" to open the standard settings menu. Click on "Units", here you see the default settings for all the units.

eet	DIPPR DIPPR DDBST	Ouick Standard Databases	Check Wizard Locking	Help WebSupport
	External	Settings	License	Data
	VLXE Blend - Set	tinas		
	nits Charts			
ſ				
	Input		Output	
	Temperature		Temperature	
	Celsius		Celsius	
	Pressure		Pressure	
	Bar		Bar	
	Composition		Composition	
	Massfraction	\checkmark	Massfraction	
	Enthalpy		Enthalpy	
	kJ/Kg	\checkmark	kJ/Kg	
	Entropy		Entropy	
	kJ/(Kg Kelvin)	$\overline{\mathbf{v}}$	kJ/(Kg Kelvin)	
I	nformation			
Tł	ne units that are sel	ected here are used as default s	ettings for new projects	
			•	
	Canco			OK

3.3 Creating a new calculation: Cloud point example

All calculations in VLXE Blend are created using the same steps as in the wizard provided. The steps below will create a cloud point calculation using the project sheet just made.

1: Select "Calculations" under "Wizards" in the "VLXE Blend" menu.

2: Leave the component part unchanged and select "Next".

3: Select "Cloud Point" on the right side and select "Next".

4: Select "Cloud P" as type and leave the other input unchanged. Note that this can easly be changed once the wizard ihas finished.

5: Click on "Units" to check that they are as required. Now click "Next".



VLXE Blend - Calculation Wizard		
Select Calculation		
🔘 Bubble Kij		Next
Cloud Point		
O Critical Point		
C Excess Enthalpy		Back
O Fitting		
◯ Flash		
O Phase Envelope		
O Properties		
🔘 Spinodal		
О Тху/Рху		
O Surface Tension		Wizard Stop
○ Viscosity		Off
O Unit Operation: Mixer		
O Unit Operation: LinkedPHFlash		<u>C</u> ancel
Project sheet: VLXE - Project	1	

6. By clicking "Next" there are two ways of calculating a cloud point: Cloud temperature and cloud pressure.

Select: Bubble T.

3

Note that in VLXE Blend a cloud and bubble point is the same.

/LXE Blend - Calculation Wizard		
Feed, In	Input	
Name Feed [Massfraction]	Pressure [Bar] 10.00	ble T
▶ 1 METHANE 0.500000	-Select Point Type	ble P
2 n-HEXANE 0.500000	VLE Dev	v T Back
	OLLE	V P
	-	Change <u>U</u> nits
		Wizard Stop
		Off
		Cancel
Project sheet: VLXE - Project		



3

7. Units can be changed by clicking on "Change Units". For this example, change the composition into mole fraction for input stream and then click "OK".

	1											
		VLXE Bler	nd - Calculat	ion Wizard								
		Feed, I	'n			Input						
			Name	Fe	ed	Pressure	[Bar]			Bubble	т	Next
/LXE E	Blend - Select	Units		-	-	100					K	
						1 manual free						
										ОК		Back
	Input				OL	utput						
	Temperatu	re			Te	emperature			C	ancel		
	Celsius		Ľ	~	Cel	sius						Ν.
	Pressure				Pr	essure						
	Bar			~	Bar			\checkmark				
	Compositio	n		-	C	omposition						Change Units
	Massfraction	1	[-	Ma	ssfraction						Wizard Stop
	To the law					alle e le co						Of
	Enthalpy		G	5	Er k10	ithaipy					1	
	Ko/Ng					vg						<u>C</u> ancel
	Entropy				Er	ntropy						
	kJ/(Kg Kelvin	1)	[~	kJ/	(Kg Kelvin)		\checkmark				
	Viscosity				Vi	scosity					-	
	centiPoise			$\overline{}$	cen	tiPoise		$\overline{}$				
	Surface Te	nsion			SL	urface Tension						
	N/m		•	-	N/n	1						
	-				Ľ							

8. At this step there are two options i.e. either output type is selected as a function row - single row output, or you can request the function range - range output. First the results for function row - single row output will be shown.

VLXE Blend - Calculation Wizard	
Select Output Type	Next
Function row (Single row output)	
O Function range (Range output)	Back
	Wizard Stop
Information	Off
Function row: The results are given in just one row. You define the output your self Function range: The output is given in a range of the sheet. The output is fixed by the program.	Cancel
Project sheet: VLXE - Project	



9. Click "Next" and following calculation wizard will appear.

VLXE Blend - Calculation Wizard			
Intensive Temperature Pressure Number of Phases System	General General Number of Results	Phase 1 Phase 2	ОК
Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mass Based) Density Volume Enthalpy Entropy Cp Average Molar Mass	Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction Mass Based Density Volume Enthalpy Entropy Cp Speed of Sound	Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mass Based) Density Volume Enthalpy Entropy Cp Spand of Sound	Back
Surface Tension	Average Molar Mass	Average Molar Mass	Wizard Stop
System: Sum of the phases First phase: Heaviest phase Last phase: Lightest phase		^ >	Cancel
Project sheet: VLXE - Project			

10. Click "OK" and the corresponding results are shown in the form of single row output.

сı				Carcula	cions					TTLarus	1		
▼ : X ✓ f _x {=BubbleT(B3:C3; D3; E3; F3; G3; H3)}													
	В	C	D	E	F	G	Н	I		K	L	М	
	METHANE	n-HEXANE 0.5	Pressure [10	Output T.D(1).H(1	Compone All	Units C(In.Mass	PointType VLE	Temperat	Density (1 0.515407	Enthalpy (-4183.99	METHANE	n-HEXANE	(2)



11. To see the result from function range - range output, go to step 8 and click on "Function range (Range output)".

VLXE Blend - Calculation Wizard	
Select Output Type Select Extra Output: Bonding fraction	ОК
	Back
Jeferra Vien	Wizard Stop
Function row: The results are given in just one row. You define the output your self Function range: The output is given in a range of the sheet. The output is fixed by the program.	Cancel
Project sheet: VLXE - Project	

12. Click on "OK" and the result will be displayed in the Excel sheet.

	* :	× v	<i>f</i> _x {=[BubbleT(B	3:C3; D3; E3	3; F3; G3; H	3)}		
4	В	С	D	E		G	н	Ι	
	METHANE	n-HEXANE	Pressure [Output	Compone	Units	►uintType		
	0,5	0,5	10	Fixed 2D	All	C(In,Mass	VLE		
	Property	System	Feed	Phase 1	Phase 2				
	Pressure [10		Time: 95 [
	Temperat	-122,15							
			\leftarrow						
	Compone								
	METHANE	0,5	0,5	0,5	1				
	n-HEXANE	0,5	0,5	0,5	1,16E-07				
	Phase Frag			1	0				
	Phase Fra			1	0				
	Compress	0,041802	0,041802	0,041802	0,83697				
	Density [g	0,515407	0,515407	0,515407	0,015267				
	Molar Vol	52,48157	52,48157	52,48157	1050,806				



3.4 How to Perform Phase Envelope Calculations

The steps below will create a phase envelope calculation. We will use the wizard so all the work in setting up the sheet is done automatically.

1. Click on the next Excel sheet and click on the cell where the calculations should start. Open the calculation wizard and click "Next".

										Methan	e + nHe	xane.:
YOUT	FORMULAS D	ATA REV.	IEW 🎽		VLXE Blend	DEVELOPE	R					
PH	∛ P		6	\$₽	-		c≡	-\$				ŀ
lash i	Properties PhaseEnvelop	e Unit	Oil And	Fitting	Calculations	Distributions	Code	Input	Output	Units	Names	Outp
PH)	(TP)	Operations	∗ Gas ×	-			Generate					
	Calculations					Wizards				Ut	ility	
	_											

2. By clicking on "Calculations" the selected components appears. For this case both methane and n-hexane can be seen.

VLXE Blend - Calculation Wizard	
Select the Components to Include:	
METHANE	Next
✓ n+HEXANE	
	Project Sheet
	Winned Stee
	wizard stop
	0
	Cancel
Project sheet: VLXE - Project	
)



3. Click "Next" and select the property (i.e. Phase envelope)

VLXE Blend - Calculation Wizard							
Select Calculation							
🔘 Bubble Kij		Next					
Cloud Point							
O Critical Point							
O Excess Enthalpy		Back					
◯ Fitting							
◯ Flash							
Phase Envelope	•						
O Properties							
🔘 Spinodal							
◯ Txy/Pxy							
O Surface Tension							
O Viscosity		Wizard Stop					
O Unit Operation: Mixer		01					
O Unit Operation: LinkedPHFlash		Cancel					
Project sheet: VLXE - Project							

4. By clicking "Next", the calculation wizard appears and displays some more functions like: Auto Phase Diagram, User Phase Diagram etc. For this example select "Auto Phase Diagram".

()	LXE BI	XE Blend - Calculation Wizard										
	Feed	, In		Input								
		Name	Feed [Massfraction]	No Input Needed Beside Feed	Auto Phase Diagram	Next						
	▶1	METHANE	0.500000	7	User Phase Diagram							
	2	n-HEXANE	0.500000		Trace Property	Back						
					Trace Phase Boundary							
					Trace Feed							
				-								
						Change <u>U</u> nits						
					Į	Wizard Stop						
						Off						
						Cancel						
	Project sheet: VI XE - Project											
L			5									



6. Click "Next" and define the output.

Intensive General Image: Temperature Number of Results Pressure Number of Results Number of Phases Composition System Feed Composition Bonding Fraction Bonding Fraction Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mole Based) Phase Fraction (Mass Based) Phase Fraction (Mole Based) Density Phase Fraction (Mass Based) Density Volume Enthalpy Enthalpy Enthalpy Enthalpy Enthalpy Enthopy Cp Cp Average Molar Mass Speed of Sound Average Molar Mass Viscosity Viscosity Viscosity Viscosity Viscosity Miscosity Viscosity	VLXE Blend - Calculation Wizard									
Last phase: Lightest phase Cancel	VLXE Blend - Calculation Wizard Intensive Temperature Pressure Number of Phases System Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mole Based) Density Volume Enthalpy Entropy Cp Average Molar Mass Surface Tension Information System: Sum of the phases	General Number of Results Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mass Based) Density Volume Enthalpy Entropy Cp Speed of Sound Average Molar Mass Viscosity	Phase 1 Phase 2 Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mass Based) Density Volume Enthalpy Entropy Cp Speed of Sound Average Molar Mass Viscosity	OK Back Wizard Stop Off						
Project sheet: VLXE - Project										

7. Click "OK" and the desired results are shown in the Excel sheet. Note: The wizard also creates a chart.





3.5 How to Change the Units Used in the Calculations

There are two ways of changing the units: 1. Manually 2. Calculation wizards

3.5.1 Manually

3

Once an output is obtained, for example, a cloud point. The units can be changed by following these steps. (As an example, temperature units are to be changed from Celsius to Kelvin).

1. Click on the units cell, input and output units are given in Celsius. To change from Celsius to Kelvin, simply type Kelvin in place of Celsius.

Note: It is case sensitive, so the first letter should be a capital and with no spelling mistakes.

• : $\times \checkmark f_x$	C(In,N	lassfractio	n);C(Out,N	lassfractio	n);T(In,Cel	sius);T(Out,Celsius);P
В	С	D	Е	F	G	
METHANE [Massfraction	n-HEXANE	Pressure [Output	Compone	Units	PointType
0,5	0,5	10	Fixed 2D	All	C(In,Mass	VLE
Property	System	Feed	Phase 1	Phase 2		
Pressure [Bar]	10		Time: 367		N	
Temperature [Celsius]	-122,15					
Components						
METHANE [Massfraction	0,5	0.5	0,5	1		
n-HEXANE [Massfractio	0,5	0,5	0,5	1,16E-07		
Dhasa Custian (Mala)						
Phase Fraction [Wole]			1	0		
Phase Fraction [Weight	0.041900	0.041903	1	0 83607		
Compressionity [-]	0,041802	0,041802	0,041802	0,015267		
Molar Volumo [cm/2/m	0,515407	52 40157	53 /0157	1050 206		
Enthalov [k]/Kg]	/102.00	/102.00	/102.00	1030,800		
Entropy [k]/(Kg Kelvin)	-4105,55	-4105,55	-4105,55	-4352,5		
Cn [k]/(Kelvin kg)]	2 598896	2 598896	2 598896	2 570219		
Cy [k]/(Kelvin kg)]	1.805184	1.805184	1.805184	1.626109		
JTCoeffient [Kelvin/Bar	2,000201	-0.04769	-0.04769	1.61779		
Velocity of Sound [m/s		1150,012	1150,012	290,3664		
MolecularWeight [g/mo	27,04939	27,04939	27,04939	16,04246		
ThermalConductivity [V		0,139579	0,139579	0,01602		
Viscosity [centiPoise]		N/A	N/A	N/A		
Surface Tension [N/m]	N/A					

The above figure shows temperature in Celsius whereas the figure shown below shows that temperature changed into Kelvin.



3

$\overline{}$: $\times \checkmark f_x$	C(In,N	lassfractio	n);C(Out,N	lassfractio	n);T(In,Kel	lvin);T(Out,	Kelvin);P(Ir
В	С	D	Е	F	G	H	I
METHANE [Massfraction	n-HEXANE	Pressure [Output	Compone	Units	PointType	
0,5	0,5	10	Fixed 2D	All	C(In,Mass	VLE	
Property	System	Feed	Phase 1	Phase 2			
Pressure [Bar]	10		Time: 23 [$-\mathbf{N}$		
Temperature [Kelvin]	150,9997						
Components						· ·	
METHANE [Massfraction	2.5	0,5	0,5	1			
n-HEXANE [Massfractio	0,5	0,5	0,5	1,16E-07			
Phase Fraction [Mole]			1	0			
Phase Fraction [Weight			1	0			
Compressibility [-]	0,041802	0,041802	0,041802	0,83697			
Density [g/cm^3]	0,515407	0,515407	0,515407	0,015267			
Molar Volume [cm^3/m	52,48157	52,48157	52,48157	1050,806			
Enthalpy [kJ/Kg]	-4183,99	-4183,99	-4183,99	-4992,3			
Entropy [kJ/(Kg Kelvin)	-3,91488	-3,91488	-3,91488	-2,77755			
Cp [kJ/(Kelvin kg)]	2,598896	2,598896	2,598896	2,570219			

Warning: Input units labels are not updated.

3.5.2 Calculation Wizard

Units can also be changed using the Units wizard. This is a simpler process since spelling and format will allways be correct.

It involves the following steps:

Select the cell with a unit that needs to be changed. Click on "Units" under "Utility". In the wizard window change temperature to "Kelvin" and click "OK". The units are now changed.

EVIE	W VIEW	VLXE	VLXE Ble	nd						
	<u>k</u>	° -		•	<u></u>	} 🐎		à 👫		DIPPR 之
ns •	Oil And Fitti Gas ▼	ng Calcul	ations Distri	butions C Ger	ode Inp nerate	out Output	Units St	nes Output	Sheet	DIPPR DDBST
	Wizards Utility External									
tion	n);T(In,Cels	ius);T(Out	,Celsius);P	(In,Bar);P(Out,Bar);H	l(In,kJ/Kg)	;H(Out,kJ/I	Kg);S(In,kJ,	/(Kg Kel	vin));S(Out,kJ/(K
	G	н	Ι	J	К	L	М	N	0	Р
				Droccuro	Output	Compone	Unite	DointTun	_	
		0,5	0,5	Pressure 10	Fixed 2D	All	C(In,Mass	s v		
r		Property	System	Feed	Phase 1	Phase 2				
	VLXE Blend -	Set Units			-					
	Temperatur	e Pressure	e Compositi	on 🛛 Enthalp	y │ Entropy	Viscosity	Surface Ter	nsion		
	-			-						
	Temperature T			Temp (ar	e Out		Converter			
	Kelvin			Kelvin		1	In [Kelvin]			
	Cels	ius		O Celsius		[100			



EW VIEW VLJ Oil And Fitting Gas * *	XE VLXE Blend	ons Code Generate	t Output Units Utility	es Output	DIPP Sheet DIPP	R DDBST		
on);T(In,Celsius);T((Out,Celsius);P(In, I	Bar);P(Out,Bar);H(J K	In,kJ/Kg);H(Out,kJ/	′Kg);S(In,kJ/	(Kg Kelvin)); O	S(Out,kJ/(P		
METHA Proper	ANE n-HEXANE Pre 0,5 0,5 rty System Fea	essure [Output 10 Fixed 2D ed Phase 1	Compone Units All C(In,Mas Phase 2	PointType s				
VLXE Blend - Set Units Temperature Pressure Composition Enthalpy Entropy Viscosity Surface Tension Temperature Temperature Out Converter								
 Kelvin Celsius 		Kelvin) Celsius	In [Kelvin]					
 Fahrenheit Rankine 	0	Fahrenheit Rankine	Out [Kelvin]					
Cancel	ity N/	Δ Ν/Δ	N/A		ок			

3.6 Change component list in a project sheet

The component list in a existing project sheet can be changed. This is often done by taking a copy of an existing sheet, renaming it and then adding or removing components using the VLXE Blend database. It is possible to perform this editing by hand, but it is far better to use the wizard.

As an example, we will take the project sheet from before and add two more components from the database. In the Excel file with Methane + n-Hexane, make a copy of the project sheet and rename it to "Project Sheet (v2)".

Then, select the sheet and click on "Edit". In the new window select "n-Octane" and "n-Nonane" and add them to the solvent list. Note how they have "New" under "Status".



VLXE | Thermodynamic Solutions | Chapter 3

X∎		5-	ै 🗚 🐺 🐺 =	Methane + nHex	ane.xls	- Excel			? 🖻 – 🗖	×
FIL	.E	HOME	INSERT PAGE LAYOUT FORM	ULAS DATA	REVIE	W VIEW	VLXE VLXE	Blend	Torben Laursen 👻	
4		4	T) (P) 🗰 🗰 🐺		3	A				
Nev	v	Edit 🛌 Bu	bbleT BubbleP Flash Flash Properties F	PhaseEnvelope Un	it	Oil And Fitting	Wizards Utility	External Settings	License Support	
			(TP) (PH) (TP)	Operat	ions *	Gas • •	* *	* *	* ÷	
Proj	ect S	Sheet 💌	Calcula	itions						
A1	¥	VLXE Blen	d databases - Select a New System						_ 0 <mark>_ X</mark>	ηĽ
4	5	Standards			Syste	m				1.8
2	ſ				Solve	ent(s)				
3		Add	Insert Remove Clear			Status	DB Index	Name		
4		VLXE I	Short Name	Formula	▶1	Old	1	METHANE		
5	8	1	n-no		2	Old	9	n-HEXANE		
7		41	n-NONANE	C9H20	3	New	23	n-OCTANE		
8		64	n-NONADECANE	C19H40	4	New	41	n-NONANE		
9	⊩	75	n-NONACOSANE	C29H60						
10	⊩	313	n-NONYLBENZENE	C15H24		· · \				2
11	⊩	635		C9H1802						
12	⊩	730		C10H20O2						
13	⊩	1049		C11H22O2						
14	⊩	1049		C19H38O2						
15	⊩	1318		C28H46O4						
17		1406	n-NONYLAMINE	C9H21N						
18										
19										
20										
21										
22	L									
23										
24		🛛 🔽 Starts	; with([Short Name], 'n-no') ∨	Edit Filter						
26		Database Co	nnection Database Format Nam	e of New Project Sheet					Cancel	
27	Lo	cal	SQLServer VLXE	- Project (v2)						
28		0				_				2
29		SU	Tace tension Lij (a) [-] METHANE	n-HEXAI	NE					
31		n-t	EXANE	0						
32										
33		No	fluid present							
3/										
4		•	VLXE - Project (v2) VLXE - Project	Sheet1 Sheet	B	(+) i I			_	
READ	DΥ							<u> </u>	+ 10	0 %

Click on "OK" to accept the changes and then "Yes" to overwrite the existing project sheet.





The existing project sheet is now overwritten by the new Mixture which now includes the 2 new components.

x 🛛 🖬 🕤	- 🔿 🐐 🐺 -	Metha	ne + nHexane.xlsx - Excel	?	承 − ■ ×
FILE HO	DME INSERT PAGE LAY	OUT FORMULAS	DATA REVIEW VIEW	VLXE VLXE Blend To	orben Laursen 👻 🔍
New Edit	BubbleT BubbleP Flash Fla (TP) (P	sh Properties PhaseEnvelo	pe Unit Oil And Fitting Operations Gas •	g Wizards Utility External Settings L	icense Support
Project Sheet		Calculations			~
A1	\bullet : \times \checkmark f_x				~
A	В	с	D	E	F 🔺
1					
2	Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal
4		14 4		PC-SAFT	DIPPN
5	Solvent Index	Name	VLXE DB. index	DDBST DB. index	Туре
6		1 METHANE	1	1051	
7		2 n-HEXANE	9	89	
8		3 n-OCTANE	23	128	
9		4 n-NONANE	41	398	
10	Columnt Index	Name	liest of formation [k]/ka]	Ideal are Cov C(4) [k1//kg Kabuip)]	Ideal res Cru Cl
12	Solvent index	1 METHANE	-4645 172872	2 075616822	1 982
13		2 n-HEXANE	-2305.2993	1.2115	4,502
14		3 n-OCTANE	-1827,477061	1,186568818	3,879
15		4 n-NONANE	-1783,476836	1,183188817	3,832
16					•
•	VLXE - Project (v2)	/LXE - Project Sheet1	Sheet3 🕂 : 🖪		•
READY				▦ ▣ ▣ -	+ 100 <u>%</u>

3.7 Working with multi-project sheets

VLXE Blend supports any number of project sheets. This is done using the "ProjectSheet" argument. This is a optional argument, so if left blank, it will use the project sheet with the default name: "VLXE - Project". Otherwise it will use the provided project sheet.

As a example we will use the file just created, it holds 2 project sheets, and create a new flash calculation.

Open the Excel file and go to a blank sheet.

3.7.1 Using the calculation wizard

Open the Excel file and go to a blank sheet. Select "Calculations" on the VLXE Ribbon. VLXE Blend will remember the last project sheet used and use that as default. So now select "Project Sheet" on the right side to change it.



3



Note the selection on the bottom and the component list. Then click "OK" in the selection window.

VLXE Blend - Calculation Wizard	
Select the Components to Include:	
METHANE	Next
	Project Sheet
	Wizard Stop
	Off
	Cancel
Project sheet: VLXE - Project (v2)	

Note how the selected project sheet name has changed and the component list has changed with it.



3

	▼ ± ⊃	X 🗸	<i>f</i> _x {=FI	ash_TP(B3:	E3; F3; G3;	H3; I3; J3;	K3;;;L3)}	~				
А	В	С	D	E	F	G	Н	I	J	К	L	1
	METHANE	n-HEXANE	n-OCTANE	n-NONAN	Temperat	Pressure [FlashType	Output	Compone	Units	Project sh	eet
	0,25	0,25	0,25	0,25	10	1	2	Fixed 2D	All	C(In,Mass	VLXE - Pro	ject (
	Property	System	Feed	Phase 1	Phase 2							
	Pressure [1		Time: 80 [
	Temperat	10										
	Compone											
	METHANE	0,25	0,25	0,000898	0,811312							
	n-HEXANE	0,25	0,25	0,286352	0,168086							
	n-OCTANE	0,25	0,25	0,353828	0,016041				·			
	n-NONAN	0,25	0,25	0,358922	0,004561							
	Phase Fra			0,283966	0,716034							

Now complete the wizard to generate the flash result. Once done, note how the "ProjectSheet" is now in use.

3.7.2 Using the Shortcut on the VLXE Blend ribbon: "Phase envelope"

If you are creating a new flash calculation using the shortcut provided on the VLXE Blend ribbon, press the "Shift" key before clicking on the "Flash" icon. This will allow you to select the project sheet. If you do not press "Shift", the default project sheet is used. In other words, the wizard will not include the "ProjectSheet" in the calculation setup.

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW VLXE VLXE New Edit Image: Constraint of the second seco	🚺 🖯 🏷 🗟 🙀	₽ 100 +
New Edit New Edit BubbleT BubbleP Flash Properties (TP) (PH)	FILE HOME INSERT	PAGE LAYOUT FORMULAS DATA REVIEW VIEW VLXE VLXE
New Edit BubbleT BubbleT Project Sheet Calculations B2 I A B I <		🖄 🖄 🚰 📑 🎯 🚮 🤽 🕂
Project Sheet Calculations W B2 I VLXE Blend - Select Project Sheet J I I I I I I I	New Edit BubbleT Bubble	P Flash Flash Properties PhaseEnvelope Unit Oil And Fitting Calculations Dis (TP) (PH) (TP) Operations * Gas * *
B2 X VLXE Blend - Select Project Sheet A B List of Project Sheets J 1 OK I 2 I OK I 3 OK I I 4 I I I I 5 I I I I 6 I I I I 7 I I I I 8 I I I I I 9 I I I I I 10 I I I I I	Project Sheet	Calculations W
B2 X VLXE Blend - Select Project Sheet 1 Ist of Project Sheets OK 2 Ist of Project Sheets OK 3 Ist of Project (v2) Cancel 6 Ist of Project (v2) Ist of Project (v2) 8 Ist of Project (v2) Ist of Project (v2) 0 VLXE - Project (v2) Ist of Project Ist of Project (v2) 0 VLXE - Project (v2) Ist of Project Ist of		
A B List of Project Sheets OK 1	B2	🛂 VLXE Blend - Select Project Sheet
1 OK 2 OK 3 OK 4 OK 5 OK 6 OK 7 OK 8 OK 9 OK 10 OK	AB	List of Project Sheets
2	1	OK
3 3 3 4 5 5 6 7 7 8 7 9 6 0 VLXE - Project (v2)	2	
4 Control (1) 5 6 7 7 8 7 9 0 10 0	3	VLXE - Project (v2)
3 3 6 7 7 7 8 7 9 0 10 0	4	Cancel
7 7 8 7 9 0 10 0	6	
8 9 0 VLXE - Project	7	
9 VLXE - Project	8	
10	9	VLXE - Project
	10	
11	11	
	12	
13	14	



R

3.8 Select Components Included in a Calculation

A calculation can pick the components to be included from the project sheet. This is done using the "Components" argument. The argument is always included and is set by default to "All". It can be changed by hand or using the built-in wizard once the calculation is created or on the first page of the calculation wizard. To illustrate, we will use the 4 component project sheet just created.

3.8.1 Change in calculation wizard

Go to a blank sheet and open the calculation wizard. In the window remove the checkmark from "n-Octane".

VLXE Blend - Calculation Wizard	
Select the Components to Include:	
METHANE	Next
✓ n+HEXANE	
I → n-NONANE	
•	
	Project Sheet
	Wizard Stop
	Off
	Cancel
	Cancel
Project sheet: VLXE - Project (v2)	<u> </u>
)

Finish the wizard to set up a flash calculation. In the output note the project that has been used, the components argument and the components included in the flash calculation.

Of the 4 components in the project, only the 3 selected are now used.

• : D	x 🗸	<i>f</i> ∞ ME	THANE,n-F	IEXANE,n-	NONANE ┥	-				
В	С	D	E	F	G	н	I	J	К	L
 METHANE	n-HEXANE	n-NONAN	Temnerat	Dressure (FlashType	Output	Compone	Units	Project sh	eet
0,333333	0,333333	0,333333	250	1	2	Fixed 2D	METHANE	C(In,Mass	VLXE - Pro	ject (v2)
Property	System	Feed	Phase 1	Phase 2						
Pressure [1		Time: 131				T		T	
 remperat	250									
Compone										
METHANE	0,333333	0,333333	0,333333	0						
n-HEXANE	0,333333	0,333333	0,333333	0						
n-NONAN	0.00333	0,333333	0,333333	0						
Dhara Far										
 Phase Frag				0						
Phase Frag			1	0						



B

3.8.2 Change after calculation is created

Once a calculation is created, the component list can be altered simply by changing the string used as the component argument. It can be changed either by hand or using the "Names" wizard.

To illustrate, click on the component cell in the calculation just created. Then hold down the shift key and click on "Names" on the VLXE Blend ribbon.

Oil And Fitting S + Gas + + Calculations Distributions Code Generate	ut Sheet	DIPPR DIPPR									
Oil And Fitting Calculations Distributions Code Input Output Units Names Outp ns • Gas • • Generate	ut Sheet	DIPPR									
Wizards Utility		Exte									
VLXE Blend - Select Project Sheet											
H I J Output Compone Units Fixed 2D METHANEC(In,N O VLXE - Project (v2) O VLXE - Project	cel	Q									

In the new window, select the first 3 components, thereby changing the components to be used in the flash calculation.

VLXE Blend - Select Components to Include		
Select the Components to Include:		
METHANE		
n-HEXANE		
n-OCTANE		
n-NONANE		
Select Output Type		
 Output as cell (string) 		
Output as column		
Output as row		
Cancel	ОК	

Select "OK" and note how the calculation is updated using the new component list.



Warning: Also note how the labels above the feed do not change. It is very important to remember to change these by hand.

	× ✓	<i>f</i> _∞ ME	THANE,n-H	IEXANE,n-	OCTANE					
В	C	D	E	F	G	Н	I	J	К	L
METHANE	n-HEXAN	n-NONAN	Temperat	Pressure [FlashType	Output	Compone	Units	Project sh	eet
0,333333	0,333333	0,333333	250	1	2	Fixed 2D	METHANE	C(In,Mass	VLXE - Pro	ject (v2
Property	System	Feed	Phase 1	Phase 2						
Pressure [[1		Time: 123							
Temperat	250									
_										
Compone										
METHANE	0,333333	0,333333	0,333333	0						
n-HEXANE	0,333333	0,333333	0,333333	0						
n-OCTAN	E 🗨 🖘 333	0,333333	0,333333	0						
_										
Phase Fra	(1	0						

3.9 Link Flash Calculations

A common use of VLXE Blend is to link 2 or more calculations, thereby creating a small simulation. VLXE Blend cannot replace a full simulator, but it makes it very easy to investigate the relevant part of the process.

To illustrate we will create a simple example using the 4 component system from before. We will link 2 flash calculations to simulate a separation. The heavy phase from the first flash is sent to the second flash. Once linked, we will use Excel's Goal-seek to solve for an inlet pressure.

In a blank sheet, create a new T/P flash using the calculation wizard. Then next to it, create a P/H flash. Now change the feed and enthalpy link for the second flash so that it uses the output from the first flash.

	• : :	× ✓	<i>f</i> _x =FI	ash_PH(E9	:E12; H6; E1	L9; 16 <mark>; J6; K</mark>	<mark>6; L6;;;M6)</mark>	K					
А	В	С	D	E	F	G	Н	1		К	L	м	
	METHANE	n-HEXANE	n-OCTAN	n-NONAN	Temperat	Pressure	FlashType	Output	Compone	Units	Project sh	eet	
	0,25	0,25	0,25	0,25	25	125	2	Fixed 2D	All	C(In,Mass	VLXE - Pro	ject (v2)	
	Property	System	Feed	Phase 1	Phase 2								
	Pressure [125		Time: 208			Pressure [FlashType	Output	Compone	Units	Project she	eet
	Temperat	25					1	2	Fixed 2D	All	C(In,Mass	VLXE - Prc	iect
							Property	System	Feed	Phase 1	Phase 2		
	Compone				1		Pressure [[1		Time: 217			
	METHANE	0,25	0,25	0,137447	0,936574		Temperat	10,03184					
	n-HEXANE	0,25	0,25	0,283714	0,044344			=Flash_PF					
	n-OCTANE	0,25	0,25	0,288938	0.012.18		Compone	1					
	n-NONAN	0,25	0,25	0,289901	0,000503		METHANE	0,137447	0,137447	0,000902	0,803119		
							n-HEXANE	0,283714	0,283714	0,305591	0,177064		
	Phase Fra			0,632323	0,367677		n-OCTANE	0,288938	0,288938	0,345038	0,015445		
	Phase Fra			0,859155	0,140845		n-NONAN	0,289901	0,289901	0,34847	0,004373		
	Compress	0,62042	0,452136	0,521621	0,790331								
	Density [g	0,359262	0,492979	0,580596	0,108035		Phase Fra	I.		0,465485	0,534515		
	Molar Vol	123,0402	89,66649	103,4467	156 367		Phase Fra	I.		0,829791	0,170209		
	Enthalpy [-2947,22	-2959,53	-2672,22	-4021,7		Compress	0,535841	0,970098	0,006527	0,996796		
	Entrony [1 27255	1 40000	1 15007	2 66020		Donaity La	0.004761	0.000600	0 606627	0.000015		

We have now created a simple separation and can work with the input to see the effect.



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4

3.10 Using Excel's Goal Seek feature to solve simulation

Once we have the calculations linked, we can use Excel's built-in Goal Seek feature to solve, for example, for outlet temperature. We can thereby converge a simulation. As an example, we will use Goal Seek to find the pressure in the first flash such that it yields a temperature of 25°C in the second flash.

Open Goal Seek under Data/"What-If Analysis".

			0.071.01		- .			<u> </u>	_			
METHANE	n-H	IEXANE	n-OCTANE	n-NONAN	Temperat	Pressure [FlashType	Output	Compone	Units	Project sh	eet
0,25		0,25	0,25	0,25	25	125	2	Fixed 2D	All	C(In,Mass	VLXE - Pro	jec
Property	Sys	tem	Feed	Phase 1	Phase 2							
Pressure [[125		Time: 195			Pressure [FlashType	Output	Compone	Units	Pro
Temperat		25					1	2	Fixed 2D	All	C(In,Mass	VL
			Goal Seek				Property	System	Feed	Phase 1	Phase 2	
Compone			Set cell	CTC			Pressure [[1		Time: 228		
METHANE		0,25	<u></u>	313.			Tanapa da	10,03184				
n-HEXANE		0,25	To <u>v</u> alue:	15								
n-OCTANE		0,25	By <u>c</u> hangir	ng cell: \$G	3		Compone					
n-NONAN		0,25		ОК	Cancel		METHANE	0,137447	0,137447	0,000902	0,803119	
							n-HEXANE	0,283714	0,283714	0,305591	0,177064	
Phase Fra				0,632323	0,367677		n-OCTANE	0,288938	0,288938	0,345038	0,015445	

Select "OK" and the solver will run for a few seconds. The cells are automatically ajusted.

0	С	D	E	F	G	Н	Ι	J	К	
·HE	XANE	n-OCTANE	n-NONAN	Temperat	Pressure [FlashType	Output	Compone	Units	Ρ
	0,25	0,25	0,25	25	84,75707	2	Fixed 2D	All	C(In,Mass	٧
/ste	em	Feed	Phase 1	Phase 2						
4,7	75707		Time: 230			Pressure [FlashType	Output	Compone	U
	25					1	2	Fixed 2D	All	С
						Property	System	Feed	Phase 1	Ρ
0					572	Pessure [1		Time: 217	
	Goal S	Seek Status		8	23	Temperat	15			
	Goal	Seeking wit	h Cell 19	Stan						
	foun	d a solution.		Step		Compone	Λ			
	Targe	t value: 1	5	Paus	e]	METHANE	086674	0,086674	0,000869	(
	Curre	ent value: 14	4,99999834			n-HEXANF	0,300705	0,300705	0,311336	(
		(OK	Cance		n-OCTANE	0,305951	0,305951	0,342591	(
		l	UK			n-NONAN	0,306669	0,306669	0,345204	(
),62	0378	0,314072	0,3974	0,845308						



4) Association Components

This chapter describes how to calculate the properties of components that form an association with each other in the liquid and vapor phases. This is described by the use of a methanol cyclohexane example. A step-by-step procedure is shown below.

1. Open an Excel sheet.

4

Click on "New" from the database.



2. Select the type of system, Equation of State and ideal gas Cp expression (solvents).

For a methanol cyclohexane mixture, PC-SAFT equation of state and standard system is selected with polynomial ideal gas Cp expression.

💵 🖯 😼 🖉 🐺 🐺 = Book1 - Excel		
FILE OME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW VLXE Blend DEVELOPER		
New Edit Bubble Flash Flash Properties PhaseEnvelope Unit Oil And Fitting Operations - Gas Calculations Distributions Code General	Input Output U	Units
VLXE Blend databases - Select a New System		Ut
System Equation of State Solvent / Polymer Solvent / coPolymer Solvent / coPolymer Modified Sanchez/Lacombe Polymer blend PC-SAFT CoPolymer blend CPA Ideal Gas Cp Expression (Standard) Polynomial DIPPR DIPPR	Next	N
Database Connection Database Format Name of New Project Sheet Local SQLServer VLXE - Project	Cancel	
9		


3. Click "Next" and add solvents from the databank to define the system. Select methanol and cyclohexane from the databank. Selected components are shown in the figure below.

4	VLXE Blen	d databases - Select a New System					l	
1	Standards			Syst	em		$ \rightarrow $	
ſ				Solv				
	Add	Insert Remove Clear			Status	DB Index	Name	
	VLXE I	Short Name	✓ Formula	▶1	New	513	METHANOL	Rack
2	1	cyclo	ne	2	New	101	CYCLOHEXANE	
5	101	CYCLOHEXA	VE C6H12		_			
	121	CYCLOHEPTA	VE C7H14			7		
	188	CYCLOHEXE	VE C6H10					
	191	CYCLOHEPTE	VE C7H12					
	300	CYCLOHEXYLBENZE	VE C12H16			•		
	499	CYCLOHEXANO	VE C6H10O					
	557	CYCLOHEXAN	DL C6H12O					
	824	CYCLOHEXYL PEROXI	C6H12O2					
	974	CYCLOHEXYLAMI	NE C6H13N					
	1052	CYCLOHEXYL MERCAPT	N C6H12S					
	1306	CYCLOHEXYL FORMA	TE C7H12O2					
	1315	CYCLOHEXYL ACETA	TE C8H14O2					
	1419	CYCLOHEXYL ISOCYANA	TE C7H11NO					
	1823	CYCLOHEXANONE OXI	IE C6H11NO					
	Starts	s with([Short Name], 'cyclohe') 🔽	Edit Filter					
	Database Co	nnection Database Format N	lame of New Project Shee					Cancel
Lo	cal	SQLServer VL	XE - Project					
		· · ·						

4. Click "Next" and all the results will be displayed in an Excel sheet.

XI	5	· C · 👍 🗱					Association -	Methanol + Cyc
FILE	Н	OME INSERT	PAGE LAYOU	JT FORMULAS	DATA REVIEW	VIEW	VLXE Blend	DEVELOPER
New Project	Edit	BubbleT BubbleP	Flash Flash (TP) (PH)	Properties PhaseEnvel (TP) Calculations	ope Unit Oil A Operations + Gas	nd Fitting	Calculations	Distributions Ge Wizards
A1		• : × ~	f_x					
	Α	В		С	D			F
1								
2		Sheet version		Number of solvents	Number of polym	ers I	Equation of st	ate
3			14		2	0	PC-SAFT	
4								
5		Solvent Index		Name	VLXE DB. index	540	DDBST DB. inc	ex
0						513		
8			2	CICLOHEAANE		101		
9		Solvent Index		Name	Heat of formation	[kJ/kg]	Ideal gas Cp: ((1) [kJ/(kg Ke
10			1	METHANOL	-627:	1,171524		1,225(
11			2	CYCLOHEXANE	-146	5,075592		0,5133
12								
13		Kij (a) [-]		METHANOL	CYCLOHEXANE			
14		METHANOL						
15		CYCLOHEXANE			0			
10		Kii (b) [KelvinA-1]		ΜΕΤΗΔΝΟΙ	CYCLOHEYANE			
18		MFTHANOI		MEMANOL	CICEONEAANE			
19		CYCLOHEXANE			0			
20	•							
21		Association, Kapp	a [-]	METHANOL	CYCLOHEXANE			
22		METHANOL		0,03517	6	0		
23		YCLOHEXANE			0	0		
24		N	Tec. 1. 1. 1					
25		Asso lation, Epsile	on Kelvin	METHANOL	CYCLOHEXANE			
1	-	VLAE - Project	SheerT	•				



5. PC-SAFT equation of state with polynomial ideal gas Cp expression will also tell whether the solvent is associated or not. Also it tells something about the association scheme.

VIEW VLXE Blend DEVELOPER Sig If Fitting Image: Calculations Distributions Code Generate Generate Wizards Image: Code GeneGenerate Wizards Image: Code Generate		Association	ı - Methanol + Cy	/cloHexane	e.xlsx - E	cel										? 📧	-
A Fitting Imput	VIEW	VLXE Blenc	DEVELOPER	2													Sig
A Fitting Calculations Distributions Code Generate Input Output Units Names Output Sheet DIPPR DDBST Quick Standard Databases License Suppo Q R S T U V W V	} ₽	-		c≡	-\$			atto mate	•		DIPPR	2	Ŧ				
Wizards Utility External Settings Q R S T U V W Image: Comparison of the comparison	Fitting	Calculation	ns Distributions	Code Generate	Input	Output	Units	Names	Output	Sheet	DIPPR	DDBST	Quick	Standard	Databases	License •	Suppo T
Q R S T U V W Image: Second constraints of the second constrated constrated constraints of the second consecond cons			Wizards				Ut	ility			Ext	ernal		Setting	15		
Q N O V V ha (5) [Kelvin^-1] epsilon [Kelvin] Volume shift [cm3/g] Association active? kappaAB [-] epsilonAB [Kelvin] Association scheme [-] Po 0 188,9 0 TRUE 0,035176 2899,5 28 0 278,11 0 FALSE 0 0 28	0		P		c			т					V		144		
na (5) [Kelvin^-1] epsilon [Kelvin] Volume shift [cm3/g] Association active? kappaAB [-] epsilonAB [Kelvin] Association scheme [-] Po 0 188,9 0 TRUE 0,035176 2899,5 2B 0 278,11 0 FALSE 0 0 2B	Q		ĸ		3			· ·			0		v		vv		
0 188,9 0 TRUE 0,035176 2899,5 2B 0 278,11 0 FALSE 0 0 2B	na (5) [Ke	elvin^-1]	epsilon [Kelvin] Volum	e shift	[cm3/g]	Ass	ociation	active?	kappa	aAB [-]	epsilor	AB [Kel	vin] As	sociation s	cheme	-] Po
0 278,11 0 FALSE 0 0 2B			188,	,9			0	TRU	E	0,	035176		28	99,5 2B			
		0	278,1	1			0	FALS	E		0			0 2B			

4.1 Bonding fraction as output

The bonding fraction can be part of the calculation output. A common reason for doing this is to compare with experimental data or simply to check how the bonding fraction moves with the input.

It is best seen as part of the standard 2D output. To illustrate, create a flash calculation using the calculation wizard. On the last page select as shown below:

VLXE Blend - Calculation Wizard	
Select Output Type Select Extra Output:	ок
Function row (Single row output)	
Function range (Range output)	Back
	Wizard Stop
Information	Off
Function row: The results are given in just one row. You define the output your self Function range: The output is given in a range of the sheet. The output is fixed by the program.	Cancel
Project sheet: VLXE - Project	

Note that the bonding fraction is now included in the output. See how it includes A and B since "2B" scheme is used plus how cyclohexane has a bonding fraction of 1 since it does not associate.



Α	В	С	D	E	F	G	H	
	METHANOL [Massfrac	CYCLOHEX	Temperat	Pressure [FlashType	Output	Compone U	Ir
	0,5	0,5	250	1	2	Fixed 2D,BondingFra	All C	(
	Property	System	Feed	Phase 1	Phase 2			
	Pressure [Bar]	1		Time: 141				
	Temperature [Celsius	250				-		
	Components							
	METHANOL [Massfrac	0,5	0,5	0,5	0			
	CYCLOHEXANE [Massf	0,5	0,5	0,5	0			
	METHANOL: X(A)		0,996979	0,996979	1			
	METHANOL: X(B)		0,996979	0,996979	1			
	CYCLOHEXANE: X(A)		1	1	1			
	CYCLOHEXANE: X(B)		1	1	1			
	Phase Fraction [Mole]			1	0			
	Phase Fraction [Weigł			1	0			
	Compressibility [-]	0,995547	0,995547	0,995547	0			
	Density [g/cm^3]	0,001072	0,001072	0,001072	0			

4.2 Txy/Pxy Calculations

1. When the system is defined and all the parameters are loaded into an Excel spreadsheet, the next step is to make some calculations.

Click on the standard wizard and go to "Calculations".

2. Select "Txy/Pxy" from the calculation wizard and click "Next".





3. Give the pressure for the Txy calculation or the temperature for a Pxy calculation. For this example a pressure of 1 Bar is given for the Txy calculation. Select an LLE type of curve, standard output and then click "Next".

VLXE Blend - Calculation Wizard		1
→ →	Input Pressure [Bar] Txy L.0 Pxy Select Line Type VLE UE OULE OUTput Type	Next A Back
→ →	Standard XY Relative Volatility	Change Units
		Wizard Stop Off Cancel
Project sheet: VLXE - Project		- \

4. Select "Temperature" and "Pressure" and click "OK".

VLXE Blend - Calculation Wizard			
Intensive Temperature Pressure Number of Phases System Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mole Based) Density Volume Enthalpy Entropy Cp Average Molar Mass Surface Tension	General General Number of Results Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mole Based) Density Volume Enthalpy Entropy Cp Speed of Sound Average Molar Mass Viscosity	Phase 1 Phase 2 Composition Bonding Fraction Phase Fraction (Mole Based) Phase Fraction (Mass Based) Density Volume Enthalpy Entropy Cp Speed of Sound Average Molar Mass Viscosity	OK Back
Information System: Sum of the phases First phase: Heaviest phase Last phase: Lightest phase			Cancel
Project sheet: VLXE - Project			



5. Bubble and dew point temperature, with respect to methanol composition, is plotted in a graph.



6. In a similar way, the VLE curve can be drawn by selecting VLE line type instead of LLE. All the other steps will remain the same as shown above.

VLXE Blend - Calculation Wizard		
\rightarrow	Input Pressure [Bar] I.0 P Select Line Type	xy Next xy Back
\rightarrow	VLE ULE Output Type Standard XY Relative Volatility	Change Units
		Wizard Stop Off Cancel
Project sheet: VLXE - Project		



7. The corresponding results in graphical form for VLE are shown below.



8. Effect of bubble point and dew point with respect to methanol composition with both LLE and VLE can also be plotted in the same graph. Just copy one graph, and paste it into the other graph with minor changes in axis in order to have a better view.



5) Polar Components

This chapter describes how to calculate the properties of components that form an association with each other in the liquid and vapor phases. This is best described by a methanol cyclohexane example. A step-by-step procedure is shown below.

Polar molecules have slightly positive and slightly negative charged ends. This section deals with the system that contains polar molecules. An example of an acetone n-hexane mixture will be described here.

1. Set up or define the system. Select "Standard", choose "PC-SAFT" equation of state, select "Polynomial" ideal gas Cp expression and click "Next".



2. Define the components from the database and click "Next".

3. All the parameters are loaded into an Excel spreadsheet. For a system containing polar compounds an Excel spreadsheet is shown below that contains three additional terms i.e. Dipole moment, Polar coordinate and Polar active.

	VLXE Ble	nd DEVELOPE	R										
e.	-		c≡	-%				-	D	IPPr 💙	1		
ing	Calculations Distributions Code Input Output		Units	Names (Output She	et Dl	PPR DDBST	Qu	uick Standard	Databases			
ľ			Generate										
	Wizards				Ut	Utility			External		Settings		
U		V		W			Х	Y		Z			AA
pa/	\В[-]ер	ilonAB [Kelvin]	Associat	tion sch	eme [-] Pola	ar active	Polar x [-] Dipc	ole momen	t [D]	Critical viso	osity (a) [uP
) 2B				TRUE	0,225	8		2,7		



5.1 Pxy Calculations

As an example, the effect of pressure with composition is shown below. Other calculations can also be performed in the same manner as was shown for other solvent systems above.

1. Start from the Calculation Wizard, click on "Calculations", then select "Txy/Pxy" from the Calculation Wizard and click "Next".



2. Click on "Pxy", provide an input temperature, select VLE line type and standard output type and then click "Next".

Input Temperature [Celsius] 40.0 Pxy Select Line Type	Next Back
O VLE	
CLE Cutput Type Standard XY Relative Volatility	ange Units
	d Stop Off Cancel
Project sheet: VLXE - Project	



3. Click "Ok" and a graph between Acetone mass fraction against pressure is plotted. From the figure below it can clearly be seen that this mixture of acetone and n-hexane forms an azeotrope.





6) Polymer

6

Polymers are the core part of VLXE Blend. As the only PVT package in the world that offers a full range of models and robust calculations.

The main advantages of VLXE Blend is that it makes polymer calculations just as simple as any other ones. Here there is no difference between a poly-disperse polymer system and a n-Hexane system. The only place where you will notice any difference is for poly-dispersity and copolymers. In these cases, a bit more in and out-put is needed.

By now you know how to use VLXE Blend, so the focus now is on the small differences in in- and out-put, and additionally an overview of the polymer calculations in VLXE Blend is provided.

6.1 Create a new Polymer Project

Create a new Excel file and select "New" on the VLXE Blend ribbon. Select as shown below.

🛂 VLXE Blend databases - S	Select a New System		
System		Equation of State	Next
O Standard		• PC-SAFT	
Solvent / Polymer		7	
Solvent / coPolymer		Modified Sanchez/Lacombe	
O Polymer blend			
O coPolymer blend		Sanchez/Lacombe	
		Ideal Gas Cp Expression (Standard)	
		O Polynomial	
		• DIPPR	
		Ideal Gas Cp Expression (Polymer)	Ī
		U DIFFR	
Database Connection	Database Format	Name of New Project Sheet	Cancel
Local	SQLServer	VLXE - Project	
)

On the next page, select Ethylene and n-Hexane as solvents and HDPE as the polymer. So as to include a distribution for the polymer, select "Distribution select".

Note that if no distribution is selected here, a default value for a mono-disperse polymer is used. The molar mass can then be changed once the project sheet is created.



4	VLXE E	lend datab	ases - S	elect a Ne	ew System					23			
S	tandard	ls Polyme	rs				Syste	m					
						٦	Solve	nt(s)					
	Add	Inse	rt R	emove	Clear				Status	DB Index	Name		
	In	Short	Long Na	ame	Distribu	싉	▶1	New		127	ETHYLENE	Back	
8							2	New		9	n-HEXANE		
Þ	▶ 1 HDPE High density pol									-	/		
	2 LDPE Low density pol												
	3 PP Polypropylene												
	4 PB Polybutene												
P	olymer												
		Туре	Pol DB	lymer Index	Polymer Name	Distrib DB In		ndex Distribution		n Distributio Pseudo Co	on Distribution unt Select		
Þ	1	Nev	v	1	HDP	=		-1	Defa	ault De	fault		
D	atabase	e Connection	1	Databas	e Format	N	lame of	New P	Cance	2			
Loc	ocal SQLServer VL				VL)	XE - Project							
_						_							

In the dialog that opens, select "From N. Koak".

VLXE Blend databases - Select a New System										
Standards Poly	Standards Poly 🛂 VLXE Blend - Select distribution for polymer: HDPE									
	Index	Short Name	Pseudo Count	Salact						
In Short	1	From Trumpi et.		7						
2	2	From Jog et. al		10	Back					
▶ 1 HD ▶	3	From N. Koak		36						
2 LD	4	From N. Koak		7						
3	5	From Tumakaka		9						
4										
Delawar					1					
Polymer					5					
Туре										
<i>0</i> .1					P					
				Cancel						
Database Connec					Cancel					
Local	SQLSE	erver VLXE - Project		ŀ.						
		1								

This distribution is now attached to the selected polymer.



Ľ	VLXE Blend databases - Select a New System									- 0					
ſ	St	Standards Polymers							System						OK
ſ	(٦	Solve	nt(s)						
		Add Insert Remove Clear								Status	DB Ir	ndex	Name		
		In	Short	Long Na	ame	Distribu	싉	▶1	New		127		ETHYLENE		Back
	9							2	New		9		n-HEXANE		Duck
	F	1	HDPE	High der	nsity pol										
		2	LDPE	Low der	nsity pol										
		3	PP	Poly	propylene										
	4 PB Polybutene						$\overline{}$								
	Polymer														
		Type Polymer Polymer DB Index Name				Distribution Distribution Distribution Distribution Distribution Select			Distribution Select						
	Ø.	1	Nev	N	1	HDP	E		3	From N. K	oak	36	5		
	1														
	Database Connection Database Format Name of New Project Sheet										Cancel				
	Local SQLServer VLXE - Project														
Ľ										-1					

Click on "OK" to create the project sheet.

All the parameters and properties of the system with the two solvents (Ethylene and n-Hexane) and the polymer (HDPE) are loaded into the Excel sheet. Take a look at the sheet to see how the polymer information is included:

	А	В	С	D	E	F
1						
2		Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas
3		14			PC-SAFT	DIPPR
4						
5		Solvent Index	Name	VLXE DB. index	DDBST DB. index	Туре
6			ETHYLENE	127	1053	
7			n-HEXANE			
8						
9		Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
10			ETHYLENE	1871,80339	1,1899	
11			n-HEXANE	-2305,2993	1,2115	
12						
13		Polymer Index 📃 🚵	Name	Block count	Pseudo count	VLXE DB. index
14		1	HDPE	1	36	
15						
16		Polymer Index	Polymer Name	Block index	Block name	Monomer name [-]
17		1	HDPE		HDPE	Ethylene
18						
19		Polymer Index	Polymer Name	Block index	Block name	c: Crystalline fractio
20			HDPE		HDPE	
21						
22		Polymer Index	Polymer Name	Block index	Block name	Heat of formation [
23		1	HDPE		HDPE	-161
24						
25		Kij (a) [-]	ETHYLENE	n-HEXANE	HDPE	
26		ETHYLENE				

The distribution information for the polymer is given at the end. Note the range of molar mass. From 3300 g/mole to 1.7E6 g/mole. VLXE Blend has no limit on molar mass.



6.2 Create a new Copolymer Project

The procedure for creating a new copolymer project sheet is the same as for a polymer system.

Select "New" on the VLXE Blend ribbon. In the database wizard select as shown below.

VLXE Blend databases - :	Select a New System				
System		Equation of State	Next		
O Standard					
O Solvent / Polymer					
💿 Solvent / coPolymer 🛛 ┥	←—	coPolymer PC-SAFT			
O Polymer blend		1			
CoPolymer blend					
		Ideal Gas Cp Expression (Standard)			
		Polynomial O DIPPR			
		Ideal Gas Cp Expression (Polymer)			
		Polynomial			
		ODIPPR			
Database Connection	Database Format Name of New Project Sheet				
Local	SQLServer	VLXE - Project			

Click "Next".

As an example, ethylene, n-hexane and PEP (polyethylenecopropylene) with a 7 pseudo-component distribution is used. Select those components as given below

VLXE Blend databases - Select a New System														
ſ	S	tandar	ds coPol	ymers			Syste	m						
						Chara	Solve	ent(s)						
	Add Insert Remove Clear						s	tatus	DB	Index	Name			
		I	Short	Long Na	me	Distrib	▶1	New		127	EI	THYLENE	llr	Back
	8						2	New		9	n-	HEXANE		
	۲	1	PEP	poly(eth	ylene-co-p									
		2	PEB	Poly(eth	ylene-co-1						Λ			
L	3 EVA Poly(ethylene-co-v													
	4 PAA Poly(ethylene-co-a													
l														
coPolymer														
l			Туре	Po DB	lymer Index	Polymer Name	Distrit DB II	oution ndex	Distributi Name	on P	Distribution Pseudo Count	Distribution Select		
L	Ø. 1 New 1 PEP 1 From Trumpi 7 ····] [
ľ	Database Connection Database Format Name of New Project Sheet									Cancel				
	Loc	cal			SQLServer		VLXE - F	roject						

Click "OK" to generate the project sheet.



Take a look at the project sheet and compare it to the one from before with a polymer. Note how extra rows are added due to the 2 blocks in the copolymer.

Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)	Ideal gas C
	1 ETHYLENE	1871,8033	9 1,1899	3,3789	
	2 n-HEXANE	-2305,299	31,2115	4,0882	
Polymer Index	Name	Block count	Pseudo count	VLXE DB. index	DDBST DB
	1 PEP		2 7	1	
Polyment for	Polymer Name	Block index	Block name	Block Mass Fraction [-]	Monomer
	1 PEP		1 HDPE	0,5	Ethylene
	1 PEP		2 PP	0,5	Propylene
De lumas la deu	DebraseMarsa	Plash index.			T-th-l-v
Polymer index	Polymer Name	BIOCK INUEX	BIOCK name	c: crystamme traction [-]	Enthalpy
	1 PEP		1 HDPE	C	
	1 PEP		2 PP	0	
Polymer Index	Polymer Name	Block index	Block name	Heat of formation [kJ/kg]	Ideal gas
	1 PEP		1 HDPE	-1613,2549	, in the second s
	1 PEP		2 PP	0	

6.3 Cloud Point Calculation

We will now set up a cloud point calculation. VLXE Blend supports robust VLE and LLE cloud point calculations for any polymer system. When we go through the steps in the Calculation Wizard note how they are the same as for Methane + n-Hexane.

Go to a new empty Excel sheet and click on "Calculations" on the VLXE Blend ribbon. Leave the component list unchanged and click "Next". Select "Cloud Point" and click "Next".

VLXE Blend - Calculation Wizard	
Select Calculation	
O Bubble Kij	Next
Cloud Point	
O Critical Point	
O Excess Enthalpy	Dack
○ Flash	
O Phase Envelope	
O Properties	
⊖ sle	
O Spinodal	
○ Tw/Pw	
O Surface Tension	Wizard Stop
O Unit Operation: Mixer	ОП
O Unit Operation: LinkedPHFlash	Cancel
Project sheet: VLXE - Project	



Note that 2 new input options are provided. We can now chose point type and temperature range. Select "Auto" for range and "0 - 300" for temperature range. VLXE Blend will look for a solution within this range only.

V	LXE BI	end - Calculation	Wizard						
	Feed,	, In		Input					
		Name	Feed [Massfraction]	Pressure [Bar]	Bubble T	Next			
	1	ETHYLENE	0.02	Select Point Type	Bubble P				
	<i>d</i> . 2	n-HEXANE	<mark>0.78</mark>	O VLE					
	3	HDPE	0.2	OLLE		Back			
				Auto					
				Temperature Range [Celsius]					
				0.0					
				Maximum					
				300.0		Change Units			
L						Wizard Stop			
L				•		Off			
						Cancel			
	Project sheet: VLXE - Project								

Under output, select "Function range" and leave "Bonding fraction" unchecked.

VLXE Blend - Calculation Wizard	
Select Output Type Select Extra Output:	ОК
Function row (Single row output)	
Function range (Range output)	Back
	Wizard Stop
Information	Off
Function row: The results are given in just one row. You define the output your self Function range: The output is given in a range of the sheet. The output is fixed by the program.	Cancel
Project sheet: VLXE - Project	

Select "OK" to create the calculation.

The output now includes distribution information but is otherwise the same as for "non-polymer" systems.



Note the distribution between the 2 phases , and also how there is 0.002 mass fraction in the second liquid phase. VLXE Blend not only finds the LLE system but will also give the distribution information.

ETHYLENE	n-HEXAN	HDPE [Ma	Pressure	[Output	Con	npone	Units	PointType	Temperat	Temperat	Project sh	eet
0,02	0,78	0,2	100	Fixed 2D	All		C(In,Mass	Auto	0	300	VLXE - Pro	ject
Property	System	Feed	Phase 1	Phase 2								
Pressure [100		Time: 899		ç—				C			
 Temperat	210,646				-			Distri	hution			+
 _					-			Distri	bution	•		
Compone					-	0.00	0 7					
ETHYLENE	0,02	0,02	0,02	0,025779	-	0.00	o	HD PF · Feed	۸			
n-HEXANE	0,78	0,78	0,78	0,972113	-	e ^{0.00}	0 -		. 1			1
HDPE [IVIa	0,2	0,2		0,002108	1	·퓐 0.00	0 -	NDFC. Flidse	± \			
Dhace Fre					d i	E 0.00	0 -		- 1 \			
Phase Fra			1		H .	0.00 g	0 -		11	\wedge		
Compress	0 49410	0 49410	0.49410	0.429060	H	o.00 ک	0 -			$\langle \rangle$		
Donsity In	0,40419	0,40419	0,40419	0.465164	H	0.00	0 -		' /			
 Molar Vol	194 7669	19/ 7669	19/ 7669	176 21//		0.00	o ——					
 Enthalov I	-19/9 28	-19/19/28	-19/19/28	-2056 12			1	100	10000	10000	000	
Entropy [0 273595	0 273595	0 273595	0 180196				Ln(I	Molar mass	5)		
Cn [k]/(Ke	3 022615	3 022615	3 022615	3 207037	ť—							-5
 Cy [k]/(Ke	2.507117	2.507117	2.507117	2.482573	-							
 ITCoeffie	2,007117	-0.00015	-0.00015	0.031384								
 Velocity o		549.6771	549.6771	458.3155	_							
Molecular	102.377	102.377	102.377	81.96861								
Mn (HDPE	55871,79	55871,79	55871,79	10042,65								
Mw (HDPE	99816,21	99816,21	99816,21	13112,86								
Mz (HDPE	185886,2	185886,2	185886,2	17254,93								
HDPE	HDPE	HDPE	HDPE	HDPE								
3300	0,00035	0,00035	0,00035	0,024701						-		
4500	0,00084	0,00084	0,00084	0,048687								
6000	0,00141	0,00141	0,00141	0,063894								
8200	0,00352	0,00352	0,00352	0,111176		F						
8800	0,0044	0,0044	0,0044	0,12594								
10900	0,00722	0,00722	0,00722	0,146421								
12300	0,00881	0,00881	0,00881	0,141996								
14400	0,01127	0,01127	0,01127	0,1287								
19300	0,01828	0,01828	0,01828	0,093423								
25900	0,027881	0,027881	0,027881	0,048245								
27900	0,030831	0,030831	0,030831	0,038425								
34200	0.040211	0.040211	0.040211	0.017825								

6.4 Flash Calculation

VLXE Blend offers the most commonly used flash calculations. They all automatically handle VLE or LLE. Not all can handle VLLE.

- Fixed Temperature & Pressure.
- Fixed Pressure & Enthalpy (Isenthalpic flash).
- Fixed Pressure & Entropy (isentropic flash).
- Fixed pressure and volume (2 phase flash only).
- Fixed temperature and volume (2 phase flash only).
- Fixed pressure and phase fraction (2 phase flash only).
- Fixed temperature and phase fraction (2 phase flash only).



6.4.1 Flash at fixed temperature and pressure

We will now set up a flash calculation. VLXE Blend supports robust VLE, LLE and VLLE flash calculations for any polymer system. When we go through the steps in the calculation wizard, note how they are the same as for Methane + n-Hexane.

Go to a new empty sheet and click on "Calculations" on the VLXE Blend ribbon. Leave the component list unchanged and click "Next". Select "Flash" and click "Next". Note that there is no additional input for a polymer flash calculation. Select "3 Phase" flash and select "Next"

V	LXE BI					
ſ	Feed	, In		Input		
	Name Feed [Massfraction]		Feed [Massfraction]	Temperature [Celsius]	Temperature/Pressure	Next
L	▶1	ETHYLENE	0.020000	Pressure [Bar]	Pressure/Enthalpy	
L	2	n-HEXANE	0.780000	1.00	Pressure/Entropy	
ı.	3	HDPE	0.200000		Temperature/Phasefraction	Back
l					Pressure/Phasefraction	
L					Temperature/Volume	
L					Pressure/Volume	
l						Change Units
L				Number of Phases to Look for		
				Automatic 2 Phases 3 Phases		
						Wizard Stop
l				· · ·		Off
						Cancel
	Projec	t sheet: VLXE - Pr	oject			

Select "Function range" as output and select "OK" to create the calculation

Select Output Type Function row (Single row output) Function range (Range output) Wizard Stop	VLXE Blend - Calculation Wizard		
Function row (Single row output) Function range (Range output) Back Wizard Stop	Select Output Type	Select Extra Output:	ОК
Function range (Range output) Back Wizard Stop	O Function row (Single row output)		
Wizard Stop	Function range (Range output)		Back
Wizard Stop	· · ·		
Wizard Stop			
Wizard Stop			
			Wizard Stop
Information Off	Information		Off
Function row: The results are given in just one row. You define the output your self Function range: The output is given in a range of the sheet. The output is fixed by the program.	Function row: The results are given in just o Function range: The output is given in a ran	one row. You define the output your self ge of the sheet. The output is fixed by the program.	Cancel
Project sheet: VLXE - Project	Project sheet: VLXE - Project		



Adjust temperature to 165°C and pressure to 19 Bar. Note how VLXE Blend finds a VLLE system and how the polymer distributes between the 3 phases.

	ETHYLENE	n-HEXANE	HDPE [Ma	Temperat	Pressure	FlashType	Output	Compone	Units	Project si	neet				
	0,02	0,78	0,2	165	19	3	Fixed 2		C(In,Mass	VLXE - Pro	oject				
	Property	System	Feed	Phase 1	Phase 2	Phase 3									
	Pressure [19		Time: 154						Dict	rihud	lion			
	Temperat	165								Dist	nbu	lion			
								0.001							
	Compone														
	ETHYLENE	0,02	0,02	0,019135	0,025259	0,182989		0.001 -	HDDE	Food					
	n-HEXANE	0,78	0,78	0,768882	0,973541	0,817011			HDFL.						
	HDPE [Ma	0,2	0,2	0,211983	0,0012	4,79E-48		0 001 -	-HD PE:	Phase 1					
\vdash										Phase 2					
	Phase Fra			0,927753	0,066875	0,005372	- 10	0.001		Phase 3					
	Phase Fra			0,943168	0,053553	0,003279		0.001							
	Compress	0,101791	0,09781	0,098752	0,088146	0,796591	- Š								
	Density [g	0,524548	0,545903	0,549679	0,485078	0,040911		0.000 -							
	Molar Vol	195,1718	187,537	189,3434	169,0086	1527,359									
	Enthalpy [-2083,77	-2084,67	-2080,12	-2195,65	-1306,82		0.000 -				~			
	Entropy []	0,014655	0,012606	0,01875	-0,07976	0,37868						\square	_		
	Cp [kJ/(Ke	2,89467	2,892589	2,881054	3,161971	2,445761		0.000	,				\sim		
	Cv [kJ/(Ke	2,346224	2,34664	2,348369	2,321687	2,130002		1	10	10 :	1000	10000	100000	1000000	10000000
	JTCoeffier		-0,0027	-0,00427	0,035565	0,964401				I	.n(Molar	mass)			
	Velocity o		567,1844	573,924	458,1795	202,8396				I					
	Molecular	102,377	102,377	104,0781	81,98244	62,48542									
	Mn (HDPE	55871,79	55871,79	55968,17	8787,47	3300									
	MW (HDPE	99816,21	99816,21	99844,75	10996,1	3300									
	MZ (HDPE)	185886,2	185886,2	185892,3	13728,56	3300									
	HDPE	HDPE	HDPE	HDPE	HDPE	HDPE									
	3300	0,00035	0,00035	0,000338	0,038192	1			-			_			
	4500	0,00084	0,00084	0,000817	0,071179	1,49E-16									
	6000	0,00141	0,00141	0,001383	0,08688	1E-75	÷								
	8200	0,00352	0,00352	0,003478	0,135433	1E-75	-								
	8800	0,0044	0,0044	0,004354	0,148806	1E-75									



6

6.4.2 Link Flash Calculation

Linking two or more flash calculations allows you to simulate a separation unit in Excel. For poly-disperse polymers the distribution will change between units since the pseudo-components will not distribute equally between the phases in the separator. VLXE Blend supports this in a very simple manner. Simply overwrite the distribution that a calculation is to use by passing it a new one using the "Distribution" argument.

As an example we will now link 2 flash calculations where we feed the heavy phase from the first flash into the second flash. This can be seen as 2 separators in series.

	ETHYLENE	n-HEXANE	HDPE [Ma	Temperat	Pressure [FlashType	Output	Compone	Units			
	0,02	0,78	0,2	250	100	2	Fixed 2D	All	C(In,Mass			
	Property	System	Feed	Phase 1	Phase 2							
	Pressure [100		Time: 178			Temperat	Pressure [FlashType	Output	Compone	Unit
	Temperat	250					250	10	- 2	Fixed 2D	All	C(In,
							Property	System	Feed	Phase 1	Phase 2	
	Compone						ressure [10		Time: 174:		
	ETHYLENE	0,02	0,02	0,014753	0,02596		Temperat	250				
	n-HEXANE	0,78	0,78	0,609218	0,973975							
	HDPE [Ma	0,2	0,2	0,376029	6,53E-05		Compone					
							ETHYLENE	0,014753	0,014753	0,000478	0,024735	
	Phase Fra			13884	0,586116		n-HEXANE	0,609218	0,609218	0,085768	0,975265	
	Phase Fra			,531792	0,468208		HDPE [Ma	0,376029	0,376029	0,913753	4,18E-31	
	Compress	0,50529	0,490593	0,559885	0,466738							
	Density [g	0,465799	0,479753	0,540137	0,40283	/	Phase Fra			0,055684	0,944316	
	Molar Vol	219,7877	213,395	243,5351	203,0186		Phase Fra			0,411522	0,588478	
	Enthalpy [-1822,82	-1826 7	-1732,79	-1925 07		Compress	0,865227	0,061603	0,321433	0,897293	
	Entropy [l	0,524794	0,51776	0,598869	0,440658		Density [g	0,034952	0,490907	0,695304	0,021003	
	Cp [kJ/(Ke	3,268219	3,225871	3,083854	3,477621		Molar Vol	3763,507	267,9573	1398,149	3902,986	
	Cv [kJ/(Ke	2,626931	2,627995	2,651163	2,599408		Enthalpy [-1609,24	-1728,89	-1428,02	-1735,97	
	JTCoeffier		0,023829	-0,00337	0,08754		Entropy [I	0,920424	0,639521	0,873337	0,953352	
	Velocity o		452,6906	543,6506	352,1476		Cp [kJ/(Ke	2,768883	3,304107	2,90346	2,674774	
	Molecular	102,377	102,377	131,5427	81,78195		Cv [kJ/(Ke	2,595142	2,636037	2,706381	2,517353	
	Mn (HDPE	55871,79	55871,79	55964,02	4741,699		JTCoeffier		0,042837	-0,0274	0,697755	
	Mw (HDPE	99816,21	99816,21	99830,63	5442,489		Velocity o		390,5313	744,1908	212,5137	
	Mz (HDPE)	185886,2	185886,2	185887,7	6363,175		wolecular	131,5422	131,5422	972,1389	81,97441	
	HDPE	HDPE	HDPE	HDPE	HDPF		Mn (HDPE	55964,02	55964,02	55964,02	3300	
	3300	0,00035	0,00035	0,000306	0,200-104		Mw (HDPE	99830,63	99830,63	99830,63	3300	
L	4500	0,00084	0,00084	0,000793	0,31132		Mz (HDPE)	185887,7	185887,7	185887,7	3300	

Use the wizard and create 2 flash calculations as shown below.

In the example above, Excel's "Trace Dependents" is activated. It visualises the links that a function is using.

Note how the second flash gets its feed and distribution from the result in the first flash. Also note how the polymer content of the phases changes. The second flash units has virtually no polymer in the vapor phase, while the first flash does.







6.5 Phase Diagram

VLXE Blend provides a method to map out the entire phase envelope, including the VLE, LLE, VLLE and SLE regions. In addition to this, lines of fixed properties can be traced in the phase diagram. In other words, a complete picture of the phase diagram can be obtained.

Phase envelope can be viewed in three different ways:

- Ordinary phase envelope.
- Polymer mass fraction versus Temperature (Tw).
- Polymer mass fraction versus Pressure (Pw).



6.5.1 Phase Envelope including VLLE region

To illustrate the robustness of the routines in VLXE Blend we will map the entire phase diagram for the previous polymer system, including the VLLE area. The routine cannot get this in one call, so you have to make 2 calculations and then combine the plots.

Start by selecting "Calculations" on the VLXE Blend ribbon. Click "Next" on the first page leaving in all 3 components. Select "Phase envelope" then "Next".

VLXE Blend - Calculation Wizard						
Select Calculation						
O Bubble Kij		Next				
O Cloud Point						
Critical Point		Back				
O Excess Enthalpy						
◯ Flash						
Phase Envelope						
O Properties						
◯ SLE						
O Spinodal						
◯ Tw/Pw						
O Surface Tension		Wizard Stop				
O Unit Operation: Mixer		Off				
O Unit Operation: LinkedPHFlash		Cancel				
Project sheet: VLXE - Project						

Select "Auto Phase Diagram" and then "Next".

1	LXE BI	end - Calculation	Wizard							
ſ	Feed, In				Input					
		Name	Feed [Massfraction]		No Input Needed Beside Feed Auto Phase Diagram	Next				
	1	ETHYLENE	0.02		User Phase Diagram					
	▶2	n-HEXANE	0.78		Trace Property					
	3	HDPE	0.2		Trace Phase Boundary	Васк				
					Trace Feed					
						Change Lipita				
						Change Onits				
						Wizard Stop				
						Off				
						Cancel				
	Proiec	t sheet: VLXE - Pr	oiect							
L										



Leave the output part unchanged. For this type of calculation, temperatue and pressure is preselected.

VLXE Blend - Calculation Wizard							
VLXE Blend - Calculation Wizard Intensive Pressure Number of Phases System Composition Bonding Fraction Polymer Massfraction Phase Fraction (Mole Based) Phase Fraction (Mass Based) Density Volume Enthalpy Enthalpy Courses	General Number of Results Feed Composition Bonding Fraction Polymer Massfraction Phase Fraction (Mole Based) Phase Fraction (Mass Based) Density Volume Enthalpy Enthalpy Entropy	Phase 1 Phase 2 Composition Bonding Fraction Bonding Fraction Polymer Massfraction Phase Fraction (Mole Based) Phase Fraction (Mole Based) Density Volume Enthalpy Enthalpy Enthopy Entropy	Back				
Cp Average Molar Mass Mn Mw Mz Surface Tension	Cp Speed of Sound Average Molar Mass Mn Mv Mz Viscosity	Cp Speed of Sound Average Molar Mass Mn Mw Mz Viscosity	Wizard Stop				
Information System: Sum of the phases First phase: Heaviest phase Last phase: Lightest phase	Cancel						
Project sheet: VLXE - Project							

Now select "OK" to generate the calculation.



Note how VLXE Blend captures the entire 2 phase area including the VLE and LLE lines. Plus it finds the LCEP where the 2 lines meet. PC-SAFT will trace the entire phase diagram. But since polymers decompose at higher temperatures, the built in stopping point is set to 600°C.



Now we want to find the VLLE area. We know it starts at the LCEP so we will use that information as an initial guess to start the routine that will calculate the VLLE line.

The LCEP is at 163°C and 19 Bar. Make a note of that and then select "Calculation" on the VLXE ribbon. Again select "Phase diagram" as the calculation type and select "Next". Now select "Trace Phase Boundary" and make the selection as given below. The starting point needs to be inside the 3-phase area and close to the phase boundary.



Select "Next" and under output select "OK" to generate the calculation.





The result is the phase boundary for the VLLE area.

Now merge the 2 charts to get the entire phase diagram. In Excel this can be done by Copy/Paste. The result is shown below:



Knowing the entire phase diagram is very important when performing process simulations. In the separation steps the 3-phase area is to be avoided, and looking at the chart above it can be seen that for this system the VLLE area is right on the separation path. The phase diagram above has been verifyed by experimental data and currently an HDPE producing company is using it to plan their separation process.



6.6 Polymer Mass Fraction vs Temperature (wT)

We have just plotted the entire phase envelope in the temperature vs. pressure space. If you imagine the polymer mass fraction of the mixture as the 3rd dimension, you get a temperature, pressure, polymer mass fraction (w) cube. The phase envelope is a "slice" of this cube in the temperature and pressure space. Now we will work with the 2 other possible slides, wT and wP.

First we will create a polymer mass fraction vs. temperature plot, from now on referred to as wT. In order to cover polymer mass fraction from 0 to 1 we have to generate 2 curves.

Select "Calculation" on the VLXE blend ribbon. Go to the page where the calculation is selected and click on "wT/wP".

VLXE Blend - Calculation Wizard					
Select Calculation					
O Bubble Kij		Next			
Cloud Point					
Critical Point		Back			
C Excess Enthalpy					
◯ Flash					
O Phase Envelope					
O Properties					
⊖ SLE					
🔿 Spinodal					
⊙ Tw/Pw					
O Surface Tension		Wizard Stop			
O Unit Operation: Mixer		Off			
O Unit Operation: LinkedPHFlash		Cancel			
Project sheet: VLXE - Project					

Select "Next" and set the input as given below.

VLXE B	lend - Calculation	Wizard		
Feed, In			Input	
	Name	Feed [Massfraction]	Our Up	Next
1	ETHYLENE	0.02	O Down	
▶ 2	n-HEXANE	0.078	Initial Mass Fraction	Back
		/ 7	Pressure [Bar] 50.0 Temperature Range for Initial Point [Celsius] Minimum 25 Maximum 800.0	Change Units
				Wizard Stop Off Cancel
Proje	ct sheet: VLXE - Pr	oject		



Note how only the solvent composition is required now. The other settings mean that the curve will start at a polymer mass fraction of 0.5 and then trace the phase boundary as a function of polymer mass fraction and temperature at a fixed pressure of 50 Bar.



Note how the curve starts at a polymer mass fraction of 0.5 and then follows the phase boundary as far as it can. PC-SAFT will model the entire curve even though it goes beyond the boundary of temperatures which are physically possible.

On the inside of the curve is the 2 phase area, and outside is the 1 phase.



In a similar way we will now repeat the calculation, only now we will go down in polymer mass fraction.

/LXE Blend - Calculation Wizard								
Feed, In	Input							
Name Fee [Massfra	d Direction in Mass Fraction Next							
▶ 1 ETHYLENE	0.02 O Down							
2 n-HEXANE	0.78 Initial Mass Fraction Back Back Change Units Back Back Back Back Back Back Back Back							
Project sheet: VLXE - Project	Wizard Stop							

Using the default output to generate the calculation, select "Next" and then "OK".



Note how the curve now starts at a polymer mass fraction of 0.5 and then follows the phase boundary down to 0 polymer mass fraction.





Now combine the 2 charts to get the entire phase boundary at 50 Bar.

The result shows how this mixture behaves at 50 Bar for a fixed ratio of solvents. Inside the curve is the 2 phase area and outside is the 1 phase.

6.7 Polymer Mass Fraction vs Pressure (wP)

The wP plot is generated just as for the wT plot. Select "Calculation" on the VLXE Blend ribbon. Select "wT/wP" as calculation and click on "Next". Set the input as shown below:

VLXE Blend - Calculation Wizard	
Feed, In	Input Disputies in Mana Facilities
Name Fe	raction Up
▶ 1 ETHYLENE	0.02 O Down
2 n-HEXANE	0.78 Initial Mass Fraction Back
7	0.5
	Tw Pw
	170
	Pressure Range for Initial Point [Bar] Minimum
	1.0 Change Units
	Wizard Stop
	Off
	Carcel
Project sheet: VLXE - Project	



Using the default output, select "Next" and then "OK". The calculation is now created.





In order to get the last part of the curve we repeat, the only change is that we now select "Down" as direction.

VLXE B	llend - Calculation	Wizard							
Feed, In			Input Direction in Mana Franking						
	Name	Feed [Massfraction]		Next					
▶ 1	ETHYLENE	0.02	O Down						
2	n-HEXANE	0.78	Initial Mass Fraction 0.5 Tw Pw	Back					
			Temperature [Celsius] 170 Pressure Range for Initial Point [Bar] Minimum 1.0 Maximum 400.0	Change Units					
				Wizard Stop					
Proje	Project sheet: VLXE - Project								

Again, select "Next" and then "OK" to generate the calculation.







Now combine the 2 plots to get the entire phase boundary.

Below the curve is the 2 phase area and above the 1 phase area. Try to verify with the phase envelope that the 2 curves meet at the right place. Keep in mind that the 2 curves are just 2 different slices of the same temperature, pressure, polymer mass fraction cube.

6.8 SLE

In this section we provide a description of Solid-Liquid calculations (SLE). It's an imperative calculation for systems containing polymers, since solid polymer is the end product. Here an assumption is made for SLE calculations, that being that the solid phase does not contain any solvent. When performing SLE calculations the thermodynamic model is not the same for the different phases. Liquid and vapor phases are modeled by using an equation of state (EOS) and the solid phase is modeled by using a separate model that can only be used for solid phases.

Two different versions of the same model are implemented:

- Original Pan & Radosz
- Full Pan & Radoz

Here the original Pan & Radoz model is used (For details see VLXE Blend Help)

VLXE Blend provides the following options for SLE calculations:

- Temperature
- Polymer Mass Fraction
- T/P Curve
- PMF/T Curve

SLE calculations need parameters which are used only for these calculations. They can be seen in the project sheet. The values used in these examples are shown below. Note the crystalline fraction.



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6.8.1 Temperature

This calculation will find the SLE temperature for a given pressure and composition. That is the temperature where the solid phase forms. This is important process information since solid deposition inside the plant is to be avoided.

Select "Calculation" on the VLXE Blend ribbon. Leave all components in and select "SLE" as the calculation type. Select "Next".



Select "Temperature" as the SLE calculation type, add feed and then select "Next". Then "Next" to get row output format and then "OK" for default output.

Feed, In Name 1 ETHYLENE 2 n-HEXANE	Feed [Massfraction]	Input Pressure [Bar] 10.00		
Name 1 ETHYLENE > 2 n-HEXANE	Feed [Massfraction]	Pressure [Bar]	Terreture	
1 ETHYLENE 2 n-HEXANE	0.00		Temperature	Next
▶ 2 n-HEXANE	0.02		Polymer Mass Fraction	
	0.78		T/P Curve	
3 HDPE	0.2		PMF/T curve	Back
Project sheet: VLXE - Pr	oject			Change Units Wizard Stop Off Cancel





The calculation is then created. Note that below 87.4°C a solid phase will form for this system.

6.8.2 Temperature/Pressure Curve

The temperature/pressure (T/P) curve will calculate the phase boundary between solid forming and not forming. Together with the phase envelope it gives a very clear picture that can be used in process design.

VLXE BI	end - Calculation	n Wizard							
Feed	, In		Input						
	Name	Feed [Massfraction]	Initial Pressure [Bar] Temperature Temperature	Next					
▶ 1	ETHYLENE	0.020000	Maximum Pressure [Bar] Polymer Mass Fraction	n					
2	n-HEXANE	0.780000	300 T/P Curve						
3	HDPE	0.200000	Step Size [Bar] 10.0 PMF/T curve	Change Units Wizard Stop					
Projec	Project sheet: VLXE - Project								

Select "Calculation" on the VLXE Blend ribbon, select SLE and then "Next".

Select "T/P Curve" and set the input as given above. Then select "Next" and then "OK" using the default output. The calculation is now created.



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Note the temperature range. The line is very vertical.

Now combine this plot with the phase diagram we made before.

The phase diagram is now complete with SLE information. For this mixture the SLE, VLE, LLE and VLLE region has now been defined, thereby facilitating process decisions to be made safely.





6.8.3 PMF/T Curve

This calculation lets the user fix pressure and obtain the phase boundary as a function of polymer mass fraction (PMF) and pressure. It is similar to what was done earlier for the wT and wP curves, except that we now look for SLE phase boundaries.

To set up this calculation, go again to the SLE calculation page in the wizard and make the selections as indicated below. Then create the calculation using the default output.



The result is shown below. Below the curve a solid phase forms, while above the curve it doesn't. Note how little the curve changes with respect to changes in the polymer mass fraction in the mixture.





6.8.4 Polymer Mass Fraction

This will calculate the polymer mass fraction where a solid phase is formed at a fixed temperature and pressure. Once the temperature range from the PMF/T curve is known, the polymer mass fraction can be calculated. It is recommended to perform a PMF/T calculation before this calculation, doing so will provide an approximate temperature value. If the temperature is defined as being outside the maximum limit, then no solution will be found.

Create the calculation as before, using the input as shown below. However, make sure to select "Function Range" as output.

VLXE Blend - Calculation Wizard							
Feed, In			Input				
	Name	Feed [Massfraction]	Temperature [Celsius]	Temperature	Next		
1	ETHYLENE	0.02	-Pressure [Bar]	Polymer Mass Fraction			
•	2 n-HEXANE	0.78	1	T/P Curve	Back		
				PMF/T curve			
					Change Units		
					Wizard Stop		
					Off		
					Cancel		
Project sheet: VLXE - Project							

Select function range (range output) and click "OK".

VLXE Blend - Calculation Wizard						
Select Output Type Select Extra Output:	ОК					
	Back					
	Wizard Stop					
Information	Off					
Function row: The results are given in just one row. You define the output your self Function range: The output is given in a range of the sheet. The output is fixed by the program.	Cancel					
Project sheet: VLXE - Project						


In the result below note how only polymer is in the heavy phase. Also note how VLXE Blend calculates the distribution and how only the heavy pseudo components are in the solid phase.



6.9 Spinodal

During the separation of components it is important to have an idea about the spinodal curve. VLXE Blend calculates the Spinodal for all supported systems. With the given thermodynamic model of system, one can calculate the set of compositions which form the boundary between the metastable and the truly unstable compositions. This set of compositions, which form a curve within the two phase area, is called the Spinodal curve.

The Spinodal is also handy if a new system is completly unknown; for polymer systems the Spinodal is often close to the phase boundary, so knowing the Spinodal gives a very good idea of the phase envelope.



Select "Calculations" on the VLXE Blend ribbon. Select "Spinodal" as calculation and select "Next".

VLXE Blend - Calculation Wizard	
Select Calculation	
O Bubble Kij	Next
Cloud Point	
Critical Point	Back
C Excess Enthalpy	
◯ Flash	
O Phase Envelope	
O Properties	
⊖ SLE	
Spinodal	
○ wT/wP	
O Surface Tension	Wizard Stop
O Unit Operation: Mixer	Off
O Unit Operation: LinkedPHFlash	Cancel
Project sheet: VLXE - Project	

Enter Feed and select "Temperature, Pressure" as the Spinodal type. Select "Next" and then "OK" using the default output.

Feed, In Input Input Curve Type (Temperature, Pressure): TP (Polymer Mass Fraction, Pressure): wP Back HDPE 0.20000 HDPE 0.20000 With the second sec	١	LXE BI	end - Calculation	Wizard	
Name Feed [Massfraction] > 1 ETHYLENE 0.020000 2 n+HEXANE 0.780000 3 HDPE 0.200000 Back Back Change Units Wizard Stop Off Cancel	ſ	Feed	, In		Input
I ETHYLENE 0.20000 (Polymer Mass Fraction, Pressure): wP Back 3 HDPE 0.20000 Ethylene			Name	Feed [Massfraction]	Curve Type Next Next
2 n+HEXANE 0.780000 3 HDPE 0.200000 Back Image: Contraction of the		▶ 1	ETHYLENE	0.020000	O (Polymer Mass Fraction, Pressure): wP
3 HDPE 0.200000 Change Units Wizard Stop Off Cancel		2	n-HEXANE	0.780000	
Change Units Change Units Wizard Stop Off Cancel		3	HDPE	0.200000	Back
Project sheet: VLXE - Project		Projec	:t sheet: VLXE - Pr	roject	Change Units Wizard Stop



The Spinodal result is shown below. Note how it has an almost vertical line at lower pressures. The lower temperatue curve will continue to a very high pressure, as illustrated here.



The best way to see the Spinodal is in combination with the phase envelope, as shown below. Note how close the Spinodal is to the phase boundary and how it does not detect the 3 phase area.





6.10 Critical Point

Critical point specifies the conditions (temperature, pressure) in which the liquid state of matter ceases to exist. It is also known as "Critical State". VLXE Blend can calculate the critical point for all supported systems. Note that a system may not have a critical point, or that it may have multiple critical points.

Select "Calculation" on the VLXE Blend ribbon. Leave all components in and under calculations, select "Critical Point".

VLXE Blend - Calculation Wizard					
Select Calculation					
O Bubble Kij		Next			
Cloud Point					
Critical Point		<u>B</u> ack			
Excess Enthalpy					
◯ Flash					
O Phase Envelope					
O Properties					
◯ SLE					
O Spinodal					
○ wT/wP					
O Surface Tension		Wizard Stop			
O Unit Operation: Mixer		Off			
O Unit Operation: LinkedPHFlash		Cancel			
Project sheet: VLXE - Project					

Select "Next" and now select "Temperature, Pressure" critical point.

Name	Feed [Massfraction]	Curve Type () (Temperature, Pressure): TP	Next
ETHYLENE	0.02	O (Polymer Mass Fraction, Pressure); wP	
n-HEXANE	0.78		
HDPE	0.2		Back
			Change <u>U</u> nits
			Wizard Stop Off Cancel
B	THYLENE THEXANE HDPE	ETHYLENE 0.02 h-HEXANE 0.78 HDPE 0.2	ETHYLENE 0.02 hHEXANE 0.78 HDPE 0.2



Select function row (single row output) as an output. On the next page simply select "OK", using the default output.

Critical temperature, pressure and number of critical points are calculated and are given below. For this solvent/polymer system with a given feed composition there is only one critical point. Note that the location of the single critical point is far outside the physical region.

Sheet		Calculations								Wizards	
	: X ECriticalPointTP(B3:D3; E3; F3; G3) 										
A	В	С	D	E	F	G	Н		J	К	L
	ETHYLENE	n-HEXANE	HDPE [Ma	Output	Compone	Units	Temperat	Pressure [Number o	f Results [·	·]
	0,02	0,78	0,2	T,P,NOR	All	C(In,Mass	1105,041	80,01921	1		



7) Properties

All the properties like: temperature, pressure, enthalpy entropy, heat capacity, compressibility factor, molecular weight etc. can be calculated with VLXE Blend. Both standard properties, like fugacy values including analytical derivatives for example, can be obtained. We will use the methanol/cyclohexane system from before as an example.

7.1 Standard Properties

Select "Properties" in the calculation wizard.

VLXE Blend - Calculation Wizard					
Select Calculation					
O Bubble Kij		Next			
O Cloud Point					
O Critical Point		Back			
O Excess Enthalpy					
O Fitting					
O Flash					
O Phase Envelope					
Properties					
🔿 Spinodal					
О Тху/Рху					
O Surface Tension					
Viscosity		Wizard Stop			
O Unit Operation: Mixer					
O Unit Operation: LinkedPHFlash		Cancel			
Project sheet: VLXE - Project					

Select "Properties" as "Calculation type" and "Temperature/Pressure" as the variable. Note how VLXE Blend allows all 3 possible combinations of Temperature/Pressure/Volume.



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Feed, In		Input		
Name 1 METHANOL 2 CYCLOHEXANE	Feed [Massfraction] 0.500000 0.500000	Temperature [Celsius] 250.0 Pressure [Bar] 1.0 Volume Type	Temperature/Pressure Temperature/Volume Pressure/Volume	<u>N</u> ext Back
	_	Auto Liquid Vapor Select Calculation Type Property Ln(Fugacity) Ln(Fugacity coefficients)		Change Units
		Chemical potentials		Wizard Stop Off Cancel

3. Click "Next" and there are two options to select output type. Here "Function range (Range output)" is selected and then click "OK".

VLXE Blend - Calculation Wizard					
Select Output Type	ОК				
Function row (Single row output)					
Function range (Range output)	Back				
	Wizard Stop				
Information	Off				
Function row: The results are given in just one row. You define the output your self Function range: The output is given in a range of the sheet. The output is fixed by the program.	Cancel				
Project sheet: VLXE - Project					



 1		carcalatio	113			
• : × ✓	f _x {=Pro	operty_TP(B3:C3; D3;	E3; F3; G3;	H3; I3)}	
В	с	D	E	F	G	н
METHANOL [Massfract	CYCLOHEX	Temperat	Pressure [VolumeTy	Output	Comp
0,5	0,5	250	1	Auto	Fixed 2D	All
Temperature [Celsius]	250					
Pressure [Bar]	1					
Molar Volume [cm^3/r	43303,68					
Compressibility [-]	0,995547					
Density [g/cm^3]	0,001072					
Enthalpy [kJ/Kg]	-3482					
Entropy [kJ/(Kg Kelvin	1,053649					
Cp [kJ/(Kelvin kg)]	2,140254					
Cv [kJ/(Kelvin kg)]	1,954751					
JTCoeffient [Kelvin/Ba	0,967046					
Velocity of Sound [m/s	318,9033					
MolecularWeight [g/m	46,413					

4. All the fixed temperature and pressure properties are calculated in an Excel spreadsheet.

5. In a similar way the result from function row requires an additional step. Select "Function row (single row output)" from step 3 above and click "Next".

VLXE Blend - Calculation Wizard	
System Temperature Pressure Volume Density Enthalpy Entropy Cp Speed of Sound Surface Tension Bonding Fraction Average Molar Mass Viscosity	QK Back Wizard Stop
Information System: Sum of the phases	Off
Last phase: Lightest phase Project sheet: VLXE - Project	Cancel



6. Click "OK" and the density at a fixed temperature and pressure is calculated and is shown in a blue cell, see below. Now by a simple Copy/Paste inside Excel this can be calculated over an entire temperature, pressure or/and composition range.

\checkmark	✓ f _x {=Property_TP(B3:C3; D3; E3; F3; G3; H3; I3)}								
	D	E	F		Н	Ι	J		
								4	
DHEX	Temperat	Pressur	volumeTy	Output	Compone	Units	Density (S	Enthalpy (S) [ŀ
0,5	250	1	Auto	D(S),H(S)	All	C(In,Mass	0,001072	-3482	



7.2 Lnfugacity Coefficients

Internal properties like fugacity can also be calculated. Use the same steps as before, but now select ln (Fugacity coefficients) and then "Next".

VLXE BI	end - Calculation	Wizard		
Feed,	, In		Input	
	Name	Feed [Massfraction]	Temperature [Celsius] Temperature/Pr	essure <u>N</u> ext
▶ 1	METHANOL	0.500000	Temperature/Vo	lume
2	CYCLOHEXANE	0.500000	Pressure [Bar] 1.0 Pressure/Volume	<u>Back</u>
			Volume Type Auto Liquid Vapor Select Calculation Type Property Ln(Fugacity) In(Fugacity)	Change Units
		/	Chemical potentials	Wizard Stop
Projec	t sheet: VLXE - Pr	oject		

Select "Function range" as output plus "Include dni" which are the analytial derivatives of the LnFc with respect to mole numbers and click "OK".

VLXE Blend - Calculation Wizard		
Select Output Type		Ōĸ
Function row (Single row output)		
Function range (Range output)		Back
	Include dni?	
	◯ No	
	⊙ Yes	
		Wizard Stop
Information		Off
Function row: The results are given in just one row. You Function range: The output is given in a range of the sh program.	eet. The output is fixed by the	Cancel
Project sheet: VLXE - Project		



7

The result is shown below. Note how all relevant derivatives are included. Please note that they are always given in internal units: Mole, bar, Kelvin and cm3.

*	: [\times	√ f _x	{=Lnfc_TP(B3:	C3; D3; E3; F3; G3;	H3; I3; J3)}			
	В		С	D	E		G	н	
MET	HAN	DL [Ma	CYCLOHEX	Temperature [C	Pressure [Bar]	Updatedni	VolumeTy	Output	Cor
		0,5	0,5	250	1	Yes	Auto	Fixed 2D	All
Resi	dual	F	Temperat	Pressure	Volume				
[mo	le]		[Celsius]	[Bar]	[cm3/mole]				
-0	,0044	49127	250	1	43303,68242				
]			
Nam	ne:		Lnfc [-]	d(Lnfc)/(dT) [Ke	d(Lnfc)/(dP) [Bar^	d(Lnfc)/(dV) [c	m3^-1]		
1: M	ETHA	NOL	-0,0042	5,23975E-05	-0,004203516	0			
2: C)	(CLOF	IEXAN	-0,00509	1,53129E-05	-0,005106855	0			
d(Ln	fc)/(d	dni) [n	1: METHAI	2: CYCLOHEXAN					
1: M	ETHA	NOL	-0,00149	0,003924542					
2: C)	(CLOF	IEXAN	0,003925	-0,010307997					



Appendix A

How Goal Seek works:

With this function, you can find a desired value for a formula in one cell by calling a different cell that then affects the first cell.

Define and solve a problem by using Goal Seek

1. On the Data ribbon, select "What-If Analysis", in the dropdown select "Goal Seek".

2. In the "Set Cell" box, enter a cell reference or name for the Set Cell. The Set Cell must contain a formula.

3. To have the Set Cell be a certain value, click "To Value", and then type the value in the box.

4. In the "By Changing Cell" box, enter a name or reference for the adjustable cell, the adjustable cell must be related directly or indirectly to the Set Cell.

5. Click "OK" to get the desired results.



Example

To understand this in a better way lets take a simple example.

1. We have an isenthalpic system, where we link 2 PH flash calculations. The feed and enthalpy are taken from the heavy phase from the first flash, see below. Note how the composition and enthalpy for the second flash is taken from the first flash calculation.

METHANE	ETHANE [n-OCTANE	n-NONAN	Temperat	Pressure [FlashType	Output	Compone	Units			
0,1	0,2	0,15	0,55	75	25	2	Fixed 2D	All	C(In,Mass			
Property	System	Feed	Phase 1	Phase 2								
Pressure [25		Time: 151			Pressure [Enthalpy [FlashType	Output	Compone	Units	
Temperat	75					1	-2121,69	2	Fixed 2D	All	C(In,Mass	ra
						Property	stem	Feed	Phase 1	Phase 2		1
Compone						Pressure	1		Time: 279			
METHANE	0,1	0,1	0,009661	0,359017		Temp rat	64,29908					
ETHANE [M	0,2	0,2	0,058799	0,604845								
n-OCTANE	0,15	0,15	0,197578	0.013585		ompone						
n-NONAN	0,55	0,55	0,733961	0,022553	7	METHANE ETHANE	0,009661	0,009661	0,00015	0,110389		
				0.500507		ETHANE [F	0,050,	0,058799	0,003873	0,640493		
Phase Fra			0,401463	0,598537			0,197578	0,197578	0,206794	0,099984		
Phase Fra	0 610057	0 100017	0,741413	0,258587		n-NONAN	0,733961	0,733961	0,789184	0,149134		
Compress Donsity In	0,012357	0,100217	0,135970	0,9318 0		Dhaco Fray			0 720520	0.260472		
Molar Vol	709 0246	116 0205	157 4427	0,0 2039		Phase Frai Dhose Frai			0,755520	0,200472		
Enthalov (-2428 52	-2/199 79	-2121.69	22/6 9/		Compress	0 262726	0.005564	0,913721	0,080273		
Entropy [-2430,32	-2400,75	-2121,05	-0.62667		Donsity [a	0,203720	0,0000004	0,000323	0,001197		
Cn [k]//Ke	2 387807	3 0/15789	2 /135121	2 2521/18		Molar Vol	7399 //22	156 1103	183 0783	27887.96		
Cy [k]/(Ke	1 970561	1 974316	2,433121	1 765743		Enthalov (-2121 69	-2149 53	-2069 38	-2675.68		
ITCoeffier	1,570501	0.03266	-0.03388	0.522705		Entropy [-0.48457	-0.61062	-0.57123	0.433151		
Velocity o		518,2766	847,9899	370.3314		Cn [k]/(Ke	2.31752	2,394954	2.352993	1.941853		
Molecular	54.0941	54.0941	99.89966	23.37042		Cy [k]/(Ke	1.986512	2.000922	2,015022	1.684581		
ThermalCo	,	0.084598	0.109855	0.03458		JTCoeffier	-,	-0.03501	-0.038	0.784108		
Viscosity [N/A	N/A	N/A		Velocity o		860,9668	918,9511	310,741		
Surface Te	N/A					Molecular	99.89966	99.89966	123,4307	33,09079		
						ThermalCo	, i	0,110257	0,123155	0,028298		
						Viscosity (N/A	N/A	N/A		
						Surface Te	N/A					

2. The goal is to adjust the pressure of the first flash in order to obtain a temperature of 45°C in the second flash.

3. Open "Goal Seek" and link the cells as shown below. Then click "OK".

IAN Temperat Pressure	[FlashType Output Compone Units	
,55 75 25	2 Fixed 2D All C(In,Mass	
1 Phase 2		
151	Pressure [Inthalpy [FlashType Output Compone Ur	nits
	1 -2121,59 2 Fixed 2D All C(In, Mass raction); C(Out, Massfraction); T(In, Ce
	Property System Feed Phase 1 Phase 2	
	Pressure [1 Time: 279	Goal Seek 2 X
561 0,359017	Temperat 64,29908	
799 0,604845		S <u>e</u> t cell: \$1\$9
578 0,013585	Compone	To <u>v</u> alue: 45
961 0,022553	METHANE 0,009661 0,009661 0,00015 0,11038	By changing cell: \$G\$3
	ETHANE [1 0,058799 0,058799 0,003873 0,640493	
463 0,598537	n-OCTANE 0,197578 0,197578 0,206794 0,099984	OK Cancel
413 0,258587	n-NONAN 0,733961 0,733961 0,789184 0,149134	
75 0.031005		



Goal seek will then run for a few seconds before it finds a solution. See below

Goal Seek Status	8 ×
Goal Seeking with Cell 19 found a solution.	Step
Target value: 45 Current value: 45,00001701	Pause
ОК	Cancel

4. The desired results are obtained and are shown below.

В	С	D	E	F	G	н	I	J	К	L	М	N
				_	_			_				
METHANE	ETHANE [n-OCTAN	n-NONAN	Temperat	Pressure	FlashType	Output	Compone	Units			
0,1	0,2	0,15	0,55	75	99,35261	2	Fixed 2D	All	C(In,Mass			
Property	System	Feed	Phase 1	Phase 2	1							
Pressure [99,35261		Time: 123			Pressure	Enthalpy	[FlashType	Output	Compone	Units	
Temperat	75					1	-2367,87	2	Fixed 2D	All	C(In,Mass	fraction);
_						Property	System	Feed	Phase 1	Phase 2		
Compone						Pressure [1		Time: 182			
METHANE	0,1	0,1	0,063857	0,447859		Temperat	45,00002					
ETHANE [I	0,2	0,2	0,169233	0,496121								
n-OCTANE	0,15	0,15	0,163748	0,017683		Compone						
n-NONAN	0,55	0,55	0,603162	0,038338		METHANE	0,063857	0,063857	0,000285	0,242897		
_						ETHANE [I	0,169233	0,169233	0,003916	0,634817		
Phase Fra			0,771547	0,228453		n-OCTAN	0,163748	0,163748	0,203595	0,051526		
Phase Fra			0,905879	0,094121		n-NONAN	0,603162	0,603162	0,792204	0,07076		
Compress	0,486017	0,372657	0,39828	0,782328								
Density [g	0,38201	0,498215	0,547325	0,097775		Phase Fra			0,37998	0,62002		
Molar Vol	141,6038	108,5758	116,0411	227,9359		Phase Fra			0,737967	0,262033		
Enthalpy [-2481,53	-2491,24	-2367,87	-3575,46		Compress	0,61964	0,97544	0,006765	0,995241		
Entropy [-0,80211	-0,83255	-0,74352	-1,36603		Density [g	0,003875	0,002461	0,689311	0,00102		
Cp [kJ/(Ke	2,631257	2,760557	2,599406	2,937811		Molar Vol	16391,1	25802,93	178,9446	26326,73		
Cv [kJ/(Ke	1,994649	1,992172	2,010821	1,838998		Enthalpy [-2367,87	-2111,51	-2114,31	-3081,99		
JTCoeffier		-0,00369	-0,02084	0,389553		Entropy [-0,42457	0,277995	-0,70753	0,372362		
Velocity o		641,4649	731,5833	368,9267		Cp [kJ/(Ke	2,186115	1,794351	2,276676	1,931067		
Molecular	54,0941	54,0941	63,51224	22,2865		Cv [kJ/(Ke	1,858262	1,65142	1,944517	1,61534		
ThermalCo		0,093858	0,099726	0,045328		JTCoeffie		1,618655	-0,04062	0,73366		
Viscosity [N/A	N/A	N/A		Velocity o		207,4572	970,3038	341,6042		
Surface Te	N/A					Molecular	63,51224	63,51224	123,3485	26,84155		
						ThermalC		0,02036	0,128354	0,027772		
						Viscosity		N/A	N/A	N/A		
						Surface Te	N/A					



Appendix B

How to Work with Array formulas

What are array formulas?

This is a Excel feature and is used extensively by VLXE Blend. It is simply a function call that gives output in more than one cell.

The use of an array function is explained with a phase envelope calculation. The method used will apply to any array function in Excel.

The figure below shows output in terms of temperature and pressure.

н	Ι	J	К	L	М	N	0	Ρ	Q
		ETHYLENE	n-HEXANE	HDPE [Ma	Output	Compone	Units		
		0,02	0,78	0,2	T,P	All	C(In,Mass	fraction);C	(Out,N
		Number:	Temperat	Pressure					
			[Celsius]	[Bar]					
		1:	-33,8786	1					
		2:	-26,1229	1,2					
		3:	-24,0255	1,257934					
		4:	-22,5083	1,300878					
		5:	-19,4574	1,389884					
		6:	-17,9383	1,435531					
		7:	-16,4172	1,482131					
		8:	-13,3541	1,578709					

Now we want to change the calculation so that density for the heavy phase becomes part of the output. In order to do this we have to expand the output area by one column more and additionally change the output argument of the function. Plus we have to change the output argument so this density is part of the result.

First we change the output. Select the cell that contains the output argument and select "Output" on the VLXE Blend ribbon.

/	VLXE VLX	E Blend					
,o	-		c	-& &			🛃 🌒
ing	Calculations [Distributions	Code Generate	Input Ou	tput Units	Names Ou	tput Sheet
		Wizards			Ut	ility	
I	J	К	L	М	N	0	Р
	ETHYLENE	n-HEXANE	HDPE [Ma	Output	Compone	Units	
	0,02	0,78	0,2	T,P	AIL	C(In,Mass	fraction);C(
	Number:	Temperat	Pressure				
		[Celsius]	[Bar]				
	1:	-33,8786	1				
	-				1	1	



Change the output by selecting the density for phase 1.



The selected density is now part of the Output. Note how the output area is too small to show the new values.

Ι	J	К	L	М	N	0	P
	ETHYLENE	n-HEXANE	HDPE [Ma	Output	Compone	Units	
	0,02	0,78	0,2	T,P,D(1)	All	C(In,Mass	fraction);C(Ou
	Number:	Temperat	Pressure				
		[Celsius]	[Bar]				
	1:	-33,8786	1				
	2:	-26,1229	1,2				
	3:	-24,0255	1,257934				
	4:	-22,5083	1,300878				
	5:	-19,4574	1,389884				
	6:	-17,9383	1,435531				



To expand the output area, select all the current output cell plus the next column (the blue area plus the column to the right).

Ι	J	К	L	М	N	0	Р
	ETHYLENE	n-HEXANE	HDPE [Ma	Output	Compone	Units	
	0,02	0,78	0,2	T,P,D(1)	All	C(In,Mass	fraction);C(
	Number:	Temperat	Pressure				
		[Celsius]	[Bar]				
	1:	-33,8786	1				
	2:	-26,1229	1,2				
	3:	-24,0255	1,257934				
	4:	-22,5083	1,300878				

Click in the formula bar and press Ctrl+Shift+Enter. The function is then recalculated and the output range extended over the entire selected range in the sheet. Density is now included in the output.

Ι	J	К	L	М	N	0	Р	
	ETHYLENE	n-HEXANE	HDPE [Ma	Output	Compone	Units		
	0,02	0,78	0,2	T,P,D(1)	All	C(In,Mass	fraction);C	(Out
	Number:	Temperat	Pressure	Density (1)			
		[Celsius]	[Bar]	[g/cm3]				
	1:	-33,8786	1	0,72501				
	2:	-26,1229	1,2	0,71838	[
	3:	-24,0255	1,257934	0,7166				
	4:	-22,5083	1,300878	0,715315				
	5:	-19,4574	1,389884	0,712738				
	6:	-17,9383	1,435531	0,711458				
	7:	-16,4172	1,482131	0,710178				
	8:	-13,3541	1,578709	0,707607				
	9:	-10,2575	1,680095	0,705015				

The new output cell does not have the correct color. So to make things look consistent, select it and then click on "Output" in the VLXE Blend Ribbon.

٧	IEW	VLXE	VLX	E Blend								
And Fitting S V V Wizards				Code Generate	input O	lutput	Units Uti	Names (Output :	Sheet	r C	
				1				Ι				
	I		J	K	L	M	1	N	• 0		Р	-
		ETH	YLENE	n-HEXAN 0,78	EHDPE [Ma	Output T,P,D(1)	Com All	pone	Units C(In,Ma	ass <mark>fracti</mark>	on);C((Oi
		Nur	nber:	Tempera	t Pressure	Density	(.)					
		1:		-33,8786	(Bai) j 1	0,7250	1					
		2: 3:		-26,1229 -24,0255) 1,2 5 1,257934	0,7183 0,716	8					



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