Prode Properties

Properties of pure fluids and mixtures

User’s Manual rel. 1.2

PRODE
www.prode.com

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License agreement

Agreement made between Prode "Prode" and "User".

- Prode is the owner of the product "Prode Properties" including , but not limited to, dynamic link libraries, static libraries, header files, sample programs, utility programs, together with the accompanying documentation collectively known as the "software",
- User desires to obtain the right to utilize the software, the parties hereby agree as follows

Personal license
A version with limited features is available for personal use at home or in educational establishments for teaching purposes, all other applications, without first obtaining a commercial license from Prode, are expressly prohibited.

Commercial license
Upon full payment of the license fee the User has full right to utilize the purchased number of units of the software, a unit is defined as one copy of the software or any portion thereof installed on one stand-alone computer, for networked computers one unit shall be applied for each user having concurrent access and one unit shall be applied for the server.

For all applications

- Prode grants the nonexclusive, nontransferable right to use the software.
- User has a royalty free right to reproduce and distribute the software as available from Prode Internet server (personal licence) provided that User doesn't remove or alter any part of the software or of the licensing codes and threat the software as a whole unit.
- You cannot decompile, disassemble or reverse engineer the files containing the licensed software, or any backup copy, in whole or in part.
- You cannot rent, lease or sublicense the Licensed Software without express agreement by Prode.
- The software is provided “as is, where is” , Prode does not warrant that software is free from defects, or that any technical or support services provided by Prode will correct any defects which might exist.
- Prode shall not be liable for any damages that may result directly or indirectly from the use of these software programs including any loss of profits, loss of revenues, loss of data, or any incidental or consequential damages that may arise out of use of these software.
- Your license is effective upon your acceptance of this agreement and installing the Licensed Software.
- This license agreement shall remain in effect until the Licensed Software will be in use.
- You may terminate it at any time by destroying the Licensed Software together with all copies. It will also terminate if you fail to comply with any term or condition of this Agreement. You agree upon such termination to destroy all copies of the Licensed Software in any form in your possession or under your control.

Customer support

Prode will provide the licensee with limited technical support by telephone, or by electronic media for a period of 60 days after delivery of the product.

How to contact Prode

you can contact Prode by phone, web page or email, the details are available at http://www.prode.com

How to obtain technical support

we welcome your comments or suggestions about our program. On request we will also provide information on the internal methods used. While the program has been tested carefully to ensure proper operation, it still may be possible for an unusual situation to result in an error. We will have a much greater chance of fixing or assisting with errors and problems if they are provided to us in a form that is repeatable.

In reporting a problem to us, the following information should be given:

- customer reference
- the version of the software
- a copy of the procedure you are running and if possible the input data
- a detailed description of what you were doing (sequence of operations) when the problem occurred
- any additional information you think may describe the problem

Introduction

Prode Properties includes a comprehensive collection of procedures to solve problems such as :

- Physical Properties Data
- Heat / Material Balance
- Process Simulation
- Process Control
- Equipment Design
- Separations
- Instrument Design
- And more ....

Technical features overview

Entirely written in C++ from the origin Properties for Windows (different versions for Android, Linux etc. are available) is released in form of Dynamic Library (DLL, Active X) for direct access from Windows applications (Microsoft Excel, , Visual Studio applications including NET, Borland applications, MATLAB, MathCad etc.).

- Windows XP, Wndows Vista, Wndows 7 / 8 etc.
- support for up to 500 different streams with up to 100 components per stream (user can redefine)
- Several compilations of chemical data and BIPs are available, the user can add new components and BIPs
- Comprehensive set of thermodynamic models
- A complete set of flash operations T-P, H-P, H-T, S-P, S-T, V-P, V-T, H-V, S-V, H-S, constant energy, phase-fraction...

‘ Functions for calculating specific properties of mixtures (critical point, Cricodentherm, Cricondenbar, cloud point etc.)

- Functions which calculates values and derivatives of fugacities, enthalpy, entropy, volume vs. temperature, pressure, composition
- Functions which return equilibrium lines at specified phase fractions (generation of phase diagrams)
- Functions for simulating operating blocks as mixer, gas separator, liquid separator, distillation column, compressor, pipe
- Functions for component property access (from database)
- Functions for stream property calcs (density, conductivity and viscosity for both gaseous and liquid phase, surface tension, speed of sound, Joule Thomson etc.)

Dynamic Link Libraries

A dynamic-link library is a binary file that acts as a shared library of functions that can be used simultaneously by multiple applications. these libraries are compatible with almost all Microsoft Windows applications and being compiled code they run very fast. They also integrate tightly with your application, allowing it to run as an autonomous program unit rather than being dependent on external modules of a different application.

Prode Properties includes file I/O , graphical interfaces etc. for a total of about 200000 lines of code, all the code (compiled with last version of Microsoft C++ compiler) resides in a library , ppp.dll of about 7 Mbytes , it’s a very compact and efficient code, easy to distribute with your application.

Reference Literature

Although Prode Properties may appear easy to utilize also to people without a background in chemical engineering a basic knowledge in this area is useful for selecting the proper methods and critically evaluate the results. There are good books available, we would suggest some titles :

- Introduction to Chemical Engineering Thermodynamics, Smith, Van Ness, Abbott , McGraw-Hill
- Chemical and Engineering Thermodynamics, Sandler, Wiley
- The Properties of Gases & Liquids, Reid, Prausnitz, Poling , McGraw-Hill

What's new

Release 1.1 [1994]
First version of Prode Properties (author Roberto Paron) as part of Prode Calculator, a tool distributed since 1994

Release 1.1f [1995]
Updated the UNIFAC model, included different options for calculating gas fugacity with liquid activity models.

Release 1.1g [1996]
User can define units of measurement via edCS() method.

Release 1.1g1 [1996]
Added a set of extended functions for direct access from spreadsheets, read the paragraph "Accessing Properties from spreadsheet's cells" for additional information.

Release 1.1h [1996]
Included a procedure for defining the path to the working directory of program, now the file Properties.dll can reside in the "system" directory of Windows while the other files on a different directory. Modified the licensing scheme, the user receives a signature file, this permits to distribute the software via internet.

Release 1.1h1 [1997]
Revised the base class for managing memory, now the users can specify the number of streams, the number of components per stream, the number of components in database etc. , additional information on paragraph "Configure Properties".

Release 1.1h2 [1997]
Included the procedure edST() which permits to define the title when accessing the Stream's dialog, included procedures for defining via software the units of measurement, modified methods setKM(), getKM().

Release 1.1i [1998]
New installation procedure.

Release 1.12 [1999]
New methods StrSGH(), StrSLH(), StrSGS(), StrSLS(), StrmCopy().

Release 1.13 [2002]
New methods AOpen, ASave, editSS, StrN, MStrN, putN, MputN, getSUMS(), MgetSUMS()

Release 1.14 [2002]
New methods StrHC, StrFML, StrFMH, EStrHC, EStrFML, EStrFMH

Release 1.15 [2005]
New methods getOM, setOM

Release 1.16 1-5 [2009]
upgraded dialog interface

Release 1.17 [2010]
included method PIPE

Release 1.18 [2010]
included methods HPFORM, HTFORM

Release 1.2 [2012]
maintenance version for porting in different platforms

Features available vs. Versions	**Personal**	**Base**	**Extended (**)**
Database with more than 1600 chemicals		x	x
Database with more than 25000 BIPs		x	x
SRK, PR (vdW mixing rules)	x	x	x
SRK, PR (WS mixing rules)	x	x	x
LKP, BWRS, GERG, AGA, Steam Tables	x	x	x
UNIFAC,UNIQUAC,NRTL,Wilson	x	x	x
CPA (with association)	x	x	x
Solid Solution Model	x	x	x
SRK, PR (HV mixing rules)			E1
SRK, PR (MHV mixing rules)			E1
SAFT (with association)			E1
GERG (2008)			E1
BWR			E1
Pitzer , NRTL (electrolytes)			E1
Derivatives vs. P,T,W of Fg, H, S, V		x	x
Properties of fluids and mixtures	x	x	x
Vapor Liquid solid isothermal flash operation	x	x	x
Vapor Liquid Pf-T, Pf-P flash operations	x	x	x
Vapor Liquid solid H-P, S-P, V-P flash operations	x	x	x
Complete set of flash operations (Pf,H,S,V)			x
Vapor-Liquid phase diagram	x(*)	x	x
Vapor-Liquid-Liquid phase diagram	x (*)	x	x
Vapor-Liquid-Solid phase diagram			E2
VLE-LLE-SLE data regression	x	x	x
Raw data regression utility	x	x	x
Characterization of petroleum fractions			E2
Hydrate formation (multiphase with std. model)	x (*)	x	x
Hydrate formation (multiphase with complex model)			E2
Multiphase (gas,liquid) pipeline with heat transfer			E2
Isentropic nozzle HEM . HNE	x	x	x
Isentropic nozzle HNE-DS , NHNE			E2
Polytropic stage, single phase (gas)	x	x	x
Polytropic stage, multi phase (gas+liquid)		x	x
Distillation column (gas-liquid)	x (*)	x	x
Distillation column (gas-liquid-liquid and liquid-liquid)			E3
Depressuring unit (blow-down)			E3
Reactions			E3

(*) simplified procedures with limited features (**) extended versions available with distribution license

Installing the program

this paraghaph provides information about system requirements, procedures on installing Prode Properties software and upgrading from previous versions.

Sistem requirements

- Microsoft Windows XP, Vista, 7, 8 or later compatible system
- 1GB of RAM installed (if used in union with Microsoft Excel or other applications)
- 20 MB of available hard-disk space

Installation procedure

1) download the last version of the program from Prode server :

http://www.prode.com

2) if there are previous installations of Prode Properties uninstall the previous version

3) run the program, the automatic installation procedure will do the work for you, follow the on-screen installation instructions note : in some operating system you must be logged as a user with administrative privileges to make the necessary changes, if you do not have administrative privileges, contact your system administrator for assistance.

To uninstall a Prode Properties installation

Use the Add / Remove Programs utility in the Windows Control Panel, the procedure does all the work for you.

Obtain the licence

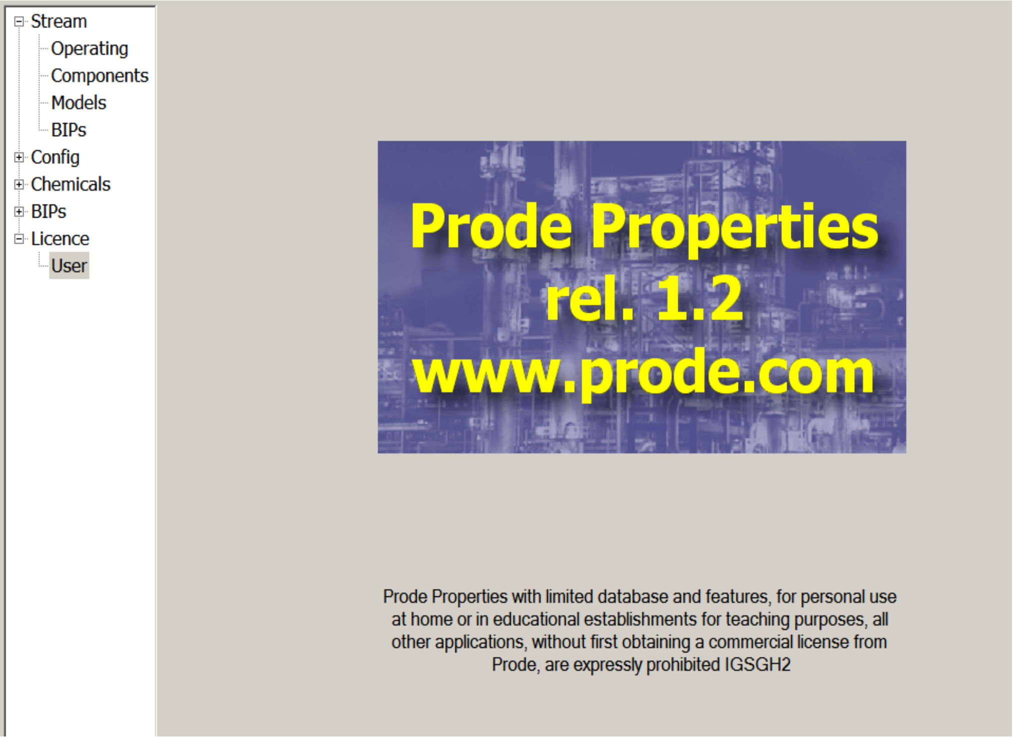
Prode Properties is copy-protected, your personal copy has limited features and to access all the features you must obtain a licence from Prode, there are se veral types of licence

- software copy protection (distribution via email, installation on a single computer identified by an installation code)
- hardware (dongle) copy protection (we ship the dongle, installation on single or multiple computers)
- network installation

Order a software copy protection licence

the licence file is based on the installation code which the program generates automatically.

- Run an applications which does access Prode PROPERTIES, once in the Properties editor the licence page will show the installation code ID (see below, it’s the string **IGSGH2**)
- when placing the order, specify the installation code



Prode Properties with limited database and features, for personal use at home or in educational establishments for teaching purposes, all other applications, without first obtaining a commercial license from Prode, are expressly prohibited IGSGH2

Order a hardware copy protection licence

There are versions for stand-alone computer and network-connected computers, please contact Prode for details

Prode Properties Quick Start

With Prode Properties you can solve complex problems with only minor programming effort. Much of the functionality is provided by the library. In this chapter you will learn step by step how to access Properties from your favourite application. This chapter is for those of you that want to skip the tutorial and immediately start using Properties. In the following sections, you will learn how to utilize the samples provided with Properties. When you run the samples you will get a broad overview of the possibilities available from using Properties, you will notice the following features:

- The Properties editor permits a simple and quick access and editing of all data including streams, units, databases.
- The user can define on each different stream : compositions, operating conditions , BIPs, thermodynamic models per property (fugacity, enthalpy, entropy, volume)
- The Properties library solves problems as multiphase equilibrium, critical points etc.
- Specific methods are provided for diagnostic / error messages
- Results of flash operations, transport properties etc. can be retrieved easily into your application

Locating and testing the sample files

As default the sample files, including data files, project files, and other associated files are supplied with the program and placed in subdirectories under Prode main directory.

MPORTANT

The installation procedure creates a directory \Prode\ and different subdirectories

\Prode\C	includes definitions and code for C / C++ applications
\Prode\Excel	includes samples for Microsoft Excel
\Prode\LIB	includes the versions of the library
\Prode\MATLAB	includes definitions and code for MATLAB applications
\Prode\MATHCAD	includes definitions and code for MATHCAD applications
\Prode\Fortran	includes definitions and sample code for Fortran applications
\Prode\NET\VBprops	includes definitions and samples for Microsoft NET VB applications
\Prode\NET\C#-props	includes definitions and samples for Microsoft NET C# applications

Data files folder

IMPORTANT

When running Properties requires to access several files, these are placed in a directory \Prode\ in user space to avoid possible conflicts with code reserved areas, the exact path depends from Windows version and settings, for example in Windows XP they could be placed in C:\Documents and Settings\All Users\Application Data, the list of files includes

chem.dat
pseudo.dat
bips.dat
mod.dat
def.ppp
res.lan
lic.dat
....

do not remove or rename these files, if Prode Properties cannot access these files (for example because they have been disseminated in different directories) an error message “Corrupted file, error reading data file” will be generated.

Getting Started from Microsoft Excel

IMPORTANT the different versions (32 or 64 bit) of Excel require different versions of Prode dll library, (Excel 32 requires Prode dll 32 bit while Excel 64 requires Prode dll 64 bit), when installing Prode Properties you must select the version suitable for your copy of Excel

IMPORTANT Microsoft Excel support files are located in the directory \Prode\Excel

IMPORTANT Define the proper separator (to be used in Macros) in Excel Reegional Settings, here we assume ‘,’ as separator, you may wish to utilize a different separator, for eample =EStrGD(1;300;1.0E5) instead of =EStrGD(1,300,1.0E5)

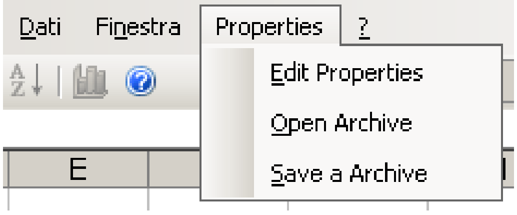
IMPORTANT as first step you must load the add-in (file properties.xla) which instructs Excel about Prode Properties library, you need to go through this procedure only once, to load the add-in

Excel 2003
open Excel and choose the Tools/Add-ins menu item, you’ll see a list of add-ins, some checked, some not checked. If Prode Properties isn’t listed (and it won’t be unless you went through this procedure earlier) browse for the properties.xla file in Excel folder then back your way out. Now Prode Properties should be listed in the list of add-ins, its box should be checked, and you should see a Prode Properties menu in Excel. If you close Excel and then reopen it Prode Properties menu must still be there. Once you installed the add-in you'll be able to access Prode Properties from within Excel (see below)

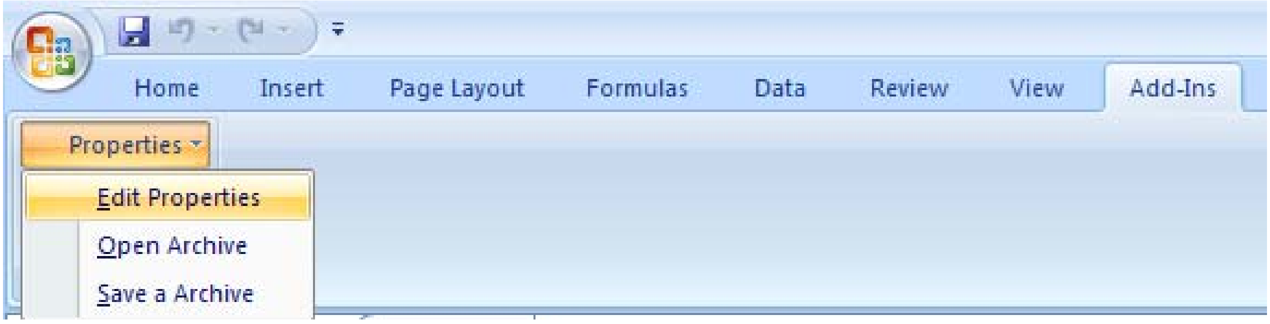
Excel 2007 and more recent versions
open Excel and choose Excel Options item, then Add-Ins, on the bottom select Manage Excel Add-Ins and click Go, you’ll see a list of add-ins, some checked, some not checked. If Prode Properties isn’t listed (and it won’t be unless you went through this procedure earlier) browse for the properties.xla file in Excel folder then back your way out. Now Prode Properties should be listed in the list of add-ins, its box should be checked. If you click on Add-Ins you should see the Properties menu (see below).

Working with Excel
The Properties Add-In creates a menu which permits direct access to Properties Editor, save and load archives.

In Excel 2003 Properties adds a new item in main menu

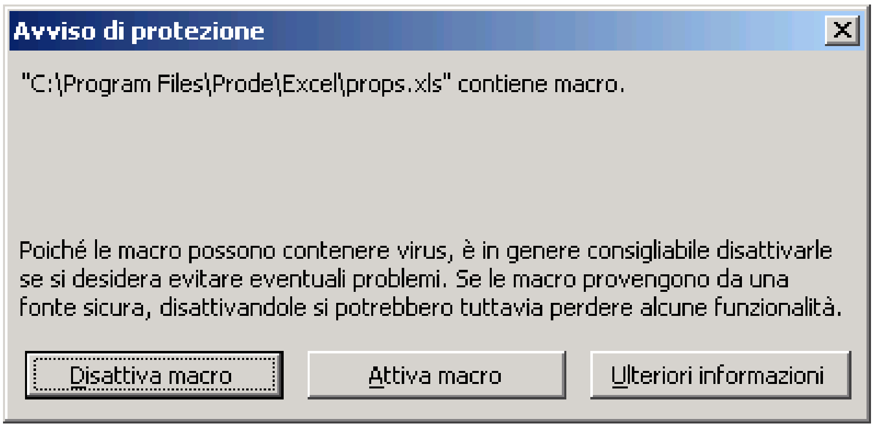


In Excel 2007 to access Properties menu click on Add-Ins and then Properties



MPORTANT

Excel 2003 , Security Alert Macro
when opening Properties files in Excel 2003 you may be requested to fix a (Macro) Security Warning (see below) issued by Excel



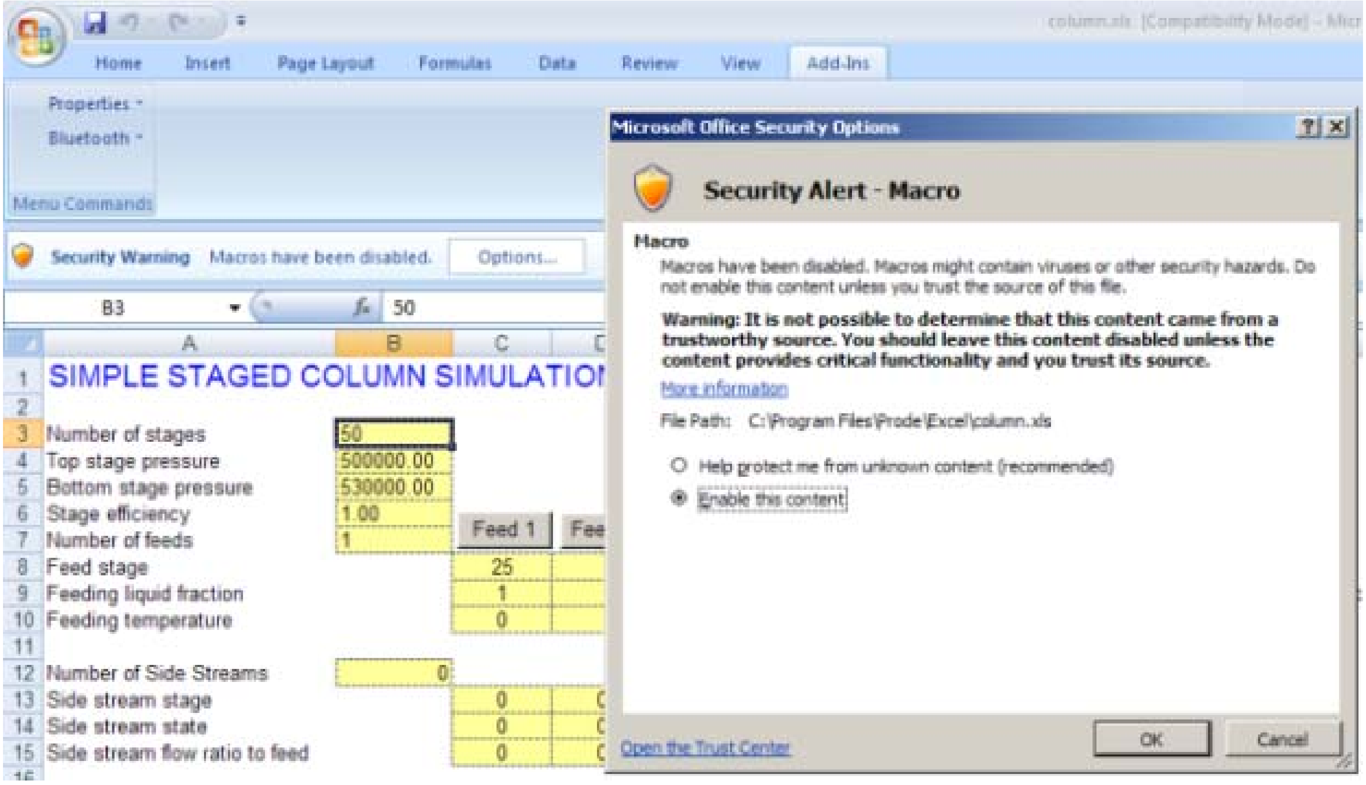
Avviso di protezione

"C:\Program Files\Prode\Excel\props.xls" contiene macro.

Poiché le macro possono contenere virus, è in genere consigliabile disattivarle se si desidera evitare eventuali problemi. Se le macro provengono da una fonte sicura, disattivandole si potrebbero tuttavia perdere alcune funzionalità.

To fix the Security Warning click Enable Macro in Security Alert dialog

Excel 2007 , Security Alert Macro
when opening Properties files in Excel 2007 you may be requested to fix a (Macro) Security Warning (see below “Security Warning Macros have been disabled”) issued by Excel



Security Warning Macros have been disabled.

SIMPLE STAGED COLUMN SIMULATIO

	A	B	C	D
3	Number of stages	50		
4	Top stage pressure	500000.00		
5	Bottom stage pressure	530000.00		
6	Stage efficiency	1.00		
7	Number of feeds	1	Feed 1	Fee
8	Feed stage		25	
9	Feeding liquid fraction		1	
10	Feeding temperature		0	
11				
12	Number of Side Streams	0		
13	Side stream stage		0	C
14	Side stream state		0	C
15	Side stream flow ratio to feed		0	C

Microsoft Office Security Options

Security Alert - Macro

Macro

Macros have been disabled. Macros might contain viruses or other security hazards. Do not enable this content unless you trust the source of this file.

Warning: It is not possible to determine that this content came from a trustworthy source. You should leave this content disabled unless the content provides critical functionality and you trust its source.

More information

File Path: C:\Program Files\Prode\Excel\column.xls

○ Help protect me from unknown content (recommended)

● Enable this content

To fix the Security Warning click the Options button and select Enable this content in Security Alert dialog

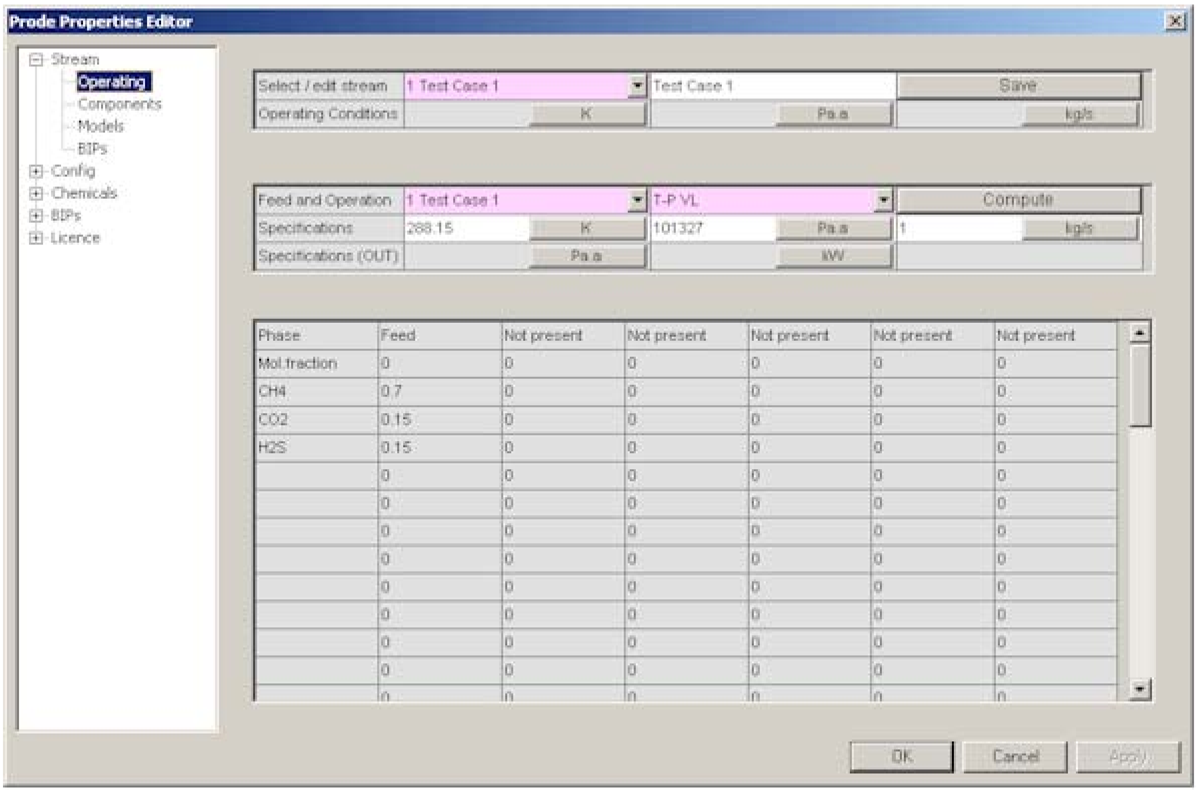
<span style="color:red">**IMPORTANT**</span>

before to evaluate the sample files read the paragraph "Working with archives, save and load data, default settings"
while working in Microsoft Excel use the commands "Open Archive" and "Save a Archive" to save and restore data

IMPORTANT

the values indicated in this manual as results of some operations can be different when calculated with software due to the different values of chemical's properties and BIP's stored in different versions of the software.

A simple way for accessing Prode Properties from Excel is to use the methods as macros within the cells, supposing we have created a worksheet for solving some problem and we need the values of gas and liquid densities at some specified temperature and pressure, first we need to define the stream and the units, from Properties menu select Edit Properties to define compositions and the units of measurement .



Select / edit stream	1 Test Case 1	Test Case 1	Save
Operating Conditions	K	Pa a	kg/s

Feed and Operation	1 Test Case 1	T-P VL	Compute
Specifications	288.15 K	101327 Pa a	1 kg/s
Specifications (OUT)	Pa a	kW	

Phase	Feed	Not present	Not present	Not present	Not present	Not present
Mol.fraction	0	0	0	0	0	0
CH4	0.7	0	0	0	0	0
CO2	0.15	0	0	0	0	0
H2S	0.15	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0

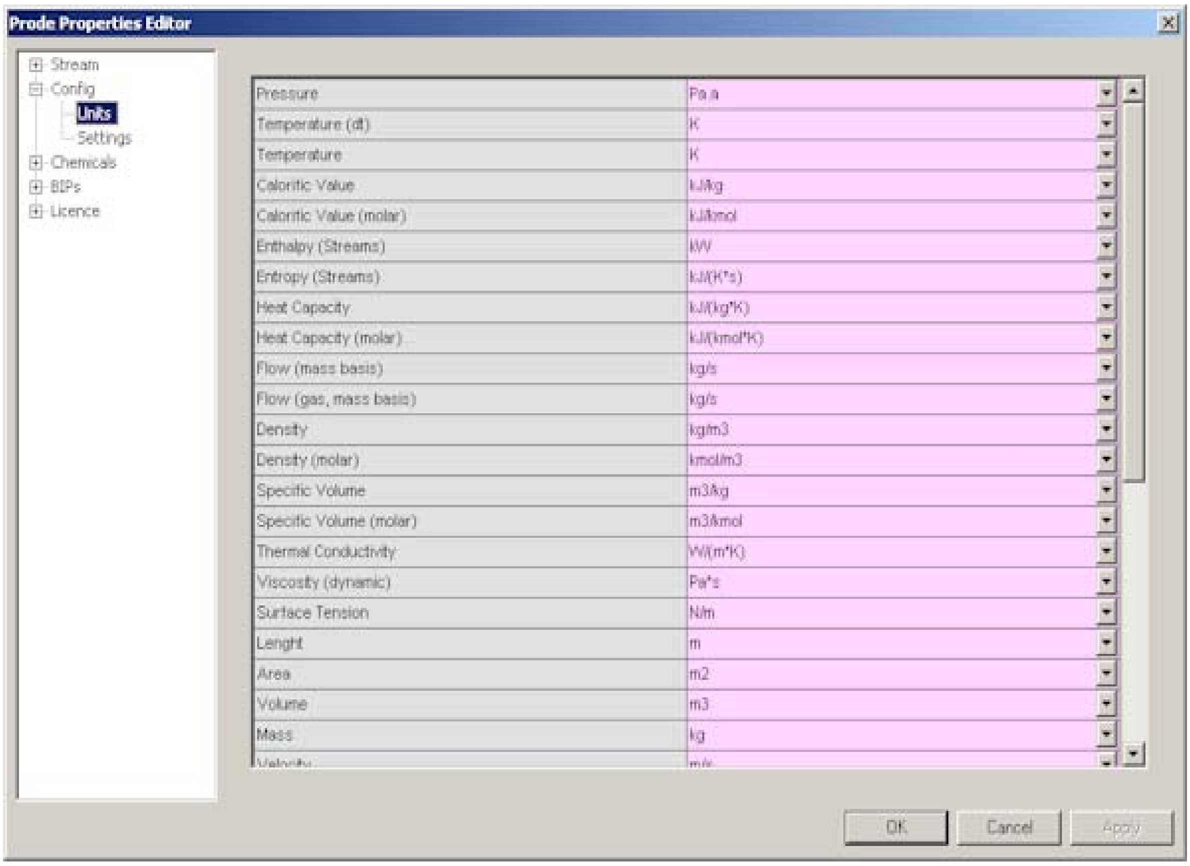
Notice that for the first stream (for editing the different streams use the Select edit stream combo) there is a mixture of three components already defined, you can change the list of components and compositions from Stream->components and models from Stream->models.

MPORTANT

Once you modify a list of components it is recommended to edit also Models and BIPs dialogs, differently Properties adopts default values.

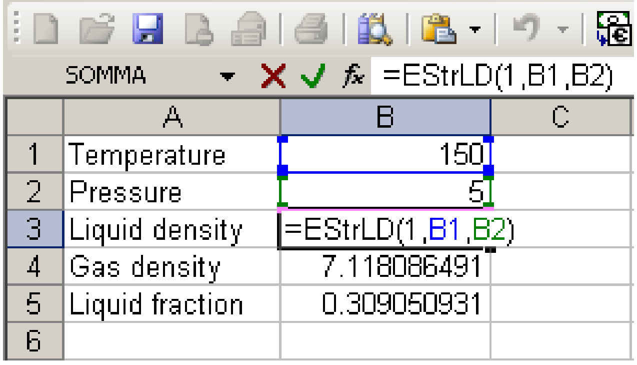
If you modify something do not forget to click the Save button before to edit a different stream or leaving the dialog ! Differently changes will be lost.

once defined the stream we need to define the units which we wish to utilize in our problem, for the pressure (first row) select Bar.a , notice that unit for temperature is K and density Kg/m3 (but you can set the units which you prefer) then click on Ok for accept changes and leaving the Properties editor



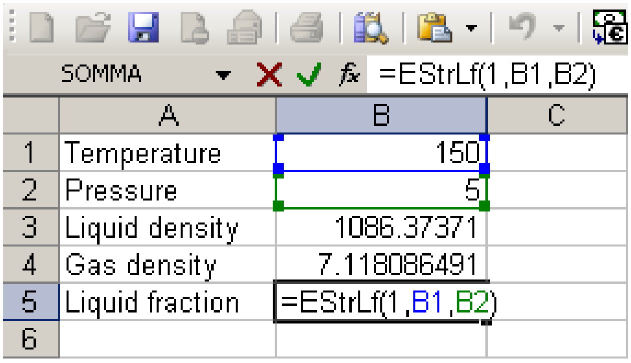
Pressure	Pa.a
Temperature (dt)	K
Temperature	K
Calorific Value	kJ/kg
Calorific Value (molar)	kJ/kmol
Enthalpy (Streams)	kW
Entropy (Streams)	kJ/(K*s)
Heat Capacity	kJ/(kg*K)
Heat Capacity (molar)	kJ/(kmol*K)
Flow (mass basis)	kg/s
Flow (gas, mass basis)	kg/s
Density	kg/m3
Density (molar)	kmol/m3
Specific Volume	m3/kg
Specific Volume (molar)	m3/kmol
Thermal Conductivity	W/(m*K)
Viscosity (dynamic)	Pa*s
Surface Tension	N/m
Lenght	m
Area	m2
Volume	m3
Mass	kg
Velocity	m/s

finally we can calculate the densities for the specified mixture directly in the cells, in B3 we enter the macro =EStrLD(1,B1,B2) , for calculating liquid density of stream 1 at temperature specified in B1 and pressure specified in B2 ,in B4 we enter the macro =EStrGD(1,B1,B2) for calculating the gas density and in B5 the macro =EStrLf(1,B1,B2) for calculating the liquid fraction



SOMMA =EStrLD(1,B1,B2)

	A	B	C
1	Temperature	150	
2	Pressure	5	
3	Liquid density	=EStrLD(1,B1,B2)	
4	Gas density	7.118086491	
5	Liquid fraction	0.309050931	
6			



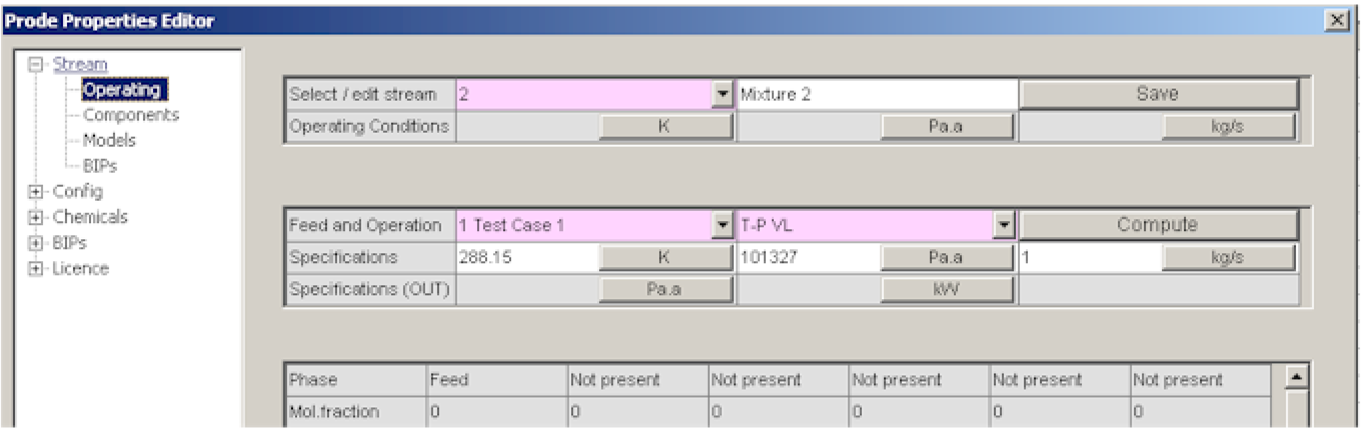
SOMMA =EStrLf(1,B1,B2)

	A	B	C
1	Temperature	150	
2	Pressure	5	
3	Liquid density	1086.37371	
4	Gas density	7.118086491	
5	Liquid fraction	=EStrLf(1,B1,B2)	
6			

In B1 we enter 200 as temperature (remember we have K as unit) and in B2 we enter 5 as pressure (remember we have set Bar.a as unit), densities are in Kg/m3 , notice that when you change B1 or B2 Prode Properties recalculates these values. Now you can modify the stream 1 (changing the list of components, the compositions or models) or the units of measurement and Prode Properties will calculate the value of ldensities and iquid fraction accordingly, in this way is very easy with Excel to solve many different problems leaving to Prode Properties the task to calculate all properties for pure fluids and mixtures.

Next example permits to calculate the phase fractions and compositions in multiphase equilibria, to show the result in Excel we'll use a predefined Excel page, from Excel menu File->open , in Excel folder (in Prode Properties installation) select the file multiphase.xls and click Ok to load the file

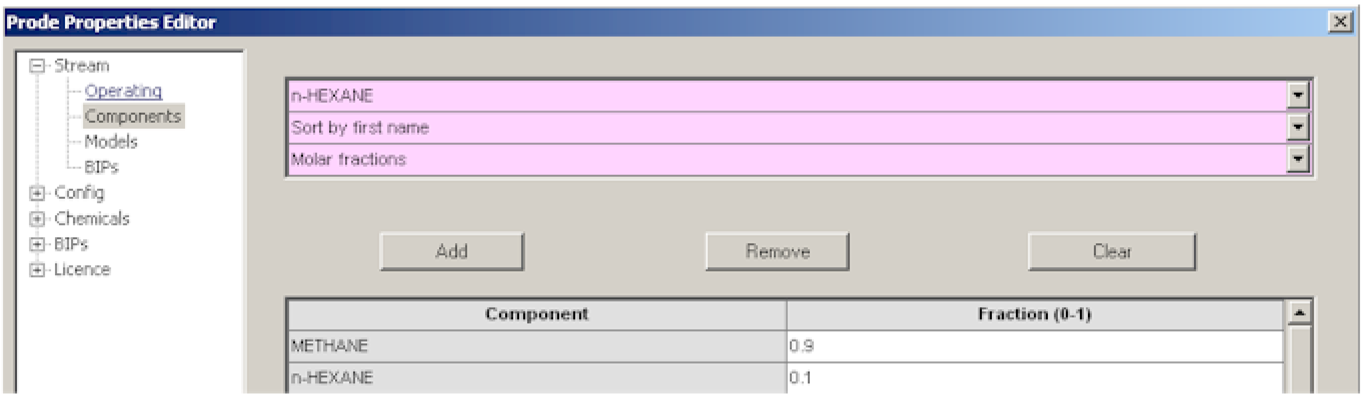
We need to define a new mixture :
a) from Properties menu select Edit Properties
b) in Stream->Operating dialog we select the stream number 2 and define the name "MIxture 2"



Select / edit stream	2		Mixture 2		Save	
Operating Conditions		K		Pa.a		kg/s
Feed and Operation	1 Test Case 1		T-P VL		Compute	
Specifications	288.15	K	101327	Pa.a	1	kg/s
Specifications (OUT)		Pa.a		kW		

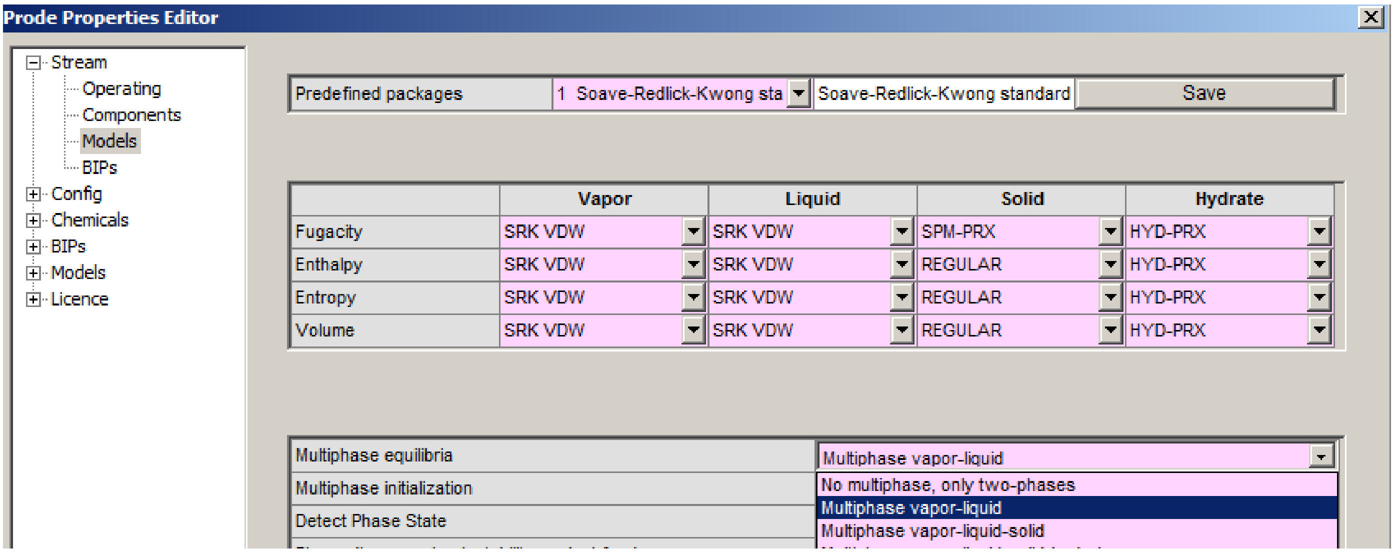
Phase	Feed	Not present	Not present	Not present	Not present	Not present
Mol.fraction	0	0	0	0	0	0

c) then we select t Stream->Components dialog and define a composition of two components with following molar fractions Methane 0.9 n-Hexane 0.1



Component	Fraction (0-1)
METHANE	0.9
n-HEXANE	0.1

d) in Stfream->Models dialog we define SRK VDW (select in predefined packages) for both gas and liquid
e) we set Multiphase equilibria to Multiphase vapor-liquid and Multiphase initialization to Standard tests

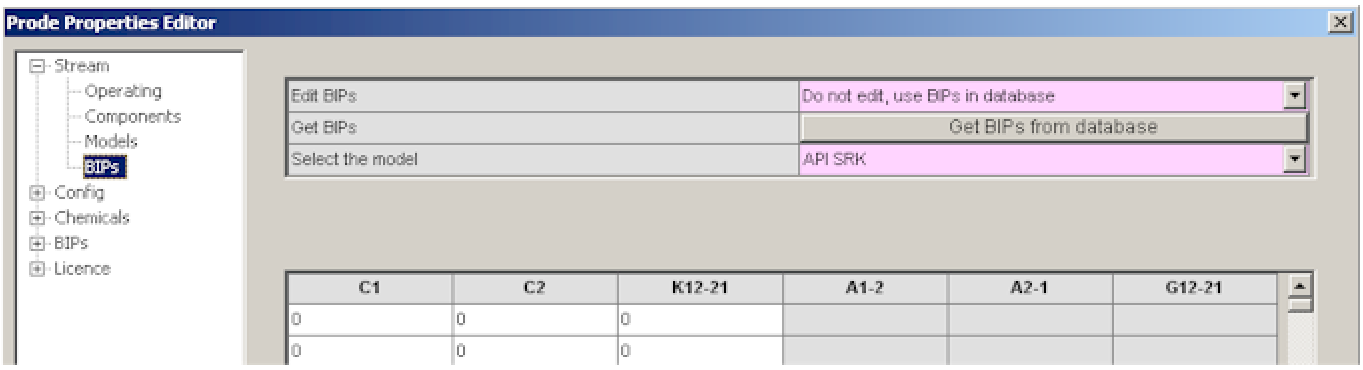


Predefined packages	1 Soave-Redlick-Kwong sta	Soave-Redlick-Kwong standard	Save

	Vapor	Liquid	Solid	Hydrate
Fugacity	SRK VDW	SRK VDW	SPM-PRX	HYD-PRX
Enthalpy	SRK VDW	SRK VDW	REGULAR	HYD-PRX
Entropy	SRK VDW	SRK VDW	REGULAR	HYD-PRX
Volume	SRK VDW	SRK VDW	REGULAR	HYD-PRX

Multiphase equilibria	Multiphase vapor-liquid
Multiphase initialization	
Detect Phase State	

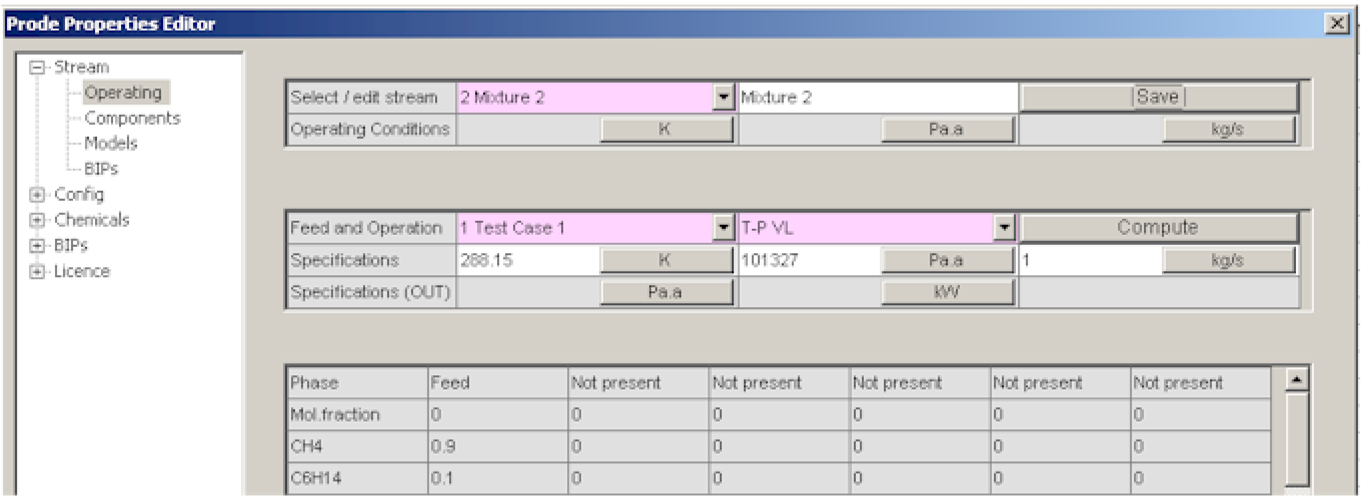
f) then we can edit BIPs, we can input data or load from database
IMPORTANT when accessing the library from an external program you must define the proper settings in stream's options for multiphase flash operation



Edit BIPs	Do not edit, use BIPs in database
Get BIPs	Get BIPs from database
Select the model	API SRK

C1	C2	K12-21	A1-2	A2-1	G12-21
0	0	0			
0	0	0			

g) and finally in Stream->Operating dialog we click on Save button to save the stream data



Select / edit stream	2 Mixture 2		Mixture 2		Save	
Operating Conditions		K		Pa.a		kg/s

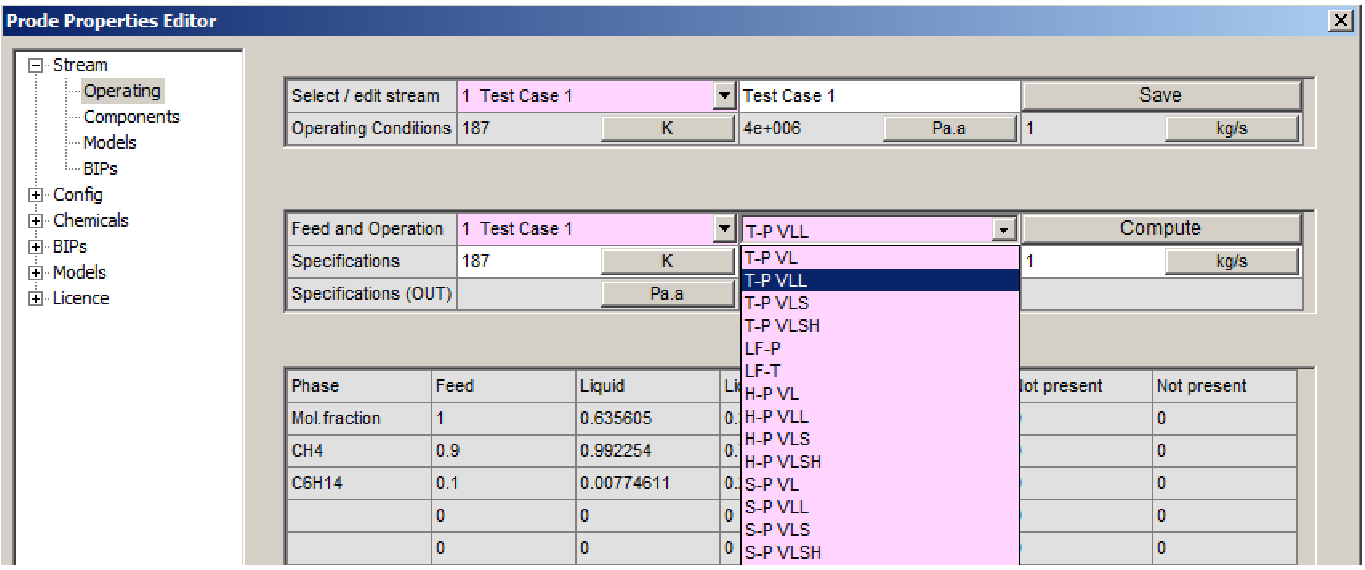
Feed and Operation	1 Test Case 1		T-P VL		Compute	
Specifications	288.15	K	101327	Pa.a	1	kg/s
Specifications (OUT)		Pa.a		kW		

Phase	Feed	Not present	Not present	Not present	Not present	Not present
Mol.fraction	0	0	0	0	0	0
CH4	0.9	0	0	0	0	0
C6H14	0.1	0	0	0	0	0

Notice that once saved the dialog shows the feed composition of the stream.
Now you can define / access diferent streams as the program remembers your data for stream 2

MPORTANT
before to leave the application remember to save all data into the archive otherways your changes will be lost read the paragraph “Working with archives, save and load data, default settings”   for additional information

From the dialog Stream->Operating you can calculate a isothermal multiphase flash, select stream 2 as feed, then T-P VLL (isothermal Vapor Liquid Liquid) , enter 187 K as temperature and 40 atm.g as pressure (this is the example provided by Michelsen in “Calculation of multiphase equilibrium”) then click on Compute, the procedure will calculate two liquid phases and show the compositions



Select / edit stream	1 Test Case 1	Test Case 1	
Operating Conditions	187 K	4e+006 Pa.a	1 kg/s

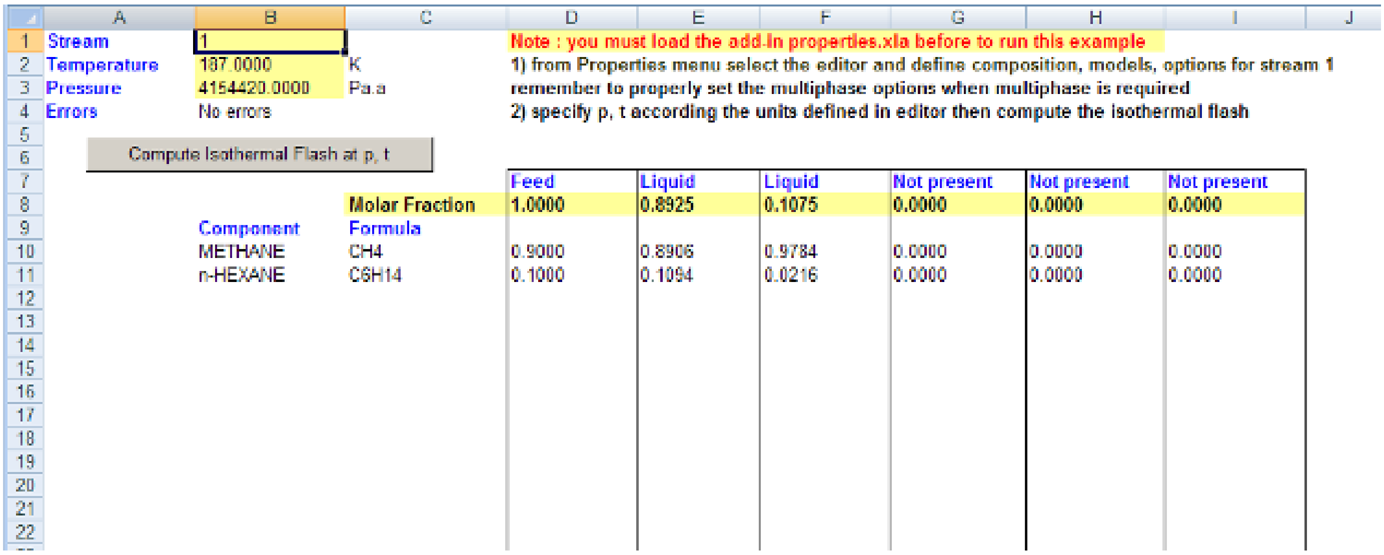
Feed and Operation	1 Test Case 1	T-P VLL	
Specifications	187 K		1 kg/s
Specifications (OUT)	Pa.a		

Phase	Feed	Liquid	Li	lot present	Not present
Mol.fraction	1	0.635605	0.		0
CH4	0.9	0.992254	0.		0
C6H14	0.1	0.00774611	0.		0
	0	0	0		0
	0	0	0		0

If you wish you can modify the units from Config->Units dialog, define Bar.a as unit for pressure.

Notice that when changing units you must close and reopen the editor to see the changes (in editor).

The results are available directly in Excel, set stream as 2, temperature as 187 K and pressure as 4154420 Pa.a (40 atm.g) the nclick on “Compute isothermal Flash at p,t”

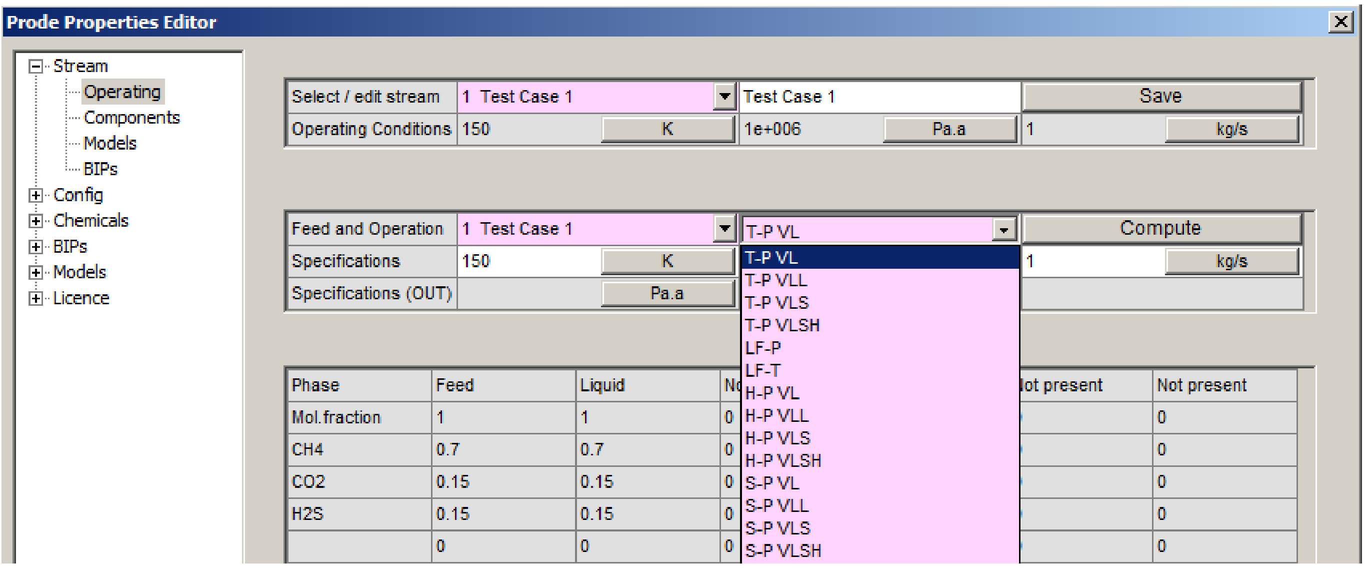


	A	B	C	D	E	F	G	H	I
1	Stream	1		Note : you must load the add-in properties.xla before to run this example					
2	Temperature	187.0000	K	1) from Properties menu select the editor and define composition, models, options for stream 1					
3	Pressure	4154420.0000	Pa.a	remember to properly set the multiphase options when multiphase is required					
4	Errors	No errors		2) specify p, t according the units defined in editor then compute the isothermal flash					
5									
6									
7				Feed	Liquid	Liquid	Not present	Not present	Not present
8			Molar Fraction	1.0000	0.8925	0.1075	0.0000	0.0000	0.0000
9		Component	Formula						
10		METHANE	CH4	0.9000	0.8906	0.9784	0.0000	0.0000	0.0000
11		n-HEXANE	C6H14	0.1000	0.1094	0.0216	0.0000	0.0000	0.0000
12									
13									
14									
15									
16									
17									
18									
19									
20									
21									
22									

Now you are able to calculate results at different operating conditions.

Altough a slow process multiphase analysis permits to discover instabilities and formation of new phases, examine the isothermal flash at 149 K 10 Bar.a with API SRK as model and a mixture of Methane 0.7 Carbon Dioxide 0.15 Hydrogen Sulfide 0.15 , this is the Mixture 1 provided as example.

a) from Properties menu select Edit Properties,
b) in Stream->Operating dialog select the stream number 1 , label "MIxture 1"
c) In Stream->Components verify the composition (Methane 0.7 Carbon Dioxide 0.15 Hydrogen Sulfide 0.15)
d) In Stream->Models we verify that model (fugacity) is SRK for gas and liquid
e) In Stream->BIPs we input BIPs or verify that procedure loads BIPs from database
f) in Stream->Components Save the stream
g) set as feed stream the first ("Mixture 1"), as operation T-P VL (isothermal, two phases flash), as specifications 150 K for temperature and 10 Bar.a for pressure, then select Compute



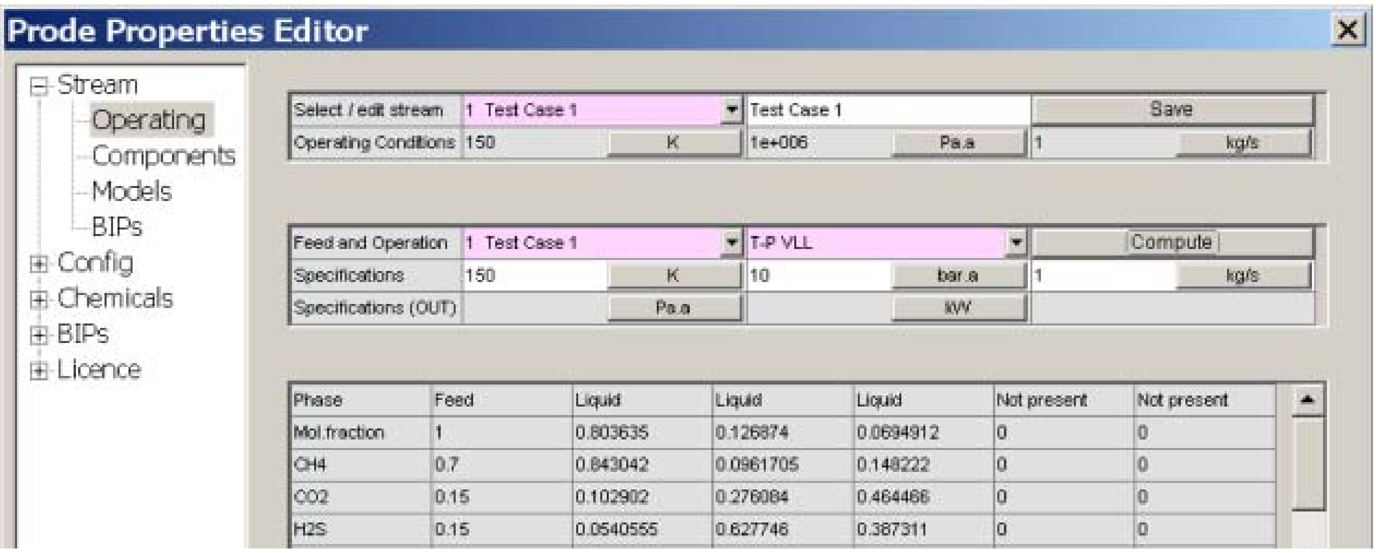
Select / edit stream	1 Test Case 1		Test Case 1			
Operating Conditions	150	K	1e+006	Pa.a	1	kg/s

Feed and Operation	1 Test Case 1		T-P VL			
Specifications	150	K			1	kg/s
Specifications (OUT)		Pa.a				

Phase	Feed	Liquid	No		ot present	Not present
Mol.fraction	1	1	0			0
CH4	0.7	0.7	0			0
CO2	0.15	0.15	0			0
H2S	0.15	0.15	0			0
	0	0	0			0

The procedure detects one liquid phase,

a) define TP-VLL (isothermal vapor-liquid-liquid) and select Compute
NOTE
<u>the procedure may detect two or three liquid phases depending from values of BIPs</u>



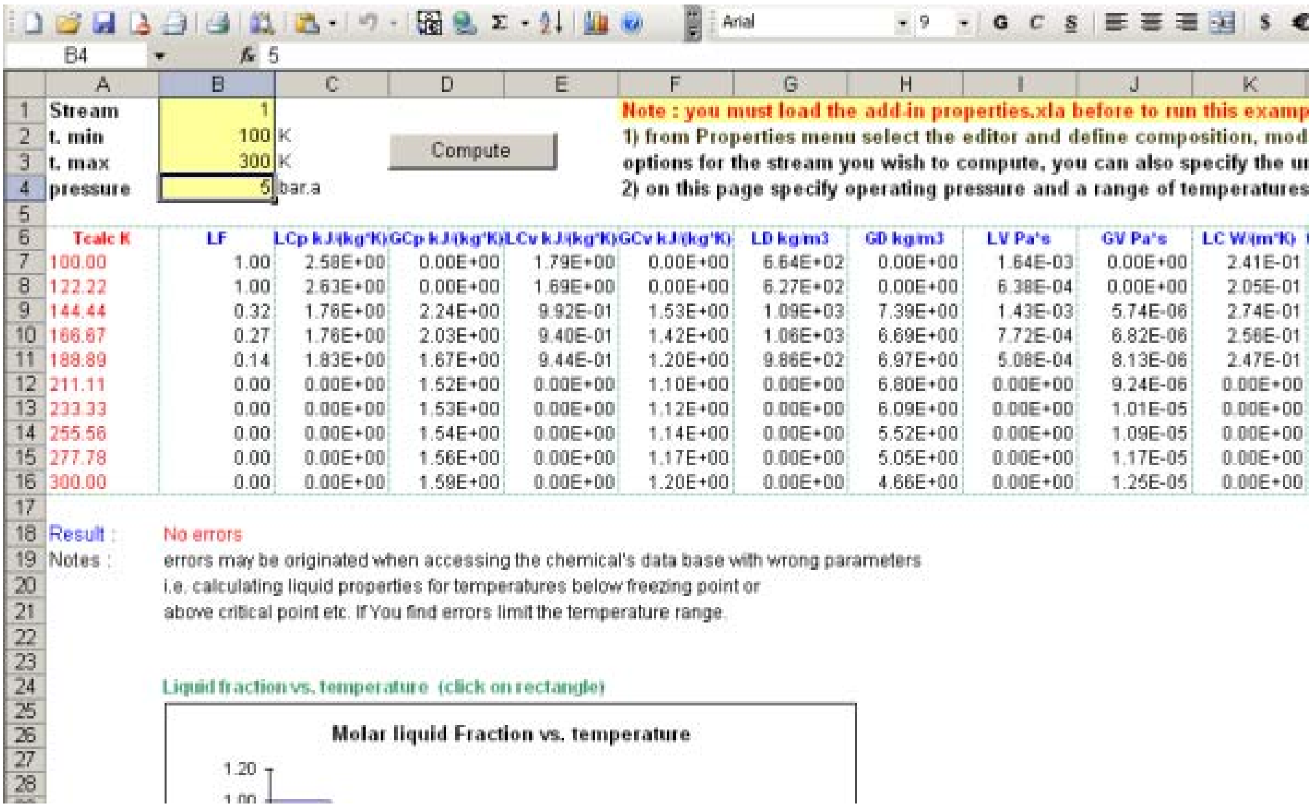
Select / edit stream	1 Test Case 1		Test Case 1			
Operating Conditions	150	K	1e+006	Pa.a	1	kg/s

Feed and Operation	1 Test Case 1		T-P VLL			
Specifications	150	K	10	bar.a	1	kg/s
Specifications (OUT)		Pa.a		kW		

Phase	Feed	Liquid	Liquid	Liquid	Not present	Not present
Mol.fraction	1	0.803635	0.126874	0.0694912	0	0
CH4	0.7	0.843042	0.0961705	0.148222	0	0
CO2	0.15	0.102902	0.276084	0.464466	0	0
H2S	0.15	0.0540555	0.627746	0.387311	0	0

Next example permits to calculate and graph tables of values in a range of temperatures for many different properties (liquid fraction, cp, cv, density, viscosity, thermal conductivity, speed of sound) and for both gas and liquid phases, for doing this we'll use a predefined Excel page, from Excel menu File->open , in Excel folder (in Prode Properties installation) select the file props.xls

If you wish you can modify the stream composition or the units of measurement , in that case, as before from Properties menu access the Properties editor and modify the previous data.
Then enter (in the proper units) the desired range of temperatures (cells B2-B3) and the operating pressure (cell B4) and click on compute button to calculate the data, Prode Properties will print the values with the desired units of measuremebt.



B4 = 5

Stream	1	
t. min	100	K
t. max	300	K
pressure	5	bar.a

Note : you must load the add-in properties.xla before to run this examp
1) from Properties menu select the editor and define composition, mod
options for the stream you wish to compute, you can also specify the u
2) on this page specify operating pressure and a range of temperatures

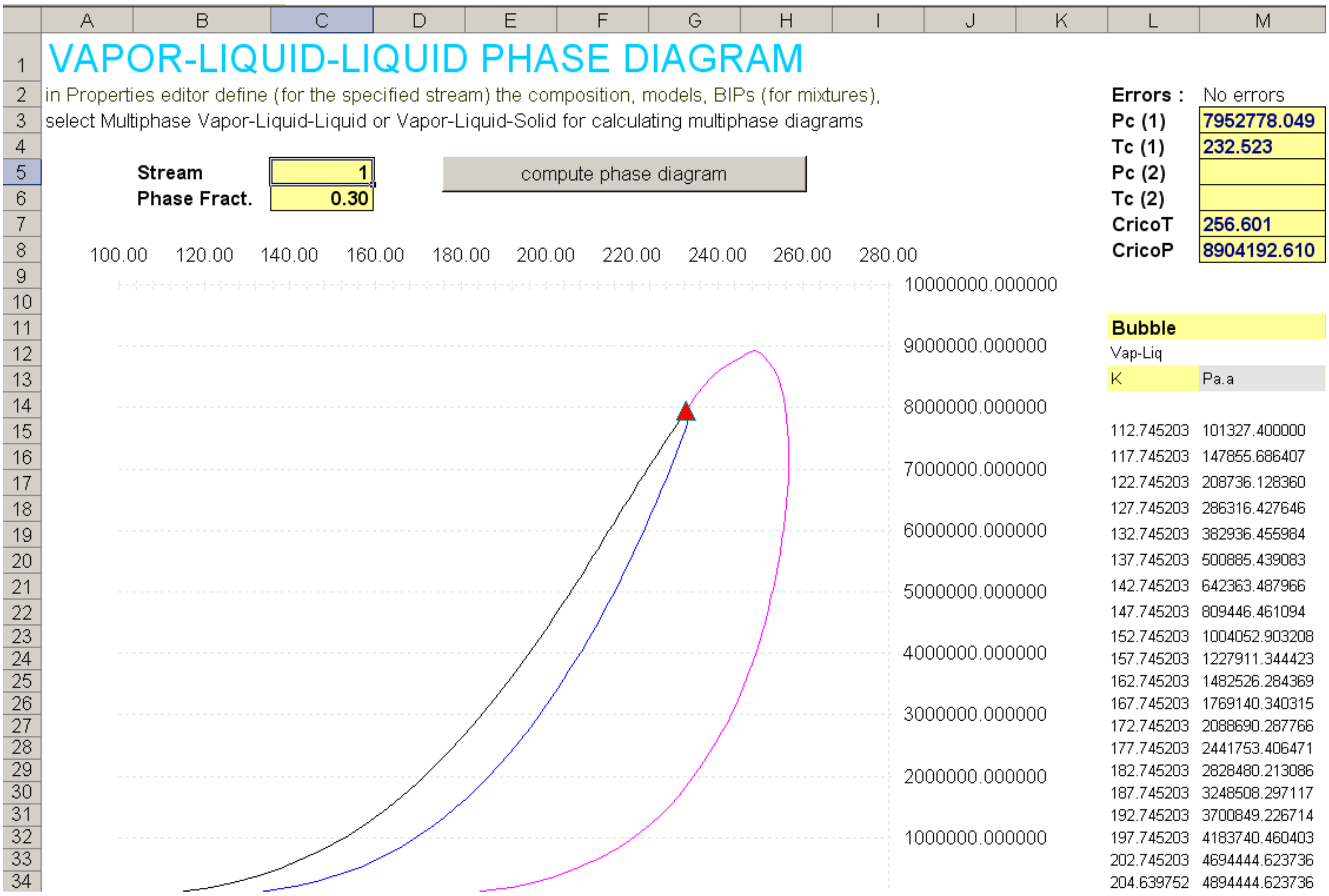
Tcalc K	LF	LCp kJ/(kg*K)	GCp kJ/(kg*K)	LCv kJ/(kg*K)	GCv kJ/(kg*K)	LD kg/m3	GD kg/m3	LV Pa*s	GV Pa*s	LC W/(m*K)
100.00	1.00	2.58E+00	0.00E+00	1.79E+00	0.00E+00	6.64E+02	0.00E+00	1.64E-03	0.00E+00	2.41E-01
122.22	1.00	2.63E+00	0.00E+00	1.69E+00	0.00E+00	6.27E+02	0.00E+00	6.38E-04	0.00E+00	2.05E-01
144.44	0.32	1.76E+00	2.24E+00	9.92E-01	1.53E+00	1.09E+03	7.39E+00	1.43E-03	5.74E-06	2.74E-01
166.67	0.27	1.76E+00	2.03E+00	9.40E-01	1.42E+00	1.06E+03	6.69E+00	7.72E-04	6.82E-06	2.56E-01
188.89	0.14	1.83E+00	1.67E+00	9.44E-01	1.20E+00	9.86E+02	6.97E+00	5.08E-04	8.13E-06	2.47E-01
211.11	0.00	0.00E+00	1.52E+00	0.00E+00	1.10E+00	0.00E+00	6.80E+00	0.00E+00	9.24E-06	0.00E+00
233.33	0.00	0.00E+00	1.53E+00	0.00E+00	1.12E+00	0.00E+00	6.09E+00	0.00E+00	1.01E-05	0.00E+00
255.56	0.00	0.00E+00	1.54E+00	0.00E+00	1.14E+00	0.00E+00	5.52E+00	0.00E+00	1.09E-05	0.00E+00
277.78	0.00	0.00E+00	1.56E+00	0.00E+00	1.17E+00	0.00E+00	5.05E+00	0.00E+00	1.17E-05	0.00E+00
300.00	0.00	0.00E+00	1.59E+00	0.00E+00	1.20E+00	0.00E+00	4.66E+00	0.00E+00	1.25E-05	0.00E+00

Result : No errors
Notes : errors may be originated when accessing the chemical's data base with wrong parameters
i.e. calculating liquid properties for temperatures below freezing point or
above critical point etc. If You find errors limit the temperature range.

Liquid fraction vs. temperature (click on rectangle)

Next example will permits to calculate and graph a phase diagram (phase envelope), to do this we'll use a predefined Excel page, from Excel menu File->open , in Excel folder (in Prode Properties installation) select the file phasenv.xls

If you wish you can modify the stream composition or the units of measurement , in that case, from Properties menu access the Properties editor and modify the previous data, <u>remember to set the same equation of state for gas and liquid fugacity and dont' forget to save the stream (button Save in first dialog) before to click "Ok" and exit</u>. Then enter the desired liquid fraction for equilibrium line (cell C6) and click on compute button to calculate the data, Prode Properties will print the calculated values with the desired units of measurement, herebelow an example with 3 components



VAPOR-LIQUID-LIQUID PHASE DIAGRAM

in Properties editor define (for the specified stream) the composition, models, BIPs (for mixtures),
select Multiphase Vapor-Liquid-Liquid or Vapor-Liquid-Solid for calculating multiphase diagrams

Stream	1
Phase Fract.	0.30

Errors :	No errors
Pc (1)	7952778.049
Tc (1)	232.523
Pc (2)	
Tc (2)	
CricoT	256.601
CricoP	8904192.610

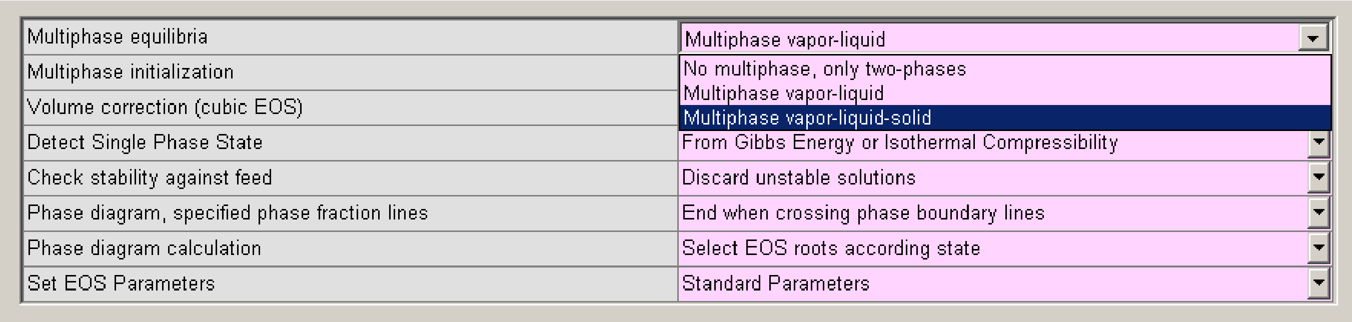
Bubble

Vap-Liq

K	Pa.a
112.745203	101327.400000
117.745203	147855.686407
122.745203	208736.128360
127.745203	286316.427646
132.745203	382936.455984
137.745203	500885.439083
142.745203	642363.487966
147.745203	809446.461094
152.745203	1004052.903208
157.745203	1227911.344423
162.745203	1482526.284369
167.745203	1769140.340315
172.745203	2088690.287766
177.745203	2441753.406471
182.745203	2828480.213086
187.745203	3248508.297117
192.745203	3700849.226714
197.745203	4183740.460403
202.745203	4694444.623736
204.639752	4894444.623736

MPORTANT

The procedure for calculating a phase diagram allows different settings, you can modify these settings from the dialog Stream->Models (in Properties editor)



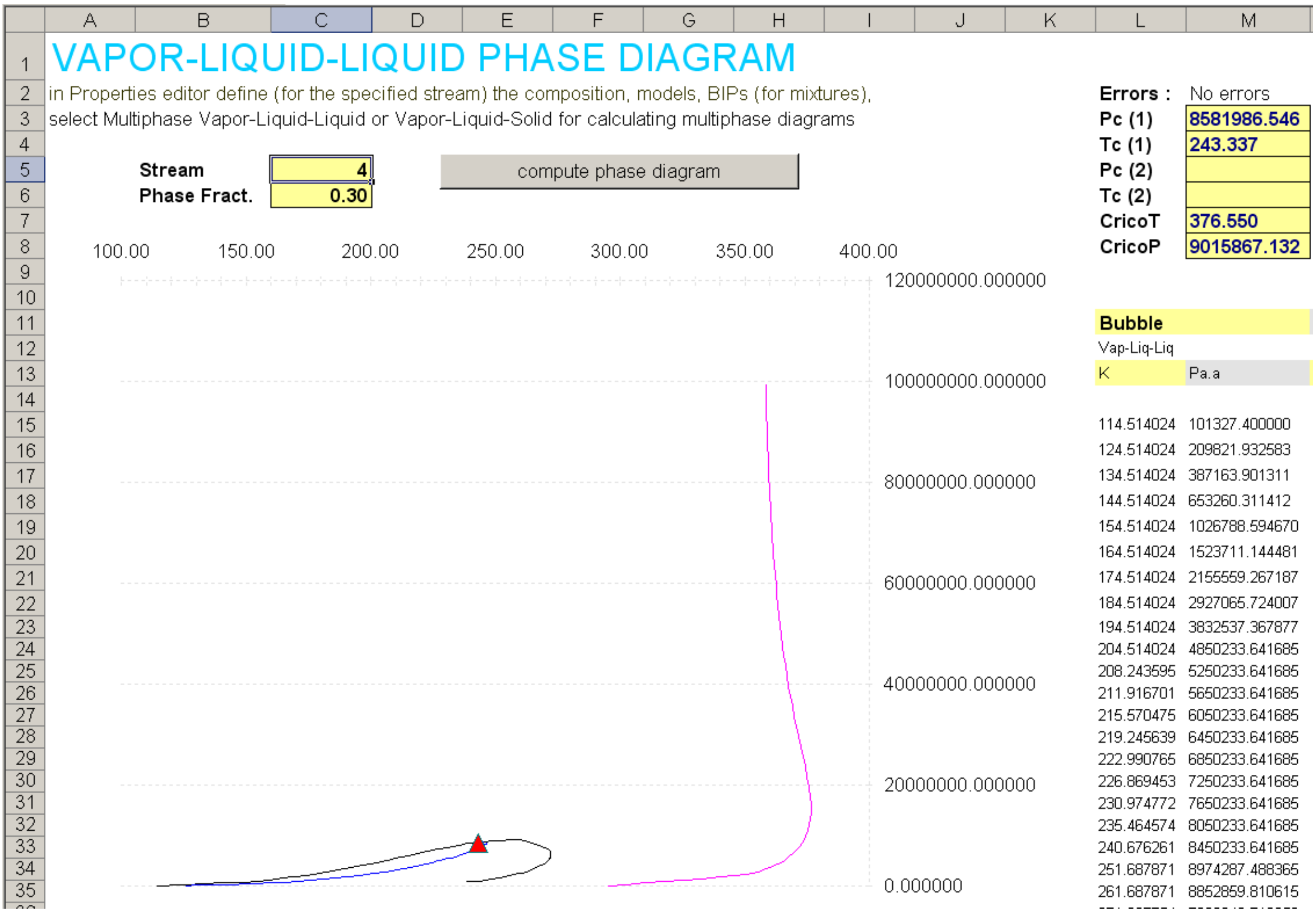
Multiphase equilibria	Multiphase vapor-liquid
Multiphase initialization	
Volume correction (cubic EOS)	
Detect Single Phase State	From Gibbs Energy or Isothermal Compressibility
Check stability against feed	Discard unstable solutions
Phase diagram, specified phase fraction lines	End when crossing phase boundary lines
Phase diagram calculation	Select EOS roots according state
Set EOS Parameters	Standard Parameters

Check stability against feed option permits to test stability of calculated points against feed, unstable points are not printed, to show all calculated points change the settings.
Phase diagram, specified phase fraction lines, allows to end (or continue) lines after crossing a phase boundary, set to end (when crossing phase boundary lines) to avoid generating lines containing inconsistent data.
Phase diagram calculation option allows to select the EOS root for minimum Gibbs energy or according the state.

Hpwever the most important setting is the multiphase equilibria oprion which allows to calculate
1) vapor-liquid phase diagrams (see above)
2) vapor-liquid-liquid phase diagrams
3) vapor-liquid-solid phase diagrams

Next example will show a vapor-liquid-liquid phase diagram

a) In Excel load the file phasenv.xls
b) select the stream 4, a predefined test case with a natural gas mixture including water
c) click on compute button to calculate the data



VAPOR-LIQUID-LIQUID PHASE DIAGRAM

in Properties editor define (for the specified stream) the composition, models, BIPs (for mixtures),
select Multiphase Vapor-Liquid-Liquid or Vapor-Liquid-Solid for calculating multiphase diagrams

Stream	4
Phase Fract.	0.30

Errors :	No errors
Pc (1)	8581986.546
Tc (1)	243.337
Pc (2)	
Tc (2)	
CricoT	376.550
CricoP	9015867.132

Bubble

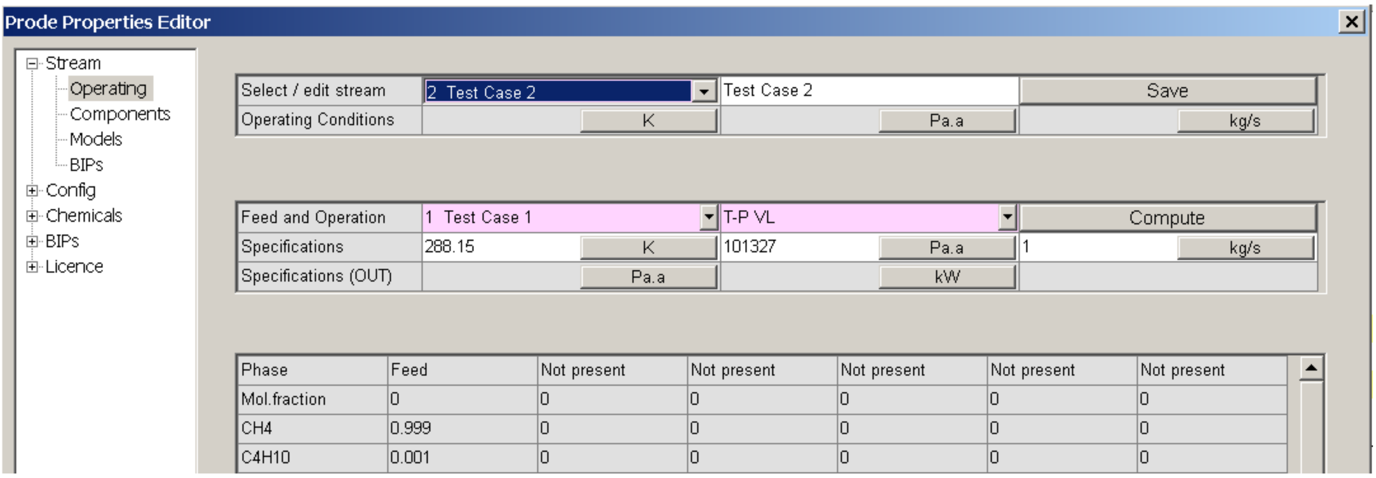
Vap-Liq-Liq

K	Pa.a
114.514024	101327.400000
124.514024	209821.932583
134.514024	387163.901311
144.514024	653260.311412
154.514024	1026788.594670
164.514024	1523711.144481
174.514024	2155559.267187
184.514024	2927065.724007
194.514024	3832537.367877
204.514024	4850233.641685
208.243595	5250233.641685
211.916701	5650233.641685
215.570475	6050233.641685
219.245639	6450233.641685
222.990765	6850233.641685
226.869453	7250233.641685
230.974772	7650233.641685
235.464574	8050233.641685
240.676261	8450233.641685
251.687871	8974287.488365
261.687871	8852859.810615

Notice the water dew point line, the red line on the right

Next example will show a phase digram with up to three dew points at the same temperature,

a) In Excel load the file phasenv.xls
b) from Properties menu select Edit Properties,
c) in Stream->Operating dialog we select the stream number 2, a predefined test case

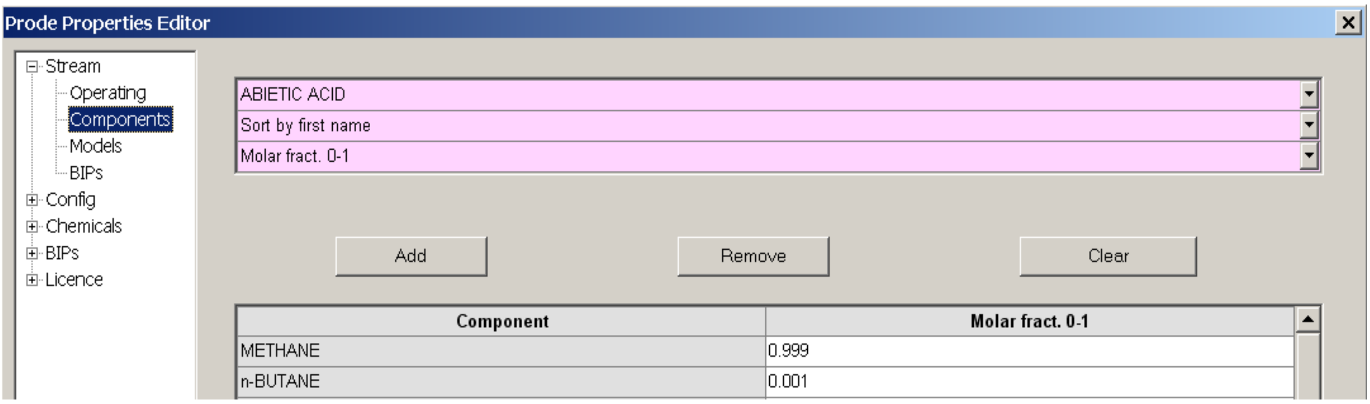


Select / edit stream	2 Test Case 2	Test Case 2	
Operating Conditions	K	Pa.a	kg/s

Feed and Operation	1 Test Case 1	T-P VL	
Specifications	288.15 K	101327 Pa.a	1 kg/s
Specifications (OUT)	Pa.a	kW	

Phase	Feed	Not present	Not present	Not present	Not present	Not present
Mol.fraction	0	0	0	0	0	0
CH4	0.999	0	0	0	0	0
C4H10	0.001	0	0	0	0	0

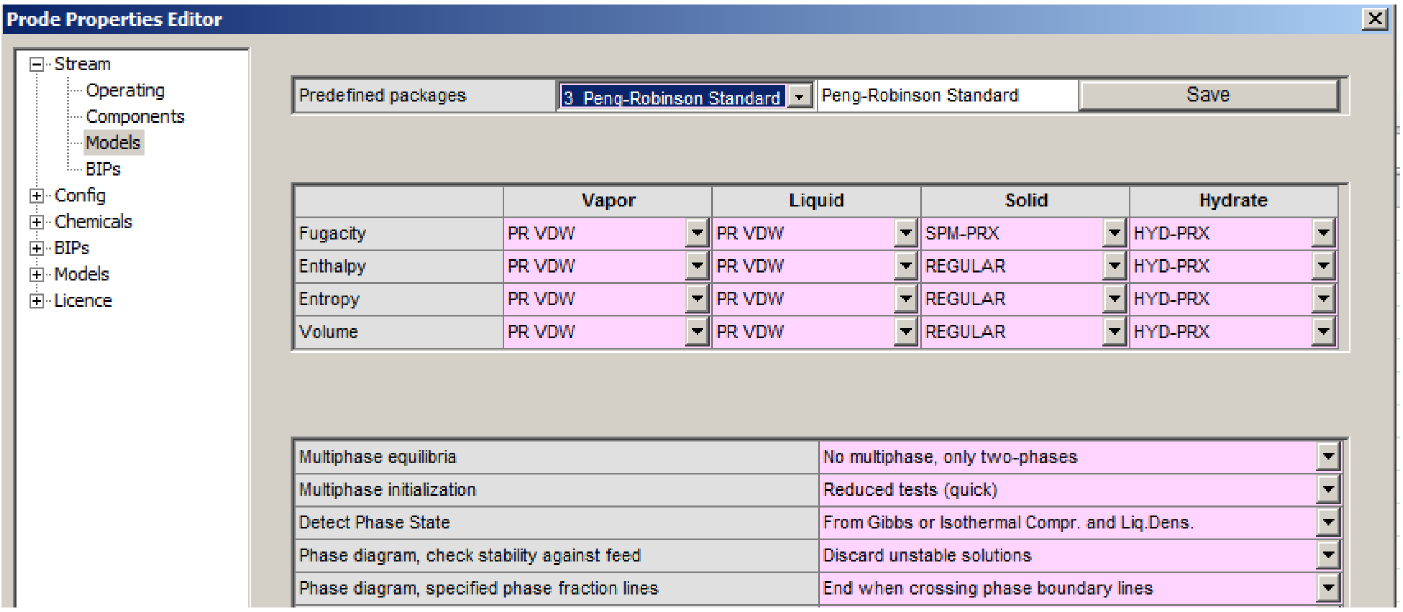
we can edit the list of components and the fraction of each component selecting the Stream->Components dialog, this mixture includes two components with molar fractions Methane 0.999 n-Butane 0.001



ABIETIC ACID
Sort by first name
Molar fract. 0-1

Component	Molar fract. 0-1
METHANE	0.999
n-BUTANE	0.001

we can modify models and options in Stream->Models dialog ,
in this test case we adopt Peng Robinson (PR-VDW) for both gas and liquid

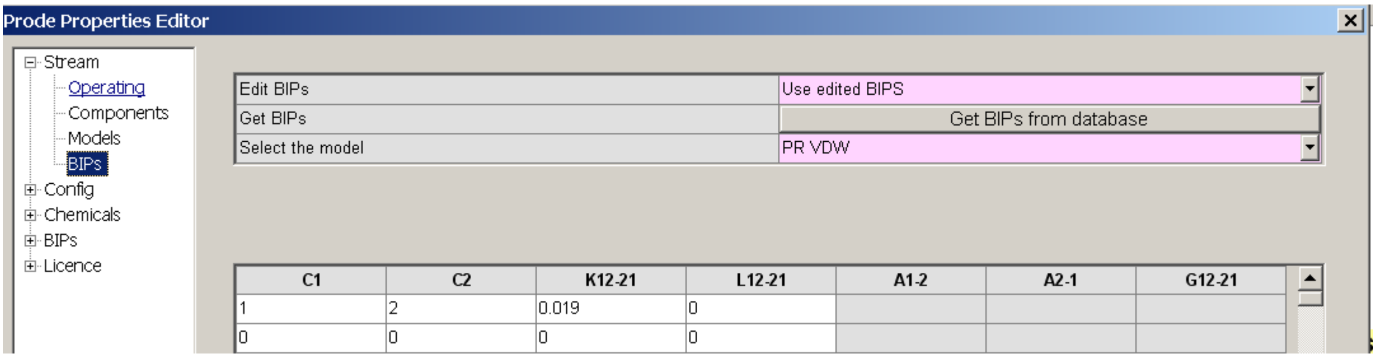


Predefined packages	3 Peng-Robinson Standard	Peng-Robinson Standard

	Vapor	Liquid	Solid	Hydrate
Fugacity	PR VDW	PR VDW	SPM-PRX	HYD-PRX
Enthalpy	PR VDW	PR VDW	REGULAR	HYD-PRX
Entropy	PR VDW	PR VDW	REGULAR	HYD-PRX
Volume	PR VDW	PR VDW	REGULAR	HYD-PRX

Multiphase equilibria	No multiphase, only two-phases
Multiphase initialization	Reduced tests (quick)
Detect Phase State	From Gibbs or Isothermal Compr. and Liq.Dens.
Phase diagram, check stability against feed	Discard unstable solutions
Phase diagram, specified phase fraction lines	End when crossing phase boundary lines

we can edit BIPs from Stream->BIPs dialog

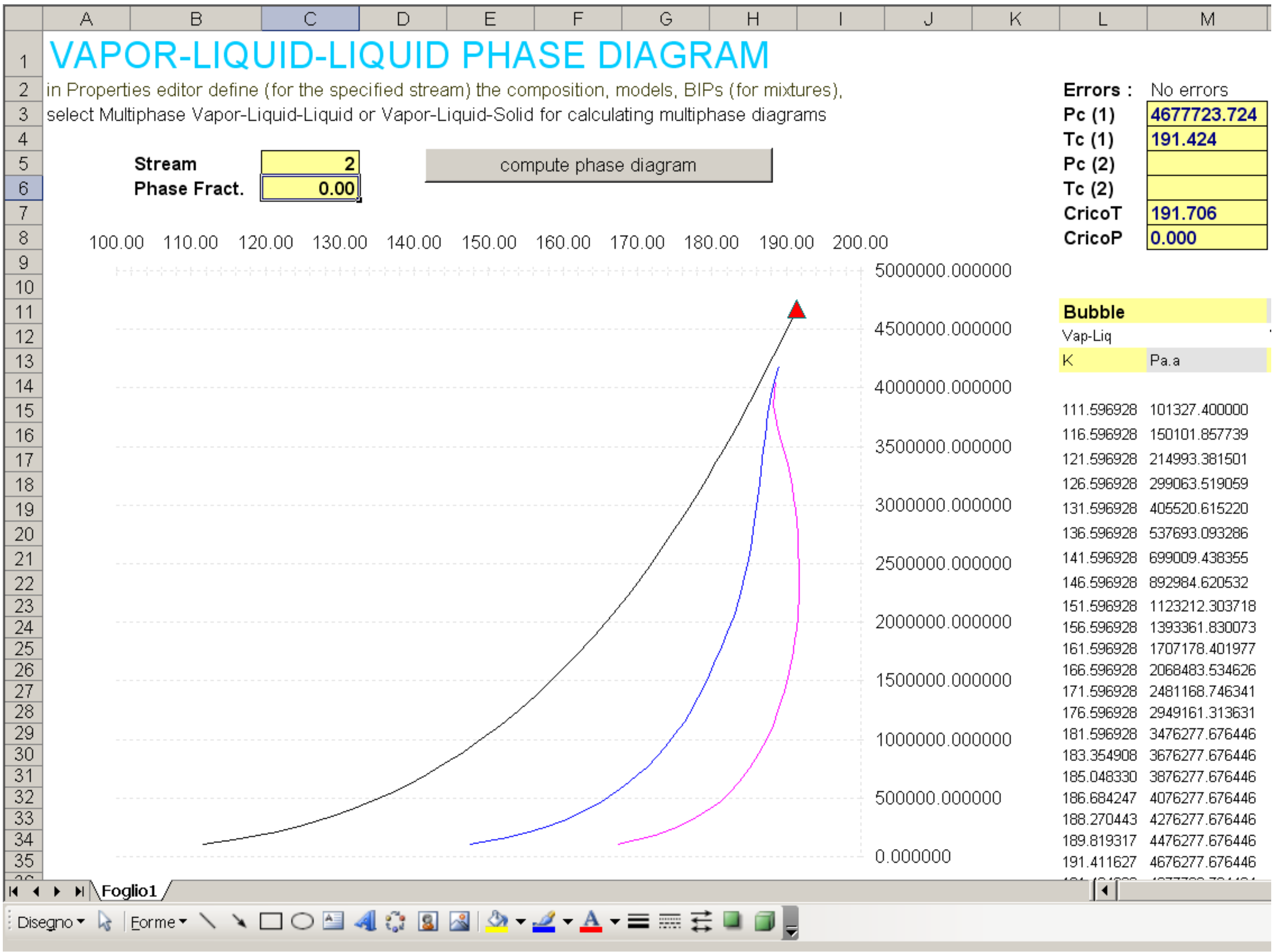


Edit BIPs	Use edited BIPS
Get BIPs	Get BIPs from database
Select the model	PR VDW

C1	C2	K12-21	L12-21	A1-2	A2-1	G12-21
1	2	0.019	0			
0	0	0	0			

Remember, if you have changed some values, in Stream->Operating dialog click on Save button to save the stream data

for canculating the phase envelope for test case 3 from Excel page phasenv.xls
enter 3 as stream and 0.001 as liquid fraction and click on button “Compute phase diagram”



VAPOR-LIQUID-LIQUID PHASE DIAGRAM

in Properties editor define (for the specified stream) the composition, models, BIPs (for mixtures),
select Multiphase Vapor-Liquid-Liquid or Vapor-Liquid-Solid for calculating multiphase diagrams

Stream	2
Phase Fract.	0.00

compute phase diagram

Errors :	No errors
Pc (1)	4677723.724
Tc (1)	191.424
Pc (2)	
Tc (2)	
CricoT	191.706
CricoP	0.000

Bubble
Vap-Liq

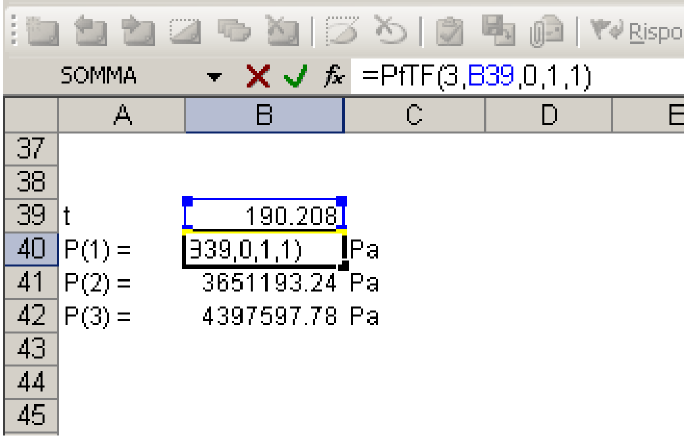
K	Pa.a
111.596928	101327.400000
116.596928	150101.857739
121.596928	214993.381501
126.596928	299063.519059
131.596928	405520.615220
136.596928	537693.093286
141.596928	699009.438355
146.596928	892984.620532
151.596928	1123212.303718
156.596928	1393361.830073
161.596928	1707178.401977
166.596928	2068483.534626
171.596928	2481168.746341
176.596928	2949161.313631
181.596928	3476277.676446
183.354908	3676277.676446
185.048330	3876277.676446
186.684247	4076277.676446
188.270443	4276277.676446
189.819317	4476277.676446
191.411627	4676277.676446

Observe that for this mixture the dew line, the red line below the critical point, shows up to three different equilibrium points at the same temperature (the area around 190 K), if you add the saturation point on the bubble line (black line) we have atotal of four saturation point pressures at a given temperature,   Prode Properties can calculate accurately all these points.

Prode Properties includes methods for calculating equilibrium points at specified conditions, see the paragraph “Methods for thermodynamic calc’ s” for details, methods LfPF(), LfTF() as the name says are based on a liquid fraction specification, they returns the first point (along the specified liquid fraction line) at the specified pressure (or temperature). Methods PfPF() and PfTF() can accept a gas or liquid fraction (solid fractions in extended edition) as specification, they can calculate up to 5 points (at specified pressure or temperature) along the line with specified phase fraction

double p = PfTF(integer stream, double t, double pf, int state, int n)

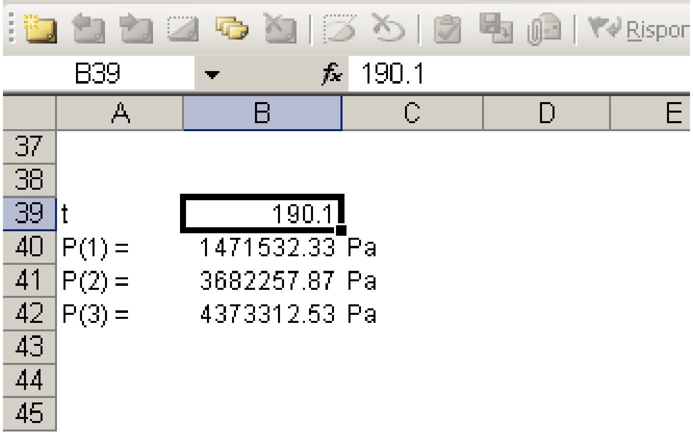
which requires the stream, the equilibrium temperature, the phase fraction (range 0-1), the state (gas, liquid, solid) and the position (1-5) of the equilibrium point
In cell B39 we define the temperature as 190.208 K , then in cells B40 , B41, B42 we enter the macros
=PfTF(3,B39,0,1,1) in cell B40
=PfTF(3,B39,0,1,2) in cell B41
=PfTF(3,B39,0,1,3) in cell B42
where the first value (3) is the stream , the second (cell B39) represents the temperature, the third (1) is the phase fraction (with 1 we specify 100% gas or a point on dew line, the same would be by setting the state as liquid and phase fraction as 0.0) the fourth (0) is the state (in Properties 0 = gas, 1 = liquid, 2 = solid) and the last is the required position (we require the points 1-3 along the dew line)



=PfTF(3,B39,0,1,1)

	A	B	C	D	E
37					
38					
39	t	190.208			
40	P(1) =	339,0,1,1)	Pa		
41	P(2) =	3651193.24	Pa		
42	P(3) =	4397597.78	Pa		
43					
44					
45					

the procedure calculates the three equilibrium points, if we change the temperature to 190.1 K we get different equilibrium pressures:



190.1

	A	B	C	D	E
37					
38					
39	t	190.1			
40	P(1) =	1471532.33	Pa		
41	P(2) =	3682257.87	Pa		
42	P(3) =	4373312.53	Pa		
43					
44					
45					

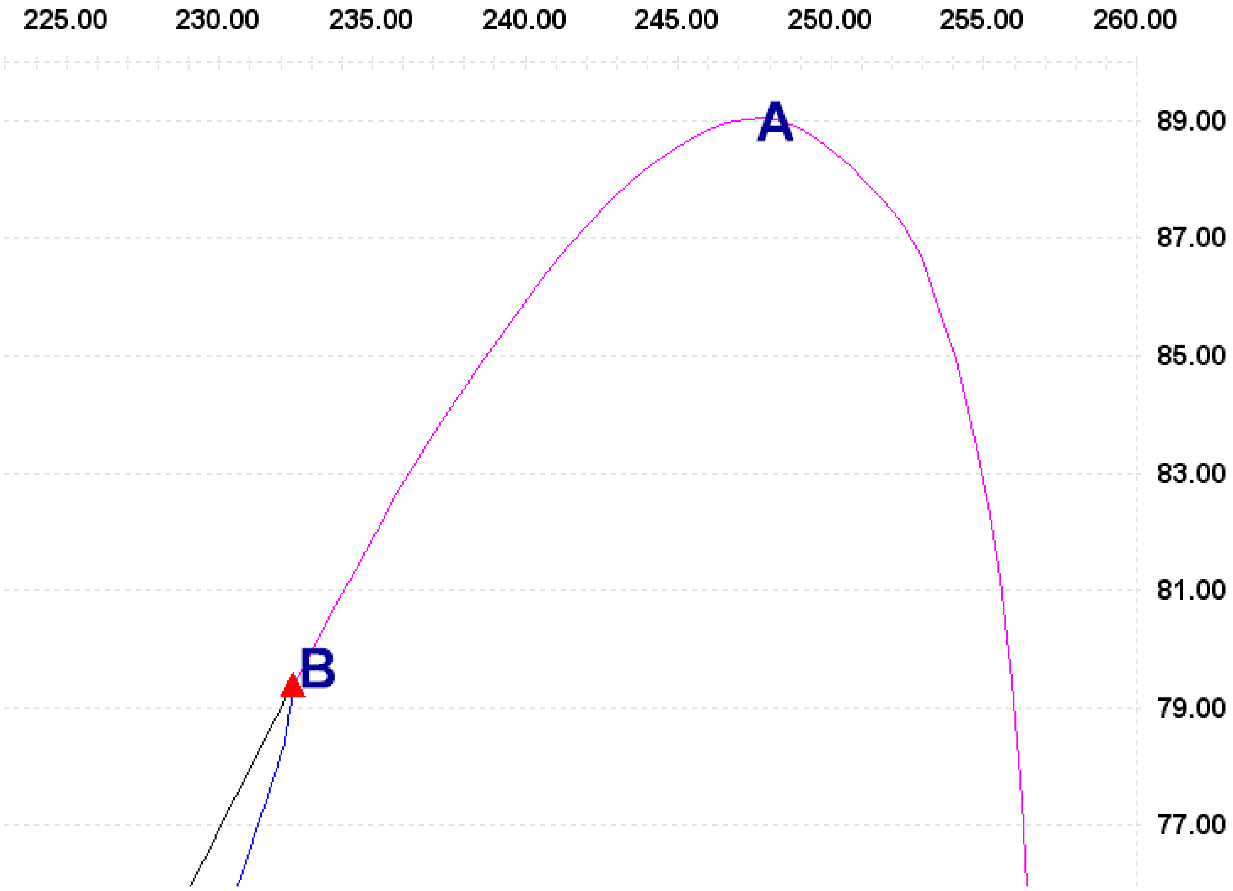
you may wish to test the method LfTF() , enter the macro
=LfTF(3,B39,0)
where 3 is the stream, B39 represents the temperature and 0 is the (liquid) phase fraction, notice that you’ll get the same values as for the first equilibrium point in PfTF()
Finally we can calculate the point on bubble line with the method LfTF()
=LfTF(3,B39,1)
where 1 is the specification (100% liquid) for a point on the bubble line ,
of course you get the same result with the method
=PfTF(3,B39,1,1,1)
where the third value (1) is the phase fraction (with 1 we specify a 100% fraction) the fourth (1) is the state (in Properties 0 = gas, 1 = liquid, 2 = solid) and the last is the required position for the point

Prode Properties includes several methods for solving multiphase (vapor-liquid-solid) phase equilibria plus enthalpy, entropy or volume specifications
-specified enthalpy or entropy or volume and pressure
-specified enthalpy or entropy or volume and temperature
-constant energy and pressure

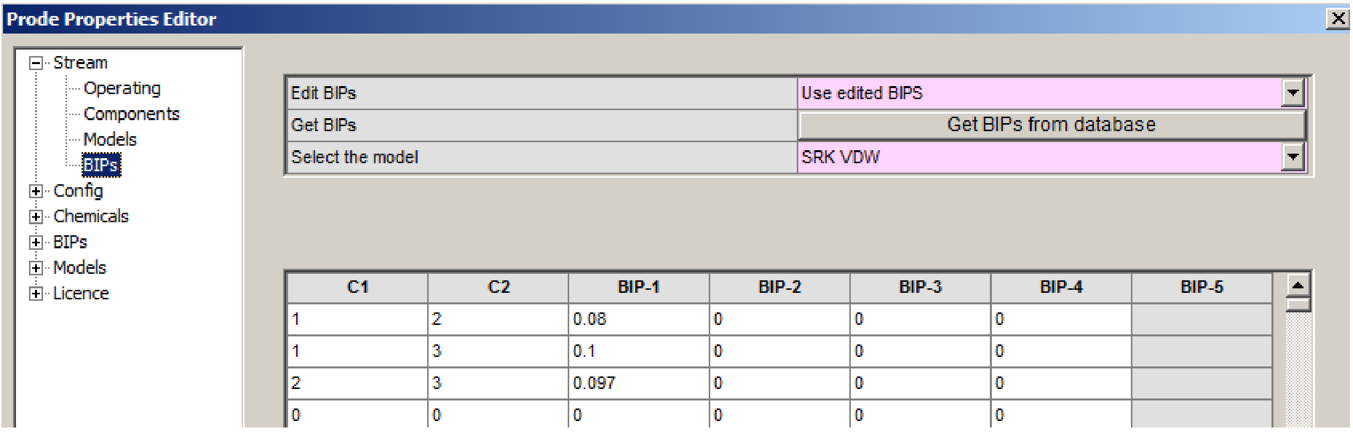
the paragraph “Methods for thermodynamic calc’ s” provides additional information.
in this example we will examine the methods HPF() and SPF() which permit to solve the enthalpy (HPF) or entropy (SPF) and pressure specifications, they return the temperature at which the calculated value of enthalpy (or entropy) equals the specified value.
These methods permit to solve many problems, for example
-model heat exchangers where you know inlet and outlet pressures and heat duty
-simulate valves where you know inlet and outlet pressures, usually valves are modeled as adiabatic processes (dh = 0)
-simulate pipelines where you know inlet and outlet pressures and heat exchanged with surrounding environment
-model pumps and compressors, when you know inlet and outlet pressures
Supposing we wish to simulate a process to cool down the mixture already examined in previous examples

Methane	0.7
Carbon Dioxide	0.15
Hydrogen Sulfide	0.15

with Soave Redlick Kwong model , from the point A in retrograde region and near the dew line (89 Bar.a and 246 K
to the point B located close to the critical point



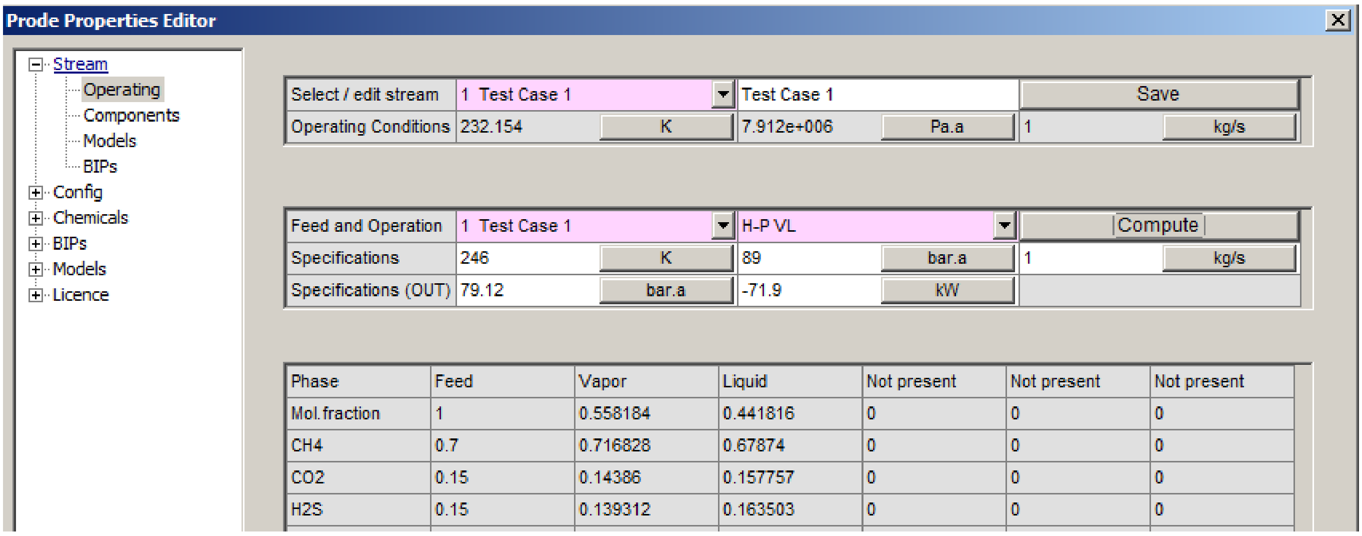
this example can represent a good test for evaluating the stability and reliability of convergence in retrograde region select stream 1 , verify the list of components and molar fractions (C1 = 0.7 CO2 = 0.15 H2S = 0.15) the models for vapor and liquid fugacity (SRK VDW) and the values for BIPs



Edit BIPs	Use edited BIPS
Get BIPs	Get BIPs from database
Select the model	SRK VDW

C1	C2	BIP-1	BIP-2	BIP-3	BIP-4	BIP-5
1	2	0.08	0	0	0	
1	3	0.1	0	0	0	
2	3	0.097	0	0	0	
0	0	0	0	0	0	

with these values the calculated p, t for critical point are 79.117 Bar.a and 232.08 K
In first dialog select the HP-VL flash operation on second grid, then set 89 Bar.a and 246 K as inlet conditions, 79.12 Bar.a as outlet condition and -71.9 KW (-61864.3 Kcal/h) as heat duty, the negative sign means that energy is subtracted
Please note that you must specify the value of energy (to add or subtract) to the total value of stream determined as specific enthalpy * mass flow the mass flow in this case has been specified as 1.0 Kg/s (see the second row)



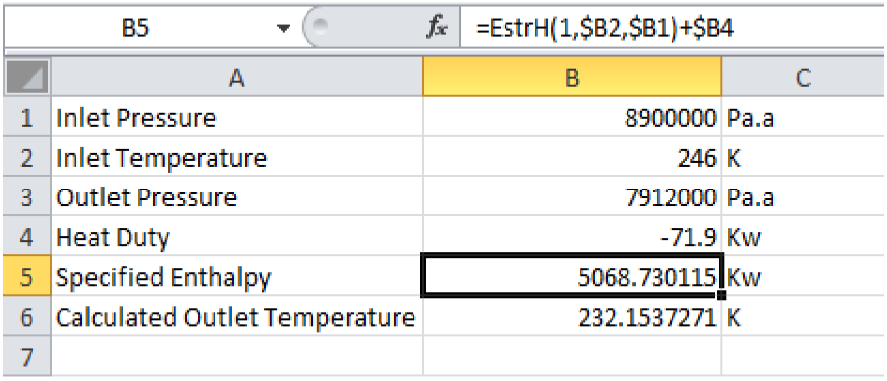
Select / edit stream	1 Test Case 1		Test Case 1		Save	
Operating Conditions	232.154	K	7.912e+006	Pa.a	1	kg/s

Feed and Operation	1 Test Case 1		H-P VL		Compute	
Specifications	246	K	89	bar.a	1	kg/s
Specifications (OUT)	79.12	bar.a	-71.9	kW		

Phase	Feed	Vapor	Liquid	Not present	Not present	Not present
Mol.fraction	1	0.558184	0.441816	0	0	0
CH4	0.7	0.716828	0.67874	0	0	0
CO2	0.15	0.14386	0.157757	0	0	0
H2S	0.15	0.139312	0.163503	0	0	0

Click on Compute buttom to solve the problem, the procedure calculates an outlet temperature (see the second row) of 232.1 K which is close to the critical point giving a idea of reliability of procedure.

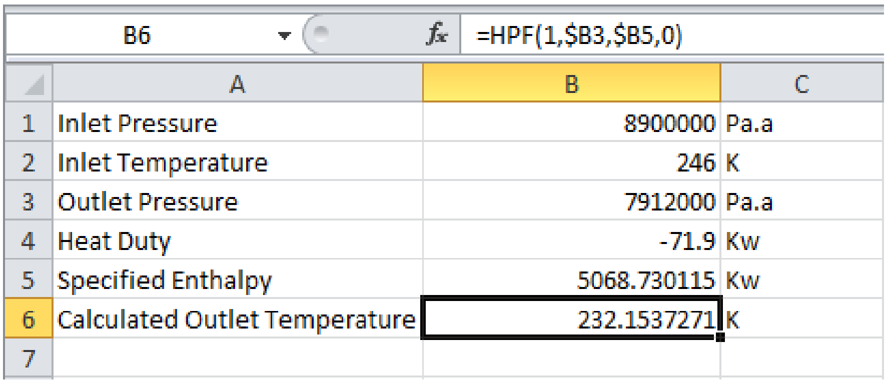
As alternative to utilize Properties Editor you can solve the problem directly in Excel,
in cell B5 enter EstrH(stream,p,t) to define the initial conditions for stream 1 at 89 Bar.a and 246 K and calculate the enthalpy
=EstrH(1,$B2,$B1)+$B4
where 1 is the stream, B2 is the operating temperature, B1 the operating pressure and B4 represents the additional duty



B5 =EstrH(1,$B2,$B1)+$B4

	A	B	C
1	Inlet Pressure	8900000	Pa.a
2	Inlet Temperature	246	K
3	Outlet Pressure	7912000	Pa.a
4	Heat Duty	-71.9	Kw
5	Specified Enthalpy	5068.730115	Kw
6	Calculated Outlet Temperature	232.1537271	K
7			

then with HPF() you calculate the final temperature at specified enthalpy (the initial enthalpy calculated at 89 Bar.a and 246 K plus -or minus- the specified heat duty)
=HPF(1,$B3,$B5,0.0)
where 1 is the stream, B3 is the outlet pressure, B5 the required heat duty and 0.0 is the estimated final temperature (set to 0.0 for automatic initialization)

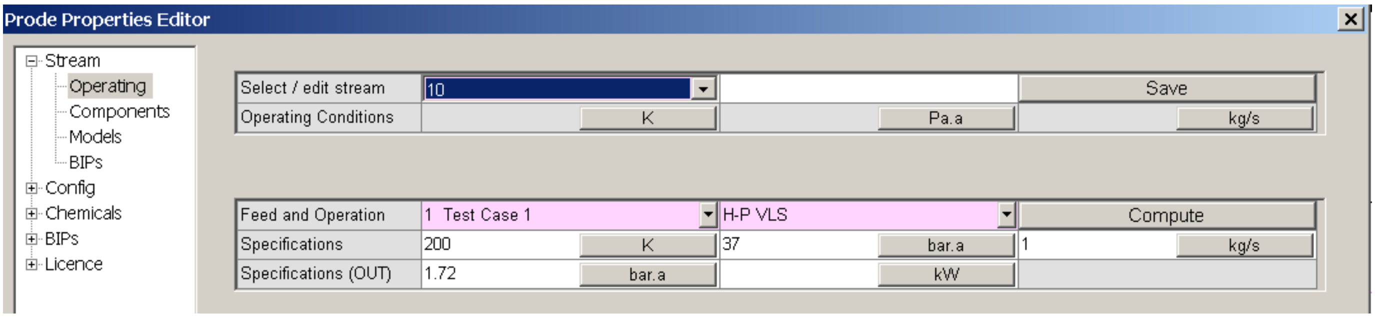


B6 =HPF(1,$B3,$B5,0)

	A	B	C
1	Inlet Pressure	8900000	Pa.a
2	Inlet Temperature	246	K
3	Outlet Pressure	7912000	Pa.a
4	Heat Duty	-71.9	Kw
5	Specified Enthalpy	5068.730115	Kw
6	Calculated Outlet Temperature	232.1537271	K
7			

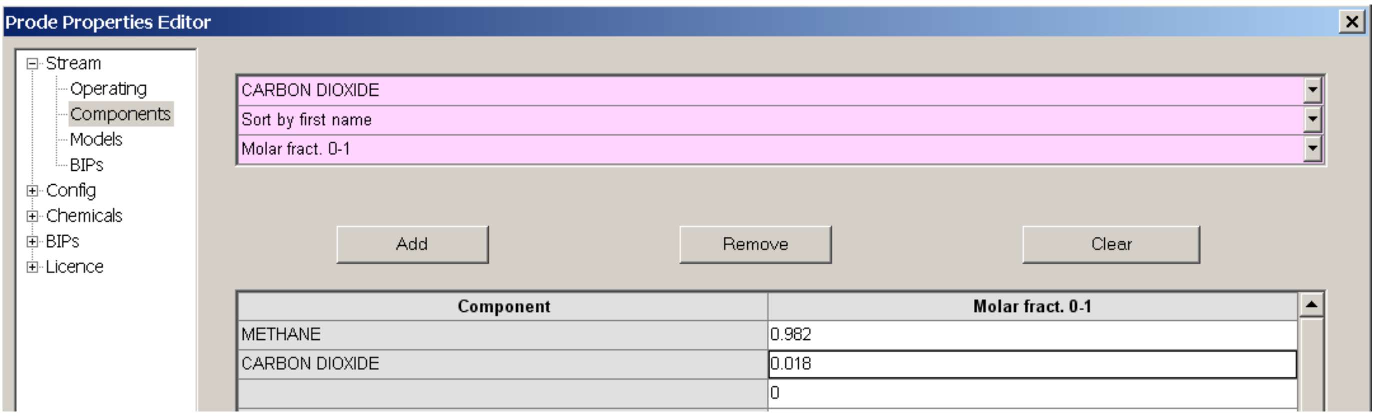
Prode Properties can solve multiphase equilibria (vapor, liquid, solid, hydrate) at specified value of enthalpy, entropy, volume pressure , temperature, additional specifications are possible.

in next example we model a pressure reducing valve (adiabatic process), the stream has composition 0.982 Methane 0.018 CO2, the valve reduces the pressure from 200 K 37 Bar.a (inlet conditions) down to 1.72 Bar.a .
We wish to investigate if at outlet conditions a solid phase is present.
As first step we define a new stream with composition 0.982 Methane 0.018 CO2,
On first page (Operating) we select (first row) the stream nr. 10



Select / edit stream	10				Save	
Operating Conditions		K		Pa.a		kg/s
Feed and Operation	1 Test Case 1		H-P VLS		Compute	
Specifications	200	K	37	bar.a	1	kg/s
Specifications (OUT)	1.72	bar.a		kW		

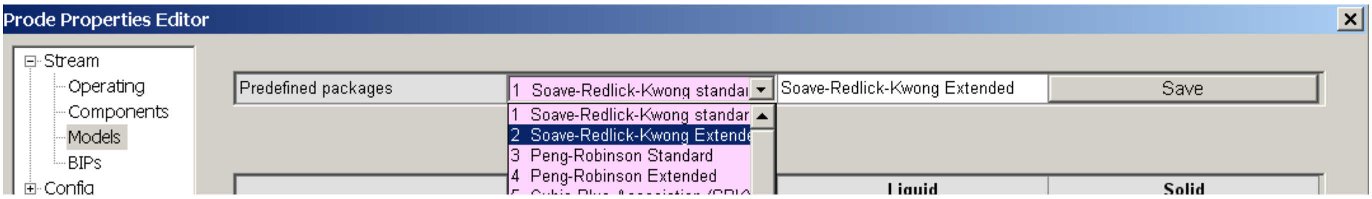
On second page (Composition) we define the composition
0.982 Methane
0.018 CO2,



CARBON DIOXIDE
Sort by first name
Molar fract. 0-1

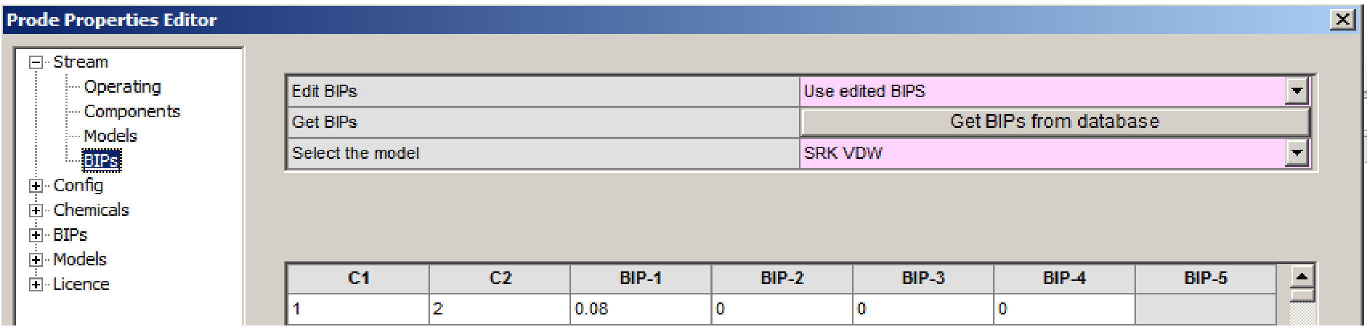
Component	Molar fract. 0-1
METHANE	0.982
CARBON DIOXIDE	0.018
	0

On third page (Models) we select the predefined package Soave Redlich Kwong Extended
the extended models available in Prode Properties include parameters calculated (data regression) for best fitting of vapor pressure, enthalpy and liquid volume of pure fluids.



Predefined packages	1 Soave-Redlick-Kwong standar	Soave-Redlick-Kwong Extended	Save

in fourth page (BIPS) click on button “Get BIPs from database” to load BIPs



Edit BIPs	Use edited BIPS
Get BIPs	Get BIPs from database
Select the model	SRK VDW

C1	C2	BIP-1	BIP-2	BIP-3	BIP-4	BIP-5
1	2	0.08	0	0	0	

We can model the pressure reducer with the predefined H-P VLS operation, this opetration solves a multiphase flash at specified pressure and enthalpy.

On first page

-click on button Save to define the new stream 10

-in second grid select the stream 10

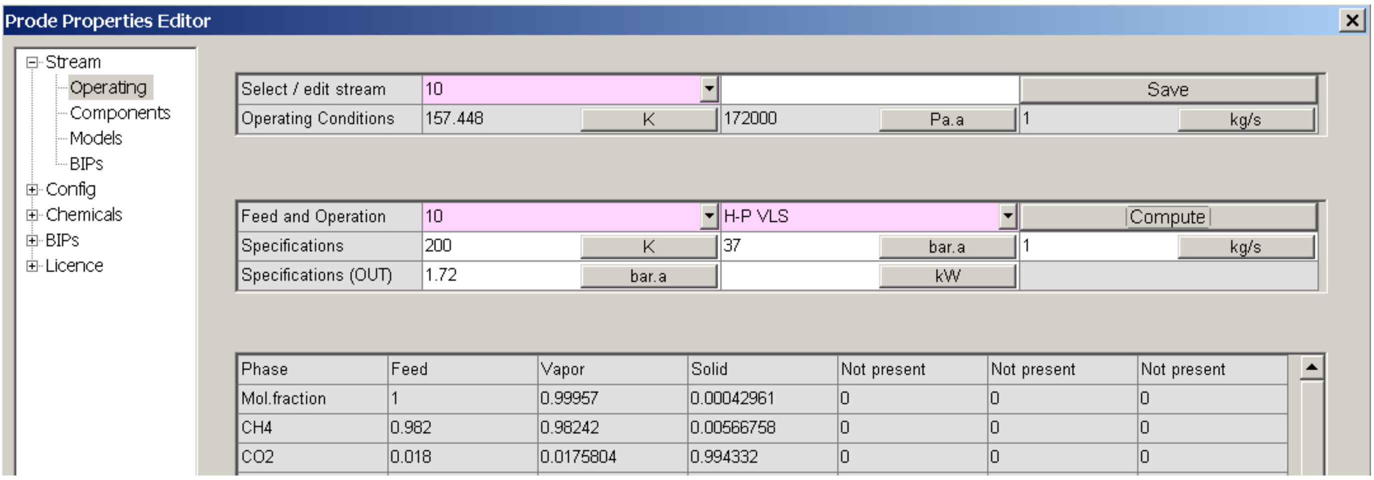
-select the H-P VLS operation

-define 200 K and 37 Bar.a as inlet conditions

-define 1.72 Bar.a as outlet pressure

-define 0 as dh (adiabatic flash)

-click on button “Compute” to get the results



Select / edit stream	10				Save	
Operating Conditions	157.448	K	172000	Pa.a	1	kg/s

Feed and Operation	10		H-P VLS		Compute	
Specifications	200	K	37	bar.a	1	kg/s
Specifications (OUT)	1.72	bar.a		kW		

Phase	Feed	Vapor	Solid	Not present	Not present	Not present
Mol.fraction	1	0.99957	0.00042961	0	0	0
CH4	0.982	0.98242	0.00566758	0	0	0
CO2	0.018	0.0175804	0.994332	0	0	0

the procedure calculates an outlet temperature of 157.45 K at 1.72 Bar.a , there is a solid phase (mainly composed by CO2)

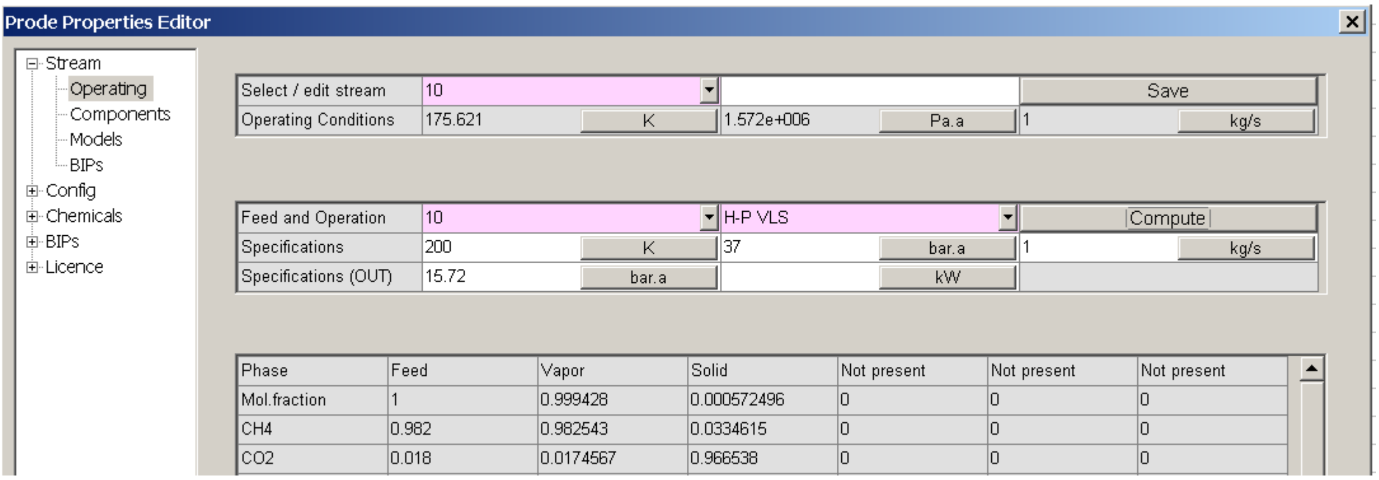
We can compare these results against vapor-solid equilibria data

Experimental data (vapor-solid equilibria)	158.12 K , 1.72 Bar.a
Calculated values	157.45 K , 1.72 Bar.a

We can examine a different case

-define 15.72 Bar.a as outlet pressure

-click on button “Compute” to get the results



Select / edit stream	10				Save	
Operating Conditions	175.621	K	1.572e+006	Pa.a	1	kg/s

Feed and Operation	10		H-P VLS		Compute	
Specifications	200	K	37	bar.a	1	kg/s
Specifications (OUT)	15.72	bar.a		kW		

Phase	Feed	Vapor	Solid	Not present	Not present	Not present
Mol.fraction	1	0.999428	0.000572496	0	0	0
CH4	0.982	0.982543	0.0334615	0	0	0
CO2	0.018	0.0174567	0.966538	0	0	0

the procedure calculates an outlet temperature of 175.6 K at 15.72 Bar.a , there is a solid phase (mainly composed by CO2)

We can compare these results against vapor-solid equilibria data

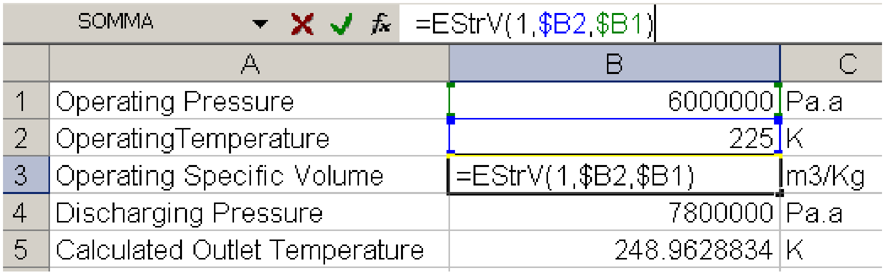
Experimental data (vapor-solid equilibria)	176.04 K , 15.72 Bar.a
Calculated values	175.6 K , 15.72 Bar.a

In next example we estimate the (initial) discharging temperature of a fluid contained in a vessel protected by a safety valve, the block valves have been closed and the fluid heated (at constant volume),
the mixture is that already examined in previous examples

Methane	0.7
Carbon Dioxide	0.15
Hydrogen Sulfide	0.15

with Soave Redlick Kwong model , the operating conditions are 60 Bar.a and 225 K
the discharging pressure is 78 Bar.a

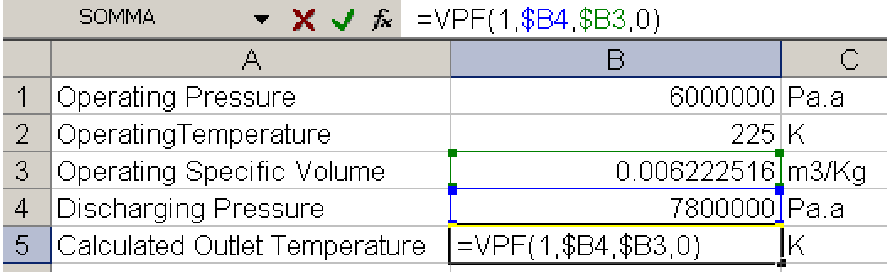
the method EStrV() in cell B3 allows to define the operating conditions and to calculate the specific volume
=EStrV(1,$B2,$B1)
where 1 is the stream, B2 is the inlet temperature and B1 is the inlet pressure



=EStrV(1,$B2,$B1)

	A	B	C
1	Operating Pressure	6000000	Pa.a
2	OperatingTemperature	225	K
3	Operating Specific Volume	=EStrV(1,$B2,$B1)	m3/Kg
4	Discharging Pressure	7800000	Pa.a
5	Calculated Outlet Temperature	248.9628834	K

to calculate the Outlet temperature for the isochoric process in celll B5 we enter
=VPF(1,$B4,$B3,0)
where 1 is the stream, B4 is the final pressure, B3 the required specific volume (equal to inlet volume) and 0.0 the estimated final temperature (the value 0.0 means we require the automatic initialization)



=VPF(1,$B4,$B3,0)

	A	B	C
1	Operating Pressure	6000000	Pa.a
2	OperatingTemperature	225	K
3	Operating Specific Volume	0.006222516	m3/Kg
4	Discharging Pressure	7800000	Pa.a
5	Calculated Outlet Temperature	=VPF(1,$B4,$B3,0)	K

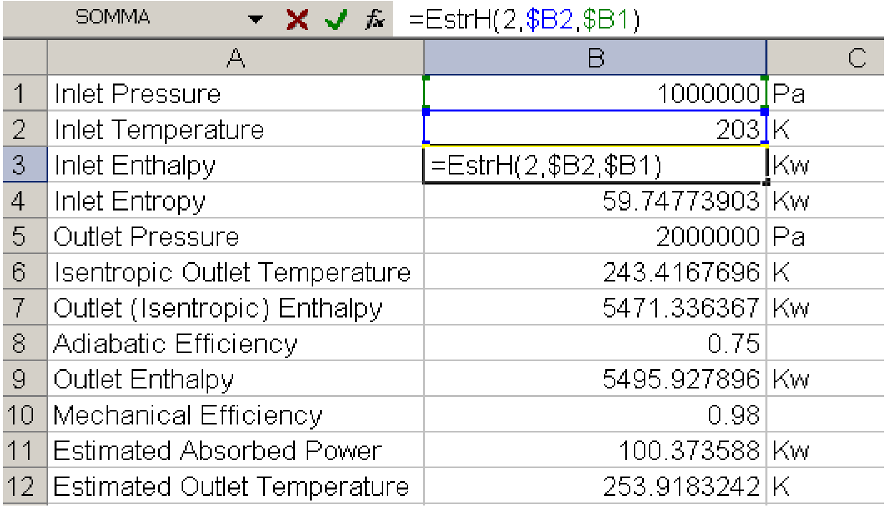
IMPORTANT due to the calling mechanism of Microsoft Excel in some cases Prode Properties may return a 0.0 value even when a solution is available, in those cases you can get the correct results by forcing the cell recalc with the Enter key

In next example we estimate the discharge temperature and the power absorbed by a single stage compressor with determined adiabatic efficiency, the theoretical power requirements can be calculated as
(enthalpy at outlet conditions - enthalpy at inlet conditions) / mechanical efficiency
The outlet temperature is calculated with four steps,
a) model the compressor as isentropic process and calculate the final temperature
b) calculate the final enthalpy for the isentropic process
c) calculate the outlet enthalpy as

$$\text{outlet enthalpy} = \text{enthalpy at inlet conditions} + \frac{\text{outlet enthalpy for the isentropic process - enthalpy at inlet conditions}}{\text{adiabatic efficiency}}$$

d) calculate the outlet temperature at given outlet enthalpy

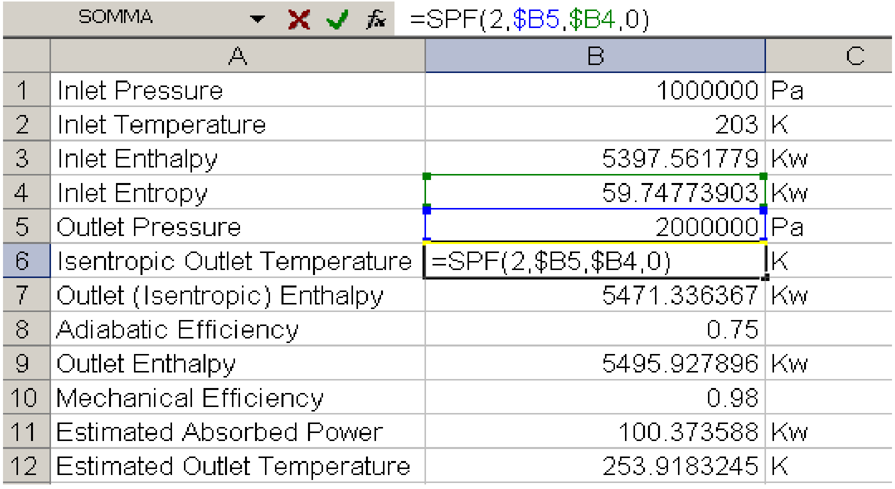
The specifications are mass flow 1 Kg/s , fluid Methane 0.999, n-Butane 0.001 (this is the Test case 2) to compress from 10 Bar.a, 203 K to 20 Bar.a, we assume 0.75 as adibatic efficiency and 0.98 as mechanical efficiency
In Excel we define the inlet conditions with macro EStrH() which forces a isothermal flash at specified pressure and temperature
=EStrH(2,$B2,$B1)
where 2 is the stream, B2 is the inlet temperature and B1 is the inlet pressure



=EstrH(2,$B2,$B1)

	A	B	C
1	Inlet Pressure	1000000	Pa
2	Inlet Temperature	203	K
3	Inlet Enthalpy	=EstrH(2,$B2,$B1)	Kw
4	Inlet Entropy	59.74773903	Kw
5	Outlet Pressure	2000000	Pa
6	Isentropic Outlet Temperature	243.4167696	K
7	Outlet (Isentropic) Enthalpy	5471.336367	Kw
8	Adiabatic Efficiency	0.75	
9	Outlet Enthalpy	5495.927896	Kw
10	Mechanical Efficiency	0.98	
11	Estimated Absorbed Power	100.373588	Kw
12	Estimated Outlet Temperature	253.9183242	K

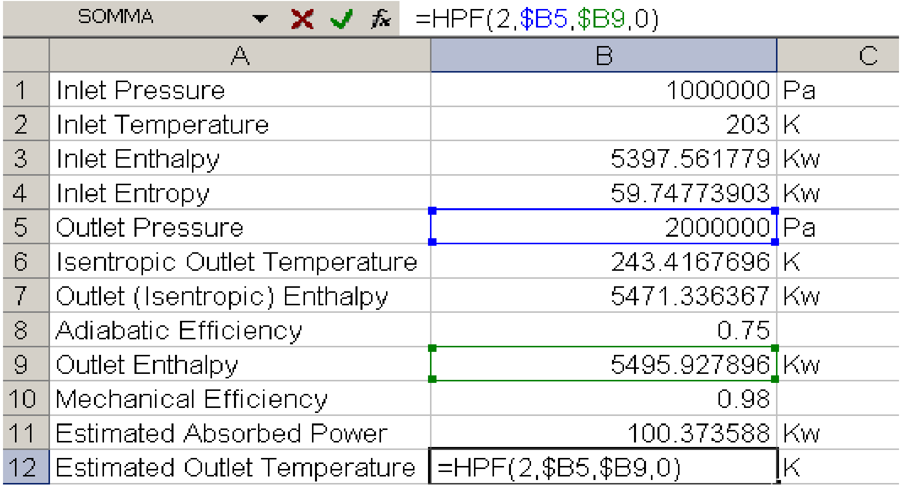
in cell B4 we calculate the initial entropy as
=EstrS(2,$B2,$B1)to calculate the outlet temperature for the isentropic process in celll B6 we enter
=SPF(2,$B5,$B4,0)
where 2 is the stream, B5 is the outlet pressure, B4 the required entropy (equal to inlet entropy being a isentropic process) and 0.0 as estimated final temperature



=SPF(2,$B5,$B4,0)

	A	B	C
1	Inlet Pressure	1000000	Pa
2	Inlet Temperature	203	K
3	Inlet Enthalpy	5397.561779	Kw
4	Inlet Entropy	59.74773903	Kw
5	Outlet Pressure	2000000	Pa
6	Isentropic Outlet Temperature	=SPF(2,$B5,$B4,0)	K
7	Outlet (Isentropic) Enthalpy	5471.336367	Kw
8	Adiabatic Efficiency	0.75	
9	Outlet Enthalpy	5495.927896	Kw
10	Mechanical Efficiency	0.98	
11	Estimated Absorbed Power	100.373588	Kw
12	Estimated Outlet Temperature	253.9183245	K

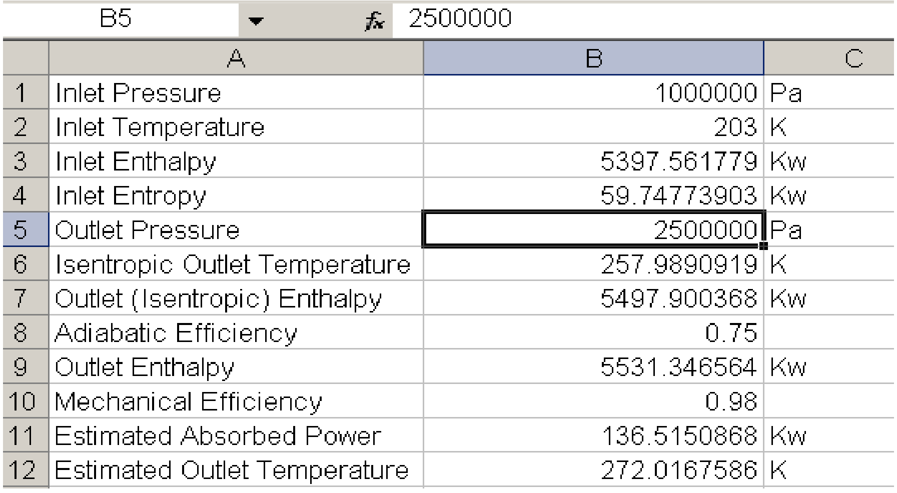
to calculate the outlet enthalpy enter in cell B7
=EstrH(2,$B6,$B5)
and in cell B9 enter
=$B3+($B7-$B3)/$B8
to calculate the final enthapy (with the adiabatic efficiency specified in cell B7),
to estimate the absorbed power in cell B11 enter
=($B9-$B3)/$B10
Since we know the enthalpy and pressure at outlet conditions we can calculate the temperature with HPF() method
=HPF(2,$B5,$B9,0)
where 2 is the stream, B4 is the outlet pressure, $B8-$B6 represents the heat duty (the difference from initial conditions calculated in cell B6) and 0.0 the estimated final temperature



=HPF(2,$B5,$B9,0)

	A	B	C
1	Inlet Pressure	1000000	Pa
2	Inlet Temperature	203	K
3	Inlet Enthalpy	5397.561779	Kw
4	Inlet Entropy	59.74773903	Kw
5	Outlet Pressure	2000000	Pa
6	Isentropic Outlet Temperature	243.4167696	K
7	Outlet (Isentropic) Enthalpy	5471.336367	Kw
8	Adiabatic Efficiency	0.75	
9	Outlet Enthalpy	5495.927896	Kw
10	Mechanical Efficiency	0.98	
11	Estimated Absorbed Power	100.373588	Kw
12	Estimated Outlet Temperature	=HPF(2,$B5,$B9,0)	K

Now if we wish to evaluate the performance at different conditions we can modify the inlet conditions, for example setting 2500000 Pa.a as outlet pressure and changing the value in cell B1 or cell B2 to force a recalc

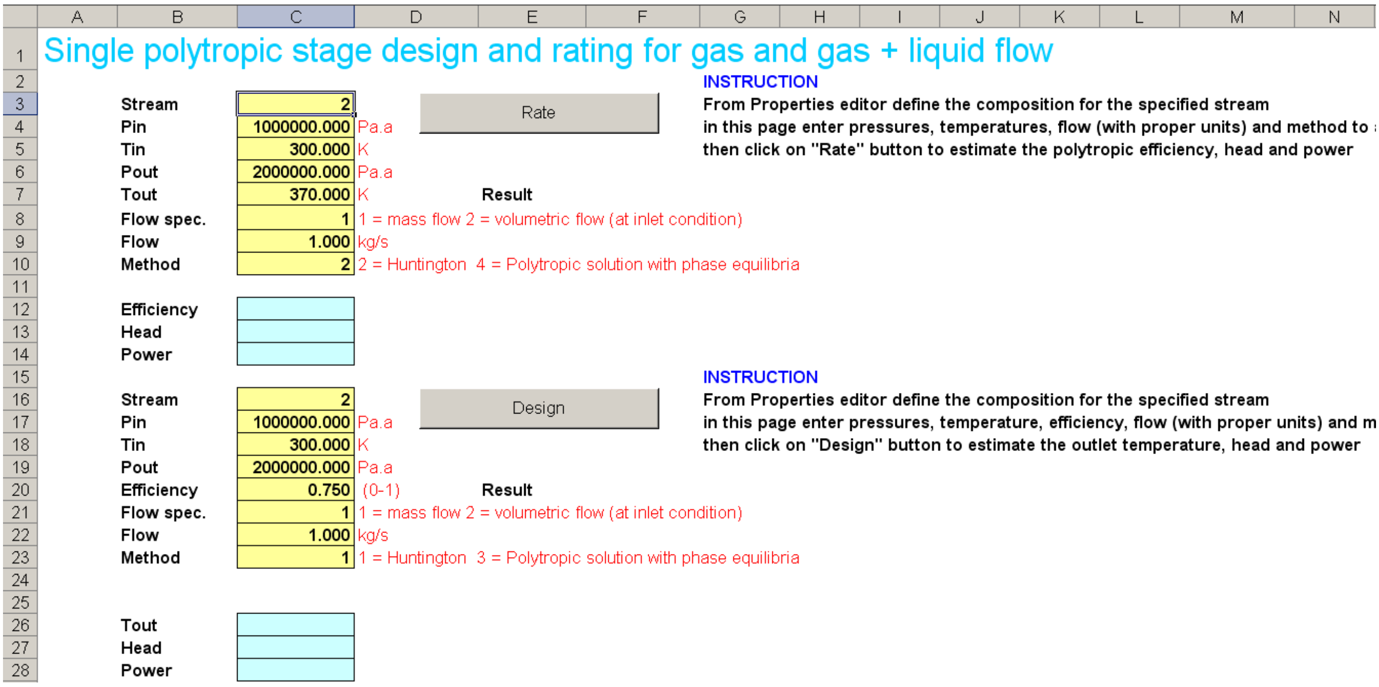


2500000

	A	B	C
1	Inlet Pressure	1000000	Pa
2	Inlet Temperature	203	K
3	Inlet Enthalpy	5397.561779	Kw
4	Inlet Entropy	59.74773903	Kw
5	Outlet Pressure	2500000	Pa
6	Isentropic Outlet Temperature	257.9890919	K
7	Outlet (Isentropic) Enthalpy	5497.900368	Kw
8	Adiabatic Efficiency	0.75	
9	Outlet Enthalpy	5531.346564	Kw
10	Mechanical Efficiency	0.98	
11	Estimated Absorbed Power	136.5150868	Kw
12	Estimated Outlet Temperature	272.0167586	K

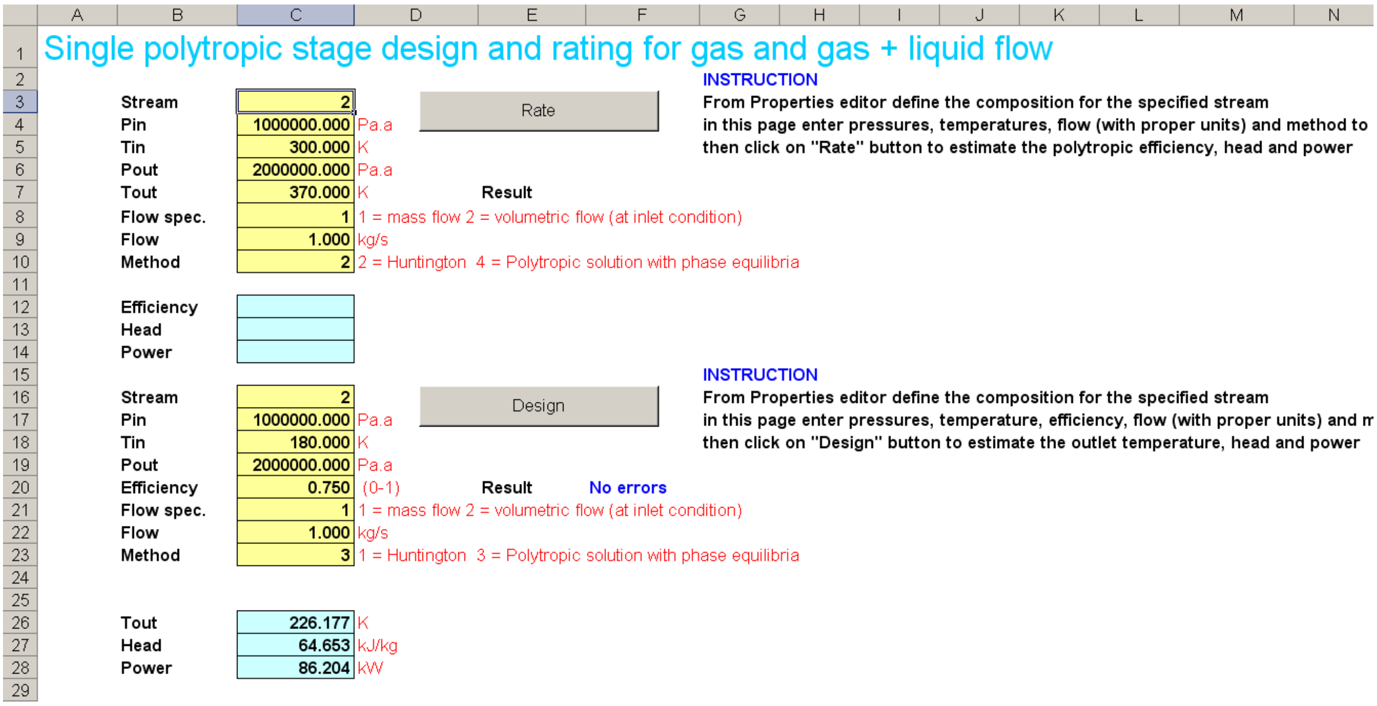
In a similar way you can define a procedure to model a polytropic process.

Next example shows how to simulate a compression stage (as polytropic process) where the inlet stream can be vapor or vapor + liquid (mixed), comparing the results of different methods, see the paragraph "Methods for solving a Polytropic operation".for additional information.
We use a predefined Excel page as interface to Prode Properties.
From Excel menu File->open , in Excel folder (in Prode Properties installation) select the file compressor.xls



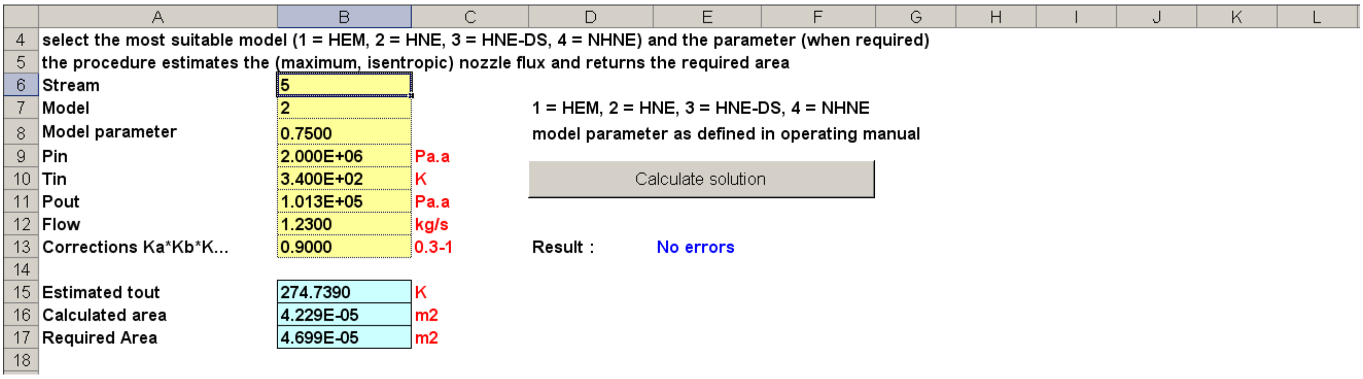
	B	C	D	E	F	H
1	Single polytropic stage design and rating for gas and gas + liquid flow					
2						INSTRUCTION
3	Stream	2		Rate		From Properties editor define the composition for the specified stream
4	Pin	1000000.000	Pa.a			in this page enter pressures, temperatures, flow (with proper units) and method to
5	Tin	300.000	K			then click on "Rate" button to estimate the polytropic efficiency, head and power
6	Pout	2000000.000	Pa.a			
7	Tout	370.000	K	Result		
8	Flow spec.	1	1 = mass flow 2 = volumetric flow (at inlet condition)			
9	Flow	1.000	kg/s			
10	Method	2	2 = Huntington 4 = Polytropic solution with phase equilibria			
11						
12	Efficiency					
13	Head					
14	Power					
15						INSTRUCTION
16	Stream	2		Design		From Properties editor define the composition for the specified stream
17	Pin	1000000.000	Pa.a			in this page enter pressures, temperature, efficiency, flow (with proper units) and m
18	Tin	300.000	K			then click on "Design" button to estimate the outlet temperature, head and power
19	Pout	2000000.000	Pa.a			
20	Efficiency	0.750	(0-1)	Result		
21	Flow spec.	1	1 = mass flow 2 = volumetric flow (at inlet condition)			
22	Flow	1.000	kg/s			
23	Method	1	1 = Huntington 3 = Polytropic solution with phase equilibria			
24						
25						
26	Tout					
27	Head					
28	Power					

the page contains two sections, the first permits to calculate the polytropic efficiency of a single compression stage given the inlet temperature and pressure.
The second section allows to estimate the discharging temperature given inlet temperature and pressure, outlet pressure and polytropic efficiency.
Notice that Prode Properties includes a specific methof for solving a polytropic stage with phase equilibria, this method permits to simulate both single phase (vapor) and mixed (vapor + liquid) processes.
The mixture Methane 0.999, n-Butane 0.001 (predefined stream 2) at 10 Bar.a shows a dew point of 187.5 K , by setting a inlet temperature of 180 K we specify vapor + liquid as inlet condition, the standard method can simulate only gas streams, however the Polytropic solution with phase equilibria method allows to solve this case.



	B	C	D	E	F	H
1	Single polytropic stage design and rating for gas and gas + liquid flow					
2						INSTRUCTION
3	Stream	2		Rate		From Properties editor define the composition for the specified stream
4	Pin	1000000.000	Pa.a			in this page enter pressures, temperatures, flow (with proper units) and method to
5	Tin	300.000	K			then click on "Rate" button to estimate the polytropic efficiency, head and power
6	Pout	2000000.000	Pa.a			
7	Tout	370.000	K	Result		
8	Flow spec.	1	1 = mass flow 2 = volumetric flow (at inlet condition)			
9	Flow	1.000	kg/s			
10	Method	2	2 = Huntington 4 = Polytropic solution with phase equilibria			
11						
12	Efficiency					
13	Head					
14	Power					
15						INSTRUCTION
16	Stream	2		Design		From Properties editor define the composition for the specified stream
17	Pin	1000000.000	Pa.a			in this page enter pressures, temperature, efficiency, flow (with proper units) and m
18	Tin	180.000	K			then click on "Design" button to estimate the outlet temperature, head and power
19	Pout	2000000.000	Pa.a			
20	Efficiency	0.750	(0-1)	Result	No errors	
21	Flow spec.	1	1 = mass flow 2 = volumetric flow (at inlet condition)			
22	Flow	1.000	kg/s			
23	Method	3	1 = Huntington 3 = Polytropic solution with phase equilibria			
24						
25						
26	Tout	226.177	K			
27	Head	64.653	kJ/kg			
28	Power	86.204	kW			
29						

Next example allows to size a relief valve comparing the results of different methods for critical and two-phase flow, see the paragraph “Methods for solving a Isentropic operation” for additional information.
We use a predefined Excel page as interface to Prode Properties.
From Excel menu File->open , in Excel folder (in Prode Properties installation) select the file nozzle.xls

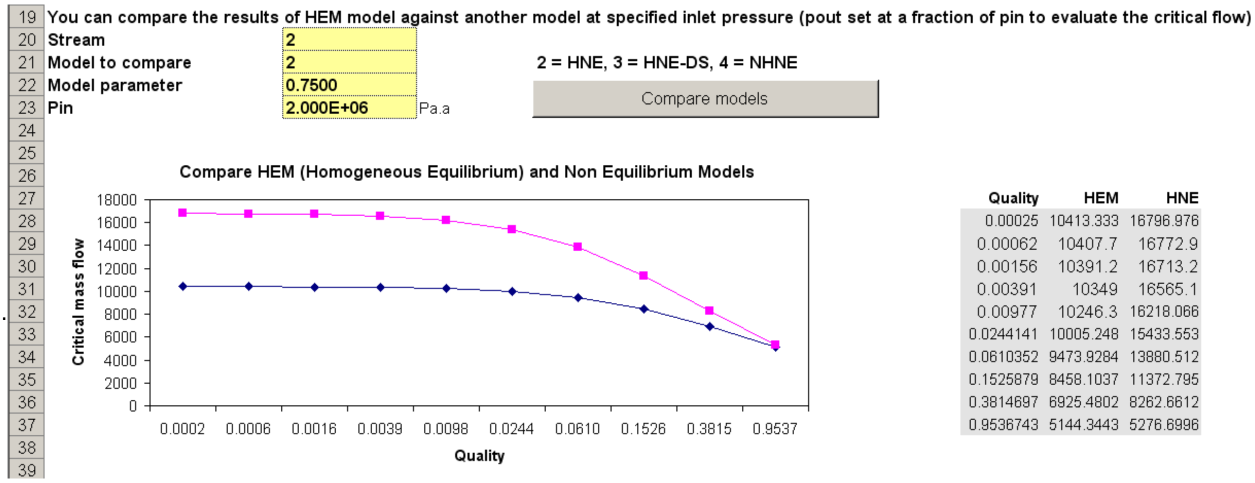


	A	B	C	D
4	select the most suitable model (1 = HEM, 2 = HNE, 3 = HNE-DS, 4 = NHNE) and the parameter (when required)			
5	the procedure estimates the (maximum, isentropic) nozzle flux and returns the required area			
6	Stream	5		
7	Model	2		1 = HEM, 2 = HNE, 3 = HNE-DS, 4 = NHNE
8	Model parameter	0.7500		model parameter as defined in operating manual
9	Pin	2.000E+06	Pa.a	
10	Tin	3.400E+02	K	Calculate solution
11	Pout	1.013E+05	Pa.a	
12	Flow	1.2300	kg/s	
13	Corrections Ka*Kb*K...	0.9000	0.3-1	Result : No errors
14				
15	Estimated tout	274.7390	K	
16	Calculated area	4.229E-05	m2	
17	Required Area	4.699E-05	m2	
18				

The steps to size a relief valve are easy to follow:
1) from Properties editor define the composition, models, BIPs (for mixtures)
2) enter the discharging temperature, pressure, flow, model, outlet pressure
3) click on button “Calculate Solution”

the procedure calculates the required area and the outlet temperature for critical and two-phase flow,
you may utilize the procedure to verify the results from a different software in applications as fluids in critical area, two-phases flow etc.

The same page includes a procedure to compare the results from HEM (Homogeneous Equilibrium) and different Non Equilibrium models for a specified pressure in a range of inlet vapor qualities
Please follow fhese steps to compare:two models,
1) from Properties editor define the composition, models, BIPs (for mixtures)
2) enter the pressure, model and parameter
3) click on button “Compare Models”



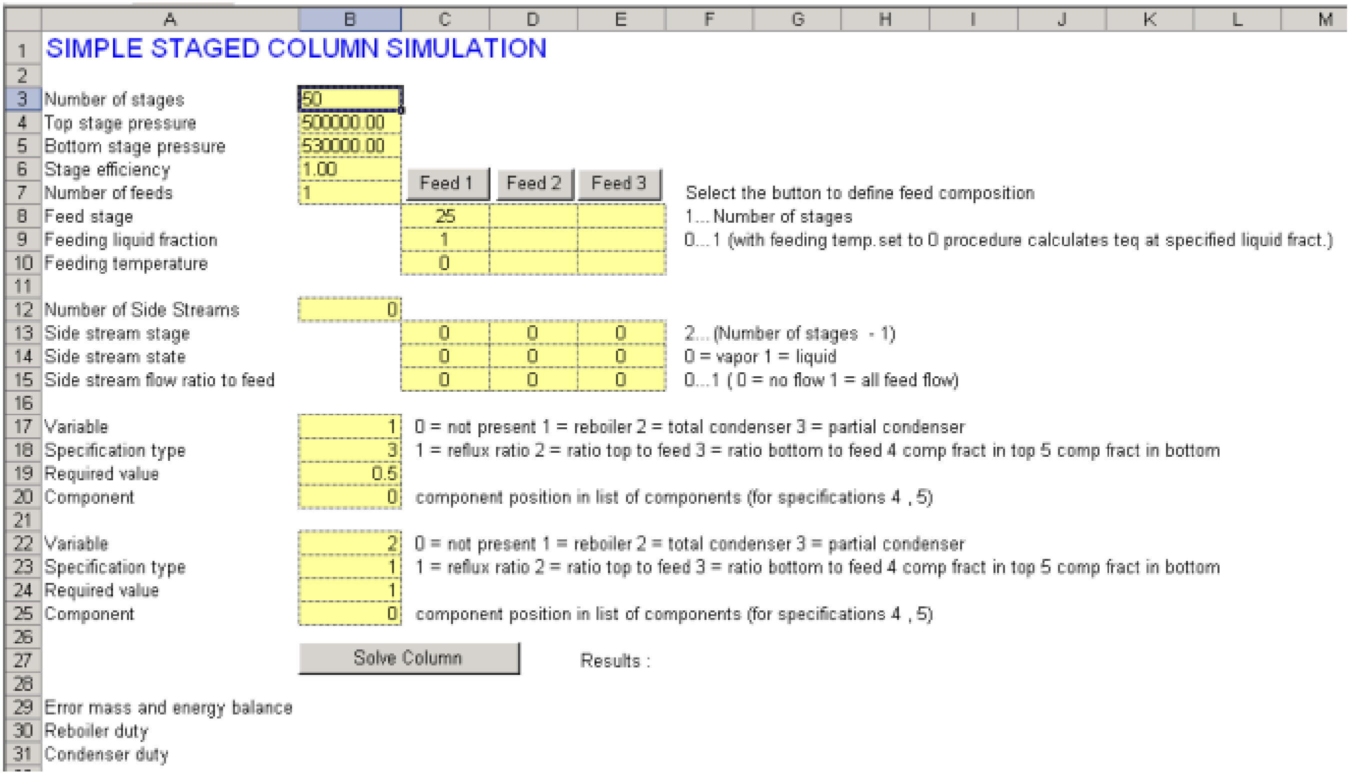
	A	B	C	D
19	You can compare the results of HEM model against another model at specified inlet pressure (pout set at a fraction of pin to evaluate the critical flow)			
20	Stream	2		
21	Model to compare	2		2 = HNE, 3 = HNE-DS, 4 = NHNE
22	Model parameter	0.7500		Compare models
23	Pin	2.000E+06	Pa.a	

Compare HEM (Homogeneous Equilibrium) and Non Equilibrium Models

Quality	HEM	HNE
0.00025	10413.333	16796.976
0.00062	10407.7	16772.9
0.00156	10391.2	16713.2
0.00391	10349	16565.1
0.00977	10246.3	16218.066
0.0244141	10005.248	15433.553
0.0610352	9473.9284	13880.512
0.1525879	8458.1037	11372.795
0.3814697	6925.4802	8262.6612
0.9536743	5144.3443	5276.6996

The Non Equlibrium models are mainly of interest for short nozzles where the final equilibrium condition (predicted by HEM models) is not reached cause the residence time of the fluid is too short.
The HNE models require specific parameters, for Prode HNE model a value of 0.75 is suggested for short nozzles but different values may be defined to fit specific data sets.

Next example permits to solve a distillation column, refer to paragraph “Methods for solving staged columns” for additional information, here we use a predefined Excel page as interface to Prode Properties methods.
From Excel menu File->open , in Excel folder (in Prode Properties installation) select the file column.xls
In this page you can define different kind of columns with reboiler, condenser , one or more feeds and one or more side streams.

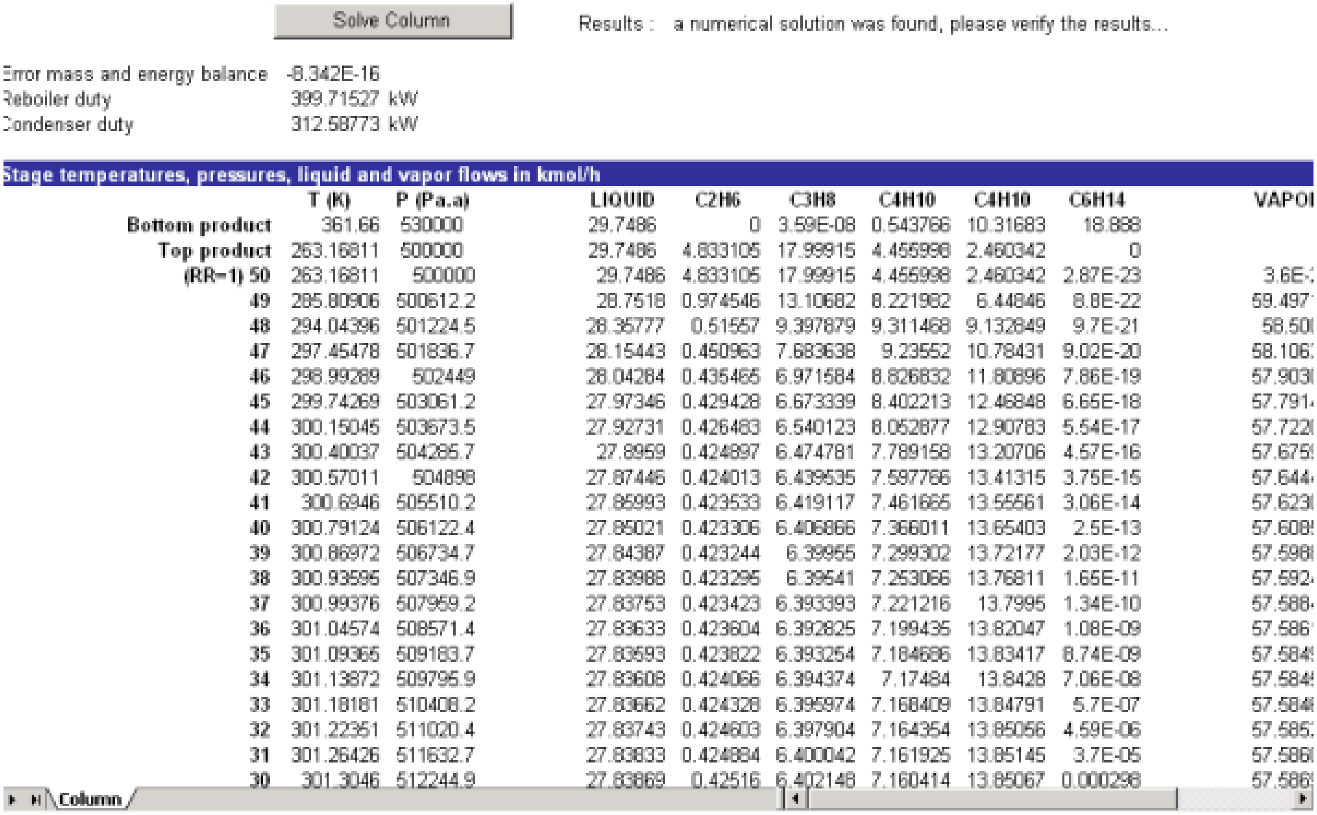


	A	B	C	D	E	F
1	SIMPLE STAGED COLUMN SIMULATION					
2						
3	Number of stages	50				
4	Top stage pressure	500000.00				
5	Bottom stage pressure	530000.00				
6	Stage efficiency	1.00	Feed 1	Feed 2	Feed 3	
7	Number of feeds	1				Select the button to define feed composition
8	Feed stage		25			1... Number of stages
9	Feeding liquid fraction		1			0...1 (with feeding temp. set to 0 procedure calculates teq at specified liquid fract.)
10	Feeding temperature		0			
11						
12	Number of Side Streams	0				
13	Side stream stage		0	0	0	2... (Number of stages - 1)
14	Side stream state		0	0	0	0 = vapor 1 = liquid
15	Side stream flow ratio to feed		0	0	0	0...1 (0 = no flow 1 = all feed flow)
16						
17	Variable	1	0 = not present 1 = reboiler 2 = total condenser 3 = partial condenser			
18	Specification type	3	1 = reflux ratio 2 = ratio top to feed 3 = ratio bottom to feed 4 comp fract in top 5 comp fract in bottom			
19	Required value	0.5				
20	Component	0	component position in list of components (for specifications 4 , 5)			
21						
22	Variable	2	0 = not present 1 = reboiler 2 = total condenser 3 = partial condenser			
23	Specification type	1	1 = reflux ratio 2 = ratio top to feed 3 = ratio bottom to feed 4 comp fract in top 5 comp fract in bottom			
24	Required value	1				
25	Component	0	component position in list of components (for specifications 4 , 5)			
26						
27		Solve Column			Results :	
28						
29	Error mass and energy balance					
30	Reboiler duty					
31	Condenser duty					

The steps to define a column are easy to follow:
1) define the number of stages
2) define pressure distribution (bottom and top stage)
3) define stage efficiency
4) define the number of feeds, each feed flow rate and compositions (click on the proper Feed button to access the stream editor), each feed stage (remember that reboiler (if present) is stage 1 and condenser (if present) is stage N, and the liquid fraction (or the temperature) of each feed.
5) Define the number of side streams (if any) , the stage, the type (vapor or liquid flow) and the flow specification
6) Define variables as condenser and reboiler and the related specifications, the procedure allows different specifications including molar fractions (and recovery) of a component in top or bottom stage

Notes :
In Stream Editor (Config->Units) you can define all the units for this project
in Stream Editor (Config->Setti gs) you can define mass units or molar units for flows in Stream Editor

Once the column has been defined it is suggested to verify the input data for inconsistent specifications, if you are sure that all is Ok run the solver (button Solve Column)



Results :   a numerical solution was found, please verify the results...

Error mass and energy balance   -8.342E-16
Reboiler duty   399.71527 kW
Condenser duty   312.58773 kW

Stage temperatures, pressures, liquid and vapor flows in kmol/h

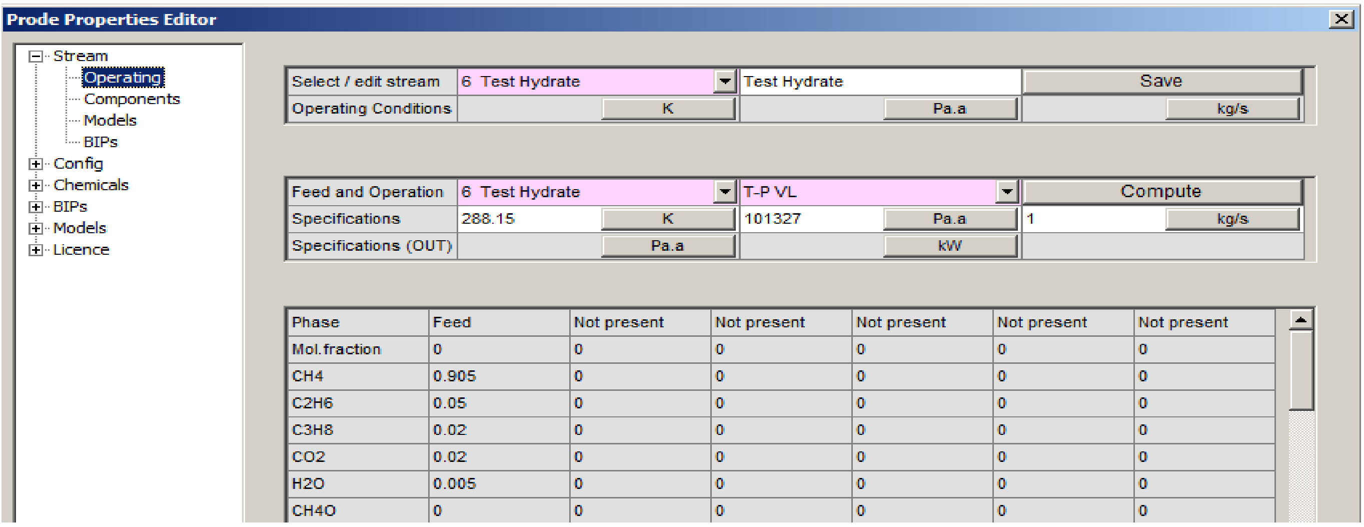
	T (K)	P (Pa.a)	LIQUID	C2H6	C3H8	C4H10	C4H10	C6H14	VAPO
Bottom product	361.66	530000	29.7486	0	3.59E-08	0.543766	10.31683	18.888	
Top product	263.16811	500000	29.7486	4.833105	17.99915	4.455998	2.460342	0	
(RR=1) 50	263.16811	500000	29.7486	4.833105	17.99915	4.455998	2.460342	2.87E-23	3.6E-
49	285.80906	500612.2	28.7518	0.974546	13.10682	8.221982	6.44846	8.8E-22	59.497
48	294.04396	501224.5	28.35777	0.51557	9.397879	9.311468	9.132849	9.7E-21	58.50
47	297.45478	501836.7	28.15443	0.450963	7.683638	9.23552	10.78431	9.02E-20	58.106
46	298.99289	502449	28.04284	0.435465	6.971584	8.826832	11.80896	7.86E-19	57.903
45	299.74269	503061.2	27.97346	0.429428	6.673339	8.402213	12.46848	6.65E-18	57.791
44	300.15045	503673.5	27.92731	0.426483	6.540123	8.052877	12.90783	5.54E-17	57.722
43	300.40037	504285.7	27.8959	0.424897	6.474781	7.789158	13.20706	4.57E-16	57.675
42	300.57011	504898	27.87446	0.424013	6.439535	7.597766	13.41315	3.75E-15	57.644
41	300.6946	505510.2	27.85993	0.423533	6.419117	7.461665	13.55561	3.06E-14	57.623
40	300.79124	506122.4	27.85021	0.423306	6.406866	7.366011	13.65403	2.5E-13	57.608
39	300.86972	506734.7	27.84387	0.423244	6.39955	7.299302	13.72177	2.03E-12	57.598
38	300.93595	507346.9	27.83988	0.423295	6.39541	7.253066	13.76811	1.65E-11	57.592
37	300.99376	507959.2	27.83753	0.423423	6.393393	7.221216	13.7995	1.34E-10	57.588
36	301.04574	508571.4	27.83633	0.423604	6.392825	7.199435	13.82047	1.08E-09	57.586
35	301.09365	509183.7	27.83593	0.423822	6.393254	7.184686	13.83417	8.74E-09	57.584
34	301.13872	509795.9	27.83608	0.424066	6.394374	7.17484	13.8428	7.06E-08	57.584
33	301.18181	510408.2	27.83662	0.424328	6.395974	7.168409	13.84791	5.7E-07	57.584
32	301.22351	511020.4	27.83743	0.424603	6.397904	7.164354	13.85056	4.59E-06	57.585
31	301.26426	511632.7	27.83833	0.424884	6.400042	7.161925	13.85145	3.7E-05	57.586
30	301.3046	512244.9	27.83869	0.42516	6.402148	7.160414	13.85067	0.000298	57.586

the report includes
1) the verified errors in mass and energy balance
2) reboiler and condenser duties
3) temperature and pressure in each stage
4) total and component vapor flows in each stage
5) total and component liquid flows in each stage

next example shows how to calculate the hydrate formation curve (temperature and pressure) for a given mixture.
From Excel menu File->open , in Excel folder (in Prode Properties installation) select the file hydrate.xls

IMPORTANT
in order to calculate phase equilibria with hydrates you must include in stream one or more fomers plus water,
when solving multiphase equilibria Prode Properties considers SI, SII and SH structures

In Properties Editor select stream "6 Test Hydrate" in both selectors of first and second window, the "6 Test Hydrate" stream includes a predefined composition C1 0.905 C2 0.05 C3 0.02 CO2 0.02 H2O 0.005 CH4O 0



Prode Properties Editor

- Stream
  - Operating
  - Components
  - Models
  - BIPs
- Config
- Chemicals
- BIPs
- Models
- Licence

Select / edit stream	6 Test Hydrate	Test Hydrate	Save
Operating Conditions	K	Pa.a	kg/s

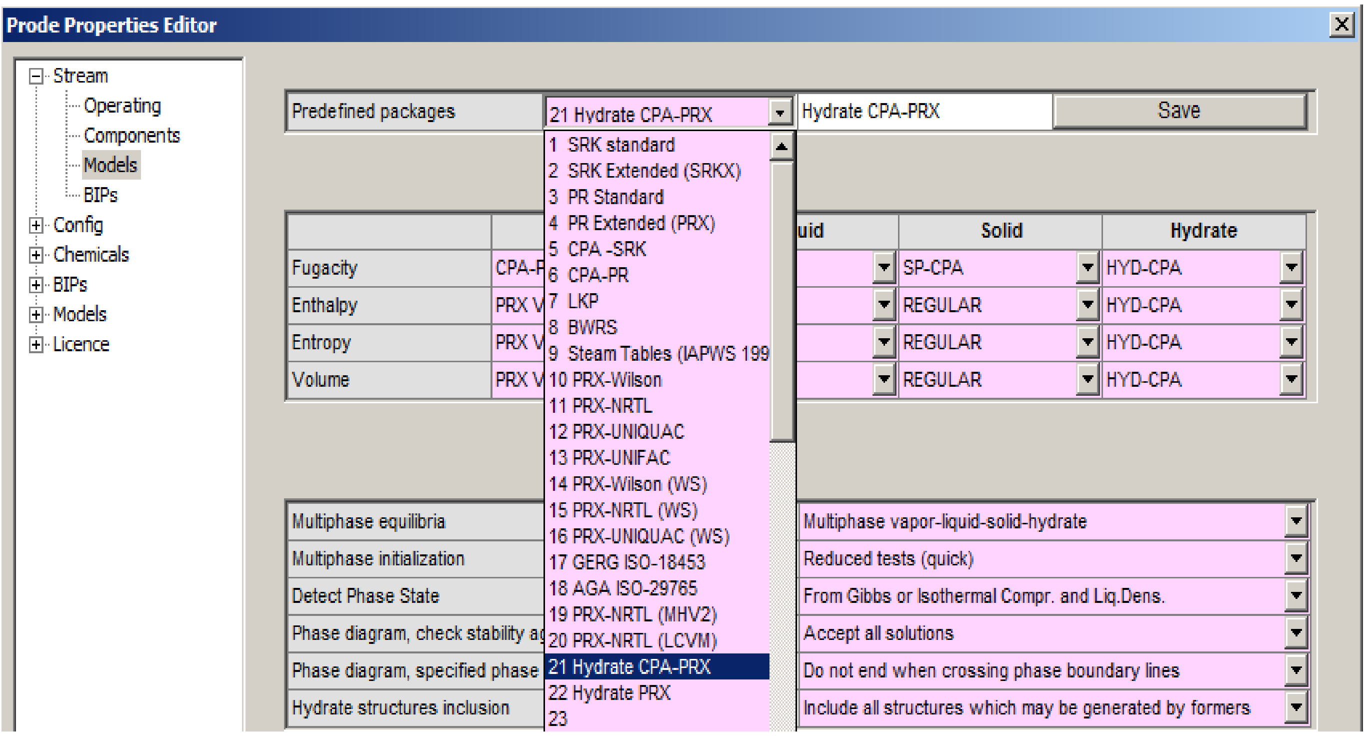
Feed and Operation	6 Test Hydrate	T-P VL	Compute
Specifications	288.15 K	101327 Pa.a	1 kg/s
Specifications (OUT)	Pa.a	kW	

Phase	Feed	Not present	Not present	Not present	Not present	Not present
Mol.fraction	0	0	0	0	0	0
CH4	0.905	0	0	0	0	0
C2H6	0.05	0	0	0	0	0
C3H8	0.02	0	0	0	0	0
CO2	0.02	0	0	0	0	0
H2O	0.005	0	0	0	0	0
CH4O	0	0	0	0	0	0

IMPORTANT
when solving phase equilibria with solids and hydrates to avoid large errors make sure to have the same model selected for vapor, liquid, solid and hydrate, you can set / inspect models from models tab in Properties Editor,
Base version allows two alternatives

1) CPA PR for vapor and liquid , SP-CPA for solid , HYD-CPA for hydrate
2) PR Extended (PRX) for vapor and liquid plus SP-PRX for solid and HPRX for hydrate

the list with predefined packages shows two opions, Hydrate CPA-PRX (based on CPA) and Hydrate PRX (based on Extended Peng Robinson) , for this example select Hydrate CPA-PRX



Prode Properties Editor

- Stream
  - Operating
  - Components
  - Models
  - BIPs
- Config
- Chemicals
- BIPs
- Models
- Licence

Predefined packages	21 Hydrate CPA-PRX	Hydrate CPA-PRX	Save

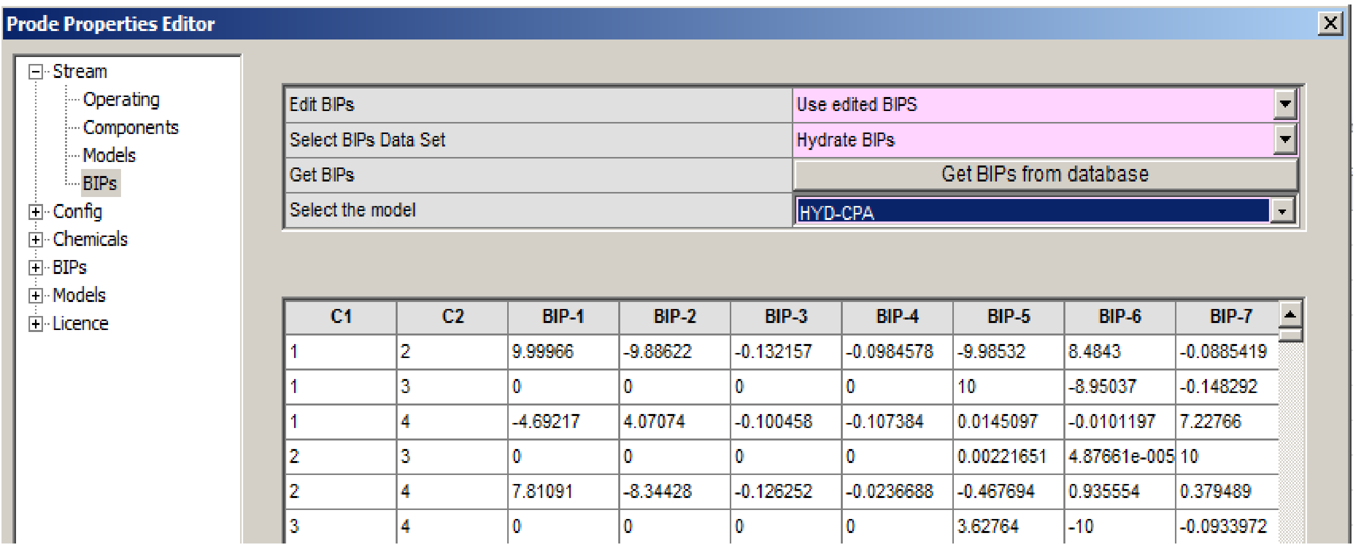
1 SRK standard
2 SRK Extended (SRKX)
3 PR Standard
4 PR Extended (PRX)
5 CPA -SRK
6 CPA-PR
7 LKP
8 BWRS
9 Steam Tables (IAPWS 199
10 PRX-Wilson
11 PRX-NRTL
12 PRX-UNIQUAC
13 PRX-UNIFAC
14 PRX-Wilson (WS)
15 PRX-NRTL (WS)
16 PRX-UNIQUAC (WS)
17 GERG ISO-18453
18 AGA ISO-29765
19 PRX-NRTL (MHV2)
20 PRX-NRTL (LCVM)
21 Hydrate CPA-PRX
22 Hydrate PRX
23

		uid	Solid	Hydrate
Fugacity	CPA-F		SP-CPA	HYD-CPA
Enthalpy	PRX V		REGULAR	HYD-CPA
Entropy	PRX V		REGULAR	HYD-CPA
Volume	PRX V		REGULAR	HYD-CPA

Multiphase equilibria	Multiphase vapor-liquid-solid-hydrate
Multiphase initialization	Reduced tests (quick)
Detect Phase State	From Gibbs or Isothermal Compr. and Liq.Dens.
Phase diagram, check stability a	Accept all solutions
Phase diagram, specified phase	Do not end when crossing phase boundary lines
Hydrate structures inclusion	Include all structures which may be generated by formers

IMPORTANT

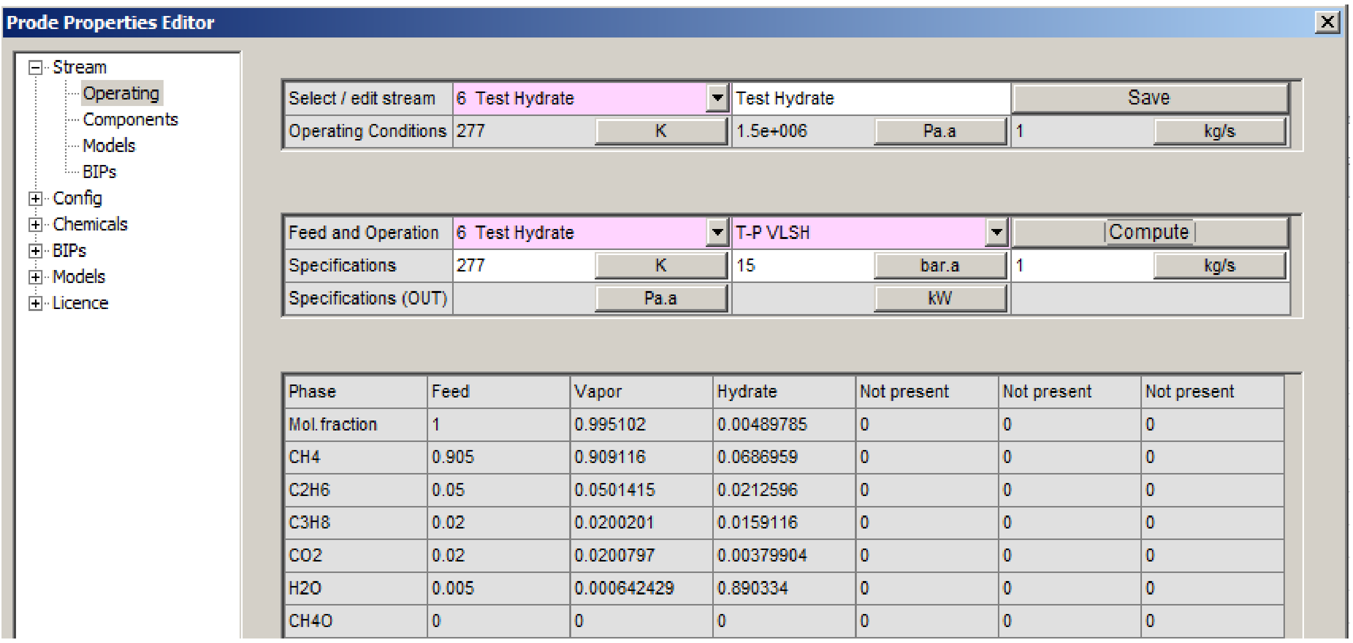
solving hydrate phase equilibria you must define BIPs ,
Prode Properties includes many precalculated BIPs for VLE, LLE, SLE and Hydrates phase equilibria,
you may utilize these values when meaured data points are not available, if there are doubts about the range of application you may inspect the database for the range of temperatures and estimated errors, see the paragraph “Binary Interaction Parameters (BIP)” for details
Consider data regression from measured data the recommended option, for the details see the paragraph “Regress VLE-LLE-SLE data”
for this example select Hydrate BIPs as Data Set and click on Get BIPs from Database button to load the values



Edit BIPs	Use edited BIPS
Select BIPs Data Set	Hydrate BIPs
Get BIPs	Get BIPs from database
Select the model	HYD-CPA

C1	C2	BIP-1	BIP-2	BIP-3	BIP-4	BIP-5	BIP-6	BIP-7
1	2	9.99966	-9.88622	-0.132157	-0.0984578	-9.98532	8.4843	-0.0885419
1	3	0	0	0	0	10	-8.95037	-0.148292
1	4	-4.69217	4.07074	-0.100458	-0.107384	0.0145097	-0.0101197	7.22766
2	3	0	0	0	0	0.00221651	4.87661e-005	10
2	4	7.81091	-8.34428	-0.126252	-0.0236688	-0.467694	0.935554	0.379489
3	4	0	0	0	0	3.62764	-10	-0.0933972

then, back to Operating tab and click on Save button to store the values in Prode Properties,
once saved you can calculate hydrate phase equilibria immediately selecting the TP VLSH flash operation, setting temperature (277 K) and Pressure (15 Bar.a) , click on Compute button to see the results, at specified condotions the model indicates that hydrates can form



Select / edit stream	6 Test Hydrate		Test Hydrate		Save	
Operating Conditions	277	K	1.5e+006	Pa.a	1	kg/s
Feed and Operation	6 Test Hydrate		T-P VLSH		Compute	
Specifications	277	K	15	bar.a	1	kg/s
Specifications (OUT)		Pa.a		kW		

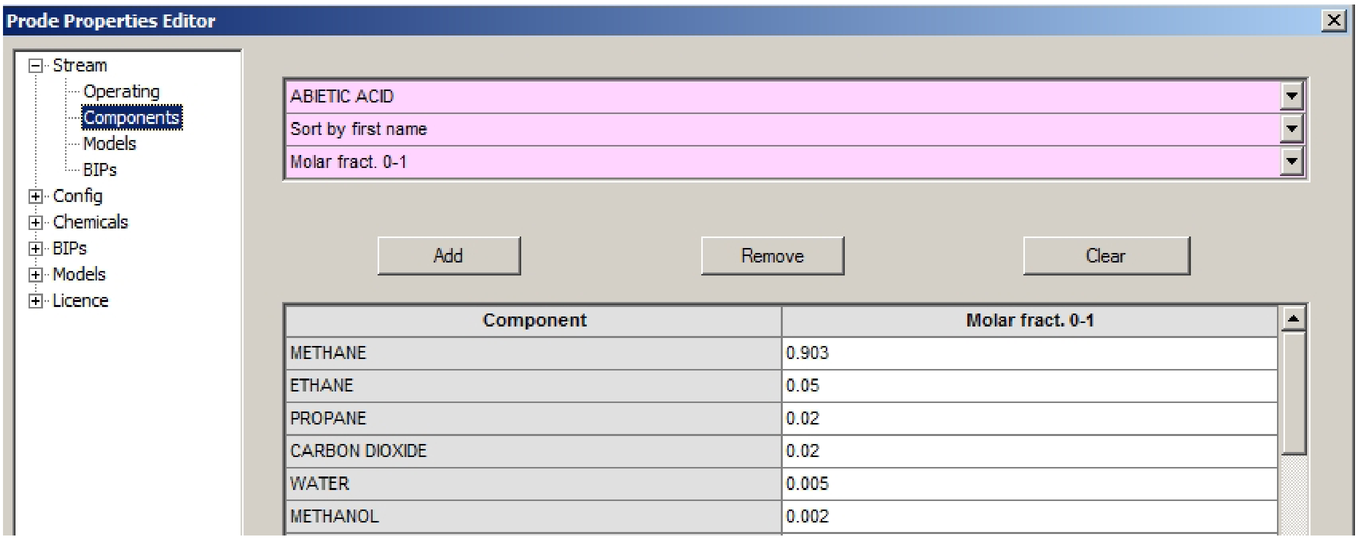
Phase	Feed	Vapor	Hydrate	Not present	Not present	Not present
Mol.fraction	1	0.995102	0.00489785	0	0	0
CH4	0.905	0.909116	0.0686959	0	0	0
C2H6	0.05	0.0501415	0.0212596	0	0	0
C3H8	0.02	0.0200201	0.0159116	0	0	0
CO2	0.02	0.0200797	0.00379904	0	0	0
H2O	0.005	0.000642429	0.890334	0	0	0
CH4O	0	0	0	0	0	0

you may decide to adopt methanol as inhibitor to avoid the formation of hydrates

IMPORTANT

depending from models BIPs for liquid-solid equilibria (water-methanol) may have limited ranges of application,
for the predefined BIPs included in Prode Properties (PRX model) the allowed range for the fraction methanol / water is 0.0-0.4 to keep the errors in calculated freezing point depression below 1.5-2 K in the range 210-273.15 K
if you wish to inject more methanol make sure to recalculate the liquid-solid BIPs with the utility available in Prode Properties, for the details see the paragraph “Regress VLE-LLE-SLE data”

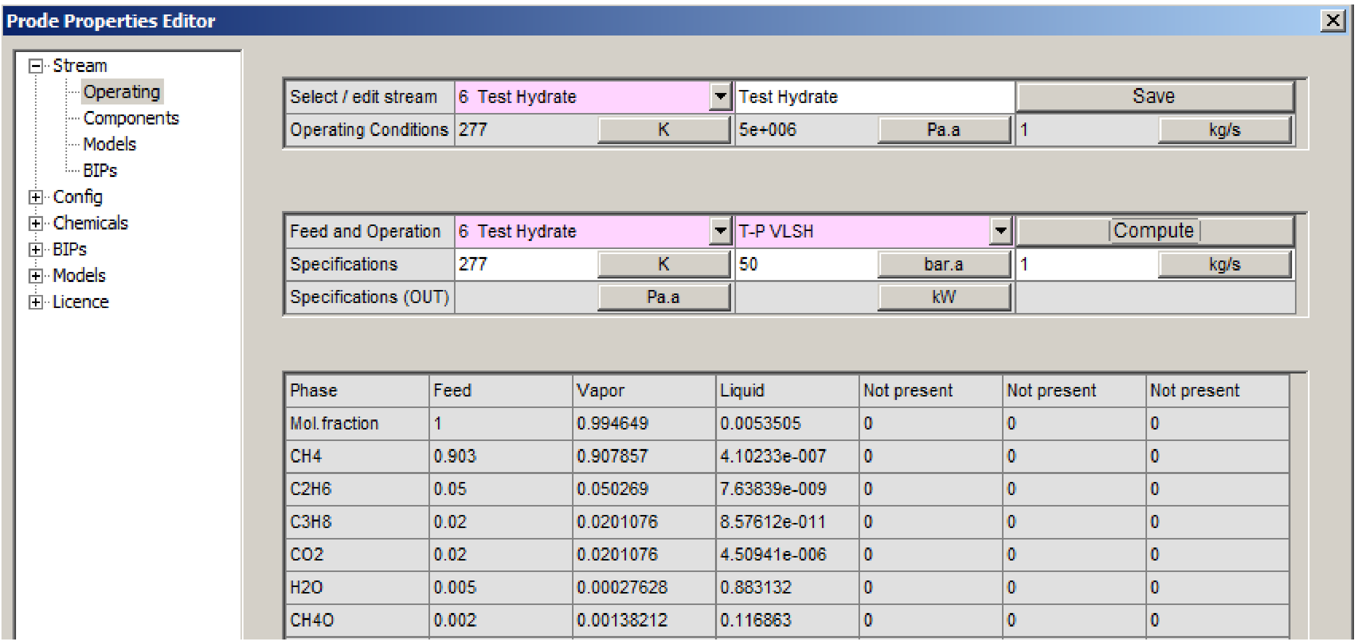
In this example we will consider a methanol fraction of 0.002 equivalent to 0.002 / 0.005 = 0.4 (the maximum allowed)
In component’s tab edit methanol fraction and methane fraction so that resulting composition will be C1 0.903 C2 0.05 C3 0.02 CO2 0.02 H2O 0.005 CH4O 0.002



ABIETIC ACID
Sort by first name
Molar fract. 0-1

Component	Molar fract. 0-1
METHANE	0.903
ETHANE	0.05
PROPANE	0.02
CARBON DIOXIDE	0.02
WATER	0.005
METHANOL	0.002

in the Operating tab click on Save button to store the new composition
then solve the TP-VLSH operation to find the predicted hydrate formation pressure
(in this case we test 277 K 50 Bar.a without finding hydrate formation)

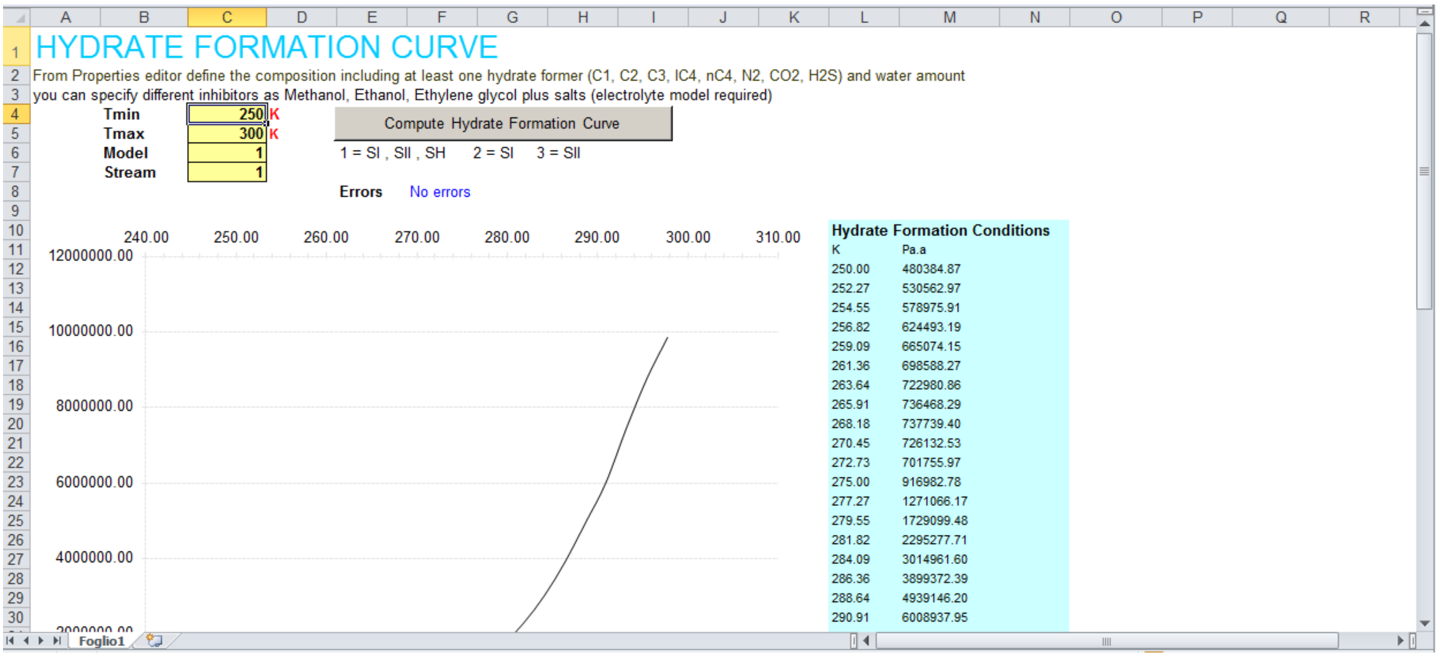


Select / edit stream	6 Test Hydrate		Test Hydrate		Save	
Operating Conditions	277	K	5e+006	Pa.a	1	kg/s

Feed and Operation	6 Test Hydrate		T-P VLSH		Compute	
Specifications	277	K	50	bar.a	1	kg/s
Specifications (OUT)		Pa.a		kW		

Phase	Feed	Vapor	Liquid	Not present	Not present	Not present
Mol.fraction	1	0.994649	0.0053505	0	0	0
CH4	0.903	0.907857	4.10233e-007	0	0	0
C2H6	0.05	0.050269	7.63839e-009	0	0	0
C3H8	0.02	0.0201076	8.57612e-011	0	0	0
CO2	0.02	0.0201076	4.50941e-006	0	0	0
H2O	0.005	0.00027628	0.883132	0	0	0
CH4O	0.002	0.00138212	0.116863	0	0	0

As alternative to solve the multiphase flash operations you can calculate the hydrate formation curve directly in Excel



HYDRATE FORMATION CURVE

From Properties editor define the composition including at least one hydrate former (C1, C2, C3, IC4, nC4, N2, CO2, H2S) and water amount
you can specify different inhibitors as Methanol, Ethanol, Ethylene glycol plus salts (electrolyte model required)

Tmin	250	K
Tmax	300	K
Model	1	
Stream	1	

Compute Hydrate Formation Curve

1 = SI , SII , SH   2 = SI   3 = SII

Errors   No errors

Hydrate Formation Conditions

K	Pa.a
250.00	480384.87
252.27	530562.97
254.55	578975.91
256.82	624493.19
259.09	665074.15
261.36	698588.27
263.64	722980.86
265.91	736468.29
268.18	737739.40
270.45	726132.53
272.73	701755.97
275.00	916982.78
277.27	1271066.17
279.55	1729099.48
281.82	2295277.71
284.09	3014961.60
286.36	3899372.39
288.64	4939146.20
290.91	6008937.95

Getting started from MATLAB

IMPORTANT Microsoft MATLAB support files are located in the directory \Prode\MATLAB

MATLAB provides two ways to access external libraries as Prode Properties
-direct access
-access through scripts and mex files

Direct Access

Direct access is through the command-line interface, this interface lets you load an external library into MATLAB memory and access functions in the library, to load Prode Properties in MATLAB enter

```
>if not(libisloaded('ppp'))
  hfile = ['C:\Program Files\Prode\MATLAB\ppp.h'];
  loadlibrary('ppp.dll', hfile);
end
libfunctions ppp
```

this command will load Prode Properties in memory and print the list of methods avaliable, you may wish to modify ‘C:\Program Files\Prode\MATLAB\ppp.h' to reflect your installation’s settings

```
Functions in library ppp:

AFOpen      CompLD      Divi        EStrLSS     PSep        StrGIC      StrLV       StrST       getAji      getPatm     putMod
AFSave      CompLV      EStrFMH     EStrLV      PfPF        StrGICp     StrLVE      StrSv       getCC       getSUMS     putN
AOpen       CompMp      EStrFML     EStrLVE     PfTF        StrGJT      StrLf       StrSvd      getCNr      getT        putZ
ASave       CompMw      EStrGC      EStrLf      SPF         StrGMw      StrMDt      StrTc       getCi       getUMC      setAc
BFsave      CompN       EStrGCp     EStrPf      STF         StrGS       StrMw       StrTcm      getCj       getUMN      setErrFlag
BPF         CompNb      EStrGCv     EStrS       StrAc       StrGSS      StrN        StrVv       getErrFlag  getUMS      setKM
BPLine      CompPc      EStrGD      EStrSCp     StrCBp      StrGV       StrPc       StrVvd      getFCNr     getW        setMFg
BRegr       CompRg      EStrGIC     EStrSD      StrCBt      StrGVE      StrPcm      StrZv       getFPNr     getWm       setMH
CompAc      CompSC      EStrGJT     EStrST      StrCPnr     StrH        StrPf       StrlnFv     getGij      getX        setMS
CompCID     CompSD      EStrGMw     EStrZv      StrCTp      StrHC       StrPt       StrlnFvd    getGji      getY        setMV
CompDm      CompSG      EStrGSS     ErrMsg      StrCTt      StrHv       StrPts      StrlnFvdv   getKji      getZ        setMw
CompF       CompSL      EStrGV      GSep        StrCopy     StrHvd      StrS        UMAU        getMBPNr    initS       setOM
CompGC      CompSS      EStrGVE     HPF         StrFMH      StrLC       StrSCp      UMCR        getMCNr     isSDef      setOp
CompGV      CompST      EStrH       HPFORM      StrFML      StrLCp      StrSD       UMCS        getMFg      loadSB      setPc
CompGf      CompSf      EStrHC      HTF         StrFv       StrLCv      StrSGH      UMRAU       getMH       putAji      setS
CompHG      CompSol     EStrLC      HTFORM      StrFvd      StrLD       StrSGS      VLLSep      getMS       putBIP      setSOp
CompHL      CompTc      EStrLCp     LFLine      StrFvdv     StrLH       StrSH       defErrMsg   getMSNr     putCC       setTc
CompHS      CompVP      EStrLCv     LSep        StrGC       StrLIC      StrSLH      edCF        getMV       putCi       setUMC
CompHV      CompVc      EStrLD      LfPF        StrGCp      StrLJT      StrSLS      edCS        getMod      putCj       setVc
CompHf      DCOL        EStrLIC     LfTF        StrGCv      StrLMw      StrSS       edS         getOM       putGij      setWm
CompID      DPF         EStrLJT     MixF        StrGD       StrLS       StrSSH      edSS        getP        putGji
CompLC      DPLine      EStrLMw     PIPE        StrGH       StrLSS      StrSSS      edST        getPNr      putKji
```

to access a method in a shared library MATLAB provides the command calllib to call functions in the library, the syntax for calllib is:

```
calllib('ppp', 'FunctionName', arg1, ..., argN)
```

the FunctionName and arguments are detailed in Prode Properties manual, for example we can call the method edSS() to edit streams with the command

```
>calllib('ppp', 'edSS')
```

in the same way you can access other methods in Prode Properties, for example to calculate cp / cv and speed of sound for vapor fraction of stream 1 at 300 K and 5 Bar

```
>> calllib(‘ppp’,’EstrGCp’1,300,500000)/’calllib(‘ppp’,’EstrGCv’1,300,500000)
>> ans = 1.3211
>> calllib(‘ppp’,’EstrGSS’1,300,500000)
>> ans = 374.1625
```

you can call even complex functions as those to plot a phase envelope or calculate a column, for these remember before to pass an array from Matlab to Prode Properties that you must allocate the memory to avoid system errors.
Finally you can use the unloadlibrary function to unload Prode Properties library from Matlab and free up memory.

```
>unloadlibrary ppp
```

Access from Matlab through scripts

In addition to direct access, you can utilize Prode Properties from Matlab with scripts or mex files (compiled scripts)
In many cases this way is more immediate since you use the original names of the functions in Prode Properties without need to write additional code.
Prode Properties includes a large number of Matlab scripts installed in directory \Prode\MATLAB\m
Before to utilize the scripts you must
-move the files into a Matlab directory (i.e. a directory where Matlab can access the scripts) , read Matlab documentation for additional information.
-edit the file pppdir.txt, this file contains a string with path and name of the header file required to instruct Matlab about the methods avalialable in Prode Properties library, once you have edited move the file on the same location of script files.

How the scripts work
Scripts act as interface between Matlab and Prode Properties, scripts have names identical to Prode Properties methods, then when you invoke the script StrGD (which is the method in Prode Properties to calculate density of vapor phase) MATLAB simply executes the commands found in the file, calls the method StrGD in Prode Properties and returns the result, by the way the script StrGD.m contains these MATLAB commands

```
function [] = StrGD(stream)
if not(libisloaded('ppp'))
fid = fopen('pppdir.txt'); hfile = fgetl(fid); fclose(fid);
loadlibrary('ppp.dll', hfile);
h = uimenu('Label','Properties');
h1 = uimenu(h,'Label','Edit Properties','Callback','edSS');
h2 = uimenu(h,'Label','Open Archive','Callback','AOpen');
h3 = uimenu(h,'Label','Save a Archive','Callback','ASave');
end
d = calllib('ppp', 'StrGD', stream)
end
```

By typing in Matlab the command

```
>>StrGD(1)
```

Matlab executes the code within the script, it loads ppp.dll (if not in memory) , creates a menu bar (with the standard Prode Properties commands) and then executes the method StrGD, to calculate the density.

Notice that the script creates a menu bar which permits to access directly Prode Properties from Matlab GUI,
there are three commands

-edit Streams
-open a archive
-save a archive

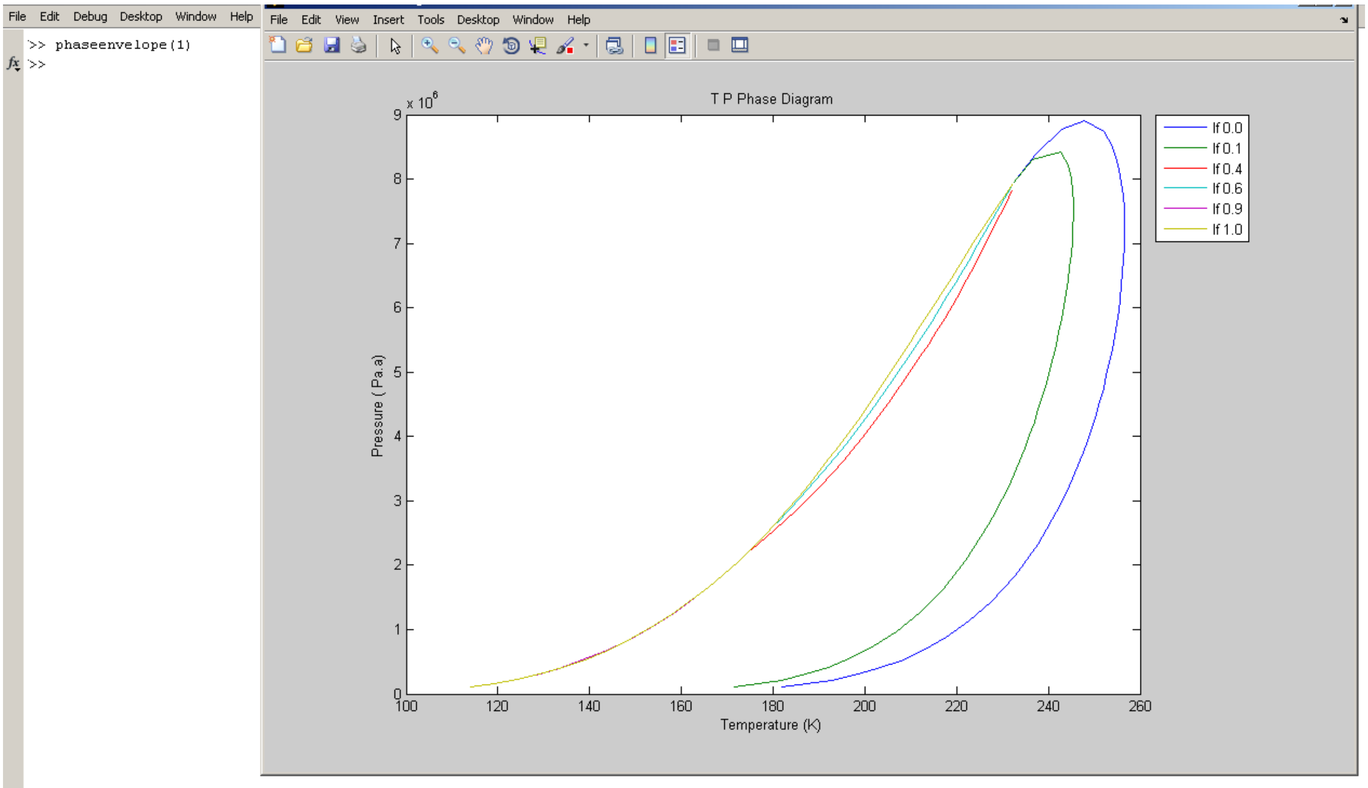
Important features of menu bar
-the characteristics may depend from Matlab version
-if you delete the associated figure the menu bar is deleted, to recreate the menu you must reenter the commands

```
h = uimenu('Label','Properties');
h1 = uimenu(h,'Label','Edit Properties','Callback','edSS');
h2 = uimenu(h,'Label','Open Archive','Callback','AOpen');
h3 = uimenu(h,'Label','Save a Archive','Callback','ASave');
```

You can write scripts to solve more complex problems, an example is the script phaseenvelope.m which prints a phase envelope, to test the script type in Matlab the command

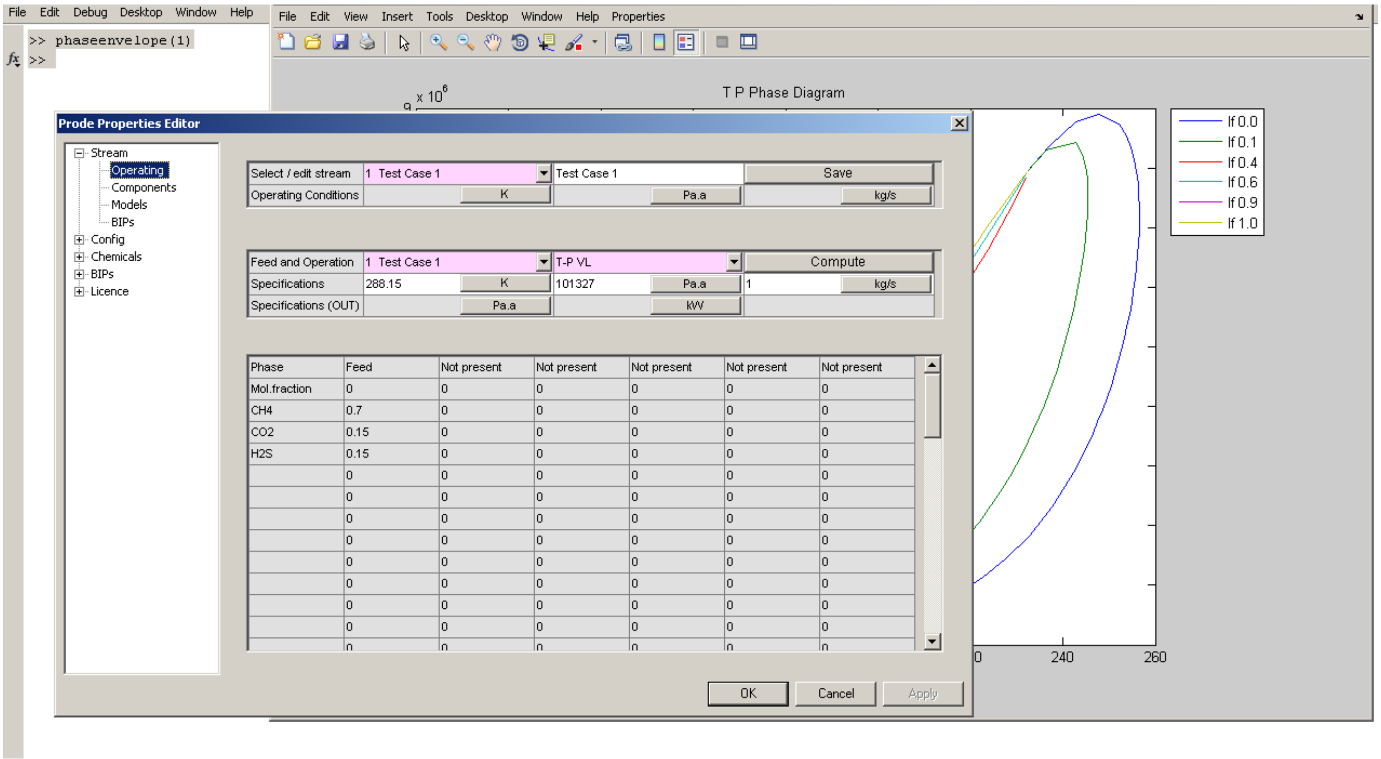
>>phaseenvelope(1)

Matlab will invoke Prode Properties to calculate the phase envelope for the stream 1 , then it plots the result



```
>> phaseenvelope(1)
>>
```

Notice that from Properties menu bar you can access Properties editor and modify the list of components or models of each stream



```
>> phaseenvelope(1)
>>
```

Prode Properties Editor

- Stream
  - Operating
  - Components
  - Models
  - BIPs
- Config
- Chemicals
- BIPs
- Licence

Select / edit stream	1 Test Case 1	Test Case 1	Save
Operating Conditions	K	Pa.a	kg/s

Feed and Operation	1 Test Case 1	T-P VL	Compute
Specifications	288.15 K	101327 Pa.a	1 kg/s
Specifications (OUT)	Pa.a	kW	

Phase	Feed	Not present	Not present	Not present	Not present	Not present
Mol.fraction	0	0	0	0	0	0
CH4	0.7	0	0	0	0	0
CO2	0.15	0	0	0	0	0
H2S	0.15	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0

File Edit Debug Desktop Window Help
File Edit View Insert Tools Desktop Window Help Properties
T P Phase Diagram
x 10^6
240
260
lf 0.0
lf 0.1
lf 0.4
lf 0.6
lf 0.9
lf 1.0
OK
Cancel
Apply

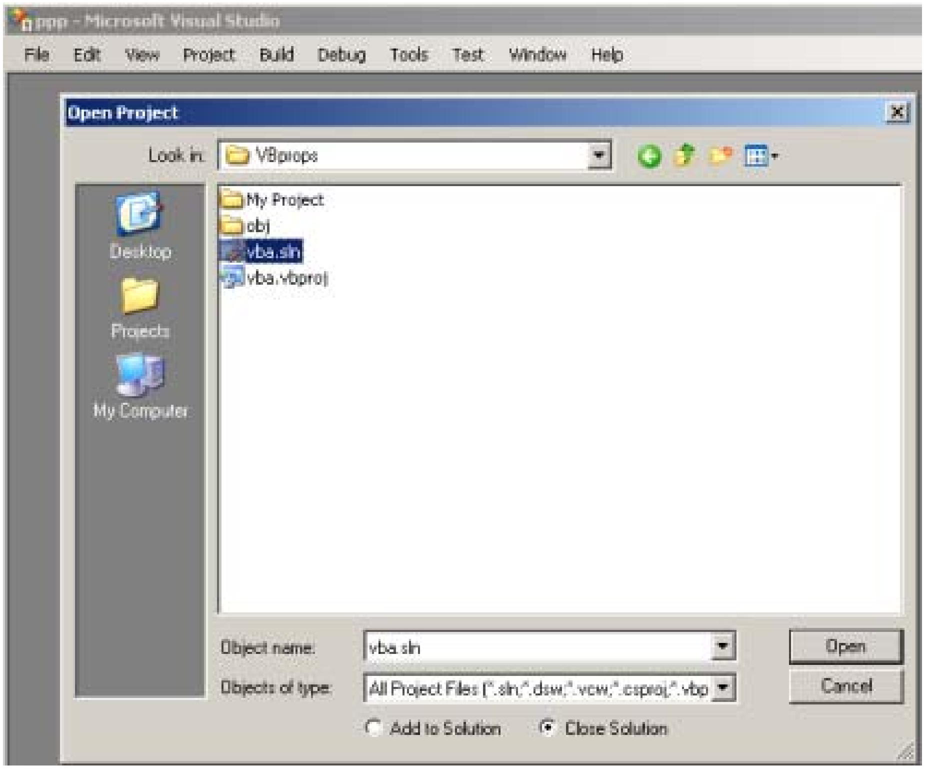
Access from MATHCAD

The files and the instructions required to link MathCad with Prode Properties are located in directory \Prode\MathCad
The MathCad support files and the documentation have been provided by Dr. Harvey Hensley

Getting started with Microsoft NET (VB , C) applications

IMPORTANT Microsoft NET support files are located in the directory \Prode\NET

Prode Properties can be easily included as unmanaged code in every Microsoft NET application, for compiling the sample code provided with Prode Properties a recent version of Microsoft Visual Studio is required.
From Microsoft Visual Studio compiler menu File->Open->Project/Solution , in NET folder (in Prode Properties installation) select the file vba.sln



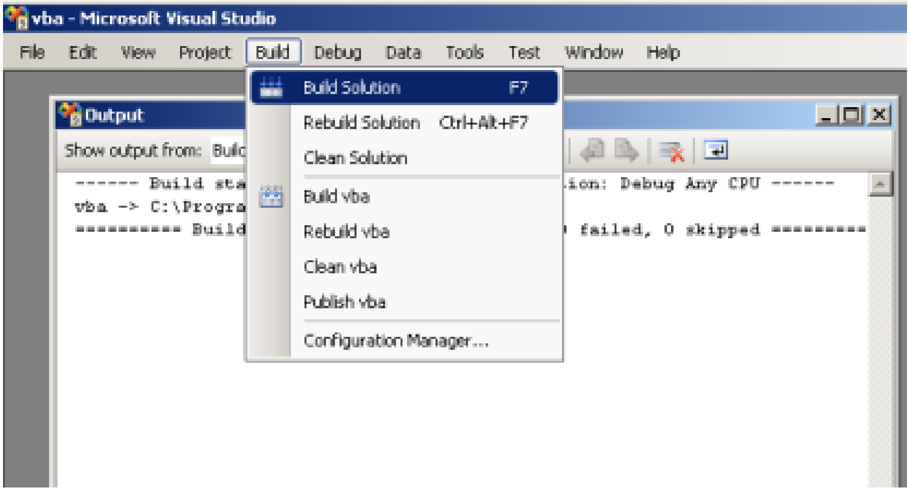
Look in: VBprops

Object name: vba.sln

Objects of type: All Project Files (*.sln;*.dsw;*.vcw;*.csproj;*.vbp

○ Add to Solution ● Close Solution

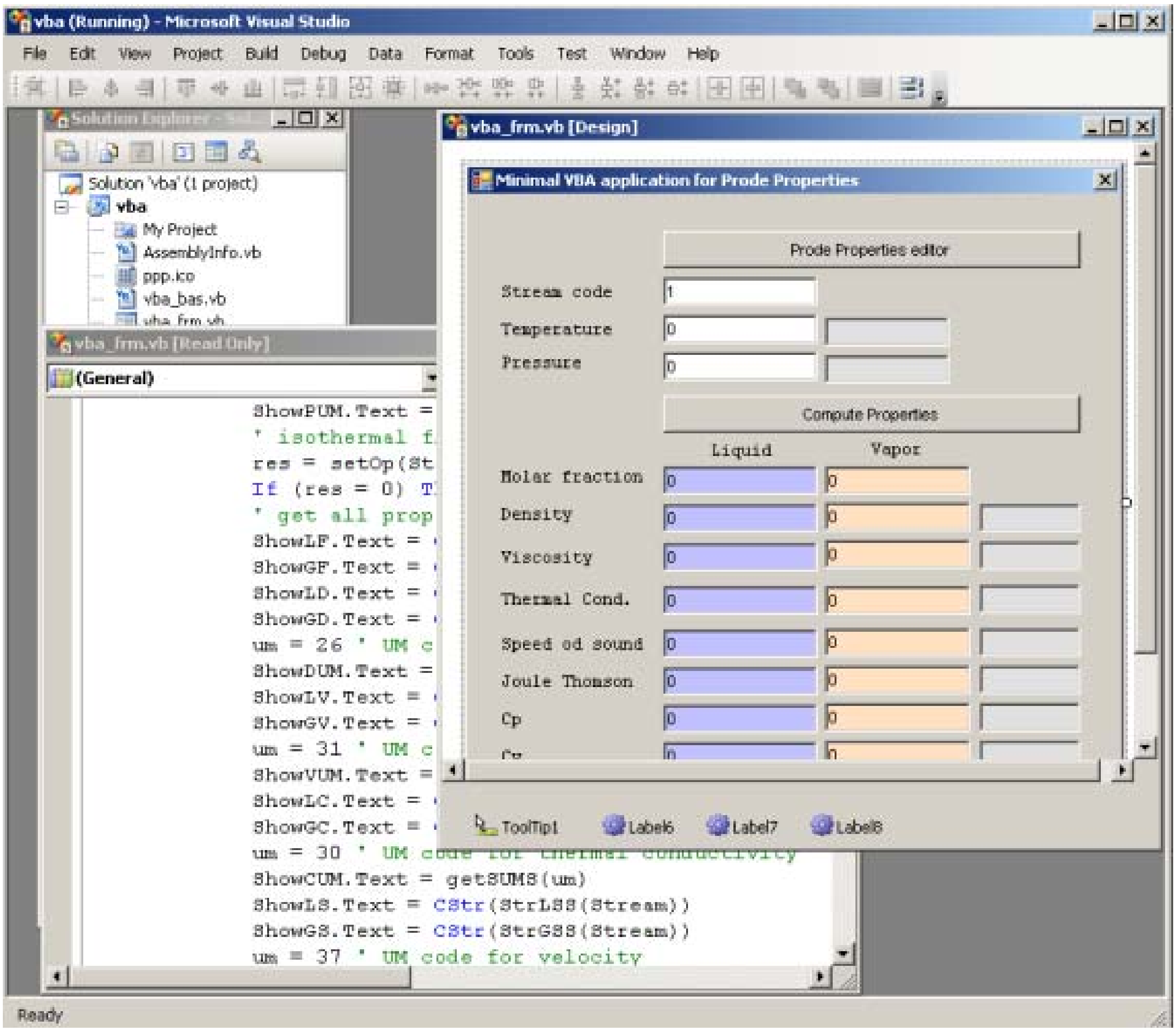
then from menu Build- select Build Solution.
Note: if desired you can edit the settings from Project->vba Properties



```
------ Build sta                          ion: Debug Any CPU ------
vba -> C:\Progra
========== Build                          failed, 0 skipped ==========
```

As next step you can test the application, from Visual Studio menu Debug->Start Debugging, then once the application is running :

1) click on the button Prode Properties editor to access the editor, define the streams and units of measurement
2) define a suitable temperature and pressure (with proper units)
3) click on button Compute Properties to print the properties



```
ShowPUM.Text =
' isothermal f
res = setOp(St
If (res = 0) T
' get all prop
ShowLF.Text =
ShowGF.Text =
ShowLD.Text =
ShowGD.Text =
um = 26 ' UM c
ShowDUM.Text =
ShowLV.Text =
ShowGV.Text =
um = 31 ' UM c
ShowVUM.Text =
ShowLC.Text =
ShowGC.Text =
um = 30 ' UM code for thermal conductivity
ShowCUM.Text = getSUMS(um)
ShowLS.Text = CStr(StrLSS(Stream))
ShowGS.Text = CStr(StrGSS(Stream))
um = 37 ' UM code for velocity
```

Stream code: 1
Temperature: 0
Pressure: 0

	Liquid	Vapor
Molar fraction	0	0
Density	0	0
Viscosity	0	0
Thermal Cond.	0	0
Speed od sound	0	0
Joule Thomson	0	0
Cp	0	0
Cv	0	0

you can then modify the code according your requirements.

Solving problems (introduction)

There are several different classes of problems which Prode Properties can help to solve but the most common are probably :

- physical properties of pure fluids and mixtures
- equipment design
- system simulation

Prode Properties provides many methods for the prediction of physical properties, in general a single instruction is required for calculating a property.

The design and rating of unit operations as distillation columns, towers, pumps, compressors, valves, heat exchangers etc. is another area where Prode Properties can result useful, the use of programming languages is generally suggested when dealing with complex problems while some formula in a worksheet can solve the usual work.

The system simulation may be used in the design stage to evaluate parameters, to help achieve an improved design or applied to existing systems for optimizing operating conditions. Generally the required solution is the list of operating conditions at the input and output of the operating blocks in the simulation block diagram. When there are no recycle streams or controls the method for solving the system is very simple : the output information from the first operating block is utilized as input for the second operating block and so on. However when there are output conditions which may interfere with input conditions some sort of iteration is required since some or all the equations governing the system may be non linear. There are two well known methods for solving such a system of non linear equations, the method of successive substitutions and Newton-Raphson, refer to good books of numerical analysis for additional information.

Streams

Most thermodynamic calcs in Prode Properties library take as reference a stream entity. For example when simulating a plant it makes sense to define different streams to represent flows in different sections, a stream usually defines compositions and operating conditions, Prode Properties supports a variable number of streams and most methods in Prode Properties require a reference to a stream, the reference is a numeric code (a progressive integer starting from 1 for first stream) .

Streams attributes

As in process simulators each stream may include following information

- a list of components and relative weights
- a value for the operating pressure
- a value for the operating temperature
- a value for the operating flow
- thermodynamic models for different properties
- a list of BIPs

Working with streams

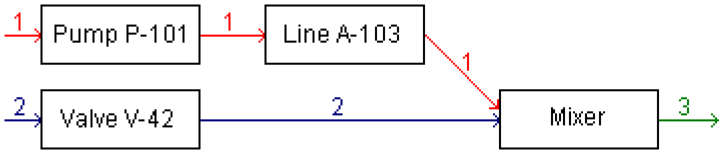
Prode Properties permits to define complex topologies as there is no limit to the number of operating blocks required for simulating a plant, with Prode Properties for simulating a plant you convert the different sections into pieces of code, to do so you can use the basic blocks available in all process simulators, for esample

- **isothermal flash**, for calculating multiphase equilibria at the specified temperature ad pressure
- **flash unit** (enthalpy, entropy or volume basis), calculates output temperature or pressure, with this unit you can simulate pipelines, valves, heat exchangers, pumps, compressors and many others operations.
- **fixed vapor fraction flash**, for constructing phase envelopes, calculating bubble and dew points etc.
- **mixer** to add the contents of two streams
- **divider** to subtract a part of flow from a stream

by putting together these blocks it is possible to simulate also complex plants.

Simulating a plant

transform the flow sheet in a simulation block diagram, fluid and energy flow diagrams are standard engineering tools, you assign a number to the different streams and identify the basic blocks which will be solved by Prode Properties.



Notice the number which identifies each stream, in this case different numbers mean (possible) different compositions (we do not consider chemical reactions here), the output of each block can be easily calculated providing the input has been defined

Working with archives, save and load data, default settings

Load and save archives

Archives are files which contain the data required by Prode Properties to work with stream's and units of measurement, when you open an archive the stream's data and units are loaded, when you choose to save an archive these data are stored in a file, in this way you can work with many different projetcs.

Prode Properties includes several methods to save and load data as archives.

The default settings

When Prode Properties starts it loads data from the archive named "def.ppp" so if you wish to use your own list of streams,units etc. just save your preferred settings under the name "def.ppp".

Properties editor

Prode Properties includes Properties editor, from the editor you have access to

- **Streams** edit operating conditions, flow, compositions, models, BIPs for all streams
- **Config** edit all units of measurement and settings
- **Chemicals** edit all chemical’s data, regress data , add new chemicals
- **BIPs** edit BIPs, regress data, add new BIPs

How to activate the Properties editor

call one of the methods edS(stream), edSS() remember that in Prode Properties each stream is referenced with a code (integer value) in the range (1... max number of streams).

Use the right method :

Use edSS() if you wish to start editing the first stream (but access all streams).

Use edS()stream if you would like to choose which stream to edit

From Microsoft VB

```
 Call edSS()
 Call edS(8) ‘ start editing stream nr. 8
```

From Microsoft Excel

```
 =edSS()
 =edS(8)  ‘ start editing stream nr. 8
```

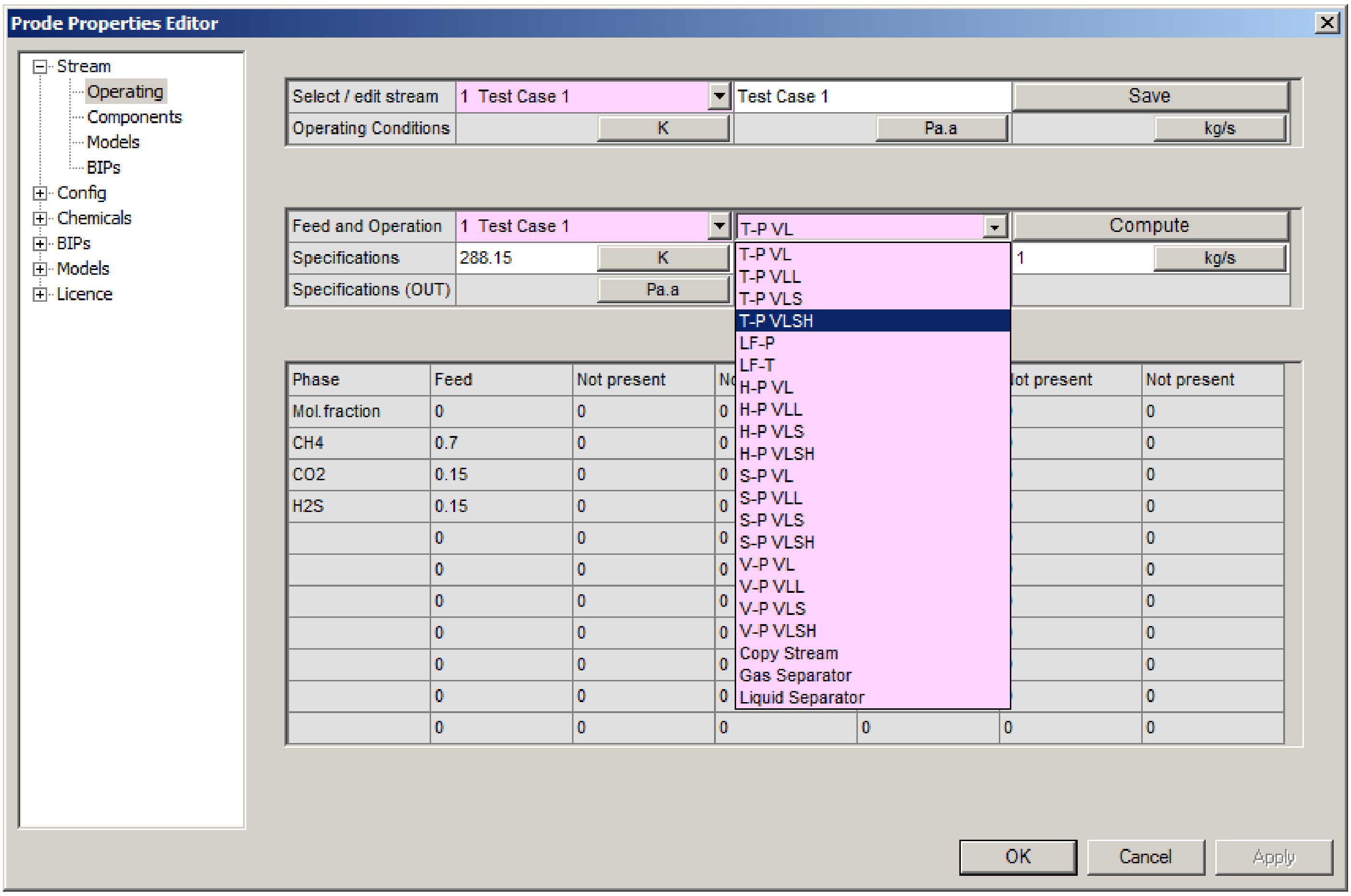
From Microsoft Visual C++

```
edSS();
edS(8);  // start editing stream nr. 8
```

Stream operating

From this page you can :

- select a stream (select / edit stream)
- define a name for the selected stream
- save edited stream data
- Compute different flash operatins



Select / edit stream: 1 Test Case 1 — Test Case 1

Operating Conditions: K — Pa.a — kg/s

Feed and Operation: 1 Test Case 1 — T-P VL

Specifications: 288.15 K — 1 kg/s

Specifications (OUT): Pa.a

Phase	Feed	Not present	No		ot present	Not present
Mol.fraction	0	0	0			0
CH4	0.7	0	0			0
CO2	0.15	0	0			0
H2S	0.15	0	0			0
	0	0	0			0
	0	0	0			0
	0	0	0			0
	0	0	0			0
	0	0	0			0
	0	0	0			0
	0	0	0	0	0	0

Define a new stream / edit existing streams

- select the stream (you wish to edit / define) from the “Select / edit stream list”
- go to page “Components”, define the list of components and relative weights
- go to page “Models”, define the models for the different properties, define settings, load BIPs
- back to page “Operating”, put a name for the stream and click on “Save”
- check that correct stream composition appears on the second grid

Compute a flash operation

- make sure a feeding stream has been properly defined (composition, models, settings) then select the feeding stream
- select the flash operation
- define the required specifications and clik on “Compute”

IMPORTANT

before to leave the application remember to save all data into the archive otherways your changes will be lost !

Predefined Flash Operations

Prode Properties allows to solve directly from editor many Flash operations

T-P VL
vapor-liquid, two phases, at specified temperature and pressure

T-P VLL
vapor-liquid-liquid, multiphase, at specified temperature and pressure

T-P VLS
vapor-liquid-solid, multiphase,at specified temperature and pressure

T-P VLSH
vapor-liquid-solid-hydrate, multiphase,at specified temperature and pressure

LF-P
equilibrium temperature at specified (liquid) phase fraction and pressure

LF-T
equilibrium pressure at specified (liquid) phase fraction and temperature

H-P VL
equilibrium temperature, two phases, at specified pressure and enthalpy

H-P VLL
equilibrium temperature, vapor-liquid-liquid, multiphase, at specified pressure and enthalpy

H-P VLS
equilibrium temperature, vapor-liquid-solid, multiphase, at specified pressure and enthalpy

H-P VLSH
equilibrium temperature, vapor-liquid-solid-hydrate, multiphase, at specified pressure and enthalpy

S-P VL
equilibrium temperature, two phases, at specified pressure and entropy

S-P VLL
equilibrium temperature, vapor-liquid-liquid, multiphase, at specified pressure and entropy

S-P VLS
equilibrium temperature, vapor-liquid-solid, multiphase, at specified pressure and entropy

S-P VLSH
equilibrium temperature, vapor-liquid-solid-hydrate, multiphase, at specified pressure and entropy

V-P VL
equilibrium temperature, two phases, at specified pressure and specific volume

V-P VLL
equilibrium temperature, vapor-liquid-liquid, multiphase, at specified pressure and specific volume

V-P VLS
equilibrium temperature, vapor-liquid-solid, multiphase, at specified pressure and specific volume

V-P VLSH
equilibrium temperature, vapor-liquid-solid-hydrate, multiphase, at specified pressure and specific volume

Copy Stream
copy a stream into another stream

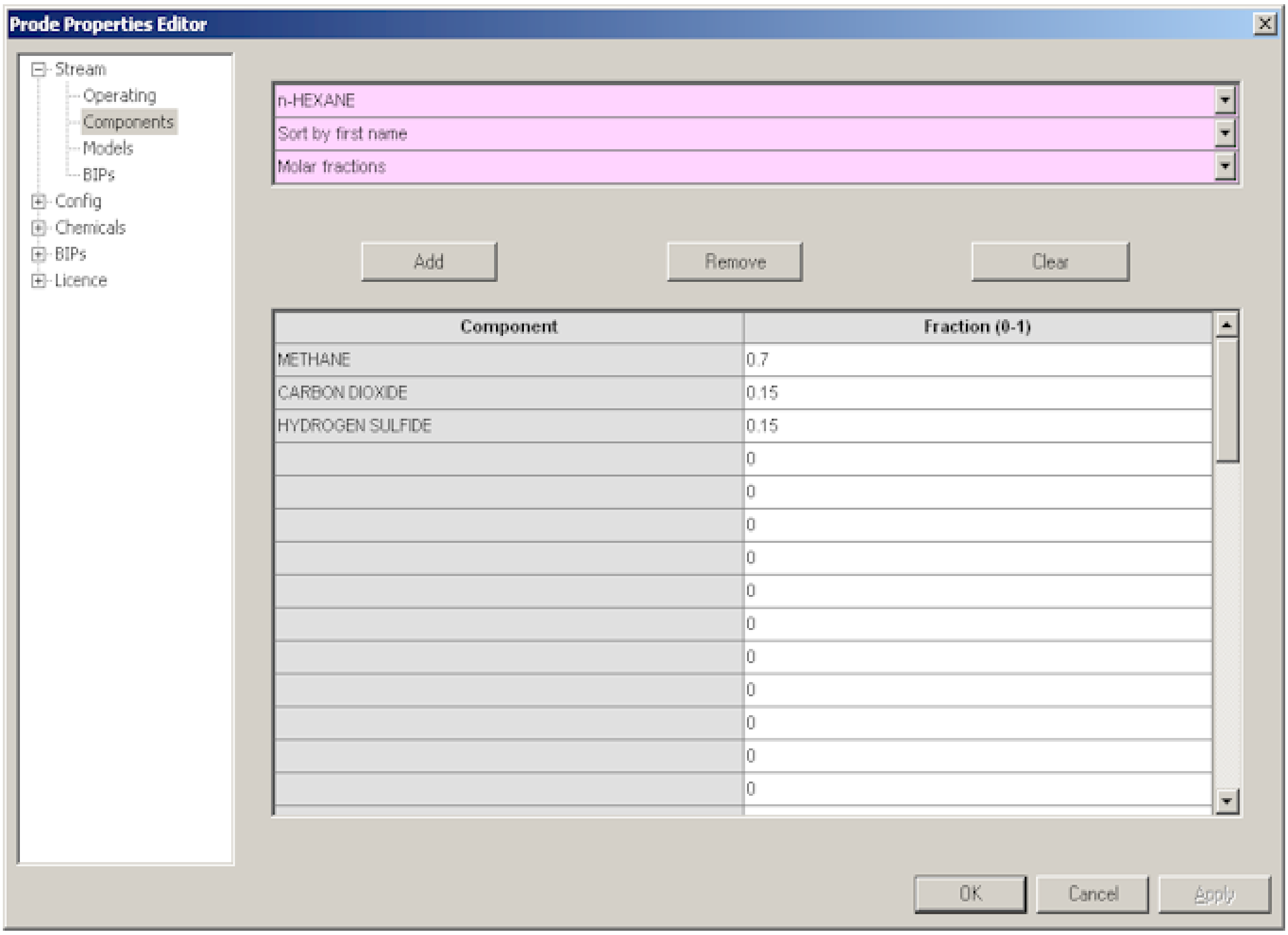
Gas Separator
simulates a gas separation at specified temperature and pressure

Liquid Separator
simulates a liquid separation at specified temperature and pressure

Stream Composition

From this page you can :

- define a list of components by selecting components from the library
- specifyi the amount of each component.



n-HEXANE

Sort by first name

Molar fractions

Component	Fraction (0-1)
METHANE	0.7
CARBON DIOXIDE	0.15
HYDROGEN SULFIDE	0.15
	0
	0
	0
	0
	0
	0
	0
	0
	0
	0
	0

Define the sorting criteria

- select the preferred criteria

Add a component to the list

- select a component from the list of components
- click on **Add** button

Remove a component from the list

- click on **Remove** button to remove the last component in the list

Clear the list

- click on **Clear** button to rclear all components in the list

Enter / normalize according Mole or Weight fractions

- select the desired Mole or Weight fractions

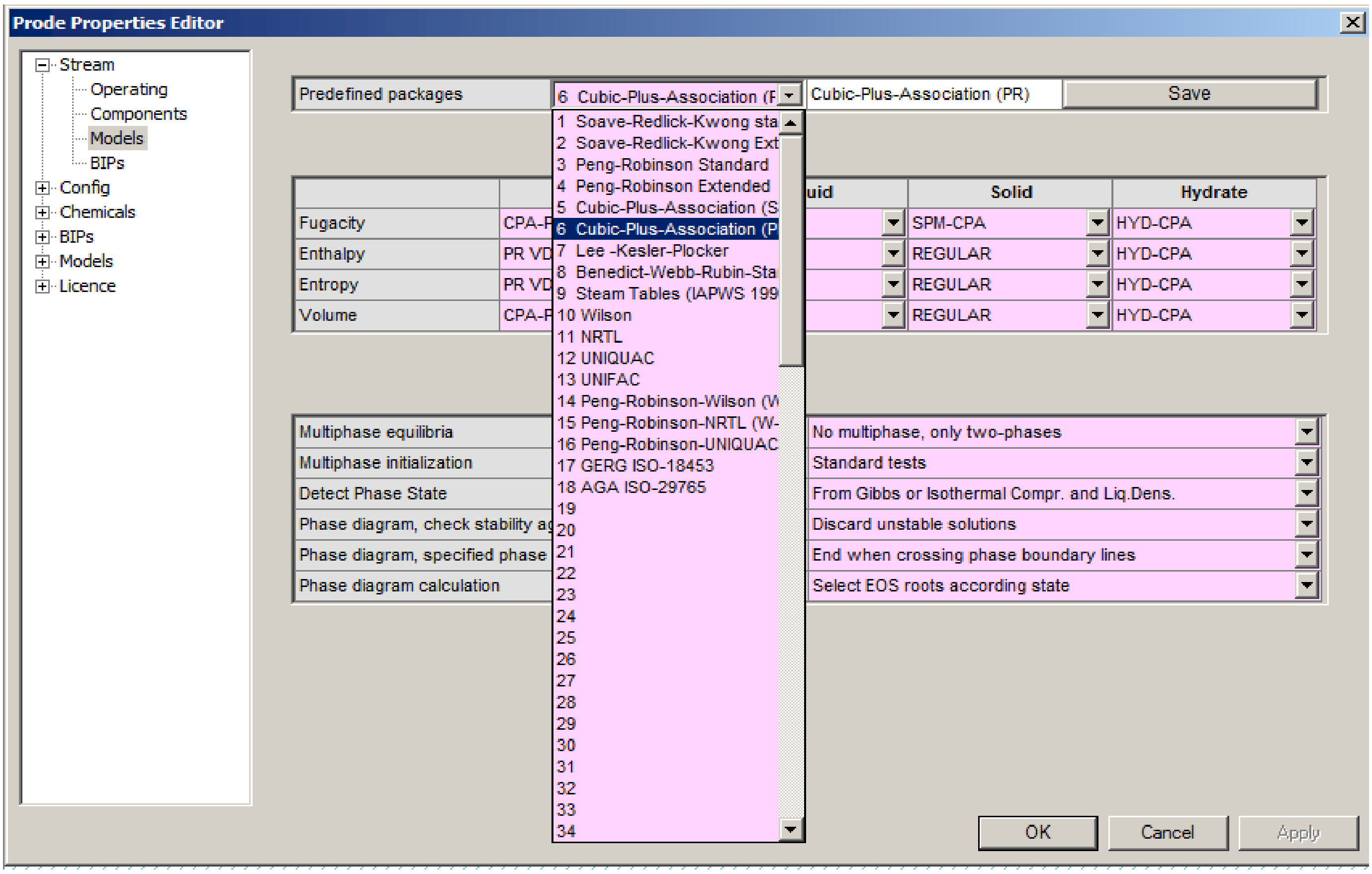
MPORTANT

to obtain the maximum accuracy solving multiphase equilibria with solid and hydrate phases it is suggested to regress BIPs from VLE + LLE data points, models such as CPA-PR can calculate accurately fugacities of solid phases with a suitable set of BIPs.

Stream Models

From this page you can :

- define up to 30 different packages with user defined models and options
- define the model per each propertty and state (gas,liquid,solid)
- set different options available for calc's



Predefined packages: 6 Cubic-Plus-Association (F

Cubic-Plus-Association (PR)

		uid	Solid	Hydrate
Fugacity	CPA-F		SPM-CPA	HYD-CPA
Enthalpy	PR VD		REGULAR	HYD-CPA
Entropy	PR VD		REGULAR	HYD-CPA
Volume	CPA-F		REGULAR	HYD-CPA

Multiphase equilibria	No multiphase, only two-phases
Multiphase initialization	Standard tests
Detect Phase State	From Gibbs or Isothermal Compr. and Liq.Dens.
Phase diagram, check stability ag	Discard unstable solutions
Phase diagram, specified phase	End when crossing phase boundary lines
Phase diagram calculation	Select EOS roots according state

Define a new package / Edit existing package

- select a package in the list
- in Models and Options Window select the models and options for this package
- define a name for the package,
- click on "Save" button to save this package

Select a package

- select a predefined package in the list

Define a model

- specify the model per each property and state

Set a option

- define multiphase as vapor + liquid or vapor +liquid+solid
- reduce the number of trial phases (in multiphase)
- use iso compressibility coeff. to detect the state of each phase
- evaluate stability of each phase in equilibrium
- in phase diagrams, end lines with specified phase fractions when crossing a phase boundary
- in phase diagrams, select EOS root for minimum energy or state

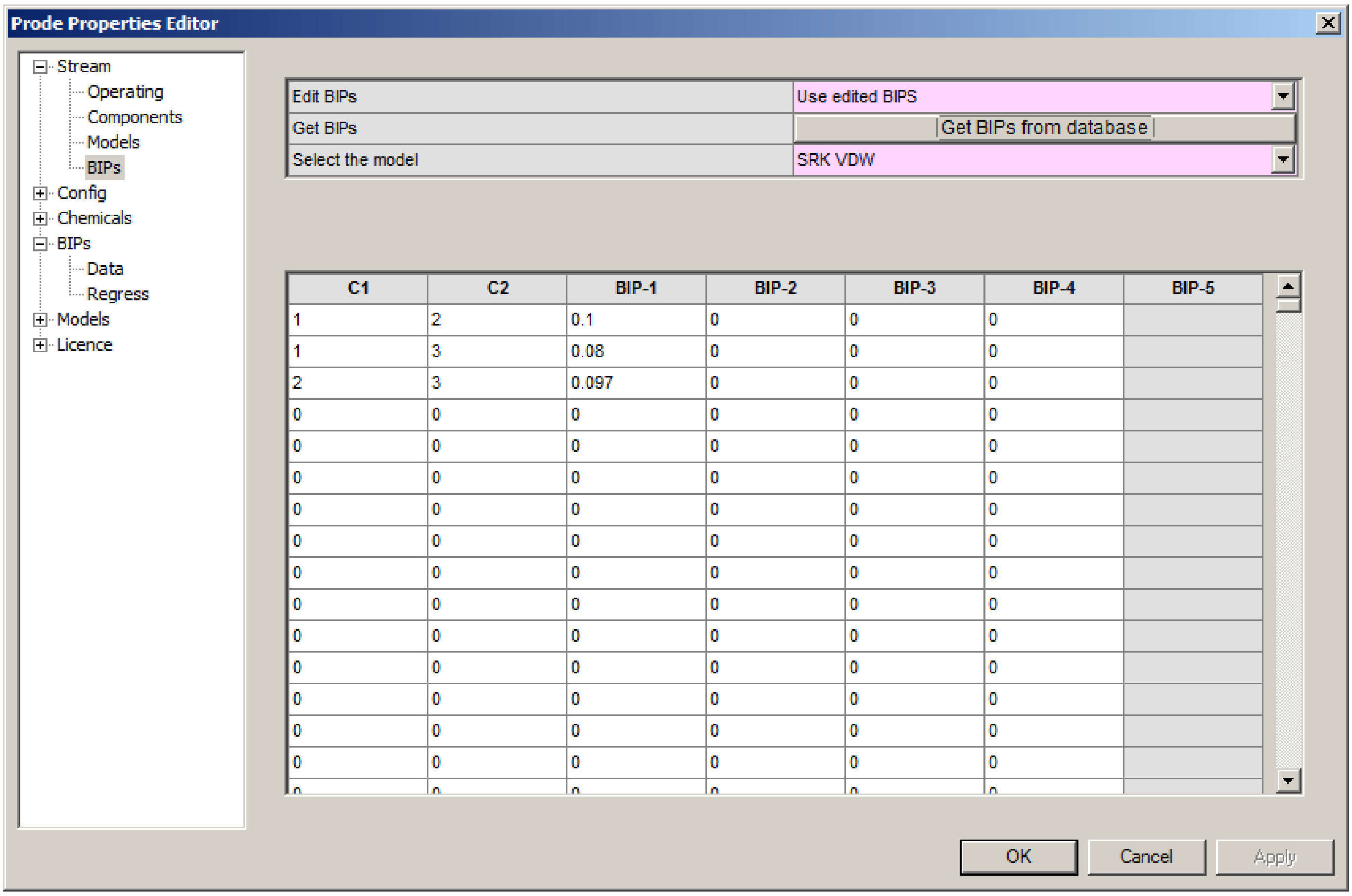
BIPs

From this page you can :

- input / edit / load BIPs for the different models

Define a list of BIPs

- click on **Get BIPs** for loading all BIPs available in library
- if required add your own specific BIPs



Edit BIPs	Use edited BIPS
Get BIPs	Get BIPs from database
Select the model	SRK VDW

C1	C2	BIP-1	BIP-2	BIP-3	BIP-4	BIP-5
1	2	0.1	0	0	0	
1	3	0.08	0	0	0	
2	3	0.097	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	
0	0	0	0	0	0	

IMPORTANT

For BIPs the first two columns Ci and Cj define the component's position in the list (i.e. 1 for the first component , 2 for second and so on), while othe colums allow to enter the values for the different BIPs required by selected model, note that some values (for example in Wilson, NRTL etc.models) have units of cal / gr.mol.

Example, binary of methanol and ethyl acetate UNIQUAC A12 : -64.1299, A21 : 644.1931 in the first two columns (c1 , c2) enter the components relative position in the list, assuming that methanol is the first component and ethyl acetate the second

c1	**c2**	**BIP-1**	**BIP-2**
1	2	-64.1299	644.1931

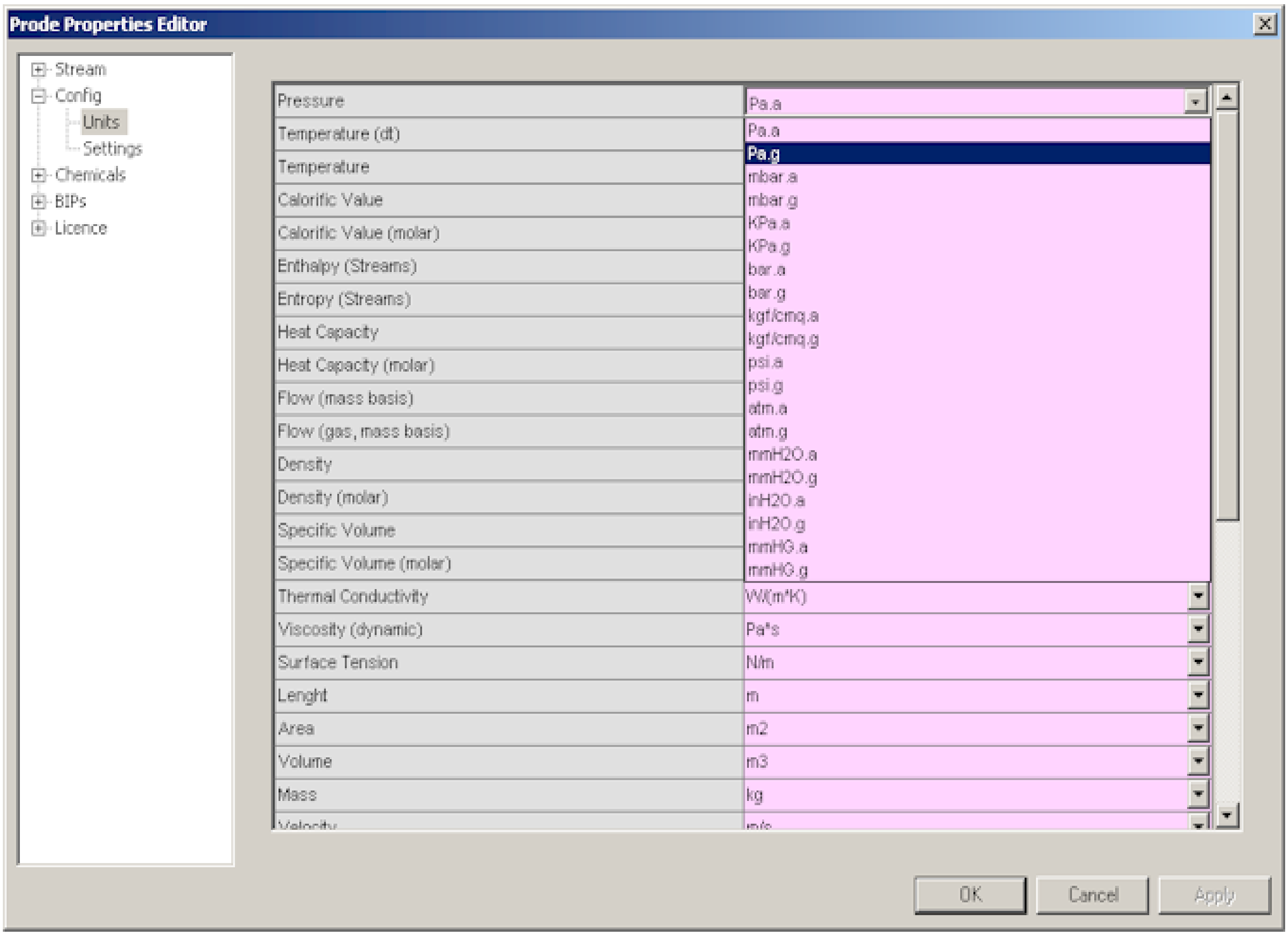
MPORTANT

Prode Properties allows to define Temperature Dependent BIPs for models as Soave or Peng Robinson, Temperature Dependent BIPs provide a better accuracy than Temperature Independent BIPs, the database includes many Temperature Dependent BIPs, BIPs in database have been calculated from VLE points at temperatures about 300 K and may not produce reliable results at temperatures far from 300 K, in those cases (a typical application could be a phase envelope) it is recommended to use Temperature Independent BIps or calculate new BIPs for the required range of temperatures.

Config Units

From this page you can :

- define the unit of measurement for the different properties



Pressure	Pa.a
Temperature (dt)	
Temperature	
Calorific Value	
Calorific Value (molar)	
Enthalpy (Streams)	
Entropy (Streams)	
Heat Capacity	
Heat Capacity (molar)	
Flow (mass basis)	
Flow (gas, mass basis)	
Density	
Density (molar)	
Specific Volume	
Specific Volume (molar)	
Thermal Conductivity	W/(m*K)
Viscosity (dynamic)	Pa*s
Surface Tension	N/m
Lenght	m
Area	m2
Volume	m3
Mass	kg
Velocity	m/s

IMPORTANT

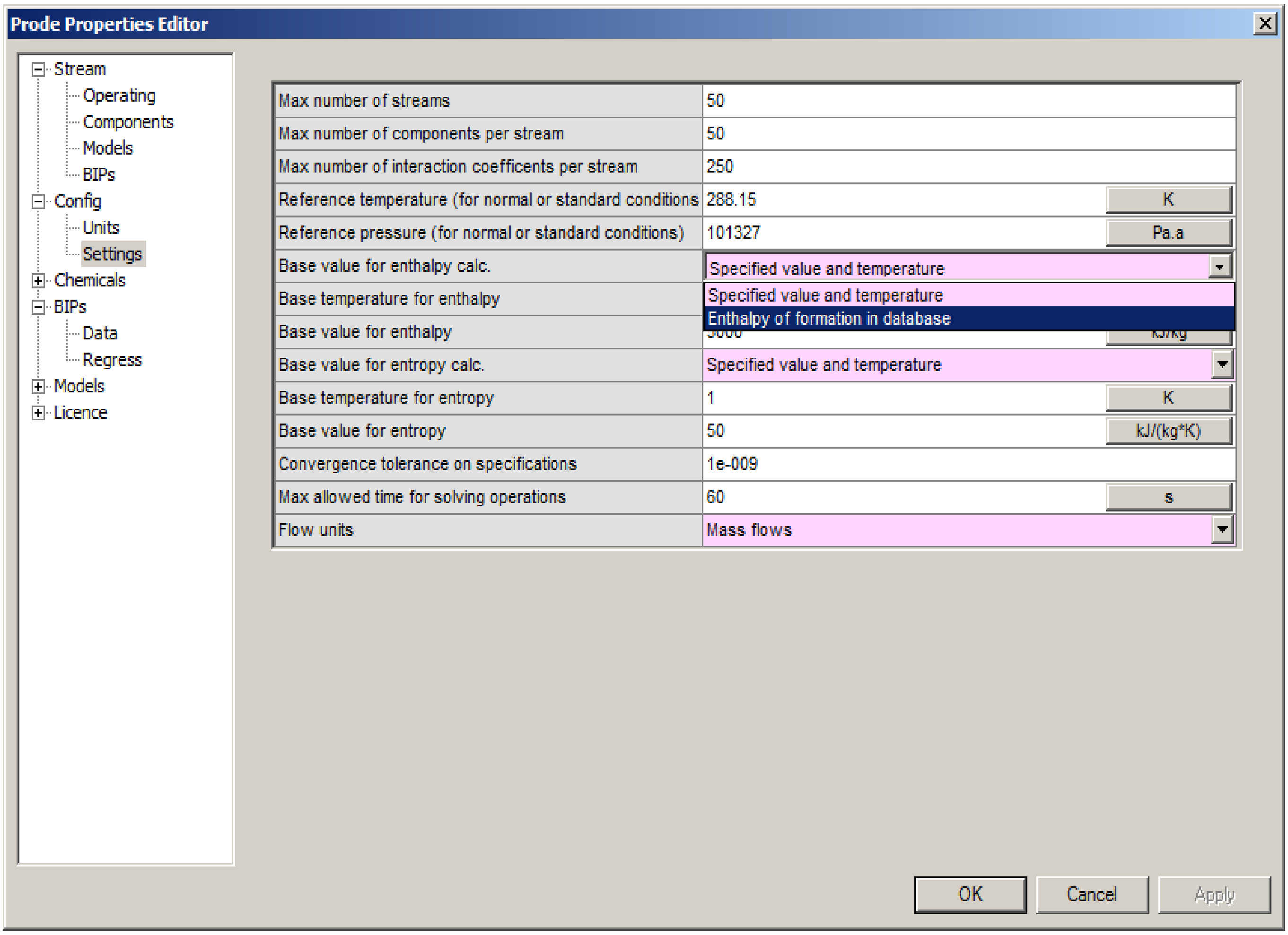
Prode Properties is a collection of functions for thermodynamic calculations, these functions receive data, of properties such as temperature or pressure, a reference to a stream etc. and perform some operations.
With Prode Properties you have complete control over the engineering units, this means that program permits to select from a list of different units for each property, and Prode Properties automatically converts the input values and the results according to the selected units.

1) if you set Bar.a as unit for pressure all inputs and outputs will be in that unit !.
2) if you wish to define your own set of units remember, before to leave the application, to save data into a archive otherways your changes will be lost !

Config Settings

From this page you can :

- define the different settings as max number of streams, the temperature and pressure at reference conditions, the base values for entalpy and entropy, convergence tolerance etc.



Max number of streams	50	
Max number of components per stream	50	
Max number of interaction coefficents per stream	250	
Reference temperature (for normal or standard conditions	288.15	K
Reference pressure (for normal or standard conditions)	101327	Pa.a
Base value for enthalpy calc.	Specified value and temperature Specified value and temperature Enthalpy of formation in database	
Base temperature for enthalpy		
Base value for enthalpy	5000	kJ/kg
Base value for entropy calc.	Specified value and temperature	
Base temperature for entropy	1	K
Base value for entropy	50	kJ/(kg*K)
Convergence tolerance on specifications	1e-009	
Max allowed time for solving operations	60	s
Flow units	Mass flows	

Prode Properties permits to define several different operating parameters, these parameters are :

- max number of streams
- max number of components per stream
- max number of interaction coefficients pairs per stream
- reference temperature and pressure
- base values for enthalpy and entropy calc's
- convergence tolerance
- max allowed time for solving a operation
- Flow units
- minimum liquid density to validate liquid phase

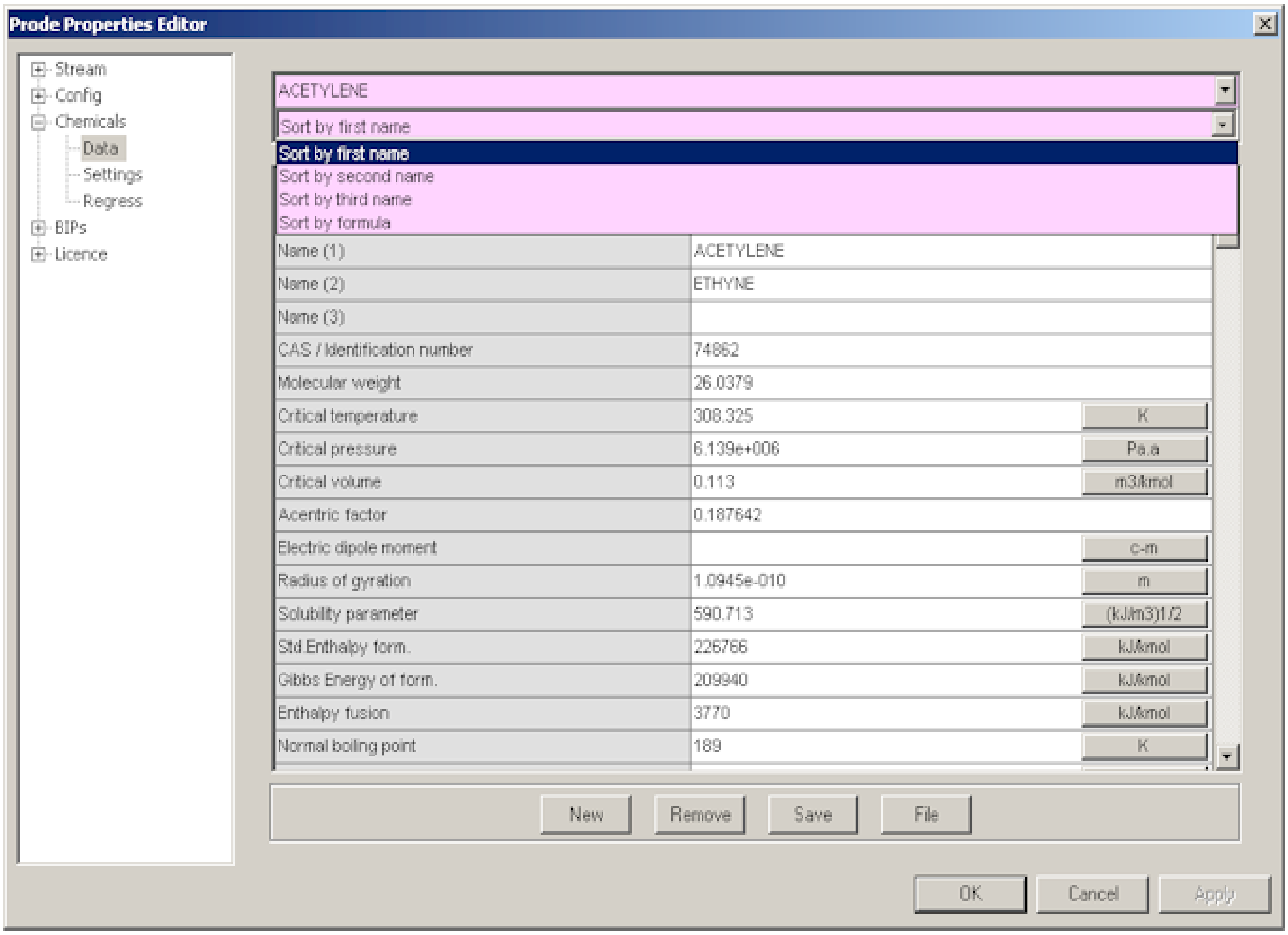
IMPORTANT

before to leave the application remember to save all data into the archive differently your changes will be lost !

Chemicals data

From this page you can :

- edit and change the physical properties data included in the databank
- save all data in a file



ACETYLENE

Sort by first name

Name (1)	ACETYLENE	
Name (2)	ETHYNE	
Name (3)		
CAS / Identification number	74862	
Molecular weight	26.0379	
Critical temperature	308.325	K
Critical pressure	6.139e+006	Pa.a
Critical volume	0.113	m3/kmol
Acentric factor	0.187642	
Electric dipole moment		c-m
Radius of gyration	1.0945e-010	m
Solubility parameter	590.713	(kJ/m3)1/2
Std.Enthalpy form.	226766	kJ/kmol
Gibbs Energy of form.	209940	kJ/kmol
Enthalpy fusion	3770	kJ/kmol
Normal boiling point	189	K

Edit / modify data :

- select a component from the component's list
- edit / modify the related fields (see also the section with description of all fields)
- select the "Save" button to save the modified data (differently new data will be discharged)

Adding a new component :

- select the "New" button
- edit the related fields (see also the following page with description of all data fields)
- select the "Save" button to save the data (differently new data will be discharged)

Remove a component :

- select a component from the component's list
- select the "Remove" button

IMPORTANT

Updating the file which contains the databank :

this option permits to store all data into a file, differently all changes will be lost when leaving the application

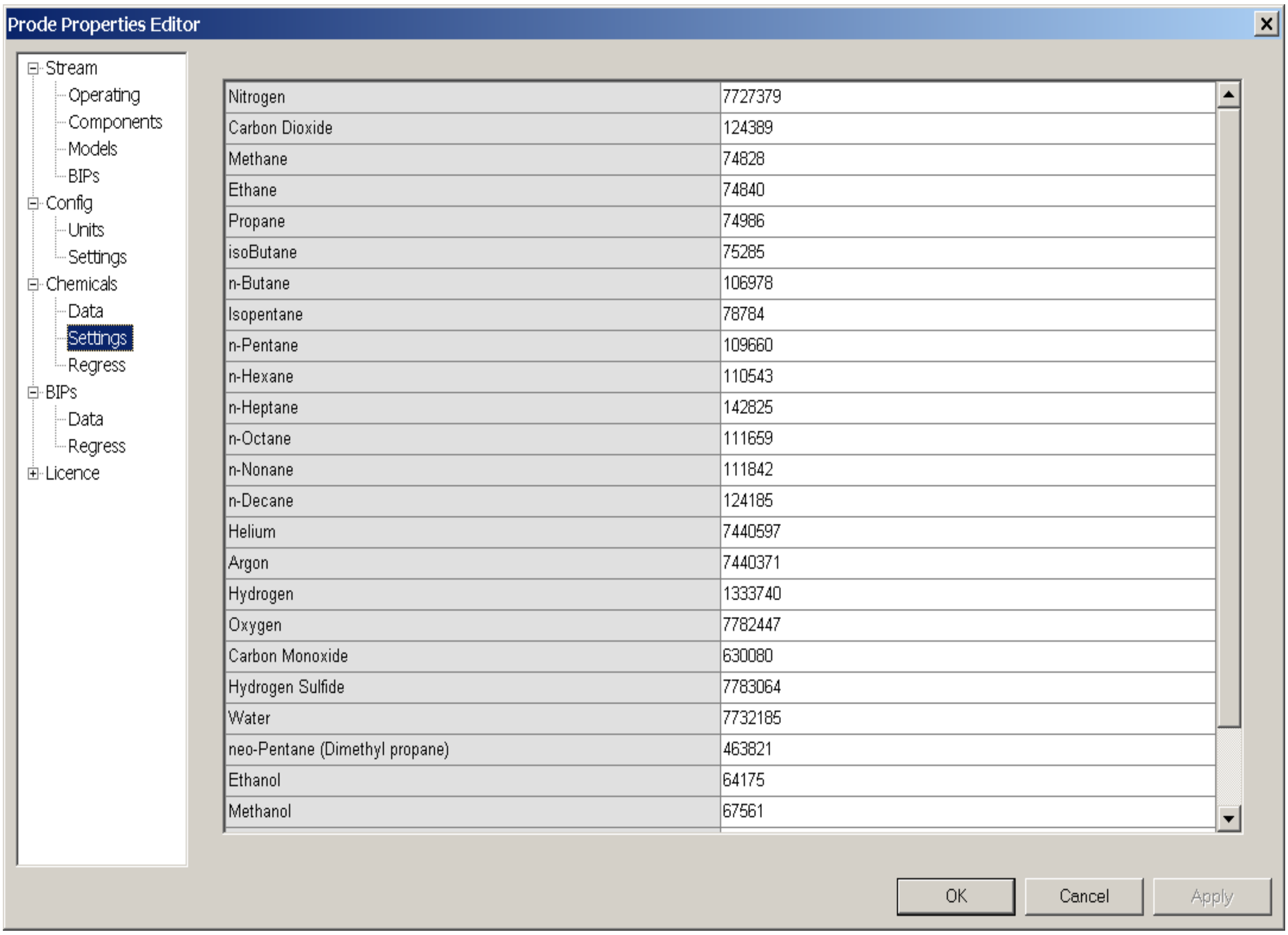
- select the "File" button

CAUTION : you may wish to create a backup of the file chem.dat before to overwrite the file

Chemicals Settings

From this page you can :

- edit informations (CAS number) required to identify some components .

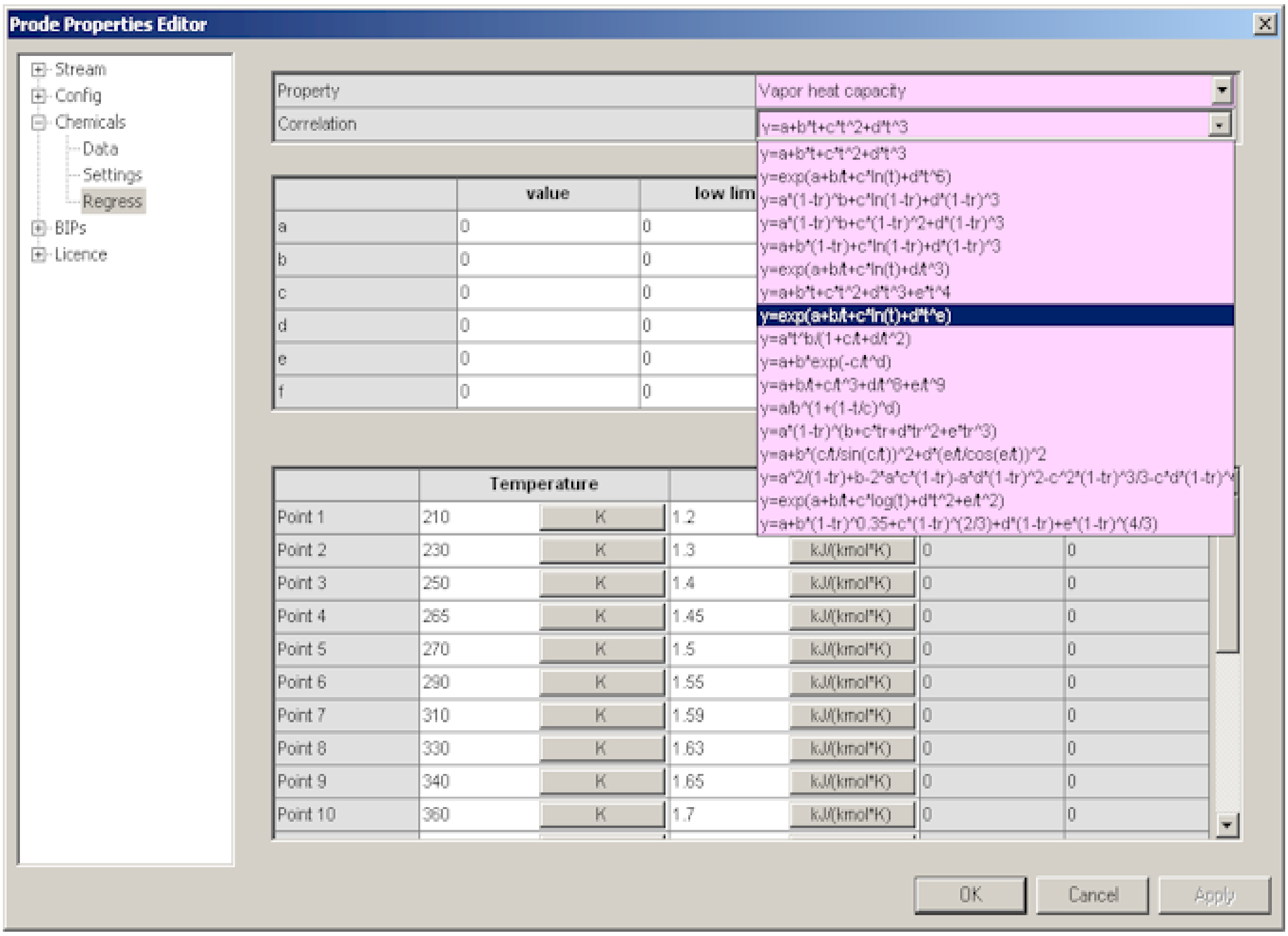


Nitrogen	7727379
Carbon Dioxide	124389
Methane	74828
Ethane	74840
Propane	74986
isoButane	75285
n-Butane	106978
Isopentane	78784
n-Pentane	109660
n-Hexane	110543
n-Heptane	142825
n-Octane	111659
n-Nonane	111842
n-Decane	124185
Helium	7440597
Argon	7440371
Hydrogen	1333740
Oxygen	7782447
Carbon Monoxide	630080
Hydrogen Sulfide	7783064
Water	7732185
neo-Pentane (Dimethyl propane)	463821
Ethanol	64175
Methanol	67561

Regress raw data

From this page you can :

- regress raw data into values compatible with chemical's database


Prode Properties Editor
Stream
Config
Chemicals
Data
Settings
Regress
BIPs
Licence
y=a+b*t+c*t^2+d*t^3
y=exp(a+b/t+c*ln(t)+d*t^6)
y=a*(1-tr)^b+c*ln(1-tr)+d*(1-tr)^3
y=a*(1-tr)^b+c*(1-tr)^2+d*(1-tr)^3
y=a+b*(1-tr)+c*ln(1-tr)+d*(1-tr)^3
y=exp(a+b/t+c*ln(t)+d/t^3)
y=a+b*t+c*t^2+d*t^3+e*t^4
y=exp(a+b/t+c*ln(t)+d*t^e)
y=a*t^b/(1+c/t+d/t^2)
y=a+b*exp(-c/t^d)
y=a+b/t+c/t^3+d/t^8+e/t^9
y=a/b^(1+(1-t/c)^d)
y=a*(1-tr)^(b+c*tr+d*tr^2+e*tr^3)
y=a+b*(c/t/sin(c/t))^2+d*(e/t/cos(e/t))^2
y=a^2/(1-tr)+b-2*a*c*(1-tr)-a*d*(1-tr)^2-c^2*(1-tr)^3/3-c*d*(1-tr)^
y=exp(a+b/t+c*log(t)+d*t^2+e/t^2)
y=a+b*(1-tr)^0.35+c*(1-tr)^(2/3)+d*(1-tr)+e*(1-tr)^(4/3)
OK
Cancel
Apply

Property	Vapor heat capacity
Correlation	y=a+b*t+c*t^2+d*t^3

	value	low lim
a	0	0
b	0	0
c	0	0
d	0	0
e	0	0
f	0	0

	Temperature					
Point 1	210	K	1.2			
Point 2	230	K	1.3	kJ/(kmol*K)	0	0
Point 3	250	K	1.4	kJ/(kmol*K)	0	0
Point 4	265	K	1.45	kJ/(kmol*K)	0	0
Point 5	270	K	1.5	kJ/(kmol*K)	0	0
Point 6	290	K	1.55	kJ/(kmol*K)	0	0
Point 7	310	K	1.59	kJ/(kmol*K)	0	0
Point 8	330	K	1.63	kJ/(kmol*K)	0	0
Point 9	340	K	1.65	kJ/(kmol*K)	0	0
Point 10	360	K	1.7	kJ/(kmol*K)	0	0

Regress raw data

- in Chemicals Data page select a chemical
- in Chemical Regress page selet a property and the correlation for fitting raw data
- enter the available data (all temperature and value pairs) with the proper units of measurement
- if required you may enter initializing values and limits for calculated parameters
- click on Calculate button, evaluate calculated values and errors, you may try different correlations for best data fitting
- click on Transfer button to copy calculated values into Chemicals Data page
- in Chemicals Data page select the "Save" button to save the data (differently new data will be discharged)

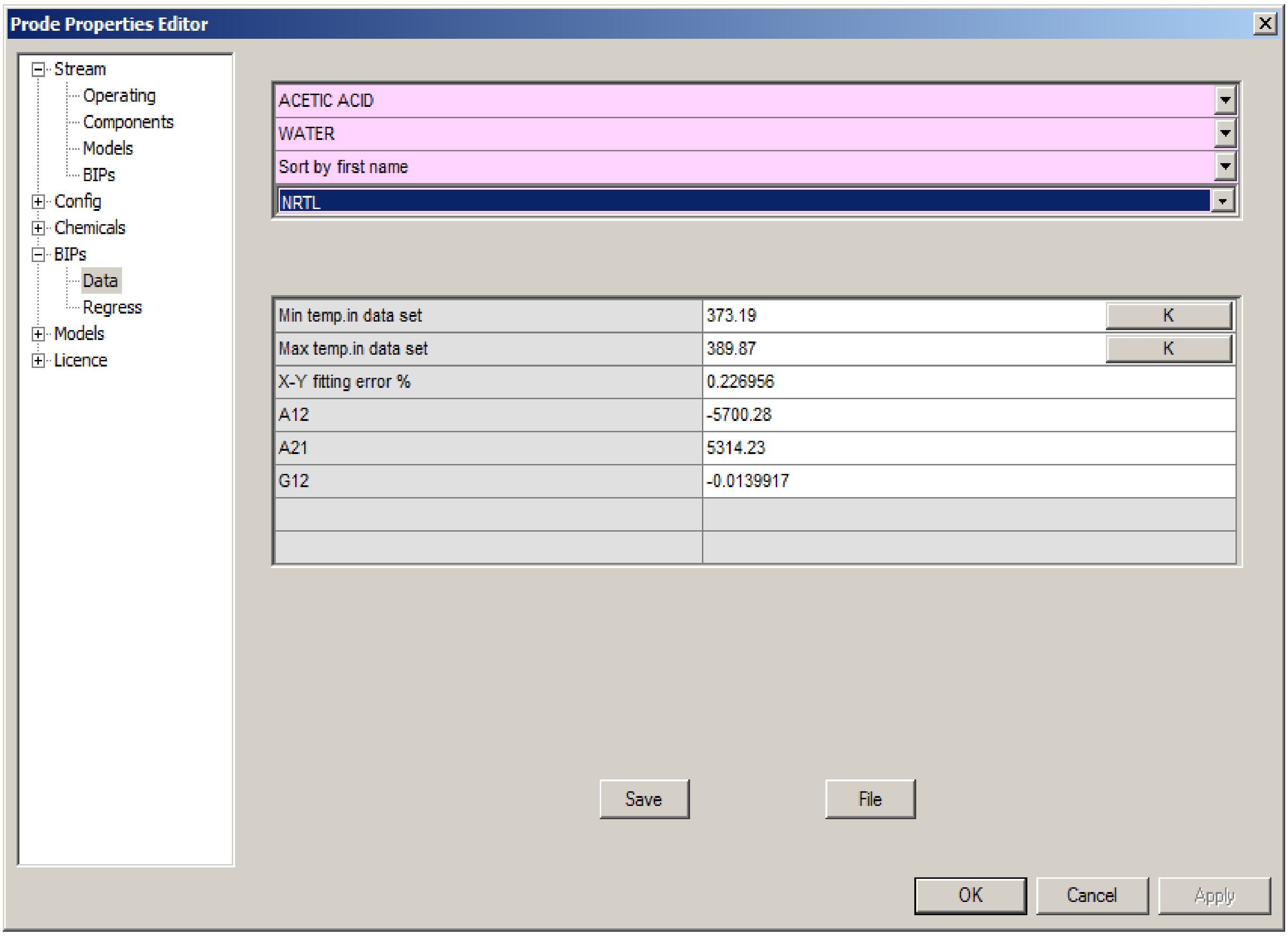
IMPORTANT

Prode Properties flexible datbase format supports more than 15 different correlations (30 in extended version), so for each property you can select the correlation which best fits experimental data.

Binary Interaction Parameters (BIP)

From these pages you can :

- edit Binary Interaction Parameters
- add / remove Binary Interaction Parameters
- regress VLE (vapor-liquid) , LLE (liquid-liquid) , SLE (solid-liquid) data points
- save all data in a file



ACETIC ACID
WATER
Sort by first name
NRTL

Min temp.in data set	373.19	K
Max temp.in data set	389.87	K
X-Y fitting error %	0.226956	
A12	-5700.28	
A21	5314.23	
G12	-0.0139917	

Edit / modify data :

- select two components from the component's lists
- edit / modify BIPs for the different models
- select the "Save" button to save the modified data (differently new data will be discharged)

IMPORTANT

Updating the file which contains the BIPs data :

this option permits to store all data into a file, differently all changes will be lost when leaving the application

- select the "File" button

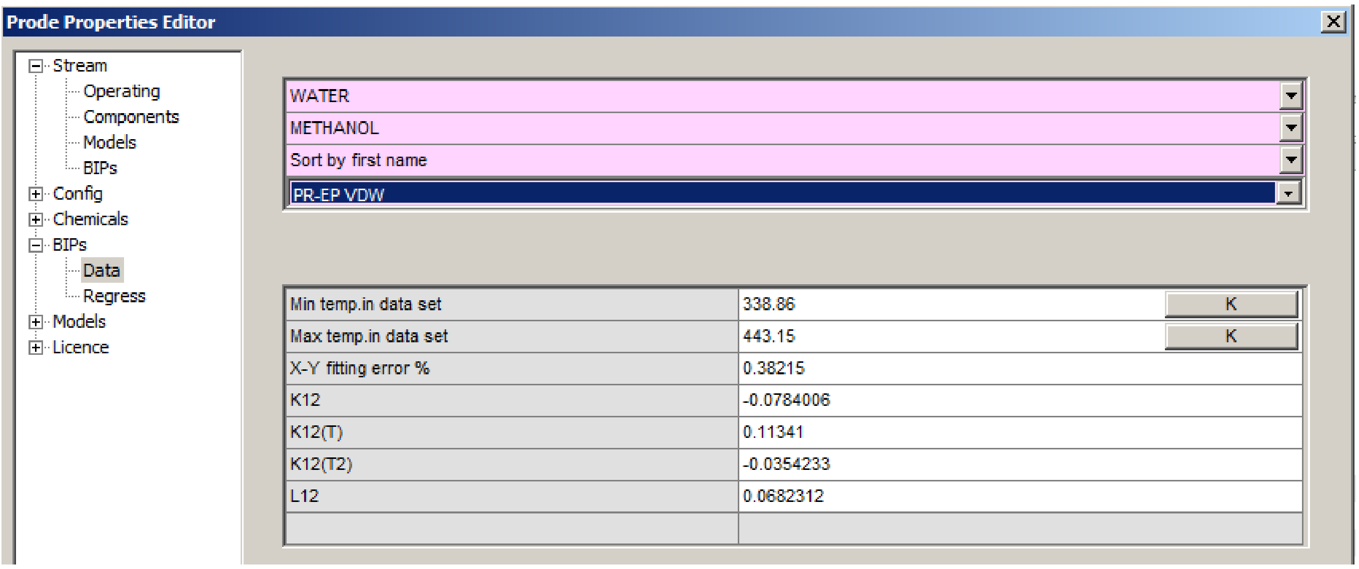
CAUTION you may wish to create a backup of the file bips.dat before to overwrite the file

Regress VLE-LLE-SLE data

From this page you can :

- regress VLE-LLE-SLE data for calculating the best fitting paraneters of different models

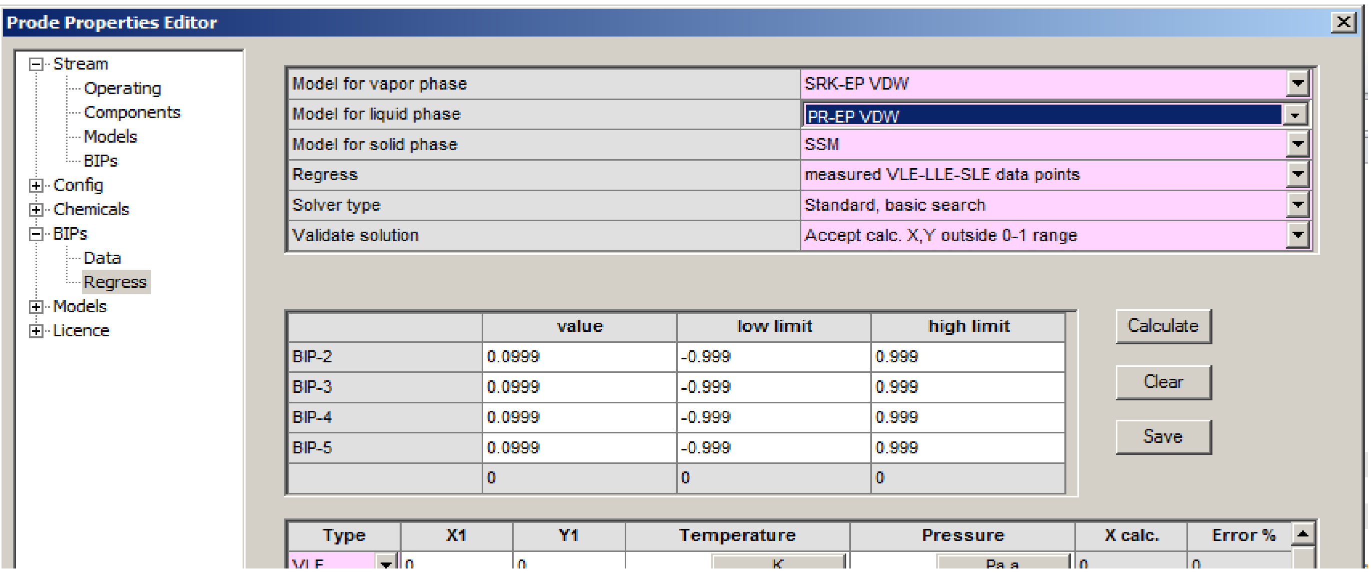
as first step in BIPs->Data page you must select two components (in this example methanol and water)



WATER
METHANOL
Sort by first name
PR-EP VDW

Min temp.in data set	338.86
Max temp.in data set	443.15
X-Y fitting error %	0.38215
K12	-0.0784006
K12(T)	0.11341
K12(T2)	-0.0354233
L12	0.0682312

The procedure permits to enter experimental (measured) VLE-LLE-SLE data points or fit automatically the model to VLE points calculated with UNIFAC.



Model for vapor phase	SRK-EP VDW
Model for liquid phase	PR-EP VDW
Model for solid phase	SSM
Regress	measured VLE-LLE-SLE data points
Solver type	Standard, basic search
Validate solution	Accept calc. X,Y outside 0-1 range

	value	low limit	high limit
BIP-2	0.0999	-0.999	0.999
BIP-3	0.0999	-0.999	0.999
BIP-4	0.0999	-0.999	0.999
BIP-5	0.0999	-0.999	0.999
	0	0	0

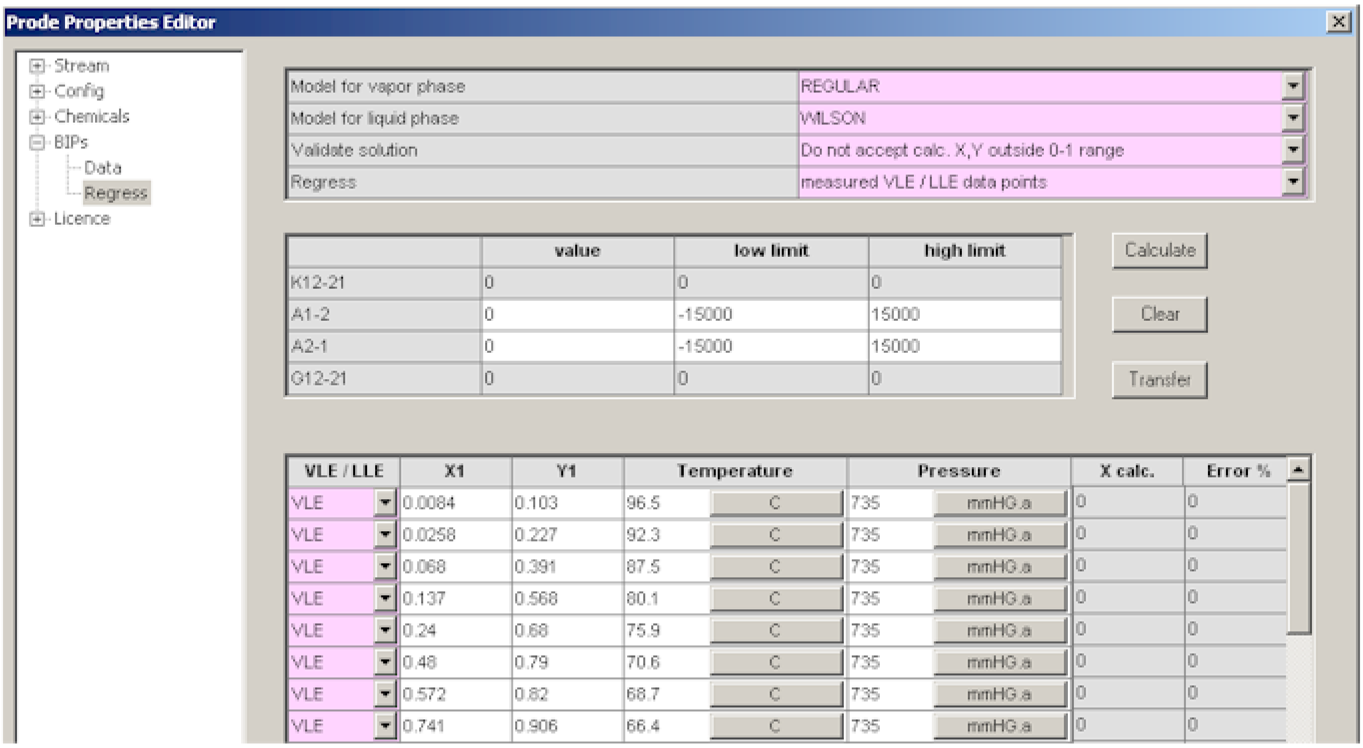
Type	X1	Y1	Temperature	Pressure	X calc.	Error %
VLE	0	0	K	Pa a	0	0

When entering measured VLE (vapor-liquid data points) on each row include in X column the measured liquid molar fraction of component 1, in Y column the measured vapor molar fraction of component 1, for LLE (liquid-liquid equilibria) include in X column the measured liquid molar fraction of component 1 in first liquid phase, and in Y column the measured liquid molar fraction of component 1 in second liquid phase, for SLE (solid-liquid equilibria) include in X column the measured liquid molar fraction of component 1 in liquid phase, and in Y column the measured solid molar fraction of component 1, finally enter the temperature and the pressure for that point.
Example of measured VLE data for Methanol-Water

VLE data for Methanol-Water at 735 mmHg

Point	X(1)	Y(1)	Temperature (C)	Pressure (mmHg)
VLE	0.008400	0.103000	96.5	735
VLE	0.025800	0.227000	92.3	735
VLE	0.068000	0.391000	87.5	735
VLE	0.137000	0.568000	80.1	735
VLE	0.240000	0.680000	75.9	735
VLE	0.480000	0.790000	70.6	735
VLE	0.572000	0.820000	68.7	735
VLE	0.741000	0.906000	66.4	735

Enter the measured data, select the models to regress (in this case Wilson for liquid phase and regulat -ideal- for vapor phase)

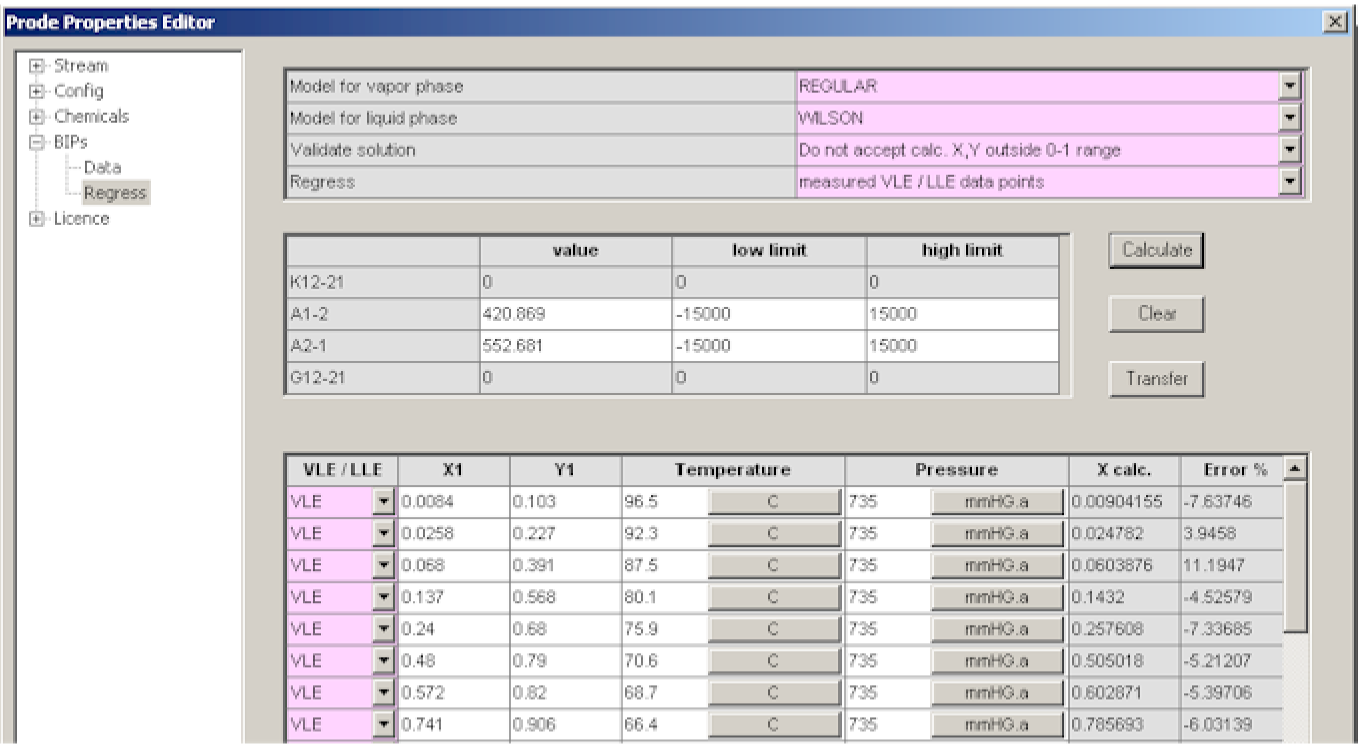


Model for vapor phase	REGULAR
Model for liquid phase	WILSON
Validate solution	Do not accept calc. X,Y outside 0-1 range
Regress	measured VLE / LLE data points

	value	low limit	high limit
K12-21	0	0	0
A1-2	0	-15000	15000
A2-1	0	-15000	15000
G12-21	0	0	0

VLE / LLE	X1	Y1	Temperature		Pressure		X calc.	Error %
VLE	0.0084	0.103	96.5	C	735	mmHG.a	0	0
VLE	0.0258	0.227	92.3	C	735	mmHG.a	0	0
VLE	0.068	0.391	87.5	C	735	mmHG.a	0	0
VLE	0.137	0.568	80.1	C	735	mmHG.a	0	0
VLE	0.24	0.68	75.9	C	735	mmHG.a	0	0
VLE	0.48	0.79	70.6	C	735	mmHG.a	0	0
VLE	0.572	0.82	68.7	C	735	mmHG.a	0	0
VLE	0.741	0.906	66.4	C	735	mmHG.a	0	0

Selecting the button Calculate the procedure calculates the best fitting parameters, shows the calculatd results and the relative errors (%)



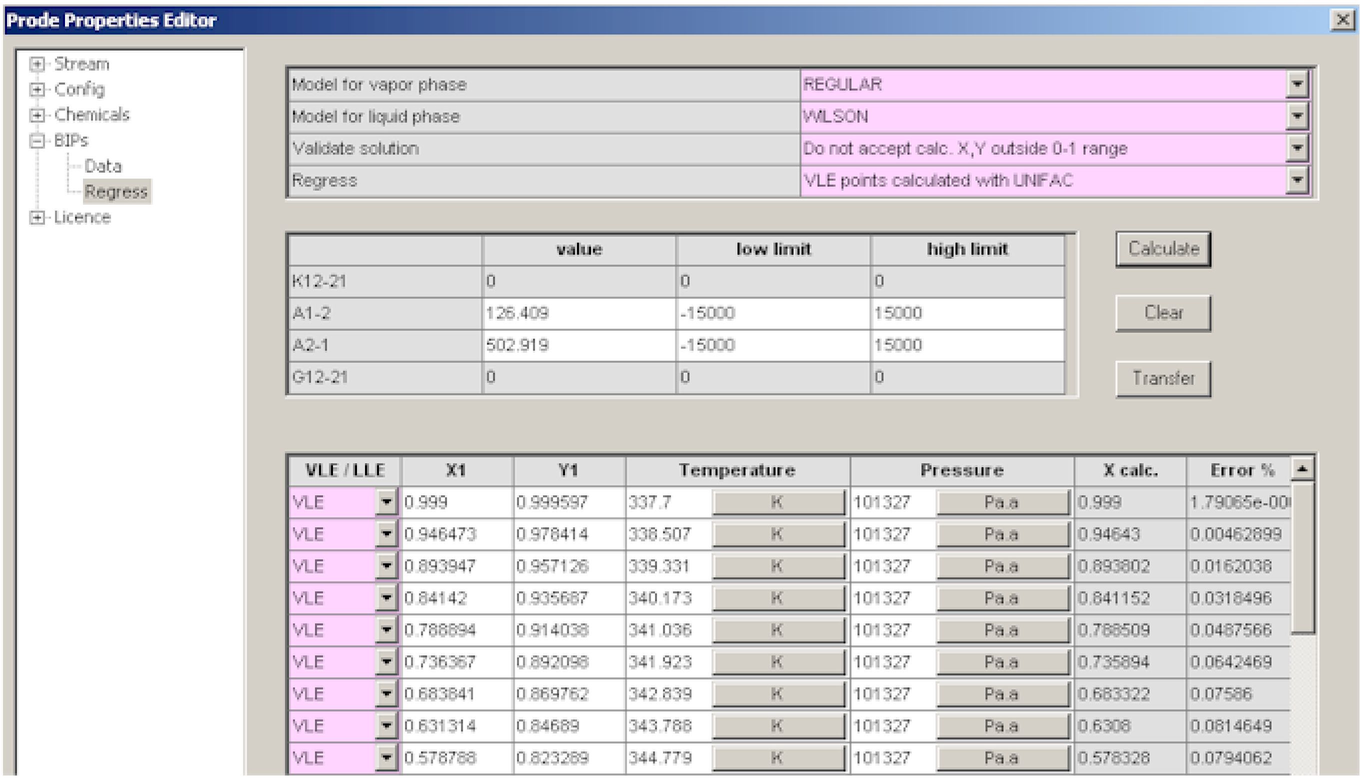
Model for vapor phase	REGULAR
Model for liquid phase	WILSON
Validate solution	Do not accept calc. X,Y outside 0-1 range
Regress	measured VLE / LLE data points

	value	low limit	high limit
K12-21	0	0	0
A1-2	420.869	-15000	15000
A2-1	552.681	-15000	15000
G12-21	0	0	0

VLE / LLE	X1	Y1	Temperature		Pressure		X calc.	Error %
VLE	0.0084	0.103	96.5	C	735	mmHG.a	0.00904155	-7.63746
VLE	0.0258	0.227	92.3	C	735	mmHG.a	0.024782	3.9458
VLE	0.068	0.391	87.5	C	735	mmHG.a	0.0603876	11.1947
VLE	0.137	0.568	80.1	C	735	mmHG.a	0.1432	-4.52579
VLE	0.24	0.68	75.9	C	735	mmHG.a	0.257608	-7.33685
VLE	0.48	0.79	70.6	C	735	mmHG.a	0.505018	-5.21207
VLE	0.572	0.82	68.7	C	735	mmHG.a	0.602871	-5.39706
VLE	0.741	0.906	66.4	C	735	mmHG.a	0.785693	-6.03139

as alternative the procedure offers the option to calculate the best fitting parameters to VLE data points calculated with UNIFAC, this entirely predictive method doesn't require experimental data and in some cases can result useful.

Select “VLE points calculated with UNIFAC” in “Regress” selector to use this method

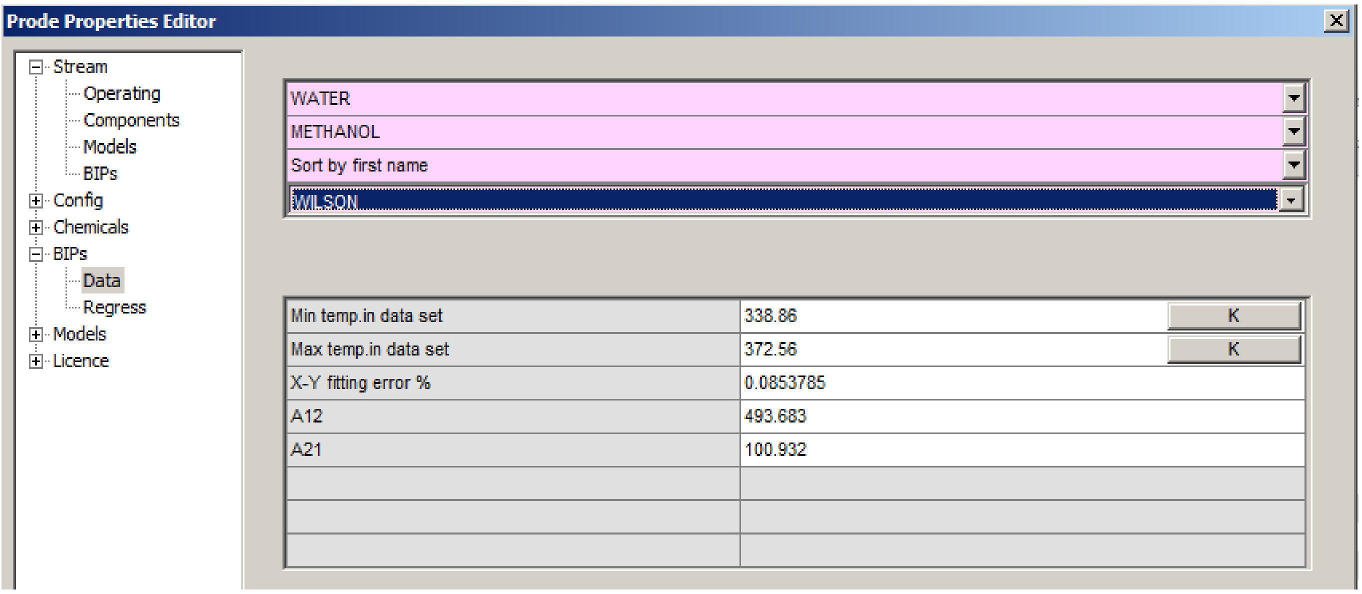


Model for vapor phase	REGULAR
Model for liquid phase	WILSON
Validate solution	Do not accept calc. X,Y outside 0-1 range
Regress	VLE points calculated with UNIFAC

	value	low limit	high limit
K12-21	0	0	0
A1-2	126.409	-15000	15000
A2-1	502.919	-15000	15000
G12-21	0	0	0

VLE / LLE	X1	Y1	Temperature		Pressure		X calc.	Error %
VLE	0.999	0.999597	337.7	K	101327	Pa.a	0.999	1.79065e-00
VLE	0.946473	0.978414	338.507	K	101327	Pa.a	0.94643	0.00462899
VLE	0.893947	0.957126	339.331	K	101327	Pa.a	0.893802	0.0162038
VLE	0.84142	0.935687	340.173	K	101327	Pa.a	0.841152	0.0318496
VLE	0.788894	0.914038	341.036	K	101327	Pa.a	0.788509	0.0487566
VLE	0.736367	0.892098	341.923	K	101327	Pa.a	0.735894	0.0642469
VLE	0.683841	0.869762	342.839	K	101327	Pa.a	0.683322	0.07586
VLE	0.631314	0.84689	343.788	K	101327	Pa.a	0.6308	0.0814649
VLE	0.578788	0.823289	344.779	K	101327	Pa.a	0.578328	0.0794062

Once the paramters have been calculated you must select the “Transfer” button to transfer the results in BIPs->Data page, from that page you can save the calculated BIPs in database (select Save button) or store permanently in file (select File button).



WATER

METHANOL

Sort by first name

WILSON

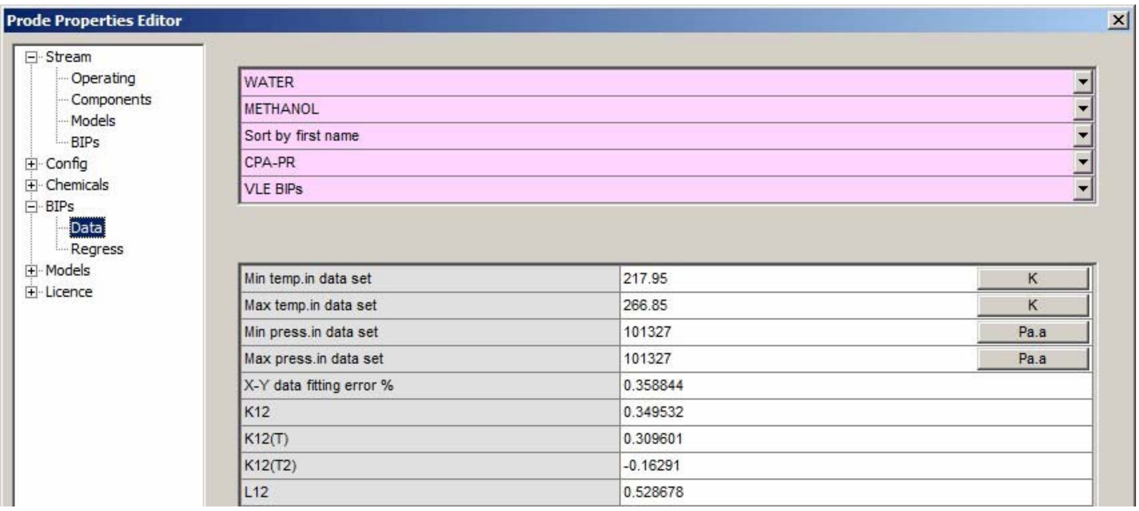
Min temp.in data set	338.86	K
Max temp.in data set	372.56	K
X-Y fitting error %	0.0853785	
A12	493.683	
A21	100.932	

Regress SLE (Water-Methanol) and test the calculated freezing point depression
This example will show how to estimate BIPs for different models from available SLE equilibrium points

SLE data for Water-Methanol atm pressure
First component is Water, second component Methanol
X1 is the water fraction in liquid phase while Y1 is solid fraction (always 0.9999... for a model based on pure fluid)

Point	X1	Y1	Temperature (K)	Pressure (Bar.g)
SLE	0.9432	0.9999	266.85	0
SLE	0.9	0.9999	259.65	0
SLE	0.87676	0.9999	257.65	0
SLE	0.80583	0.9999	246.85	0
SLE	0.8	0.9999	242.95	0
SLE	0.728	0.9999	233.45	0
SLE	0.641	0.9999	217.95	0
SLE	0.636	0.9999	214.95	0
SLE	0.6	0.9999	208.15	0

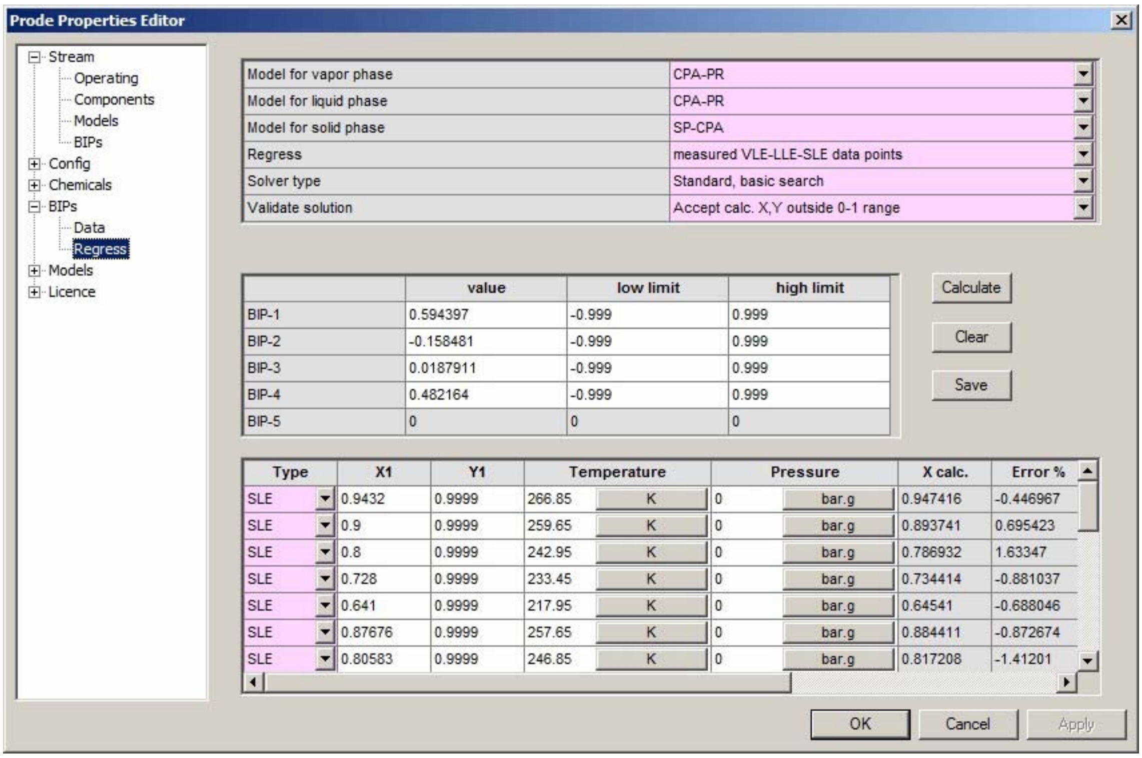
as first step in BIPs->Data page you must select the components (in this example methanol and water)



WATER
METHANOL
Sort by first name
CPA-PR
VLE BIPs

Min temp.in data set	217.95	K
Max temp.in data set	266.85	K
Min press.in data set	101327	Pa.a
Max press.in data set	101327	Pa.a
X-Y data fitting error %	0.358844	
K12	0.349532	
K12(T)	0.309601	
K12(T2)	-0.16291	
L12	0.528678	

then in BIPs->Regress page select models (CPA-PR for vapor, CPA-PR for liquid, SP-CPA for solid) options, enter all data points and click on Calculate button to get the results

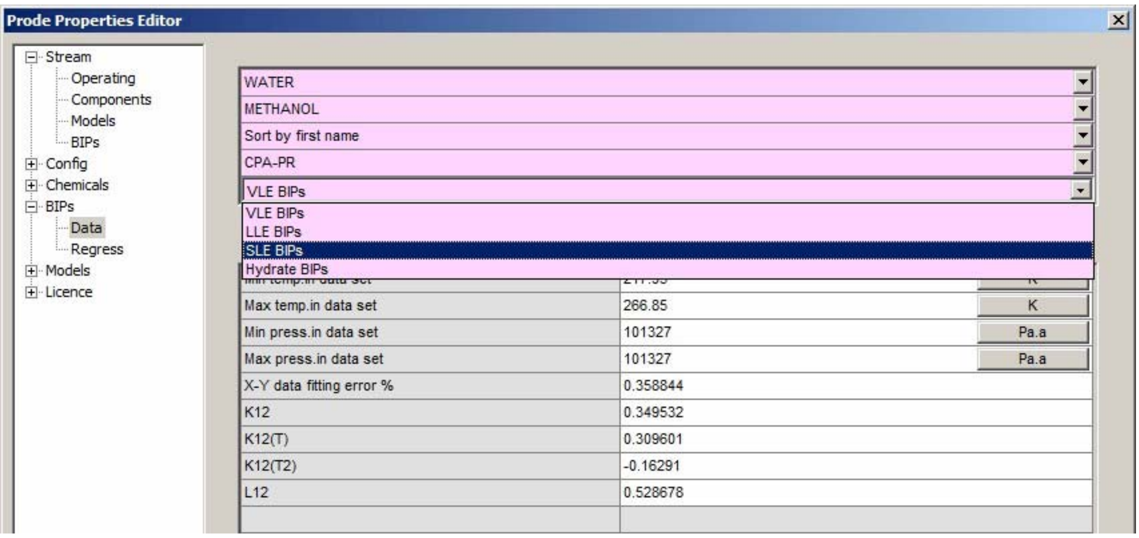


Model for vapor phase	CPA-PR
Model for liquid phase	CPA-PR
Model for solid phase	SP-CPA
Regress	measured VLE-LLE-SLE data points
Solver type	Standard, basic search
Validate solution	Accept calc. X,Y outside 0-1 range

	value	low limit	high limit
BIP-1	0.594397	-0.999	0.999
BIP-2	-0.158481	-0.999	0.999
BIP-3	0.0187911	-0.999	0.999
BIP-4	0.482164	-0.999	0.999
BIP-5	0	0	0

Type	X1	Y1	Temperature		Pressure		X calc.	Error %
SLE	0.9432	0.9999	266.85	K	0	bar.g	0.947416	-0.446967
SLE	0.9	0.9999	259.65	K	0	bar.g	0.893741	0.695423
SLE	0.8	0.9999	242.95	K	0	bar.g	0.786932	1.63347
SLE	0.728	0.9999	233.45	K	0	bar.g	0.734414	-0.881037
SLE	0.641	0.9999	217.95	K	0	bar.g	0.64541	-0.688046
SLE	0.87676	0.9999	257.65	K	0	bar.g	0.884411	-0.872674
SLE	0.80583	0.9999	246.85	K	0	bar.g	0.817208	-1.41201

Then click on Save button to move calculated values on Data tab,
in Data dialog select SLE BIPs as database and click on Save button to store data, you may use File button to store (permanently) data in bips.dat file

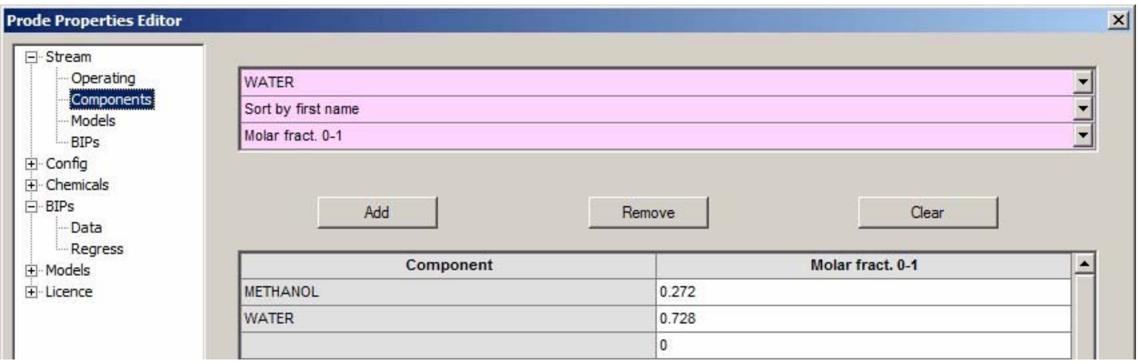


WATER
METHANOL
Sort by first name
CPA-PR
VLE BIPs

Max temp.in data set	266.85	K
Min press.in data set	101327	Pa.a
Max press.in data set	101327	Pa.a
X-Y data fitting error %	0.358844	
K12	0.349532	
K12(T)	0.309601	
K12(T2)	-0.16291	
L12	0.528678	

to test the accuracy of calculated BIPs in estimating freezing point depression in Prode Properties Editor select a new stream and define as composition H2O 0.728 CH4O 0.272 to test this point in the series

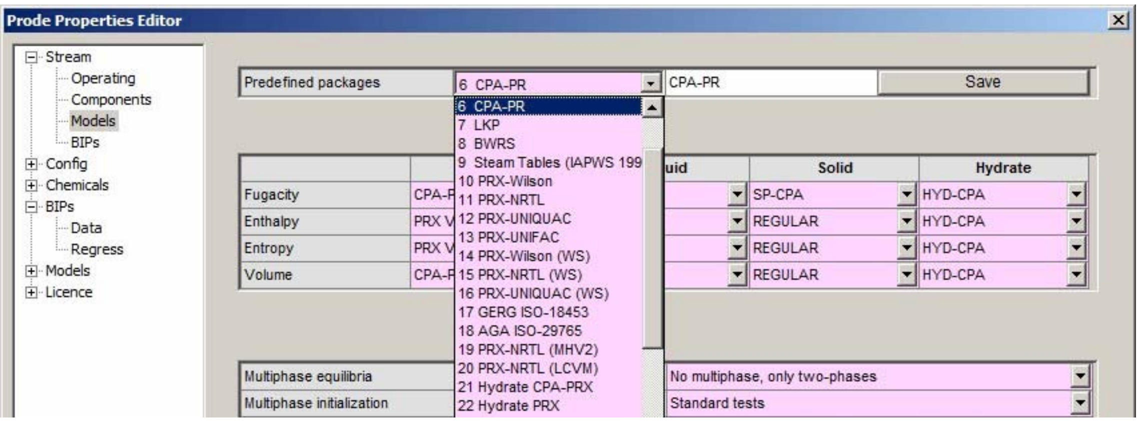
	X1	Y1	T(K)	P(Bar.g)
SLE	0.728	0.9999	233.45	0



WATER
Sort by first name
Molar fract. 0-1

Component	Molar fract. 0-1
METHANOL	0.272
WATER	0.728
	0

then in Models tab select the same models adopted in data regression, CPA-PR for vapor, CPA-PR for liquid, SP-CPA for solid

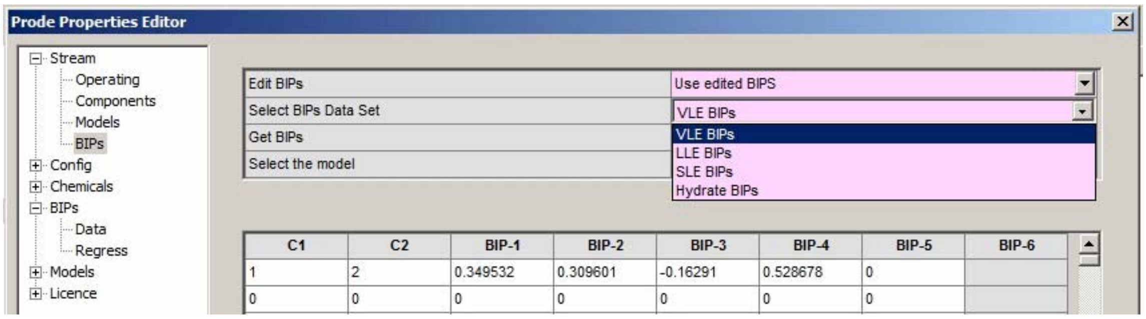


Predefined packages	6 CPA-PR	CPA-PR

		uid	Solid	Hydrate
Fugacity	CPA-F		SP-CPA	HYD-CPA
Enthalpy	PRX V		REGULAR	HYD-CPA
Entropy	PRX V		REGULAR	HYD-CPA
Volume	CPA-F		REGULAR	HYD-CPA

Multiphase equilibria	No multiphase, only two-phases
Multiphase initialization	Standard tests

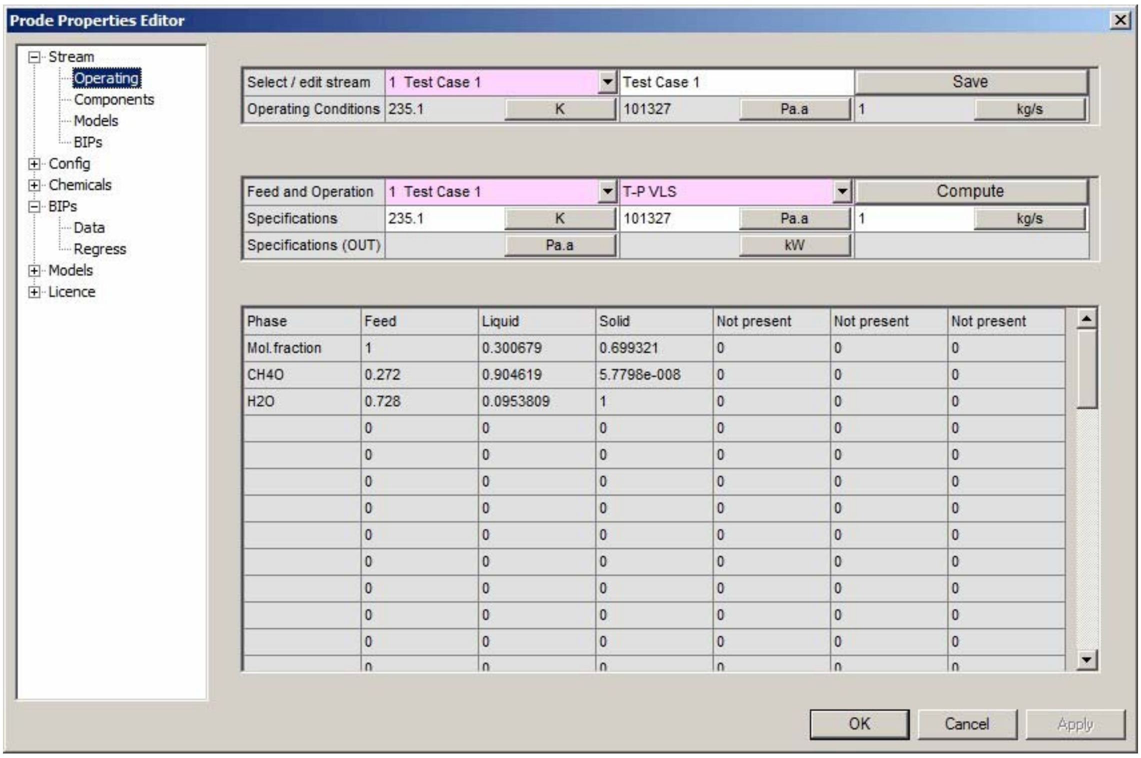
In BIPs tab select SLE BIPs Data set and click on Load BIPs button to get BIPs,
make sure that values shown on window are those previously calculated



Edit BIPs	Use edited BIPS
Select BIPs Data Set	VLE BIPs
Get BIPs	
Select the model	

C1	C2	BIP-1	BIP-2	BIP-3	BIP-4	BIP-5	BIP-6
1	2	0.349532	0.309601	-0.16291	0.528678	0	
0	0	0	0	0	0	0	

Finally in Operating tab click Save Button to define the stream and solve a TP-VLS flash operation to evaluate the point of incipient solidification



Select / edit stream	1 Test Case 1		Test Case 1		Save	
Operating Conditions	235.1	K	101327	Pa.a	1	kg/s

Feed and Operation	1 Test Case 1		T-P VLS		Compute	
Specifications	235.1	K	101327	Pa.a	1	kg/s
Specifications (OUT)		Pa.a		kW		

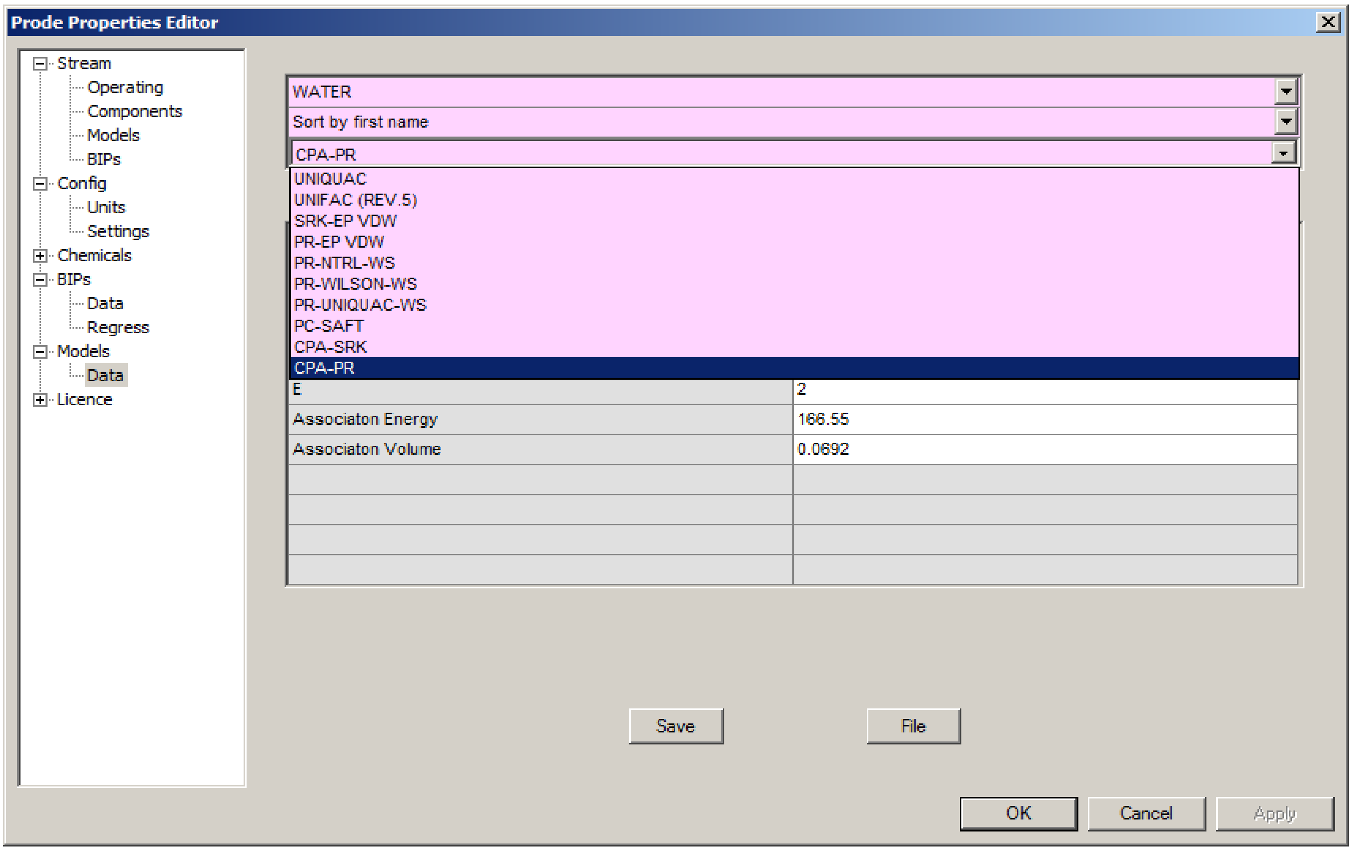
Phase	Feed	Liquid	Solid	Not present	Not present	Not present
Mol.fraction	1	0.300679	0.699321	0	0	0
CH4O	0.272	0.904619	5.7798e-008	0	0	0
H2O	0.728	0.0953809	1	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0

the calculated point is about 235.1 K ,
compare this value with the experimental data (233.45 K) utilized in data regression,
error is about 1.6 K

Parameters of models

From this page you can :

- edit the parameters required by the different models available in library



WATER

Sort by first name

CPA-PR

E	2
Associaton Energy	166.55
Associaton Volume	0.0692

Edit / modify data :

- select the components from the component's lists
- select the model
- edit / modify the parameters
- select the "Save" button to save the modified data (differently new data will be discharged)

IMPORTANT

Updating the file which contains the Model data :

this option permits to store all data into a file, differently all changes will be lost when leaving the application

- select the "File" button

CAUTION you may wish to create a backup of the file bips.dat before to overwrite the file

Accessing Prode Properties library

The technique for accessing the methods available in Prode Properties library will depend on which programming language You use. Languages such as FORTRAN , C, C++ or Microsoft NET (VB,C) exhibit differences in parameter passing in and out of functions. This may require you to adapt your code from the examples shown here. The calling convention determines how a program makes a call and where the parameters are passed. PROPERTIES does use of standard calls of Windows API, it pushes parameters on the stack, in reverse order. When accessing PROPERTIES You must also consider :

- Prode Properties real type is 8 bytes
- Prode Properties integer type is 4 bytes
- parameters are passed by value (with exception of strings which are arrays of characters)

IMPORTANT
C / C++ support files are located in the directory \Prode\C
FORTRAN support files are located in the directory \Prode\FORTRAN
Microsoft NET support files are located in the directory \Prode\NET
Microsoft EXCEL support files are located in the directory \Prode\Excel

Fortran

add ppp.lib file to the list of the files in Your project and include ppp.f90 to instruct the compiler about the methods available in Prode Properties then access the methods as they were included in your code

```
C   this procedure returns the critical temperature of a compound
INTERFACE TO REAL*8 FUNCTION TC ([C,ALIAS:'CompTc'] comp)
INTEGER*4 comp [VALUE]
END

REAL*8 tc
INTEGER*4 id
C   define the id value  here
tc = TC(id)
```

C / C++

- include the ppp.h header
- add ppp.lib file to the list of the files in Your project
- make sure you use the calling convention of ppp.h header file,
- access the Prode Properties methods

```
char *name;
name  = CompN(1);  // returns the name of the first component in the chemical's file
```

Microsoft NET (VB)

see the samples provided with Prode Properties for additional information

- include properties.vba to instruct the compiler about the methods available in Prode Properties and access the methods

```
CompName = MCompN(1)
```

Microsoft Excel

Microsoft Excel supports *macros* and VBA language for defining procedures; both of these can be used to access the functions in Prode Properties, see the samples provided with Prode Properties for additional information

- include properties.vba to instruct Microsoft Excel about the methods available in Prode Properties and access the methods

CompName = MCompN(1)

Translate resources to different languages

A large part of the resources are stored in the file res.lan , see the paragraph “**Data files folder**” for additional information about how to locate the file. The file res.lan is a text file, easily editable by the user.

Example

in English language
N2_NAME = “Nitrogen”;

in French language
N2_NAME = “Azote”;

in Italian language
N2_NAME = “Azoto”;

IMPORTANT

When editing a string take care to modify only the parts enclosed within the braces ”” and do not alter/modify the data structures composed by special characters as for example ::

Microsoft Applications and Strings

Prode Properties utilizes the standard API calling convention for Microsoft Windows applications. This assures that almost all Windows compatible applications which support DLLs will also support Prode Properties. There are, however, some exceptions in passing strings (arrays of characters) since Microsoft utilizes proprietary data formats. Prode Properties includes Microsoft specific methods in addition to the standard methods supporting the ANSI C standard, Microsoft specific methods are compatible with almost all Microsoft applications.

Define models, compatibility with old verions

Prode Properties includes many methods for defining (via software) the thermodynamic models and the related options, see the paragraph “Methods to set / access different options” for additional information

Units of measurement

Prode Properties allows to define via software the units of measurement, there are methods for defining the units and methods for retrieving codes and strings, see paragraph “Methods for accessing / defining the units of measurement” and the samples provided with the package for additional information, in Prode Properties to reference a unit must use a numeric code

QUANTITY	**UNIT**	**CODE**	**DEFAULT UNIT**
Pressure (abs)	CONV_P	15	“Pa.a”
Pressure (rel)	CONV_DP	16	“Pa”
Temperature (abs)	CONV_T	17	“K”
Temperature(rel)	CONV_DT	18	“K”
Calorific Value (weight)	CONV_HM	19	“Kj/Kg”
Calorific Value (molar)	CONV_HMM	20	“Kj/Kmol”
Power	CONV_HS	21	“KW”
Entropy (Streams)	CONV_SS	22	“KJ/(K*s)”
Heat Capacity (weight)	CONV_CP	23	“kJ/(kg*K)”
Heat Capacity (molar)	CONV_CPM	24	“kJ/(kmol*K)”
Flow (mass basis)	CONV_W	25	“Kg/s”
Flow (gas, mass basis)	CONV_WG	26	“Kg/s”
Density (weight)	CONV_D	27	“Kg/m3”
Density (molar)	CONV_DM	28	“Kmol/m3”
Specific Volume (weight)	CONV_SV	29	“m3/Kg”
Specific Volume (molar)	CONV_SVM	30	“m3/Kmol”
Thermal Conductivity	CONV_TC	31	“W/(m*K)”
Viscosity (dynamic)	CONV_V	32	“Pa*s”
Surface Tension	CONV_ST	33	“N/m”
Lenght	CONV_L	34	“m”
Area	CONV_A	35	“m2”
Volume	CONV_VOL	36	“m3”
Mass	CONV_M	37	“Kg”
Velocity	CONV_VL	38	“m/s”
Acceleration	CONV_ACC	39	“m/s2”
Force	CONV_FOR	40	“N”
Time	CONV_TM	41	“s”
Heat Flux	CONV_HF	42	“KW/m2”
Thermal Resistance	CONV_TR	43	“K*m2/KW”
Heat Transfer Coefficent	CONV_HTC	44	”KW/(m2*C)”
Flow (volume basis)	CONV_VW	45	“m3/s”
Viscosity (kinematic)	CONV_VK	46	“m2/s”
Energy	CONV_EN	47	“KJ”
Dipole moment	CONV_EDM	48	“c-m”
Solubility parameter	CONV_SP	49	“(J/m3)^1/2”
Flow Coefficient	CONV_CV	50	“Cv”
Compressibility coefficient	CONV_CC	51	“1/Pa”
Joule Thomson coefficient	CONV_JTC	52	“K/Pa”
Flow (molar basis)	CONV_WM	53	“Kmol/s”
Volume expansivity	CONV_VE	54	“1/K”

Introducing Prode Properties library methods

Prode Properties library includes a range of methods to deal with problems in chemical engineering and to achieve tight control over the calculations .

A non-inclusive list would include

- Thermodynamic calcs (flash operations, enthalpy, entropy, volume, energy, unit operations)
- Streams data access and calcs (set and retrieve operating conditions, critical and transport properties calcs)
- Chemicals library access (retrieve data from chemicals file)
- Error messages (management of errors messages)

Methods for thermodynamic calc' s

Prode Properties includes a complete set of methods for solving all the standard flash operations with specified final temperature or pressure and entropy or enthalpy or volume or energy basis, phase fraction with temperature or pressure basis plus mixers, dividers, gas,liquid phase separation operations etc.

integer result = setOp(integer stream, double t, double p)
Given a stream, operating pressure and temperature, performs an isothermal flash and sets operating conditions.

integer result = setSOp(integer stream)
Given a stream performs an isothermal flash at (user defined) standard conditions.

double t = PfPF(integer stream, double p, double pf, int state, int n)
Given a stream, the pressure , phase fraction (range 0-1), state (gas, liquid, solid) and position n calculates and returns the nth (n : 1-5) equilibrium temperature along the specified phase fraction line

double p = PfTF(integer stream, double t, double pf, int state, int n)
Given a stream, the temperature , phase fraction (range 0-1), state (gas, liquid, solid) and position n calculates and returns the nth (n : 1-5) equilibrium pressure along the specified phase fraction line

double t = LfPF(integer stream, double p, double lf)
Given a stream, the pressure and Liquid fraction (range 0-1) calculates and returns the first equilibrium temperature along the specified phase fraction line

double p = LfTF(integer stream, double t, double lf)
Given a stream, the temperature and Liquid fraction (range 0-1) calculates and returns the first equilibrium pressure along the specified phase fraction line

double t = HPF(integer stream, double p, double h, double et)
Given a stream, final pressure, the required (final) enthalpy (see the method StrH() for the definition) and a estimated value for final temperature (or 0 for automatic estimate), method solves the flash operation (enthalpy basis) and returns final temperature

double p = HTF(integer stream, double t, double h, double ep)
Given a stream, final temperature, the required (final) enthalpy (see the method StrH() for the definition) and a estimated value for final pressure (or 0 for automatic estimate), method solves the flash operation (enthalpy basis) and returns final pressure

double t = SPF(integer stream, double p, double s, double et)
Given a stream, final pressure, the required (final) entropy (see the method StrS() for the definition) and a estimated value for final temperature (or 0 for automatic estimate), method solves the flash operation (entropy basis) and returns final temperature.

double p = STF(integer stream, double t, double s, double ep)
Given a stream, final temperature, the required (final) entropy (see the method StrS() for the definition) and a estimated value for final pressure (or 0 for automatic estimate), method solves the flash operation (entropy basis) and returns final pressure.

double t = VPF(integer stream, double p, double v, double et)
Given a stream, final pressure, the required specific volume (see the method StrV() for the definition) and a estimated value for final temperature (or 0 for automatic estimate), method solves the flash operation (volume basis) and returns final temperature.

double p = VTF(integer stream, double t, double v, double ep)
Given a stream, final temperature, the required specific volume (see the method StrV() for the definition) and a estimated value for final pressure (or 0 for automatic estimate), method solves the flash operation (volume basis) and returns final pressure.

integer result = HVF(integer stream, double h, double v, double et, double ep)
Given a stream, the required (final) enthalpy (see the method StrH() for the definition) the required (final) specific volume (see the method StrV() for the definition) and estimated values for final temperature and pressure (or 0 for automatic estimate), method solves the flash operation

integer result = SVF(integer stream, double s, double v, double et, double ep)
Given a stream, the required (final) entropy (see the method StrS() for the definition) the required specific volume (see the method StrV() for the definition) and estimated values for final temperature and pressure (or 0 for automatic estimate), method solves the flash operation

integer result = HSF(integer stream, double h, double s, double et, double ep)
Given a stream, the required (final) enthalpy (see the method StrH() for the definition) the required (final) entropy (see the method StrS() for the definition) and estimated values for final temperature and pressure (or 0 for automatic estimate), method solves the flash operation

double t = EPF(integer stream, double p, double E, double aout, double et)
Given a stream, final pressure, outlet area, the term E (equal to Hin + 1/2Vin^2) and a estimated value for final temperaure (or 0 for automatic estimate) method solves the constant energy flash and returns final temperature.
Hin + 1/2Vin^2 = Ho + 1/2Vo^2
this method permits to model adiabatic, irreversible expansions when the contribute of kinetic energy cannot be neglected.

integer result = MixF(integer stream1, integer stream2, double et)
Given two streams, stream1 and stream2 and a estimated value for final temperature (or 0 for automatic estimate) method solves a mixer operation and returns the result on stream1, the feed streams are adiabatically flashed to the lowest inlet stream pressure

integer result = Divi (integer stream1, integer stream2, double wdiv)
Given two streams (stream1 and stream2) and a flowrate fraction (0-1) performs a divider operation so that stream 1 is shifted into two streams (stream1, stream2) of the same composition, temperature and pressure, flowrate fractions are subdivided as specified by wdiv (stream2 = wdiv, stream1 = 1- wdiv)

integer result = psep(integer stream1, integer stream2, integer phase)
Given a stream (stream1) performs an isothermal flash to simulate a phase type (vapor,liquid,solid) separator and returns the result as stream2.

Methods for stream’ s data access

Prode Properties includes a set of functions for accessing stream parameters and calculating transport properties. Note that when calculating transport properties the program performs a VLE flash and returns 0 (zero value) when no associated liquid or gas phase is found.

integer res = isSDef(integer stream)
given a stream returns TRUE (integer = 1) if stream has been defined, otherwise returns FALSE (0)

double t = getT(integer stream)
given a stream returns stream’s operating temperature

double p = getP(integer stream)
given a stream returns stream’s operating pressure

integer nr = getPNr()
returns the maximum number of phases that procedure can detect

integer type = StrPt(integer stream, int phase)
given a stream and position in range 1- getPNr() returns the phase type (vapor,liquid,solid)

char *description = StrPts(integer stream, int phase)
given a stream and position in range 1- getPNr() returns a ANSI C string with the description of type for detected phase

VARIANT description = MStrPts(integer stream, int phase)
given a stream and position in range 1- getPNr() returns a string with the description of type of detected phase, this is the Microsoft specific method

double lf = StrLf(integer stream)
given a stream returns the total liquid fraction (molar basis) in stream

double pf = StrPf(integer stream, integer phase)
given a stream and phase position in range 1- getPNr() returns the phase fraction

double w = getW(integer stream, integer phase, integer pos.)
given a stream, the phase position and component’s position (in component’s list) returns the component molar fraction in that phase

double Zi= getZ(integer stream, integer pos.)
given a stream and component’s position (in component’s list) returns the comp’s Z (weight percentage, molar basis)

integer res = putZ(integer stream, integer pos., double Zi)
given a stream, comp’s position and Z , sets the comp’s pos. in Z vector (composition, molar basis) for that stream

integer nr = getCNr(integer stream)
given a stream returns the number of components defined in that stream

integer nr = getMCNr()
returns the maximum number of components in a stream

double zv = StrZv(integer stream)
given a stream returns the relevant compressibility factor (gas phase)

double mw = StrMw(integer stream)
given a stream returns the averaged molecular weight (all phases)

double v = StrV(integer stream)
given a stream returns the specific volume as sum of specific volumes of all phases

double mw = StrGMw(integer stream)
given a stream returns the averaged molecular weight (gas phase)

double mw = StrLMw(integer stream)
given a stream returns the averaged molecular weight (liquid phase)

double h = StrH(integer stream)
given a stream returns the total (stream) enthalpy (gas + liquid + solid phases)

double h = StrGH(integer stream)
given a stream returns the total (stream) enthalpy (gas phase)

double h = StrSGH(integer stream)
given a stream returns the specific (unit weight) enthalpy (gas phase)

double h = StrLH(integer stream)
given a stream returns the total (stream) enthalpy (liquid phase)

double h = StrSLH(integer stream)
given a stream returns the specific (unit weight) enthalpy (liquid phase)

double h = StrSH(integer stream)
given a stream returns the total (stream) enthalpy (solid phase)

double h = StrSSH(integer stream)
given a stream returns the specific (unit weight) enthalpy (solid phase)

double cp = StrGICp(integer stream)
given a stream returns the ideal gas heat capacity

double cp = StrGCp(integer stream)
given a stream returns the specific heat capacity (constant pressure, gas phase)

double cv = StrGCv(integer stream)
given a stream returns the specific heat capacity (constant volume, gas phase)

double cp = StrLCp(integer stream)
given a stream returns the specific heat capacity (constant pressure, liquid phase)

double cv = StrLCv(integer stream)
given a stream returns the specific heat capacity (constant volume, liquid phase)

double cp = StrSCp(integer stream)
given a stream returns the specific heat capacity (constant pressure, solid phase)

double ss = StrMSS(integer stream)
given a stream returns the speed of sound (gas, liquid) as calculated with HEM model for mixed phases

double ss = StrGSS(integer stream)
given a stream returns the speed of sound in gas phase

double ss = StrLSS(integer stream)
given a stream returns the speed of sound in liquid phase

double jt = StrGJT(integer stream)
given a stream returns the Joule Thomson coefficient in gas phase

double jt = StrLJT(integer stream)
given a stream returns the Joule Thomson coefficient in liquid phase

double ic = StrGIC(integer stream)
given a stream returns the isothermal compressibility coefficient - (1 / V) * dV / dP in gas phase

double ic = StrLIC(integer stream)
given a stream returns the isothermal compressibility coefficient - (1 / V) * dV / dP in liquid phase

double v = StrGVE(integer stream)
given a stream returns the volumetric expansivity coefficient - (1 / V) * dV / dT in gas phase

double ic = StrLVE(integer stream)
given a stream returns the volumetric expansivity coefficient - (1 / V) * dV / dT in liquid phase

double s = StrGS(integer stream)
given a stream returns the total (stream) entropy (gas phase)

double s = StrSGS(integer stream)
given a stream returns the specific (unit weight) entropy (gas phase)

double s = StrLS(integer stream)
given a stream returns the total (stream) entropy (liquid phase)

double s = StrSS(integer stream)
given a stream returns the total (stream) entropy (solid phase)

double s = StrSLS(integer stream)
given a stream returns the specific (unit weight) entropy (liquid phase)

double s = StrSSS(integer stream)
given a stream returns the specific (unit weight) entropy (solid phase)

double s = StrS(integer stream)
given a stream returns the total (stream) entropy (gas + liquid + solid phases)

integer res = setWm(integer stream, double W)
given a stream and flow (mass basis), sets the flow

double w = getWm(integer stream)
given a stream returns the flow specified for that stream.

double hc = StrHC(integer stream)
given a stream returns the calculated net heat of combustion (gas phase).

double fl = StrFML(integer stream)
given a stream returns the calculated flammability lean limit (gas phase).

double fl = StrFMH(integer stream)
given a stream returns the calculated flammability rich limit (gas phase).

double d = StrLD(integer stream)
given a stream returns the calculated liquid density (at operating conditions).

double d = StrGD(integer stream)
given a stream returns the calculated gas density (at operating conditions).

double tc = StrLC(integer stream)
given a stream returns the calculated liquid thermal conductivity (at operating conditions).

double tc = StrGC(integer stream)
given a stream returns the calculated gas thermal conductivity (at operating conditions).

double v = StrLV(integer stream)
given a stream returns the calculated liquid viscosity (at operating conditions).

double v = StrGV(stream)
given a stream returns thecalculated gas viscosity (at operating conditions).

double st = StrST(integer stream)
given a stream returns the calculated surface tension (at operating conditions).

Integer cpnr = StrCPnr(integer stream)
given a stream returns the number of critical points detected and calculated, to get a critical point use the methods StrPc() and
StrTc() setting value of pos in the range 1-cpnr

double p = StrPc(integer stream, Integer pos)
given a stream and the critical point position in the list (see method StrCPnr()) returns the critical pressure

double t = StrTc(integer stream, Integer pos)
given a stream and the critical point position in the list (see method StrCPnr()) returns the critical temperature.

double p= StrCBp(integer stream)
given a stream returns the cricodenBar pressure.

double t= StrCBt(integer stream)
given a stream returns the cricodenBar temperature.

double p= StrCTp(integer stream)
given a stream returns the cricodenTherm pressure.

double t= StrCTt(integer stream)
given a stream returns the cricodenTherm temperature.

double ac = StrAc(integer stream)
given a stream returns the acentric factor (mole fraction average).

Methods for stream’ s definition

Prode Properties includes a set of functions to define a stream by program (as alternative to utilize the Properties Editor) typical application

- call initS()
- define the list of components with putCC()
- define the mole fraction of each component with putZ()
- call setS() to define the stream
- utilize the methods described in paragraph “Methods to define thermodynamic models” to define the models
- call setW() to define the flow
- call loadSB() to load the BIPs from database
- as alternative to define specific BIPs utilize the methods PutCi(), PutCj(), PutMB(), PutBIP()

integer res = initS (integer stream)
given a stream initializes all data for successive data transfer operations. This method must be called before restoring stream’s data from archives (files etc.)

integer res = putCC (integer stream, integer pos, integer compcode)
given a stream, component’s position (in component’s list) and component code sets the code in component’s list.

integer res = putZ(integer stream, integer pos., double Zi)
given a stream, comp’s position and Z , sets the comp’s pos. in Z vector (composition, molar basis) for that stream

integer res = setS(integer stream)
given a stream performs a sequence of validating operations on data. This method must be called after to have restored stream’s data from archives (files etc.)Methods to define a initial condition for a stream

nteger res = loadSB(integer stream, integer btype)
given a stream loads all BIP available in database. This method must be called after the stream has been defined since it requires the list of components. Codes for btype are 0 for VLE, 1 for LLE, 2 for SLE, 3 for Hydrates

double Zi= getZ(integer stream, integer pos.)
given a stream and component’s position (in component’s list) returns the comp’s Z (molar fraction)

integer cc = getCC(integer stream, integer pos)
given a stream and component’s position (in component’s list) returns the component code (a integer that identifies the component in chemical’s file).

integer nr = getMBPNr()
returns the maximum number of (interaction coefficients) binary pairs in a stream

int ci = getCi(integer stream, integer pos)
given a stream and position (in interaction’s coeff. list) returns the first component reference (a integer that identifies the component in component’s list).

integer res = PutCi (integer stream, integer pos, integer ci)
given a stream, position (in interaction coefficients list) and first component reference sets the component’s reference in interaction coefficient’s list.

int cj = getCj(integer stream, integer pos)
given a stream and position (in interaction’s coeff. list) returns the second component reference (an integer that identifies the component in component’s list).

integer res = PutCj (integer stream, integer pos, integer cj)
given a stream, position (in interaction coefficients list) and second component reference sets the component’s reference in interaction coefficient’s list.

int model = getMB(integer stream, integer pos)
given a stream and position (in interaction’s coeff. list) returns the related model (an integer that identifies the model).

integer res = PutMB(integer stream, integer pos, integer model)
given a stream, position (in interaction coefficients list) and a model identifier sets the model in interaction coefficient’s list.

double BIP = getBIP(integer stream, integer pos, integer id)
given a stream, position (in binary coeff. list) and BIP identifier (0-max nr. of BIPs for that model) returns BIP.

integer res = PutBIP(integer stream, integer pos, integer id. double Kji)
given a stream, position (in binary coeff. list) BIP identifier (0-max nr. of BIPs for that model) and value stores BIP in that position of the list.

Methods to define stream’s operating conditions

Prode Properties includes a set of functions to define the intial (operating) condition of a stream, these can be utilized as alternative to the standard initialization via setOp() method
typical application

- call rstValidSop()
- define compostion in phase 1 with putW()
- define phase fraction with putPF()
- define phase type with putPT()
- set phase 1 as valid , setValidPhase()
- continue with another phase (2...n)
- define temperature with putT()
- define pressure with putP()
- set conditions as valid with setValidSop()

integer result = rstValidSop(integer stream)
Given a stream clears the compostions of different phases at operating conditions

integer result = setValidSop(integer stream)
Given a stream sets the compostions of different phases at operating conditions.as valid.

integer result = setValidPhase(integer stream, integer phase)
Given a stream and phase sets the phase compostion.as valid.

integer result = putW(integer stream, integer phase, int compnr, double w)
Given a stream, phase, component number and component’s molar fraction in that phase stores the value

integer result = putPF(integer stream, integer phase, double fraction)
Given a stream, phase and phase fraction stores the phase .fraction value

integer result = putPT(integer stream, integer phase, int type)
Given a stream, phase and phase type (vapor,liquid,solid) stores the phase type

nteger result = putT(integer stream, double t)
Given a stream and operating temperature stores the value

nteger result = putP(integer stream, double p)
Given a stream and operating pressure stores the value

Copy of streams

to make a copy of a stream utilize the method

integer res = StrCopy(integer stream1, integer stream2)
Given two streams (stream1 and stream2) copies the stream 2 into stream 1

Methods for solving staged columns

Note : this method utilizes the standard ANSI C convention for exchanging parameters (see the samples provided with the software)

Properties includes a procedure for solving staged columns, the column is modeled with stgnr equilibrium stages, column may include a condenser and a rebolier, stage numbering is bottom up, the bottom stage (reboiler, if specified) is number one and the top stage (condenser, if specified) is number stgnr
There may be one or more feeds, a feed is modeled by entering liquid on the specified stage and vapor portion to the stage above (with exception of top stage).
There may be one or more side streams
Heat added/removed on each stage can be specified
Efficiency parameter on each stage can be specified

```
integer res = DCOL(int csep, int stgnr, int init, double *stgt,double *stgp,double *stgef,double *stgdH,
                   int prod_h, int btm_h,int fnr,int *fstr,int *fpos,int snr,int *sstr,int *spos,int *sft,
                    double *sflow,int vnr,double *vrv,int *vtype,int *ptype,int *piv,double *prv,
                    double*flows)
```

Parameters :

csep	(int)	column type : 1 VLE , 2 VLLE , 3 LLE (some features available in extended versions)
stgnr	(int)	number of stages
init	(int)	0 for automatic initialization, 1 temperatures and flows are defined by user
stgt	(double*)	vector (stgnr) with stage temperatures
stgp	(double*)	vector (stgnr) with specified stage pressures
stgef	(double*)	vector (stgnr) with specified stage efficiency, permitted range 0,1-1
stgdH	(double*)	vector (stgnr) with specified dH (heat added, removed)
prod_h	(int)	stream for top product/distillate
btm_h	(int)	stream for bottom product
fnr	(int)	number of feeds
fstr	(int*)	vector (fnr) with the feeding streams
fpos	(int*)	vector (fnr) with feeds positions 1-stgnr
snr	(int)	number of side streams
sstr	(int*)	vector (snr) with the list of side streams
spos	(int*)	vector (snr) with side streams positions (1-stgnr)
sft	(int*)	vector (snr) with specified flow type (GAS_PHASE, LIQ_PHASE, see Codes used in Prode library)
sflow	(double*)	vector (snr) with the specified (on each side stream) side product to feed flow ratio
vnr	(int)	number of variables to solve
vtype	(int*)	vector (vnr) with type of variable (seebelow)
vrv	(double*)	vector (vnr) with calculated values for variable
ptype	(int*)	vector (pnr) with type of specification (see below)
piv	(int*)	vector (pnr) with integer values as the position of components in the list
prv	(double*)	vector (pnr) with values of the specifications to solve
flows	(double*)	vector with calculated values for vapor/liquid flows in all stages, dimension nrphases*nrc*stgnr when a condenser is present the reflux is the liquid flow on top stage

Codes for variables

reboiler	1
total condenser	2
partial condenser	3

Codes for specifications

reflux ratio	1
product to feed ratio (molar fract.)	2
bottom to feed ratio (molar fract.)	3
component (molar fract.) in top product	4
component (molar fract.) in bottom product	5
component recovery in top product	6
component recovery in bottom product	7

Notes :
When passing / returning paramenters the first element in vectors is the element 0
Main variables (1-vnr) are (when specified) reboiler and condenser (partial or total), each variable (of type defined in vtype) requires a suitable specification (in ptype, piv, prv), usually for reboiler the specification is the product to feed ratio and for a condenser the reflux ratio, but specifications based on component's fractions on top and bottom products are permitted, in these cases specify in piv the position of selected component in the list and in prv the value of the fraction required
Secondary variables are side streams (1-snr), each side stream (defined in sstr, spos) requires (in sflow) a specification for the side product to (total) feed flow ratio.

The column is modeled with thermodynamics and options defined for the first feed in the list.

Initialization

in most cases the procedure doesn't require to initialize values, when required set the variable init to 1 and define the proper initial values in vectors stgt and flows, note that in a sequence of similar operations (for example when controlling the operating point of a column) it may result useful to reintroduce the calculated values as starting point for the new calculus

Examples

Column with 8 stages, 1 feed (stage 4), pressure reboiler 12.5 Bar, pressure top 12 Bar, efficiency 1, dH = 0

```
csep            = 1
stgnr           = 8
init            = 0
stgp[0]         = 12.5
......
stgp[7]         = 12
stgef[0]        = 1
......
stgef[7]        = 1
stgdH[0]        = 0
......
stgdH[7]        = 0
prod_h          = stream1
btm_h           = stream2
fnr             = 1
fstr            = stream3
fpos            = 4

variables       : reboiler and  total condenser
specifications  : component 2 fraction in top product and bottom product to to feed ratio

vnr             = 2
vtype[0]        = 1
ptype[0]        = 4
piv[0]          = 2
prv[0]          = 0.96
vtype[1]        = 2
ptype[1]        = 3
piv[1]          = 0
prv[1]          = 0.4


variables       : reboiler , partial  condenser and 2 side streams (liquid and gas phases)
specifications  : component 2 fraction in top product ,  bottom product to feed ratio, side streams flow to feed ratio

vnr             = 2
vtype[0]        = 1
ptype[0]        = 4
piv[0]          = 2
prv[0]          = 0.96
vtype[1]        = 3
ptype[1]        = 3
piv[1]          = 0
prv[1]          = 0.4

snr             = 2
sstr[0]         = stream4
spos[0]         = 4
sft[0]          = LIQ_PHASE
sflow[0]        = 0.12
sstr[1]         = stream5
spos[1]         = 7
sft[1]          = GAS_PHASE
sflow[1]        =  0.078
```

Methods for Reactors

Note : this method utilizes the standard ANSI C convention for exchanging parameters (see the samples provided with the software)

simulation of reactors

int res = REACT(int streamIn, streamOut, int model, int NrReactions, double **Conv, double Pout, double dHeat)

Parameters :

streamIn	(int)	inlet stream
streamOut	(int)	outlet stream
model	(int)	model for reactor (see below)
NrReactions	(int)	number of reactions
Conv	(double**)	matrix (NrComponents, NrReactions) to specify reactions
Pout	(double)	output pressure
dHeat	(double)	heat added, removed

Codes for models

Gibbs	1
Equilibrium Reactor	2
additional models on request	

Methods for fluid flow problems

simulation of single phase, two-phases, multiphase flow on circular pipes

int res = PIPE(int stream, int model, double diam, double rough, double length, double dHeight, double dHeat)

Parameters :

stream (int)	inlet stream
model (int)	model for fluid flow and phase equilibria (see below)
diam (double)	pipe internal diameter
rough (double)	parameter defining relative pipe roughness
length (double)	lenght of this segment
dHeight (double)	height difference (inlet, outlet)
dHeat (double)	heat added, removed

Codes for models

Beggs & Brill / Hazen-Williams / AGA	1
additional models on request	

Methods for Hydrates phase equilibria

methods for calculating hydrate formation pressure (or temperature)

double p = HPFORM(int stream, double t, int method)
double t = HTFORM(int stream, double p, int method)

Parameters :

stream (int)	inlet stream
t (double)	operating temperature (or operating pressure)
method (int)	1 = include SI , SII , SH
	2 = SI
	3 = SII

Methods for solving a Polytropic operation

Polytropic stage (compression and expansion)

double val = PSPF(int stream, double pout, int model, double param)

Parameters :

stream (int)	inlet stream
pout (double)	outlet pressure
model (int)	model, see below codes 1-4
param (double)	for model 1 and 3 specified polytropic efficiency (range 0-1)
	for model 2 and 4 (measured) outlet temperature

the procedure can model compression and expansion units such as centrifugal compressors, expansion turbines etc.
the procedure returns

-calculated temperature	options 1,3
-calculated efficiency	options 2,4

models available (**)

1 given initial condition, pout and polytropic efficiency calculates outlet condition,
R.A. Huntington “Evaluation of Polytropic calculation Methods for Turbomachinery Performance”,
method applicable to gas phase only

2 given initial condition, pout and tout calculates polytropic efficiency,
R.A. Huntington “Evaluation of Polytropic calculation Methods for Turbomachinery Performance”,
method applicable to gas phase only

3 given initial condition, pout and polytropic efficiency calculates outlet condition
R.Paron “Polytropic solution with phase equilibria”
method applicable to gas and mixed (gas + liquid) phases

4 given initial condition, pout and tout calculates polytropic efficiency,
R.Paron “Polytropic solution with phase equilibria”
method applicable to gas and mixed (gas + liquid) phases

(**) additional models available from Prode

Methods for relief valves design / rating

This unit models a relief valve with different methods

double area = ISPF(int stream, double pout, int model, double *param)

Parameters :

stream (int)	inlet stream
pout (double)	outlet pressure
model (int)	model, see below codes 1-4
param(double)	correction parameter, see below the range of values

the procedure models a relief valve at specified operating conditions and returns the calculated area

models available   (**)

1	HEM Homogeneous Equilibrium (Solution of Mass Flux integral)
2	HNE Homogeneous Non-equilibrium (HEM with Boling Delay and Gas-Liquid Slip Contributes)
3	HNE-DS , Homogeneous Non-equilibrium
4	NHNE Non-homogeneous Non-equilibrium

model	recommended range of values for correction parameter
HEM	not required
HNE	0.7-0.8 for safety valves
HNE-DS	see the paper
NHNE	0.7-0.8 for safety valves

(**) additional models available from Prode

Methods for calculating equilibrium lines in phase diagrams

Note : these methods utilize the standard ANSI C convention for exchanging parameters, the distribution includes samples to show how to utilize these methods in different languages

Prode Properties includes methods for calculating different types of phase diagrams
vapor-liquid
vapor-liquid-liquid
vapor-liquid-solid (**)

(**) feature available in extended versions

typical application

- define the stream, set the required phase equilibria (vapor-liquid, vapor-liquid-liquid, vapor-liquid-solid)
- call PELnr() to calculate the phase diagram and obtain the number of lines available
- on each line call PELP(), PELT(), PELine() to obtain the data for the different lines
- if required call PFLine() to calculate a line with specified phase fraction ad state

integer lnr = PELnr(integer stream)
Given a stream calculates the phase diagram and returns the number of equilibrium lines available

integer lnr = PELT(integer stream, integer line)
Given a stream and the line, returns the line type (see below)

1 = bubble line
2 = dew line
3 = three phase line

integer lnr = PELP(integer stream, integer line)
Given a stream and the line, returns the line property (see below)

1 = vapor-liquid
2 = vapor-liquid-liquid
3 = vapor-solid
4 = liquid-solid

integer nrpt =PELine(integer stream, integer line, double *P, double *T, int maxpt)
Given a stream, the line and two arrays (0 -maxpt elements) the procedure returns nrpt < maxpt equilibrium points in specified line

integer nrpt =PVLine(integer stream, integer line, double *P, double *T, double *H, double *S,double *V,int maxpt)
Given a stream, the line and five arrays (0 -maxpt elements) the procedure returns nrpt < maxpt equilibrium points in specified line,
in additions to t,p values this method returns enthalpy, entropy and volume values calculated at equilibrium points

this method allows to calculate a line with specified phase fraction in specified state (gas,liquid,solid)

integer nrpt =PFLine(integer stream,int line, double pf, double *P, double *T, int maxpt)
Given a stream, the line, a specified phase fraction and two arrays (0-maxpt elements) the procedure returns nrpt < maxpt equilibrium points in specified phase fraction line

Methods for direct access to properties (F,H,S,V) and derivatives (T,P,W)

Prode Properties includes methods for fast access to the procedures for calculating thermodynamic properties, to access these methods create one or more processes with method DPinit() passing a integer as process code (permitted range of values 1..5) to identify each process and a stream (caution: must define the stream, i.e. the list of components and molar fractions, before to call DPinit), then call in sequence the methods for calculating thermodynamic properties passing as first parameter the process code, the methods will return the properties calculated for the stream associated with that specific process.
Note: Base version allows to define up to 5 iindependent processes

example of application
DPinit(1,stream);
StrHv(1,0,t ,p,X,&HL);
StrHv(1,1,t ,p,Y,&HV);

integer res = DPinit(integer process,integer stream)
Given a process (code 1-5) and a stream the method loads all data

integer res = StrFv(integer process,integer state,double t ,double p, double *w,double *fg)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the vector of fugacities (Pa)

integer res = StrFvd(integer process,integer state,double t ,double p, double *w,double *fg, double *dfgt, double *dfgp, double **dfgw)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the vector of fugacities (Pa) and related derivatives vs. temperature (K), pressure (Pa), composition (note : derivatives vs. composition as matrix [n][m])

integer res = StrFvdv(integer process,integer state,double t ,double p, double *w,double *fg, double *dfgt, double *dfgp, double *dfgw)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the vector of fugacities (Pa) and related derivatives vs. temperature (K), pressure (Pa), composition (note : derivatives vs. composition as vector [n*m])

integer res = StrHv(integer process, integer state,double t ,double p, double *w,double *H)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the molar enthalpy (Kj/Kmol)

integer res = StrHvd(integer process,integer state,double t ,double p, double *w,double *H, double *dHt, double *dHp, double *dHw)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the molar enthalpy (Kj/Kmol) and related derivatives vs. temperature, pressure, composition

integer res = StrSv(integer process,integer state,double t ,double p, double *w,double *S)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the molar entropy (Kj/Kmol-K)

integer res = StrSvd(integer process,integer state,double t ,double p, double *w,double *S, double *dSt, double *dSp, double *dSw)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the molar entropy (Kj/Kmol-K) and related derivatives vs. temperature, pressure, composition

integer res = StrVv(integer process,integer state,double t ,double p, double *w,double *V)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the molar volume (M3/Kmol)

integer res = StrVvd(integer process,integer state,double t ,double p, double *w,double *V, double *dVt, double *dVp, double *dVw)
Given a predefined stream the required state (vapor, liquid, solid)) and operating conditions returns the molar volume (M3/Kmol) and related derivatives vs. temperature, pressure, compositionMethods for stream’ s data access

Extended methods for accessing stream’s properties

These functions (which are otherways equivalent to standard methods) permit in addition to set the operating conditions at which the required property must be evaluated. This may result useful in many cases, for example when utilizing Prode Properties methods as macros from Excel cells. Caution : the isothermal flash will reset any previous settings and you should use with care these methods in sequential calculus.

double mw = EStrGMw(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the molecular weight for gas phase

double mw = EStrLMw(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the molecular weight for liquid phase

double lf = EStrLf(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns liquid fraction (molar basis) in stream

double pf = EStrPf(integer stream, integer state, double t, double p)
given a stream , state (gas, liquid, solid) pressure and temperature performs an isothermal flash and returns the phase fraction (molar basis) in specified state

double zv = EStrZv(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the relevant compressibility factor (gas phase)

double h = EStrH(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the enthalpy (gas + liquid phase)

double v = EStrV(integer stream, double t, double p)
given a stream, pressure and temperature performs an isothermal flash and returns the specific volume as sum of specific volumes of all phases

double cp = EStrGCp(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the specific heat capacity (constant pressure, gas phase)

double cv = EStrGCv(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the specific heat capacity (constant volume, gas phase)

double cp = EStrLCp(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the specific heat capacity (constant pressure, liquid phase)

double cv = EStrLCv(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the specific heat capacity (constant volume, liquid phase)

double c = EStrGIC(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the isothermal compressibility in gas phase

double c = EStrLIC(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the the isothermal compressibility in liquid phase

double ss = StrMSS(integer stream, double t, double p)
given the stream pressure and temperature performs an isothermal flash and returns returns the speed of sound (gas, liquid) as calculated with HEM model for mixed phases

double ss = EStrGSS(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the speed of sound in gas phase

double ss = EStrLSS(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the speed of sound in liquid phase

double jt = EStrGJT(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the Joule Thomson coefficient for gas phase

double jt = EStrLJT(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the Joule Thomson coefficient for liquid phase

double ic = EStrGIC(integer stream double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the isothermal compressibility coefficient - (1 / V) * dV / dP in gas phase

double ic = EStrLIC(integer stream double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the isothermal compressibility coefficient - (1 / V) * dV / dP in liquid phase

double v = EStrGVE(integer stream double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the volumetric expansivity coefficient - (1 / V) * dV / dT in gas phase

double v = EStrLVE(integer stream double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the volumetric expansivity coefficient - (1 / V) * dV / dT in liquid phase

double hc = EStrHC(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the net heat of combustion (gas phase).

double fl = EStrFML(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the flammability lean limit (gas phase).

double fl = EStrFMH(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the flammability rich limit (gas phase).

double s = EStrS(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the relative entropy (gas + liquid phase)

double d = EStrLD(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the calculated liquid density (at operating conditions).

double d = EStrGD(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the calculated gas density (at operating conditions).

double tc = EStrLC(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the calculated liquid thermal conductivity (at operating conditions).

double tc = EStrGC(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the calculated gas thermal conductivity (at operating conditions).

double v = EStrLV(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the r calculated liquid viscosity (at operating conditions).

double v = EStrGV(stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the calculated gas viscosity (at operating conditions).

double st = EStrST(integer stream, double t, double p)
given the stream, pressure and temperature performs an isothermal flash and returns the calculated surface tension (at operating conditions).

Methods for chemical's file access

Prode Properties includes a set of functions for chemical data file access. Components are referenced via a component code which is an integer with value in the range 1 to getFCNR()

Integer nr = getFCNr()
returns the number of components in Chemical's File

VARIANT str = MCompF(integer code)
given the component code returns the relevant component formula (eventually truncated to string maximum lenght) , this is the Microsoft specific method

char *str = CompF(integer code)
given the component code returns the relevant component formula (eventually truncated to string maximum length) , this is the ANSI C compatible method

VARIANT str = MCompN(integer code)
given the component code returns the relevant component name (eventually truncated to string maximum length) , this is the Microsoft specific method

char *str = CompN(integer code)
given the component code returns the relevant component name (eventually truncated to string maximum length) , this is the ANSI C compatible method

int id = CompID(integer code)
given the component code returns component's ID (it's the CAS number)

int cc = CompCID(integer id)
given the component ID returns the component's code

double mw = CompMw(integer code)
given the component code returns the relevant molecular weight

double tc = CompTc(integer code)
given the component code returns the relevant critical temperature

double ac = CompAc(integer code)
given the component code returns the relevant acentric factor

double vc = CompVc(integer code)
given the component code returns the relevant critical volume

double pc = CompPc(integer code)
given the component code returns the relevant critical pressure

double dm = CompDm(integer code)
given the component code returns the dipole moment

double rg = CompRg(integer code)
given the component code returns the radius of gyration

double sol = CompSol(integer code)
given the component code returns the solubility parameter

double hf = CompHf(integer code)
given the component code returns the std. enthalpy of formation

double gf = CompGf(integer code)
given the component code returns the Gibbs energy of formation

double sf = CompSf(integer code)
given the component code returns the enthalpy of fusion

double nb = CompNb(integer code)
given the component code returns the normal boiling point

double mp = CompMp(integer code)
given the component code returns the melting point

double p = CompVP(integer code, double t)
given the component code and a temperature, returns the calculated saturation pressure (calculated via Chemical’s file temperature dependent correlation)

double h = CompHG(integer code, double t0, double t1)
given the component code , initial and final temperatures for integration, returns the calculated ideal gas enthalpy (calculated via Chemical’s file temperature dependent correlation)

double s = CompSG(integer code, double t0, double t1)
given the component code , initial and final temperatures for integration, returns the calculated ideal gas entropy (calculated via Chemical’s file temperature dependent correlation)

double h = CompHL(integer code, double t0, double t1)
given the component code , initial and final temperatures for integration, returns the calculated ideal liquid enthalpy (calculated via Chemical’s file temperature dependent correlation)

double s = CompSL(integer code, double t0, double t1)
given the component code , initial and final temperatures for integration, returns the calculated ideal liquid entropy (calculated via Chemical’s file temperature dependent correlation)

double h = CompHS(integer code, double t0, double t1)
given the component code , initial and final temperatures for integration, returns the calculated ideal solid enthalpy (calculated via Chemical’s file temperature dependent correlation)

double s = CompSS(integer code, double t0, double t1)
given the component code , initial and final temperatures for integration, returns the calculated ideal solid entropy (calculated via Chemical’s file temperature dependent correlation)

double h = CompHV(integer code, double t)
given the component code and a temperature, returns the calculated latent heat (calculated via Chemical’s file temperature dependent correlation)

double v = CompLV(integer code, double t)
given the component code and a temperature, returns the calculated liquid viscosity (calculated via Chemical’s file temperature dependent correlation)

double v = CompGV(integer code, double t)
given the component code and a temperature, returns the calculated gas viscosity (calculated via Chemical’s file temperature dependent correlation)

double d = CompLD(integer code, double t)
given the component code and a temperature, returns the calculated liquid density (calculated via Chemical’s file temperature dependent correlation)

double tc = CompLC(integer code, double t)
given the component code and a temperature, returns the calculated liquid (thermal) conductivity (calculated via Chemical’s file temperature dependent correlation)

double tc = CompGC(integer code, double t)
given the component code and a temperature, returns the calculated gas (thermal) conductivity (calculated via Chemical’s file temperature dependent correlation)

double st = CompST (integer code, double t)
given the component code and a temperature, returns the calculated surface tension (calculated via Chemical’s file temperature dependent correlation)

double d = CompSD(integer code, double t)
given the component code and a temperature, returns the calculated solid density (calculated via Chemical’s file temperature dependent correlation)

double tc = CompSC(integer code, double t)
given the component code and a temperature, returns the calculated solid (thermal) conductivity (calculated via Chemical’s file temperature dependent correlation)

Methods to set / access different options

To set / access the different options available in Prode Properties the library includes two methods, getOM() and setOM(), these methods accept / return a 32 bit integer, each bit in the integer represents a different option, see below a short list of the most important options available.

int om = getOM(integer stream)
given a stream returns a code (integer) which defines the settings

integer res = setOM (integer stream, integer option)
given a stream and model code sets the options.

Codes used in Prode library

Table of codes to specify the different options

reference : methods getOM(), setOM() ...

Caution! The codes may change in different versions.

Bit	Decimal value	Option
1	1	set multiphase vapor + liquid
2	2	set multiphase vapor + liquid + solid
3	4	set multiphase vapor + liquid + solid + hydrate
4	8	reduce the number of trial phases (in multiphase)
5	16	use iso compressibility coeff. to detect single phase state
6	32	evaluate stability of each phase in equilibrium
7	64	end specified phase fraction lines when crossing phase boundary lines
8	128	includeall hydrate structures (also those not normally generated by formers)

to set one or more options call setOM() passing as value a integer with the sum (decimal values) of all required options.

Table of codes to specify the different states

reference : methods setMP() , PfTF() , PfTF() , StrFv(), StrFvd() ...

Code	State
0	Vapor phase
1	Liquid phase
2	Solid phase
3	Hydrate phase

Table of codes to specify the different models

reference : methods setMP(), getMP() ...

Caution! Some models may not be available and/or the codes may change in different versions (contact Prode for details).

Code	**Model**
1	Regular
11	Pitzer
21	Hayden-O'Connell
31	Wilson
32	NRTL
33	Uniquac
40	Unifac
50	Soave-Redlich_Kwong (VDW)
51	Soave-Redlich_Kwong Extended (VDW)
60	Peng Robinson (VDW)
61	Peng Robinson Extended (VDW)
62	Peng Robinson-Wilson (WS)
63	Peng Robinson-UNIQUAC (WS)
64	Peng Robinson-NRTL (WS)
65	Peng Robinson-UNIFAC (WS)
66	Peng Robinson-Wilson (MHV2)
67	Peng Robinson-UNIQUAC (MHV2)
68	Peng Robinson-NRTL (MHV2)
69	Peng Robinson-NRTL (LCVM)
70	BWR
71	BWRS
75	Lee Kesler
76	Lee Kesler (Plocker)
80	Solid Pure (based on Peng Robinson Extended)
81	Solid Pure (based on CPA-Peng-Robinson)
82	Solid Pure Regular (solid pressure)
83	Solid Solution (based on Peng Robinson Extended)
85	Hydrate (based on CPA-Peng-Robinson)
86	Hydrate (based on Peng Robinson Extended)
87	Hydrate (based on CPA-Electrolyte)
90	PC SAFT
95	CPA-Soave-Redlich-Kwong
96	CPA-Peng-Robinson
97	CPA-Electrolyte
100	Steam tables (IAPWS 1995)
101	GERG (ISO 18453)
102	GERG (2008)
105	AGA (ISO 20765)
111	COSTALD
112	VT PR

Methods to define thermodynamic models

To define or retrieve the thermodynamic models associated with a stream the library includes several methods setKM() works with predefined packages while setMP(), getMP() allow to define specific models on each property (Fg, H, S,V..).

integer res = setKM (integer stream, integer Kcode)
given a stream and the code for the predefined package (contact Prode for the list of predefined packages available in different versions) sets the package.

integer res = setMP(integer stream, integer mp, integer model, integer state)
given a stream, property (Fg,H,S..) model and state (Vapor,Liquid,Solid,Hydrate) this method sets the specified model for that property and returns TRUE in case of success, otherwise returns FALSE

integer m = getMP(integer stream, integer mp, integer state)
given a stream, related property (Fg,H,S..) and state (Vapor,Liquid,Solid,Hydrate) this method returns the specified model for that property and state

<u>Table of codes to specify the different properties in setMP() and getMP()</u>

reference : methods setMP(), getMP() ...

Code	**Property**
1	Fugacity
2	Enthalpy
3	Entropy
4	Volume
5	Viscosity
...	(additional properties available in extended versions)

Methods to define base values for Enthalpy and Entropy

The library allows to define the base values (the temperature and initial value from which to start integration) for entropy and enthalpy from Properties Editor, in setting's page, these values are stored in archive and restored when program starts.
In addition it is possible to modify these value by code with the following methods,

integer res = setHB(integer mod, double t, double val)
given a code to identify the procedure (see the table with codes), the temperature and initial value sets base value for enthalpy .

integer res = setSB(integer mod, double t, double val)
given a code to identify the procedure (see the table with codes), the temperature and initial value sets base value for entropy .

<u>Table of codes to specify the different base values in setHB() and setSB()</u>

reference : methods setHB(), setSB() ...

Code	**Procedure**
1	initial values specified by user (values of t and val)
2	initial values are enthalpy of formation (or entropy of formation) and temperature 25 C

Methods to set / access stream’s names

In Prode Properties streams have several properties including a label (name) which could match (for example) the name of a line in your project, you can easily set / access these labels through a series of methods.

VARIANT str = MStrN(integer stream)
given a integer (that identifies a stream) method returns a string identifying that stream   this is the Microsoft specific method

char *str = StrN(integer stream)
given a integer (that identifies a stream) method returns as ANSI C type the string identifying that stream.

integer res = putN(integer stream, char *str)
given a integer (that identifies a stream) and a ANSI C string identifying that stream this method sets the label.

Methods to access Model’s data

Prode Properties includes models for calculating properties as fugacities, enthalpies, entropies, volumes, viscosities etc. these methods allow to access the models available

integer nr = getMDnr()
returns the number of models available in this version

char *str = getMDN(int model)
given the model position (in the range 1-number of models available) method returns as ANSI C type the string identifying that model.

integer res = getMDP(int model, int prop, int state)
given the model position (in the range 1-number of models available) the required property and state returns TRUE if model can calculate the specified property, otherwise returns FALSE

integer code = getMDC(int model)
given the model position (in the range 1-number of models available) returns the code of the model

Methods to control error’s messages

PROPERTIES includes a set of functions to control the error messages. By default PROPERTIES produces an error message via a Microsoft Windows Dialog Box every time an error is discovered. This approach can slow down the process when a long sequence of errors occurs in an extended calculation sequence, such as an iterative convergence calculation. A better solution in that situation is to provide a status flag that can be interrogated and used by the users at convenient points in the sequence.

setErrFlag (integer state)
given a Boolean (state) sets the error flag to TRUE or FALSE. The flag should be cleared (state = FALSE) before each sequence of calculations and tested (method getErrFlag()) after the calcs. If this is done, then a flag state of TRUE indicates that an error has occurred somewhere in the calculation sequence).

integer res = getErrFlag ()
a value of TRUE means that an error has been found, please note that PROPERTIES doesn’t clear the error flag state, You should clear the error flag (via setErrFlag()) before each sequence of calc’s.

defErrMsg (integer state)
a value TRUE for variable state sets on the Microsoft Windows Dialog Box and a message will appear every time an error is discovered. A value FALSE sets off the dialog box (no messages of error).

VARIANT str = MErrMsg()
Returns the last error message generated, this is the Microsoft specific method

char *str = ErrMsg()
Returns the last error message generated, this is the ANSI C compatible method

Methods for accessing data-editing windows

Prode Properties includes two predefined methods for activating Properties editor

integer res = edS(nteger stream)
given a integer (that identifies a stream) method activates the Properties Editor on the specified stream

integer res = edSS()
this method activates the Properties Editor on first stream

Methods to load / save archives

Archives are files which contain a copy of the data used by Prode Properties to manage stream's and units of measurement, when you open an archive the stream's data and units are loaded, when you choose to save an archive these data are stored in a file. Archives are useful to create copies of your work otherways all data will be lost when leaving the application, Prode Properties includes methods for operations on archives.

integer res = AOpen()
open a file as archive (browse for file)

integer res = AFOpen(char *path)
open the file specified in *path as archive

integer res = ASave()
save a file as archive (browse for file)

integer res = AFSave(char *path)
save the file specified in *path as archive

Methods for accessing / defining the units of measurement

Prode Properties includes methods for accessing and defining the units of measurement, these methods utilize a numeric code for identifying the correspondent quantities, refer to the paragraph "Access via software to the units of measurement" for a list of these codes.

integer res = getUMC(integer UM)
given a integer (that identifies a quantity) method returns the selected UM for that quantity.

integer res = setUMC(integer UM, integer sel)
given two integers (the first identifies a quantity and the second the selection) method selects a UM for that quantity.

integer res = getUMN(integer UM)
given a integer (that identifies a quantity) method returns the number of different units of measurement available for that quantity.

VARIANT str = MgetUMS(integer UM, integer sel)
given two integers (the first identifies a quantity and the second the selection) method returns a string identifying the selected UM, this is the Microsoft specific method

char *str = getUMS(integer UM, integer sel)
given two integers (the first identifies a quantity and the second the selection) method returns as ANSI C type the string identifying the selected UM.

VARIANT str = MgetSUMS(integer UM)
given a integer UM for quantity this method returns a string identifying the selected UM, this is the Microsoft specific method

char *str = getSUMS(integer UM)
given a integer UM for quantity this method returns as ANSI C type the string identifying the selected UM.

double res = UMCR(double value, integer UM, integer SEL)
given a value, the code for quantity and selection converts to reference and returns the result

double res = UMCS(double value, integer UM, integer SEL)
given a value, the code for quantity and selection converts from reference and returns the result

integer res = UMAU(double a, double b, char *name, integer UM)
given the code for a quantity, the parameters a, b required for conversion and the name adds a new (user defined, temporary) unit.

integer res = UMRAU(integer UM)
given the code for a quantity removes all additional (temporary) units

Additional methods

double p = getPatm()
returns the internal reference (user defined) for atmosferic pressure quantity.

Application examples

We present here some notes about Prode Properties applications in form of FAQ that should assist users to easily extend features or add interfaces.

Tips on creation of Prode Properties applications

- Include a command (menu', button etc.) for accessing the Properties Editor (method edS(stream))
- Ensure that units of measurement are those defined in Prode Properties or include methods to set the units.
- Use isSDef() method to test a streams validity before accessing the stream. Accessing an undefined stream generates a large numbers of errors.
- Include functions for controlling error messages if you have extended calculation sequences. When managing error messages ensure that you test at the end of the calculation sequence to capture any problems that may have occurred.
- When debugging always attempt to limit the complexity of problems and expand progressively to the full application, retesting at intervals as you expand the scope of your problem.

User defined ID for accessing the components in chemical's file

In Prode Properties each component in chemical's file includes a ID which permits to access that component, this feature permits to maintain a unique identification number also when the chemical file changes. The ID must be a integer type, as default the CAS number has been adopted but the user may edit and change this value from theProperties Editor. The functions for accessing components in Prode Properties require the component code, this code may vary in different versions of chemical file, to convert the ID to the component code utilize the method CompCID() and CompID() to convert from code to ID

```
‘ this example shows how to access data
‘ with  ID code
Dim code As Long , ID As Long, Pc As Double
ID       = 74840               ‘ CAS code for Ethane (but the user may define his own list of values)
code   = CompCID(ID)      ‘ get the code
Pc  = CompPc(code)        ‘ and the critical pressure
```

How to define directly a stream (without accessing the Properties Editor)

Prode Properties includes methods to access (read and write) each different value in a stream, making it possible for the user to create procedure to define / edit / update directly each value without going through the Properties editor
Following list presents the methods for accessing all items

	read the value	**set the value**
• operating pressure,	getP()	setOp()
• operating temperature,	getT()	setOp()
• flow,	getW()	setW()
• vector [getMCNr() elements] with components codes	getCC()	putCC()
• vector [getMCNr() elements] Z vector, mole basis	getZ()	putZ()
• thermodynamic model (and related options)	getMP()	setMP()
• vector[getMBPNr() elements] of Ci	getCi()	putCi()
• vector[getMBPNr() elements] of Cj	getCj()	putCj()
• vector[getMBPNr() elements] of BIP matrix	getBIP()	putBIP()

When defining a stream one must follow these steps.

- call initS() method to clear all stream’s data
- definedata
- call setS() method to validate the data

The following example shows how to define a 2 components stream

```
Call initS(Stream)
Call setMP(Stream, Fg, SRK, 0)   ‘ see the paragraph “Codes used in Prode library”
Call setMP(Stream, Fg, SRK, 1)
..........................       ‘ define the models for all required properties and states
Call putZ(Stream, 1, z1)
Call putCC(Stream, 1, cc1)
Call putZ(Stream, 2, z2)
Call putCC(Stream, 2, cc2)
Call setS(Stream)                ‘ validates stream

Call setW(Stream, W)             ‘ flow

Call loadSB(Stream,0)                  ‘ load VLE BIPS from database
```

How to save and restore streams to / from a file

Archives are files which contain a copy of all compositions, operating conditions, units of measurement, settings etc. , archives are useful for creating copies of your work otherways all data will be lost when leaving the application.
The library includes methods to load and save archives , see the paragraph “Methods to load / save archives” for the list.

```
Call AOpen()                     ' open a file as archive (browse for file)

Call AFOpen(“e:/def.ppp”)        ' open the specified file as archive

Call ASave()                     ' save a file as archive (browse for file)

Call AFSave(“e:/def.ppp”)        ' save the specified file as archive
```

Error messages

PROPERTIES may generate the following error messages. For some of these, an action is suggested

Memory allocation error
A limit in resources allocation (close applications, release memory and restart)

Corrupted file, error reading data file
PROPERTIES cannot access a file, this may depend from the file not being in the proper directory or being corrupted, it is suggested that You reinstall PROPERTIES.

Internal error
This error may depend from several different conditions, the most common is a wrong parameter in a function (i.e. an attempt to pass a value out of permitted range). Check Your code.

too many local variables
too many variables
a limit in resources allocation (see above)

calc. on undefined stream data
an undefined stream found while executing calc's (edit and define the stream)

undefined stream' s operating conditions
pressure, temperature or flow are undefined (edit and define the stream)

error calling thermo calc. procedure
wrong input value (calcs cannot converge) or calcs outside temperature range (check chemical's file for limits in temperature correlation's).

cannot converge calc' s loop
A wrong convergence condition has been specified (i.e in an adiabatic flash calcs a thermal condition that cannot be reached by varying temperature, pressure or liquid fraction ; a parameter is outside range limits etc.)

T, P values outside H, S range calcs
A wrong condition has been specified and a parameter in enthalpy /entropy calcs is outside range limits

too many comp' s in a stream
when two or more streams are mixed the total nr. of components may exceed the maximum
some inconsistences in stream's data

error accessing component' s data archive
unavailable data (a unspecified component) or calc's outside temperature range.

Stack error (no memory), reload procedure
a limit in resources allocation (see above)

Method not available in this version
Attempt to define a method not available in that version, edit the stream and define a new method

A stream with Steam Tables model must have only 1 component
You should specify a stream with one component only in order to apply ASME Steam Tables model

Calculation basis

The user can specify which method to use selecting the models.
Please refer to the paragraph “reference literature” and “Models” for additional information about the methods.

Fugacity	calculated according selected model
Enthalpy	calculated according selected model
Entropy	calculated according selected model
Volume	calculated according selected model

Viscosity

gas
low pressure mixing rule according Wilke (1950) , operating conditions correction according Stiel and Thodos (1964).
liquid
logarithmic average mixing rule, pressure correction according Lucas (1981)

Thermal conductivity

gas
low pressure mixing rule according Mason and Saxena (1958), operating conditions correction according Stiel and Thodos (1964)
liquid
mixing rule according Li (1976)

Surface tension

mixing rule according MacLeod-Sugden

Heat of combustion

weight average mixing rule according ISO std. (database contains values in Kj/Kg)

Flammability limits

mixing rule according Le Chatelier as discussed by Coward & Jones (1952)

Limits in thermodynamic calc’s

Enthalpy, Entropy calc’s

In Prode Properties the user can specify different initial conditions for enthalpy and entropy, see the paragraph “Config settings” for additional details.

Temperature, pressure ranges

Temperature range	1 K - 5000 K
Pressure range	1 Pa – 1000 Bar

Chemical’s File format

Note : all data dependent correlation’s in chemicals file have a range of temperature for application, outside this range they may provide inconsistent results. Prode Properties checks for this range (as defined by high and low limits in chemicals file) and attempts to extend data when required (when operating conditions are outside the range of application of correlations), this may produce in some cases inconsistent results with simple models and properties which require differentiation, for example specific heat capacity.

Flexible data format

Prode Properties utilizes proprietary code which allows up to 30 correlations and custom units to define each temperature dependent property, all major standards including DIPPR and others are supported.

Chemical’ s data file

Prode Properties base version adopts the following format

```
Formula string 12 chars max
Name (1) (main list) string 40 chars max
Name (2) (user defined list) string 40 chars max
Name (3) (user defined list) string 40 chars max
Identification number (CAS as default)
Molecular weight
Critical temperature
Critical pressure
Critical volume
Acentric factor
Dipole Moment
Radius of Gyration
Solubility parameter
Standard enthalpy of formation (298 K)
Gibbs free energy of formation (298 K, 1 atm)
Normal boiling point
Enthalpy of fusion
Melting point
Flammability lean limit % (range 0-100)
Flammability rich limit % (range 0-100)
Autoignition temperature
Net heat of combustion

Gas heat capacity correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Vapor viscosity correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Vapor thermal conductivity correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Heat of vaporization correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)
```

```
Liquid vapor pressure correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Surface tension
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Liquid density correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Liquid viscosity correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Liquid thermal conductivity correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Liquid heat capacity correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Solid vapor pressure correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Solid density correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)
```

Solid thermal conductivity correlation
type of equation
unit for property
unit for temperature
low temperature limit
high temperature limit
A-E (5 parameters)

Solid heat capacity correlation
type of equation
unit for property
unit for temperature
low temperature limit
igh temperature limit
A-E (5 parameters)

Sources of data

Data in chemical data file come from several sources including :

- “Dechema Chemistry Data ser.” text books
- “DIPPR data collection” text books
- “Technical Data Book, Petroleum Refining”

Due to the large differences in critical and transport properties found in different sources, DIPPR (AICHE Design Institute for Physical PRoperty Data) reference has been selected as a default.

Component’s identification

Components are identified by name (from DIPPR list) , chemical formula and Identification number.

Regression procedures and results

Coefficients in correlations have been calculated with a custom program that uses a modified version of Levenberg-Marquardt algorithm , reported errors (at each fitting point) are usually lower than 1 % of input values for the most complex correlations (i.e. vapor pressure),), however in some cases they may be higher.

Consistency tests

When relations exist between thermodynamic properties (i.e. acentric factor and critical pressure and temperature, vapor pressure and heat of vaporization etc.) a consistency test has been performed.

Comparing Prode Properties results against those of different process simulators

When comparing data from different tools one must verify that

- the different tools do use the same thermodynamic models
- properties in databanks have siimilar values
- lists and values of BIPs and other parametres which can influence results have similar values

Models

Standard versions include a complete set of thermodynamic models, additional models are available in extended versions

Regular
Properties calculated according ideal fluid law

Wilson
Properties calculated according Wilson (G.M.Wilson 1964)

NRTL
Properties calculated according NRTL (Renon and Prausnitz, 1968)

UNIQUAC
Properties calculated according UNIQUAC (Abrams and Prausnitz, AICHE J. 1975)

UNIFAC
Liquid activity coefficient calculated according UNIFAC (Fredeslund, Jones, Prausnitz, AICHE J. 1975)

Soave-Redlich-Kwong
Different variants of Soave Redlich Kwong model (Giorgio Soave, 1972) are available,
base version includes standard and extended version of Soave Redlich Kwong model, extended version includes (for each fluid) 5 parameters calculated to fit the set of experimental data (saturation pressures, densities, latent heats) available in DIPPR or DECHEMA pure fluid data collections.

PR , Peng Robinson
Different variants of Peng Robinson model (D.Y.Peng, D.B. Robinson, 1976) are available,
base version includes standard and extended version of Peng Robinson model , extended version includes (for each fluid) 5 parameters calculated to fit the set of experimental data (saturation pressures, densities, latent heats) available in DIPPR or DECHEMA pure fluid data collections.

BWRS , Benedict-Webb-Rubin-Starling
Properties calculated according Benedict-Webb-Rubin Starling Han (1972)

LKP , Lee Kesler Plocker
Properties calculated according Lee-Kesler-Plocker (1978)

AGA (ISO 20765)
Gas volume calculated according AGA report (ISO 20765)

GERG (ISO 18453)
Fugacity   calculated according GERG report (ISO 18453)

CPA SRK
Properties calculated as Q = Qphys + Qass where Qphys is derived from Soave Redlich Kwong model and Qass is the association term (G.M. Kontogeorgis, E. Voutsas, I. Yakoumis, D.P. Tassios 1996)
The model includes (for each fluid) 5 + 2 (ass.) parameters calculated to fit the set of experimental data (saturation pressures, densities, latent heats) available in DIPPR or DECHEMA pure fluid data collections.

CPA PR
Properties calculated as Q = Qphys + Qass where Qphys is derived from Peng Robinson model and Qass is the association term (G.M. Kontogeorgis, E. Voutsas, I. Yakoumis, D.P. Tassios 1996)
The model includes (for each fluid) 5 + 2 (ass.) parameters calculated to fit the set of experimental data (saturation pressures, densities, latent heats) available in DIPPR or DECHEMA pure fluid data collections.

SPM Solid Pure Model
solid phase treated as single component, solid fugacity derived from liquid fugacity calculated according selected model

SSM Solid Solution Model
solid phase treated as homogeneous solution, solid fugacity derived from liquid fugacity calculated according selected model

Steam tables (IAPWS 1995)
Water / steam properties calculated according IAPWS 1995 formulation for the thermodynamic properties of Water for general and scientific use, issued by the International Association for the Properties of Water and Steam

Hydrates
Multiphase equilibria, fugacities calculated according Van der Waals and Plateeuw, two models available (simplified model, in Base version, and complex model, in Extended versions)

UNIFAC functional groups

The underlying idea in UNIFAC method is that a molecule can be considered as a collection of functional groups. The main advantage of this approach is that from a relatively small number of functional groups the properties of many different molecules can be predicted. The UNIFAC model is useful for estimating solution behaviour in the absence of experimental data. Prode Properties incorporates the UNIFAC Group Contribution revision 5 (January 1992, J.P.Baker).
Following the main groups and subgroups table :

Code	Main	Subgroup	Example
1	CH2	CH3	Hexane
2		CH2	n-Hexane
3		CH	2-Methylpropane
4		C	Neopentane
5	C=C	CH2=CH	1-Hexene
6		CH=CH	2-Hexene
7		CH2=C	2-Methyl-1-butene
8		CH=C	2-Methyl-2-butene
70		C=C	2,3-Dimethylbutene
9	ACH	ACH	Naphthaline
10		AC	Styrene
11	ACCH2	ACCH3	Toluene
12		ACCH2	EthylBenzene
13		ACCH	Cumene
14	OH	OH	n-Propanol
15	CH3OH	CH3OH	Methanol
16	H2O	H2O	Water
17	ACOH	ACOH	Phenol
18	CH2CO	CH3CO	Butanone
19		CH2CO	Pentanone-3
20	CHO	CHO	Propionic aldehyde
21	CCOO	CH3COO	Butyl acetate
22		CH2COO	Methyl propionate
23	HCOO	HCOO	Ethyl formate
24	CH2O	CH3O	Dimethyl ether
25		CH2O	Diethyl ether
26		CHO	Diisopropyl ether
27		THF	Tetrahydrofuran
28	CNH2	CH3NH2	Methylamine
29		CH2NH2	Ethyl amine
30		CHNH2	Isopropylamine
31	CNH	CH3NH	Dimethylamine
32		CH2NH	Diethyl amine
33		CHNH	Diisopropylamine
34	(C)3N	CH3N	Trimethylamine
35		CH2N	Triethylamine
36	ACNH2	ACNH2	Aniline
37	Pyridine	C5H5N	Pyridine
38		C5H4N	2-Methyl pyridine
39		C5H3N	2,3-Dimethylpyridine
40	CCN	CH3CN	Acetonitrile
41		CH2CN	Propionitrile
42	COOH	COOH	Acetic acid
43		HCOOH	Formic acid
44	CCl	CH2Cl	Butane-1-chloro
45		CHCl	Propane-2-chloro
46		CCl	2-Methylpropane-2-chloro
47	CCl2	CH2Cl2	Methane-dichloro
48		CHCl2	Ethane-1,1-dichloro
49		CCl2	Propane-2,2-dichloro
50	CCl3	CHCl3	Chloroform
51		CCl3	Ethane-1,1,1-trichloro
52	CCl4	CCl4	Methane-tetrachloro
53	ACCl	ACCl	Benzene-chloro
54	CNO2	CH3NO2	NitroMethane
55		CH2NO2	Propane-1-nitro
56		CHNO2	Propane-2-nitro

Code	Main	Subgroup	Example
57	ACNO2	ACNO2	Benzene-nitro
58	CS2	CS2	Carbon Disulfide
59	CH3SH	CH3SH	Methanethiol
60		CH2SH	Ethanethiol
61	Furfural	Furfural	Furfural
62	DOH	DOH	1,2-Ethanediol
63	I	I	Iodoethane
64	Br	Br	Bromoethane
65	C-C	CH-C	Hexyne-1
66		C-C	Hexyne-2
67	DMSO	DMSO	Dimethylsulfoxide
68	ACRY	Acrylnitril	Acrylnitrile
69	ClCC	Cl-(C=C)	Ethene-trichloro
71	ACF	ACF	Hexafluorobenzene
72	DMF	DMF-1	N,N-Dimethylformamide
73		DMF-2	N,N-Diethylformamide
74	CF2	CF3	Perfluorohexane
75		CF2	
76		CF	Perfluoromethylcyclohexane
77	COO	COO	Methyl acrylate
78	SiH2	SiH3	Methylsilane
79		SiH2	Diethylsilane
80		SiH	Heptamethyltrisiloxane
81		Si	Heptamethyldisiloxane
82	SiO	SiH2O	1,3-Dimethyldisiloxane
83		SiHO	1,1,3,3-Tetramethyldisiloxane
84		SiO	Octamethylcyclotetrasiloxane
85	NMP	NMP	N-methylpyrrolidone
86	CClF	CCl3F	Trichlorofluoromethane
87		CCl2F	Tetrachloro-1,2-difluoroethane
88		HCCl2F	Dichlorofluoromethane
89		HCClF	1-Chloro-1,2,2,2,-tetrafluoroethane
90		CClF2	1,2-Dichlorotetrafluoroethane
91		HCClF2	Chlorodifluoromethane
92		CClF3	Chlorotrifluoromethane
93		CCl2F2	Dichlorodifluoromethane
94	CON	CONH2	Acetamid
95		CONHCH3	N-Methylacetamid
96		CONHCH2	N-Ethylacetamid
97		CON(CH3)2	N,N-Dimethylacetamid
98		CONCH3CH2	N,N-methylethylacetamid
99		CON(CH2)2	N,N-Diethylacetamid
100	OCCOH	C2H5O2	2-Ethoxyethanol
101		C2H402	2-Ethoxy-1-propanol
102	CH2S	CH3S	Dimethylsulfide
103		CH2S	Diethylsulfide
104		CHS	Diisopropylsulfide
105	Morpholine	MORPH	Morpholine
106	Thiophene	C4H4S Thiophene	
107		C4H3S	2-Methylthiophene
108		C4H2S	2,3-Dimethylthiophene