
**DWSIM - Process Simulation, Modeling and Optimization
User Guide**

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1 Introduction

This document provides DWSIM users with information about how to setup, run, modify and view results of a basic process simulation. The document is organized according to the sequence of execution of the simulation simulation. Each step/task is explained with the help of images and descriptions of the associated windows.

For details about the models used for calculation of thermodynamic, transport and thermal properties, please read the **Technical Manual**. Detailed Unit Operations and Utilities' descriptions can be found in the **Unit Operations and Utilities Guide**.

2 Welcome screen

When DWSIM is opened, the welcome screen is shown (Figure 1):

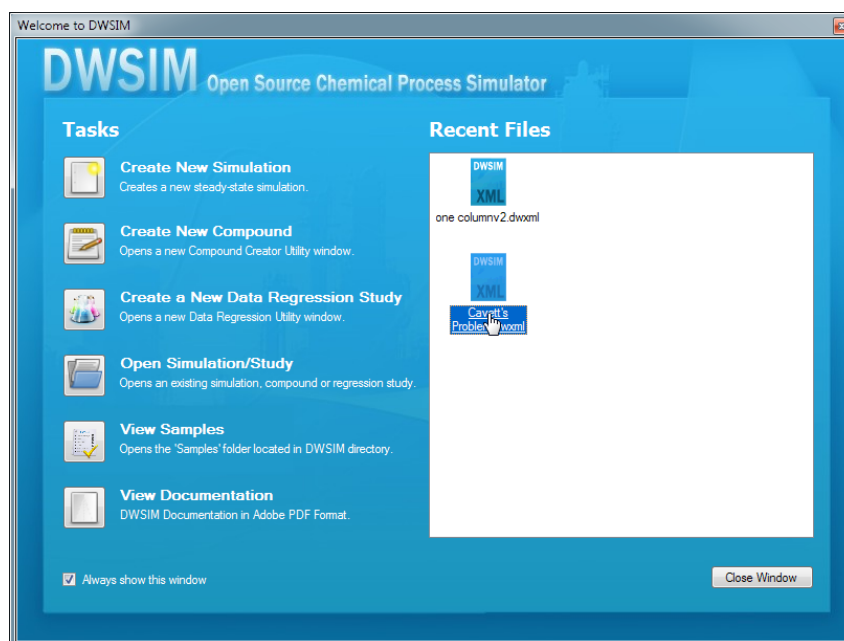


Figure 1: DWSIM's welcome screen.

The welcome screen provides the user with shortcuts to open existing simulations, create new ones, create new compound creator and data regression cases and open the samples folder. To prevent this window from showing after initialization, uncheck the "Always show this window" box. The "Close Window" button closes the window and shows the main DWSIM interface:

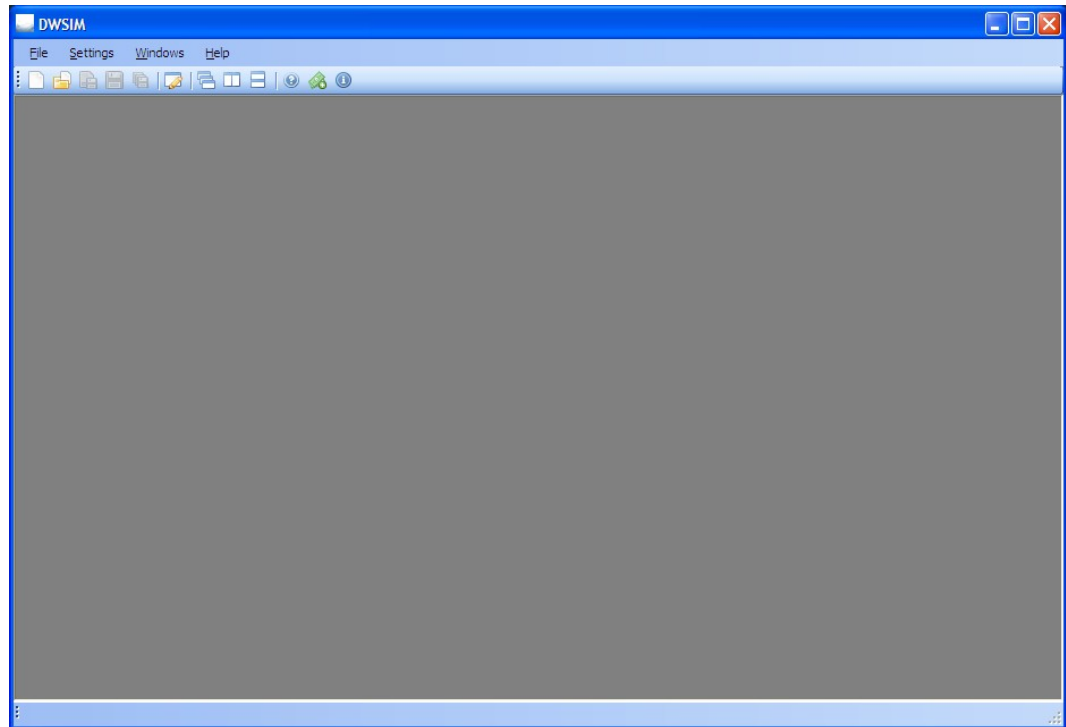


Figure 2: DWSIM's main window.

In the main DWSIM window (Figure 2), one can visualize the following items:

- **Menu bar**, with buttons to open/save/create simulations, component creator and data regression cases, configure the active simulation, general preferences, launch tools, configure the child windows view mode, etc.;



If a simulation is active in DWSIM, the menu bar is filled with other specific items.

- **Button strip**, to open, save and create new steady-state simulations, component creator and data regression cases.

There are various options to access the most commonly operations with simulation files and component creator/data regression cases - open, save and create. In the next sections you will be guided through some necessary steps to create and configure a steady-state simulation, a compound creator and/or a data regression case.

3 Simulation

3.1 User Interface

The "Create a new steady-state simulation" button in the welcome window can be used to create a new simulation. After the simulation is created, the **configuration window** (Figure 3) is shown. The simulation configuration interface consists in a lateral menu composed by tabs which, by themselves, are divided in *sections*:

- ➔ **Compounds** - Compound addition to and removal from the simulation, petroleum fractions (pseudocompounds) utilities.
- ➔ **Thermodynamic and Reactions** - Property Package configuration and Chemical Reactions management.
- ➔ **Tools** - Creation and management of user-created components.
- ➔ **Options** - Unit systems management and number formatting.
- ➔ **Description** - Simulation info (title, author and description).

3.2 Configuration

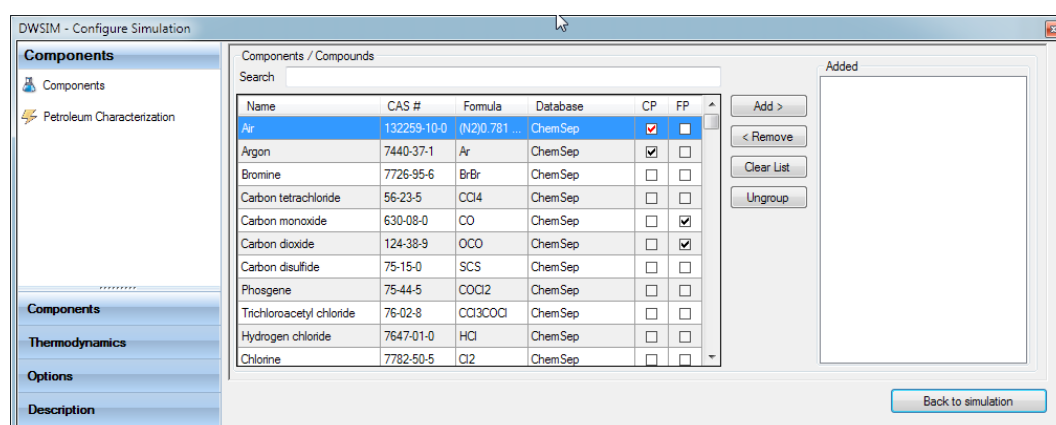


Figure 3: Simulation configuration window.

The simulation configuration window (Figure 3) is the interface where all the functions for configuration and personalization of a simulation in DWSIM can be found. In this window, the user can manage the simulation components, the property package (thermodynamic model), units system and number format, among other options.



The configuration window can be accessed at any time during the simulation, and the changes made on it have immediate effect on the simulation.

3.2.1 Components

There are two essential information required by DWSIM in order to correctly start a simulation. The first refers to the available **components** (or **compounds**). Operations with the

components in a simulation can be done in the submenus in the "Components" tab. There are three types of components which can be managed in DWSIM - the first type are the components present in the database. The second, **hypotheticals**, and the third, **pseudocomponents**, are components which can be added by the user through the **Compound Creator** or the **Petroleum Characterization** utilities. These user-created components will be available in the end of the component list inside the "Components" tab for inclusion or removal from the simulation as necessary.



View the section 3.8 for information about the hypothetical and pseudocomponent generation utilities.

3.2.2 Property Package

The Property Package consists in a set of methods and models for the calculation of physical and chemical properties of material streams in the simulation. It is composed of a thermodynamic model - an equation of state or a hybrid model - and methods for property calculation, like the surface tension of the liquid phase. It is shown in Figure 4 the interface for configuration of the property package ("Thermodynamic and Reactions" tab, "Property Package" section).

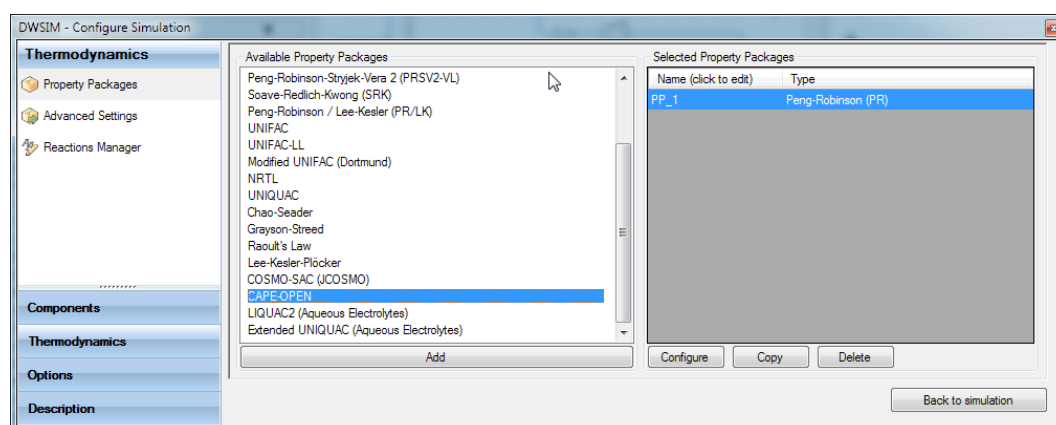


Figure 4: Property Package configuration interface.

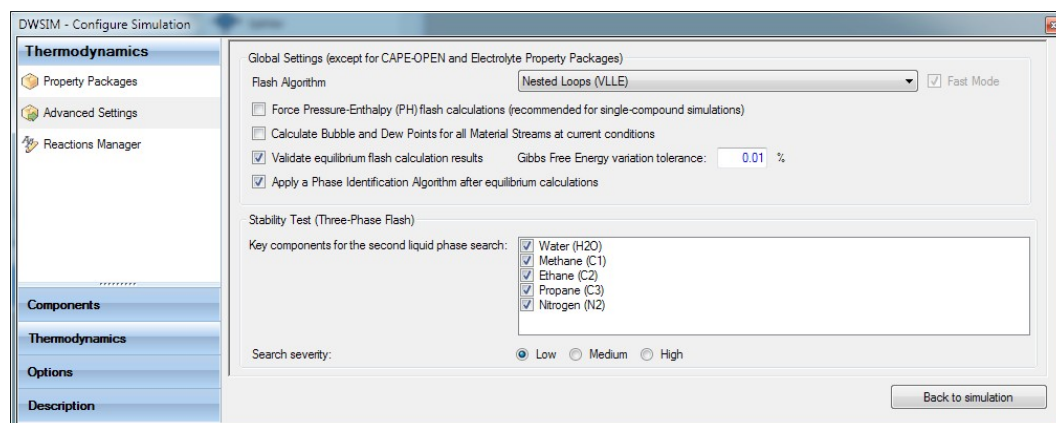


Figure 5: Property Package configuration interface.

Advanced Settings You can define some parameters which will be used throughout all Property Packages, in all simulation objects. They are:

➔ *Flash Algorithm*

Defines the flash algorithm to be used by all Property Packages which have its Flash Algorithm option set to "Global" (default).

1. **Nested Loops (default):** recommended for the vast majority of VLE systems;
2. **Inside-Out (2 or 3-Phase):** recommended for petroleum simulations with many pseudo-components. The 3-phase option must be used when a second liquid phase is expected (i.e. free water);
3. **Gibbs Minimization (2 or 3-phase):** recommended for difficult chemical systems;
4. **Nested Loops for Eutectic Solid Systems:** Calculates Solid-Liquid Equilibria for eutectic systems considering the solid phase as being ideal.
5. **Nested Loops for Solid Solution Systems:** Calculates Solid-Liquid Equilibria for solid solution systems considering the solid phase as being ideal.
6. **Nested Loops (3-phase immiscible VLLE):** For systems with an immiscible second liquid phase (VLLE). The first compound selected in the key compound list will be the immiscible one.

The "Fast Mode" switch enables some optimizations in the IO code in order to improve calculation times.

➔ *Force Pressure-Enthalpy (PH) Flash calculations*

If enabled, all requests by unit operations for PT Flashes will be replaced by PH ones. This option must be activated if you are working with only one component (steam simulation, for example), otherwise you won't have partial vaporization/liquefaction in valves, compressors and expanders, if that is the case.

➔ *Calculate Bubble and Dew points at stream conditions*

Check this box if you want the DWSIM to calculate bubble and dew points at conditions specified on each material stream. The calculated values will be shown only if the stream is at VLE equilibrium. The calculations are not exactly fast, so use this option with caution and only if needed.

→ *Validate Equilibrium Flash Calculation Results*

If enabled, DWSIM will check the mixture Gibbs energy before and after the equilibrium flash calculation. If the gibbs energy *increases* after the calculation (it should always *decrease* when there is a phase split), an error message will be shown and the flowsheet calculation will be aborted.

→ *Apply a Phase Identification Algorithm after Equilibrium Calculations*

Check this to apply an identification algorithm to each phase after the equilibrium calculation is finished. This can be useful for supercritical compounds which behave as liquid at high pressures and temperatures, or special mixtures which exhibit LLE behavior at low temperatures, incorrectly identified as VLE by the flash algorithms.

This procedure is enabled by default and will override the flash result regarding phase identification. For instance, the result of a flash calculation may give an all-vapor solution and, after the phase identification algorithm is applied, the phase may, in fact, behave as liquid. In this case, DWSIM will show this phase as liquid in the Material Stream property window.

Visit DWSIM's wiki for more information about the phase identification algorithm.

→ *Stability Test*

When a flash algorithm with a three-phase capability is selected, DWSIM needs to know which components are most likely to be present in a second liquid phase. You can do that by selecting the ones you think that will be in a higher amount - that is, the key components for the second liquid phase. That doesn't necessarily imposes that the other, unselected components cannot be present in the second liquid phase - only the equilibrium calculation will tell you that.

The search severity setting controls how much effort DWSIM should put into searching for a second liquid phase. In the *Low* setting, only one trial phase is created with a mixture of the key components and the convergence tolerance is somewhat high. In the *High* setting, DWSIM will include additional trial phases, one for each key component and do additional checks using incipient phases' gibbs energy, with the smallest convergence tolerance value (1E-06).

Multiple Property Packages Since DWSIM 1.5, the user can add multiple Property Packages to a single simulation, which can be associated to each unit operation and material stream on a individual basis. Each property package has its own settings, even if two or more packages are of the same type.

Property Package configuration If the selected property package has any editable property, the "Configure" button becomes clickable and the user can click on it to show the property package configuration window. For instance, with the SRK property package the editable parameters are the binary interaction parameters (Figure 6) and some convergence/tolerance values for flash calculations (Figure 7).

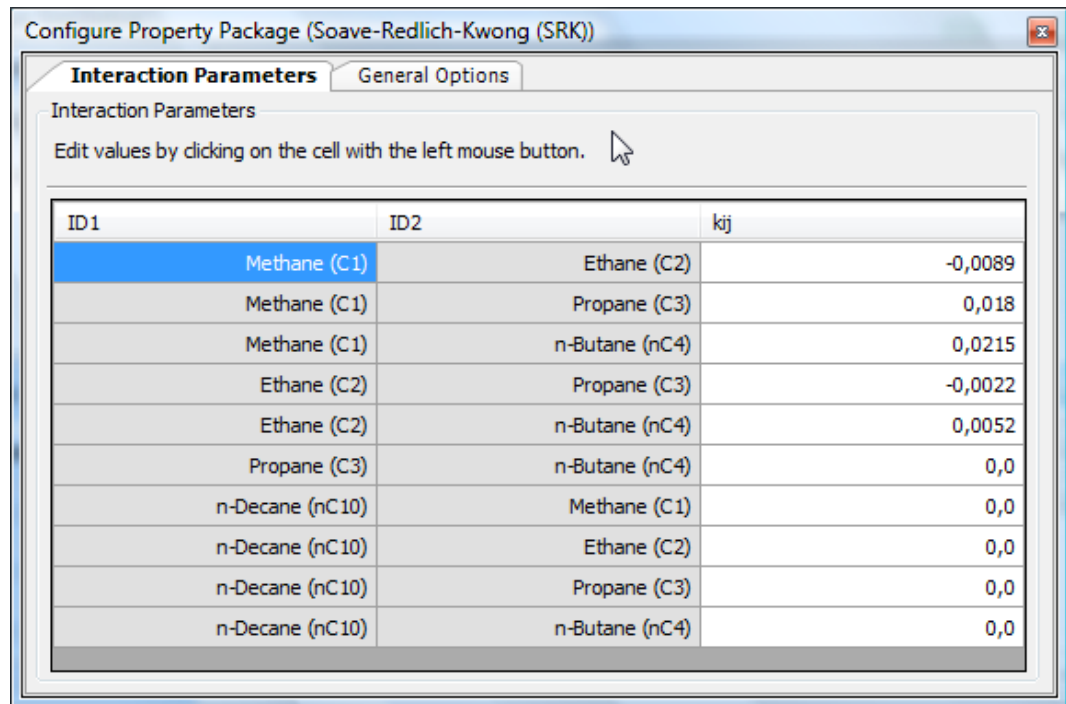


Figure 6: Property package configuration window (1).

→ *Use Ideal Mixing Rule for Liquid Phase Density*

If the liquid phase has small amounts of supercritical components, the default calculation method may fail. If that is the case, change this option to 1 to force an ideal mixing rule for the liquid density (use a molar weighted average of individual component liquid densities).

→ *Flash Algorithm*

Use this option to override the global setting for the Flash Algorithm. Default is 2 (use the global setting).

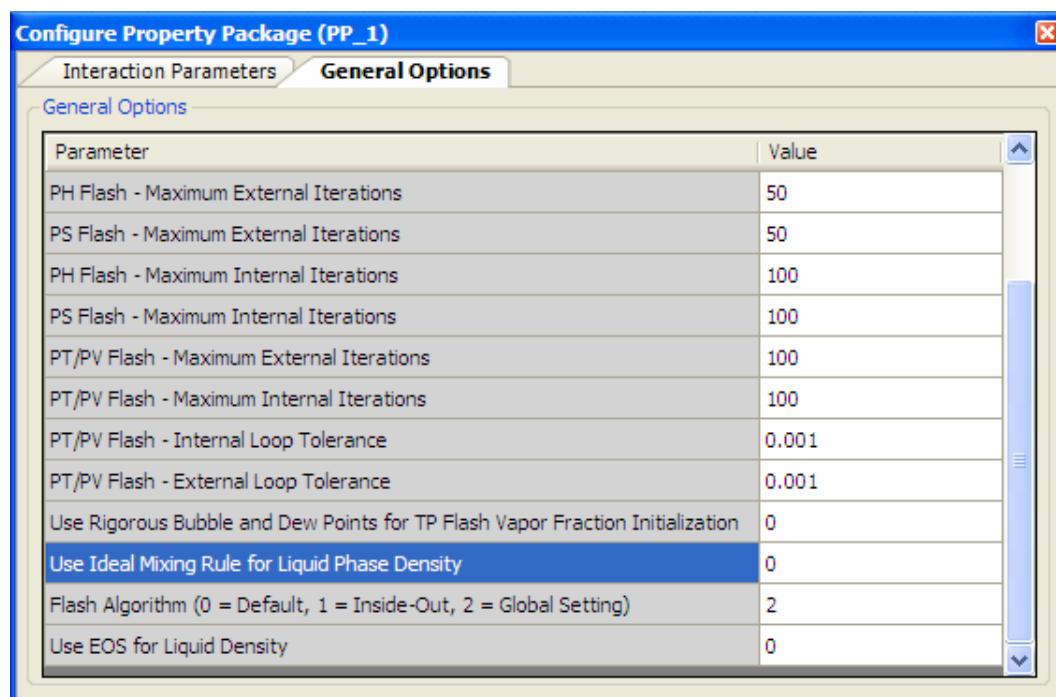


Figure 7: Property package configuration window for EOS-based models.

Additional Property Package configuration options Some Property Packages have extra configuration options in order to allow a deeper control of the thermodynamic calculations for the user. They are:

→ *Use Rigorous Bubble and Dew Points for TP Flash Vapor Fraction Initialization*

By default, DWSIM uses a simple rule based on Raoult's law to estimate an initial value for the vapor fraction in the TP Flash calculation. This works well for most cases and helps improving calculation speed but, sometimes, with very non-ideal mixtures, this can lead to a very erroneous initial value, far from the solution, which ultimately leads to non-convergence of the algorithm and consequently, the stream/operation isn't calculated as expected. With this option you can force the calculation of rigorous bubble and dew point pressures for the estimation of the vapor fraction. It will take more time than usual, but helps the Flash calculation to converge in difficult situations.

Use 0 to disable, 1 to enable this option.

→ *Use EOS for Liquid Density*

This option forces the calculation of the liquid densities based on the compressibility factor given by the EOS. When disabled, DWSIM will use the Rackett correlation to calculate the liquid density. Please note that this also affects the calculation of partial molar volumes, and, consequently, component liquid volumetric fractions and flow rates.

Use 0 to disable, 1 to enable this option.

→ *Use Peneloux Volume Translation correction*

This option is available for PR and SRK Property Packages. It enables correction of EOS-calculated densities by the inclusion of a correction factor named *volume translation coefficient*. This option will be effective only if the *Use EOS for Liquid Density* option is enabled.

Use 0 to disable, 1 to enable this option.

→ *Use Experimental Liquid Density Data*

This option affects ChemSep database compounds only. It forces usage of experimental coefficients present in the database to calculate liquid phase densities.

Use 0 to disable, 1 to enable this option.

→ *Use Experimental Liquid Thermal Conductivity Data*

This option affects ChemSep database compounds only. It forces usage of experimental coefficients present in the database to calculate liquid thermal conductivities.

Use 0 to disable, 1 to enable this option.

3.2.3 Units systems and Number formatting

Three basic units systems are present in DWSIM: **SI System** (selected by default), **CGS System** and **English System**. The simulation's units system can be viewed/modified in the "Units System" section of the "Options" tab in the simulation configuration window (Figure 8).

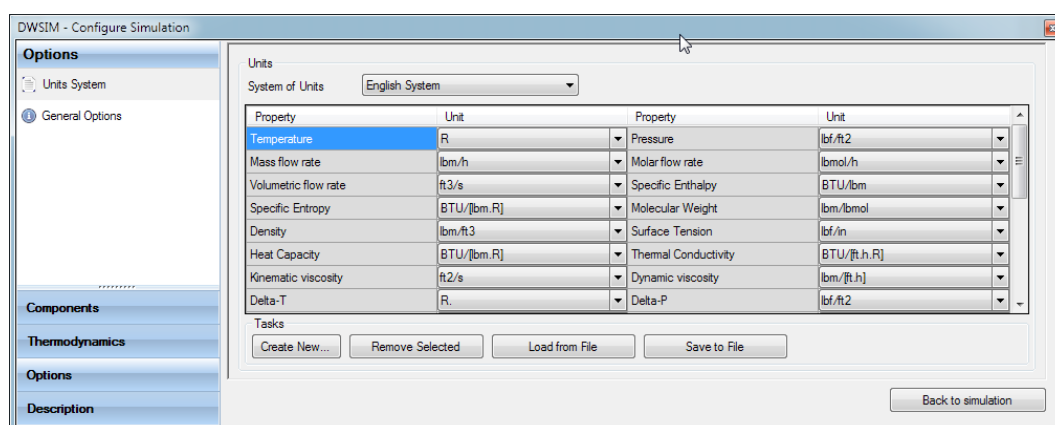


Figure 8: Units system configuration interface.

There are buttons available on this interface to create custom units systems and save/load them. It is worth remembering that the units systems can also be modified at any time during the simulation - the changes are applied immediately.

In the "General Options" section it is possible to define the number formatting in the simulation (Figure 9).

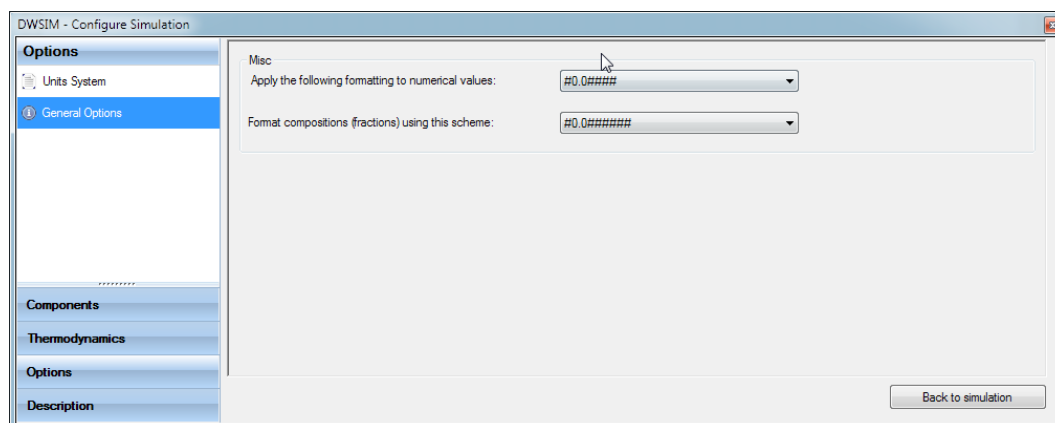


Figure 9: Number formatting selection interface.

3.2.4 Other options

The "Tools" tab contains hypothetical and pseudocomponents creation and management tools (Section 3.8). In the "Description" tab it is possible to edit some information about the active simulation (title, author and description). You can also define a password to prevent the simulation of being opened by anyone, but this feature only works with the binary simulation file format (*.dwsim) (Figure 10).

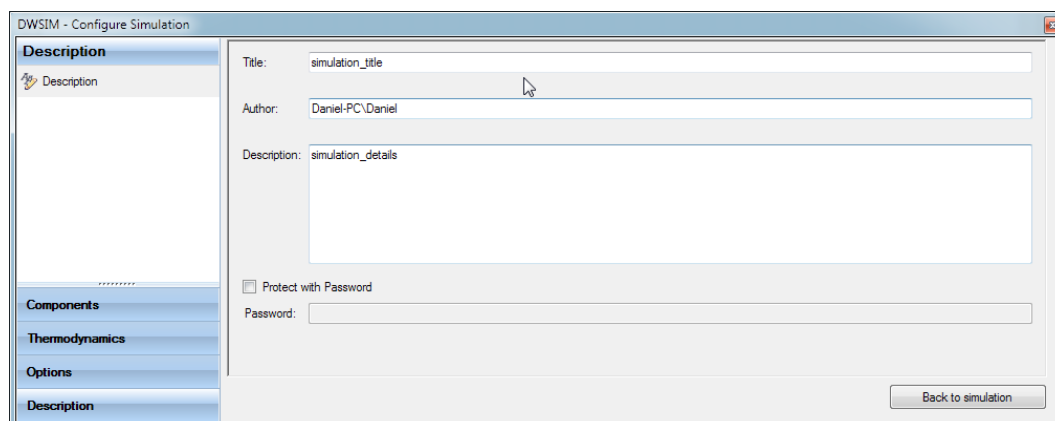


Figure 10: Simulation description editing interface.

If all simulation parameters are correctly configured, the "Back to simulation" button can be clicked to take the user to the main simulation window, where the flowsheet can be built and the simulation itself can be executed.

3.3 Process modeling (Flowsheeting)

After configuring the simulation, the user is taken to the main simulation window (Figure 11). In this window we can highlight the following areas:

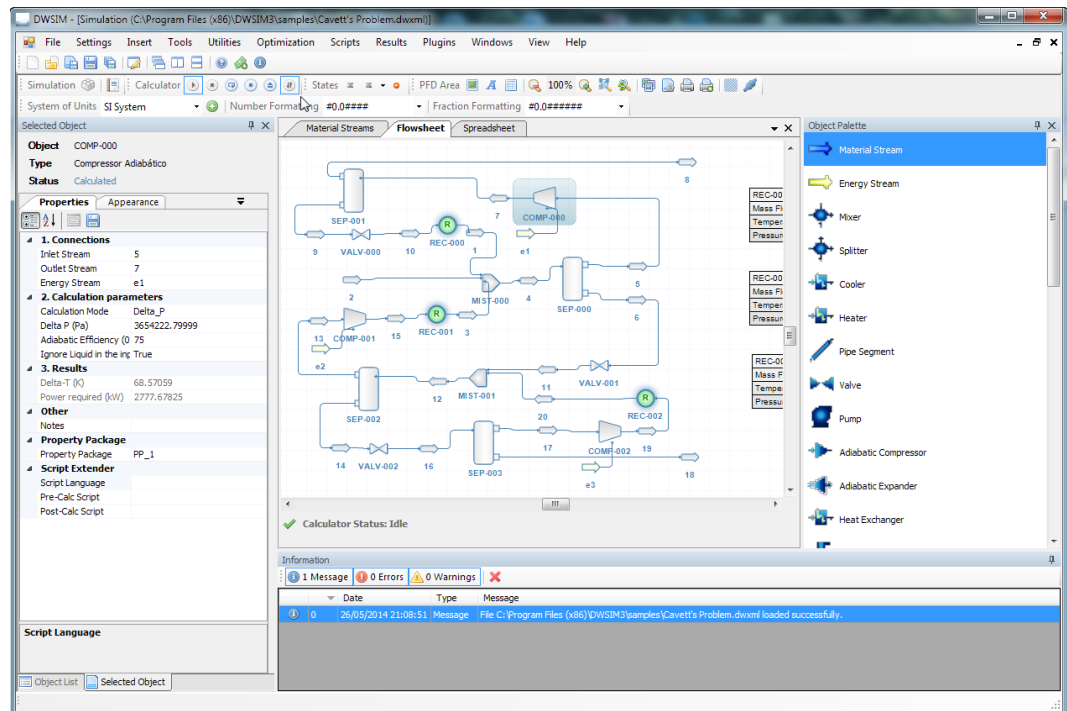


Figure 11: Simulation interface.

- ➔ **Menu bars** (left-right / up-down): simulation configuration, results viewer, image and text insertion, zoom controls and flowsheet printing; unit ops and streams insertion buttons;
- ➔ **Object Palette** window: shows objects which can be added by dragging them into the PFD;
- ➔ **Selected Object** window: show information about the selected object in the flowsheet;
- ➔ **Material Streams** window: lists the material streams in the flowsheet and their calculated properties;
- ➔ **Flowsheet** window: process flowsheet building and editing area;
- ➔ **Information** window: general information about the active simulation;
- ➔ **Object List** window: information tree about the objects in flowsheet according to their type - can be used to find and center objects in large flowsheets;
- ➔ **Spreadsheet** window: shows the spreadsheet, a utility to do math operations with data provided by the objects in the current simulation;
- ➔ **Help** window: shows useful tips during a simulation.

The simulation windows can be freely repositioned, with the arrangement information being saved together with the rest of simulation data. To reposition a window, the user should click with the left mouse button in the window's top bar and drag it to the desired place. A preview of how the window will be is shown in blue (Figure 12).

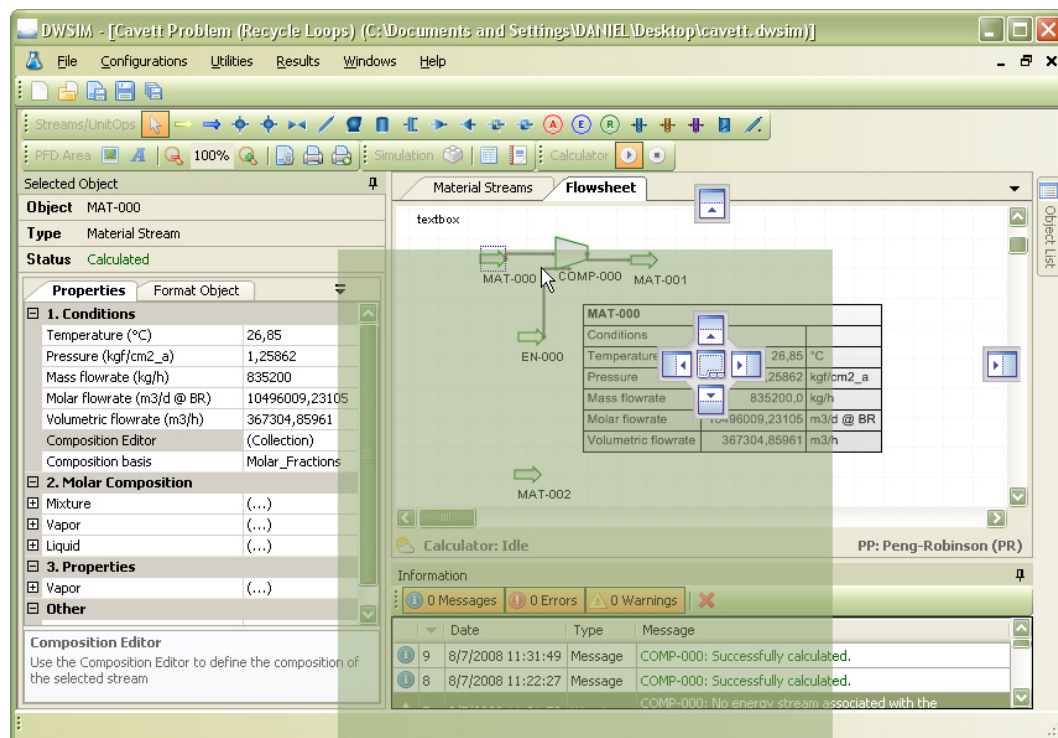


Figure 12: Window repositioning.

3.3.1 Objects

The elements of a simulation (objects) which can be added to the flowsheet are:

- ➔ **Material Stream**: used to represent matter which enters and leaves the limits of the simulation and passes through the unit operations. The user should define their conditions and composition in order for DWSIM to calculate their properties accordingly;
- ➔ **Energy Stream**: used to represent energy which enters and leaves the limits of the simulation and passes through the unit operations;
- ➔ **Mixer**: used to mix up to three material streams into one, while executing all the mass and energy balances;
- ➔ **Splitter**: mass balance unit operation - divides a material stream into two or three other streams;
- ➔ **Valve**: works like a fixed pressure drop for the process, where the outlet material stream properties are calculated beginning from the principle that the expansion is an isenthalpic process;
- ➔ **Pipe**: simulates a fluid flow process (mono or two-phase). The pipe implementation in DWSIM provides the user with various configuration options, including heat transfer to environment or even to the soil in buried pipes. Two correlations for pressure drop calculations are available: Beggs & Brill and Lockhart & Martinelli. Both reduce to Darcy equation in the case of single-phase flow;

- **Pump**: used to provide energy to a liquid stream in the form of pressure. The process is isenthalpic, and the non-idealities are considered according to the pump efficiency, which is defined by the user;
- **Tank**: in the current version of DWSIM, the tank works like a fixed pressure drop for the process;
- **Separator Vessel**: used to separate the vapor and liquid phases of a stream into two other distinct streams;
- **Compressor**: used to provide energy to a vapor stream in the form of pressure. The ideal process is isentropic (constant entropy) and the non-idealities are considered according to the compressor efficiency, which is defined by the user;
- **Expander**: the expander is used to extract energy from a high-pressure vapor stream. The ideal process is isentropic (constant entropy) and the non-idealities are considered according to the expander efficiency, which is defined by the user;
- **Heater**: simulates a stream heating process;
- **Cooler**: simulates a stream cooling process;
- **Conversion Reactor**: simulates a reactor where conversion reactions occur;
- **Equilibrium Reactor**: simulates a reactor where equilibrium reactions occur;
- **PFR**: simulates a Plug Flow Reactor (PFR);
- **CSTR**: simulates a Continuous-Stirred Tank Reactor (CSTR);
- **Shortcut Column**: simulates a simple distillation column with approximate results using shortcut calculations;
- **Distillation Column**: simulates a distillation column using rigorous thermodynamic models;
- **Absorption Column**: simulates an absorption column using rigorous thermodynamic models;
- **Refluxed Absorber**: simulates a refluxed absorber column using rigorous thermodynamic models;
- **Reboiled Absorber**: simulates a reboiled absorber column using rigorous thermodynamic models.
- **Heat Exchanger**: simulates a countercurrent heat exchanger using rigorous thermodynamic models.
- **Orifice Plate**: model to simulate an orifice plate, used for flow metering.
- **Component Separator**: model to simulate a generic process for component separation.
- **Custom Unit Operation**: an user-defined model based on IronPython/IronRuby scripts.

- **CAPE-OPEN Unit Operation:** External CAPE-OPEN Unit Operation socket for adding CO Unit Operations in DWSIM.
- **Solids Separator:** model to simulate a generic process for solid compound separation.
- **Continuous Cake Filter:** continuous cake filter model for solids separation.

Additionally, the following logical operations are available in DWSIM:

- **Adjust:** used to make a variable to be equal to a user-defined value by changing the value of other (independent) variable;
- **Specification:** used to make a variable to be equal to a value that is a function of other variable, from other stream;
- **Recycle:** used to mix downstream material with upstream material in a flowsheet,
- **Energy Recycle:** used to mix downstream energy with upstream energy in a flowsheet.

Adding objects to the flowsheet Objects can be inserted into the flowsheet by dragging and dropping items from the **Object Palette** or by using the corresponding toolbar menu items (**Insert** menu item).

To insert objects into the flowsheet by using the toolbar menu items:

1. With the left mouse button, click in the desired object menu item.
2. With the left mouse button, click in the flowsheet area, at the point where you want to position the object.

To insert objects from the Object Palette, drag and drop the items into the PFD (Figure 13):

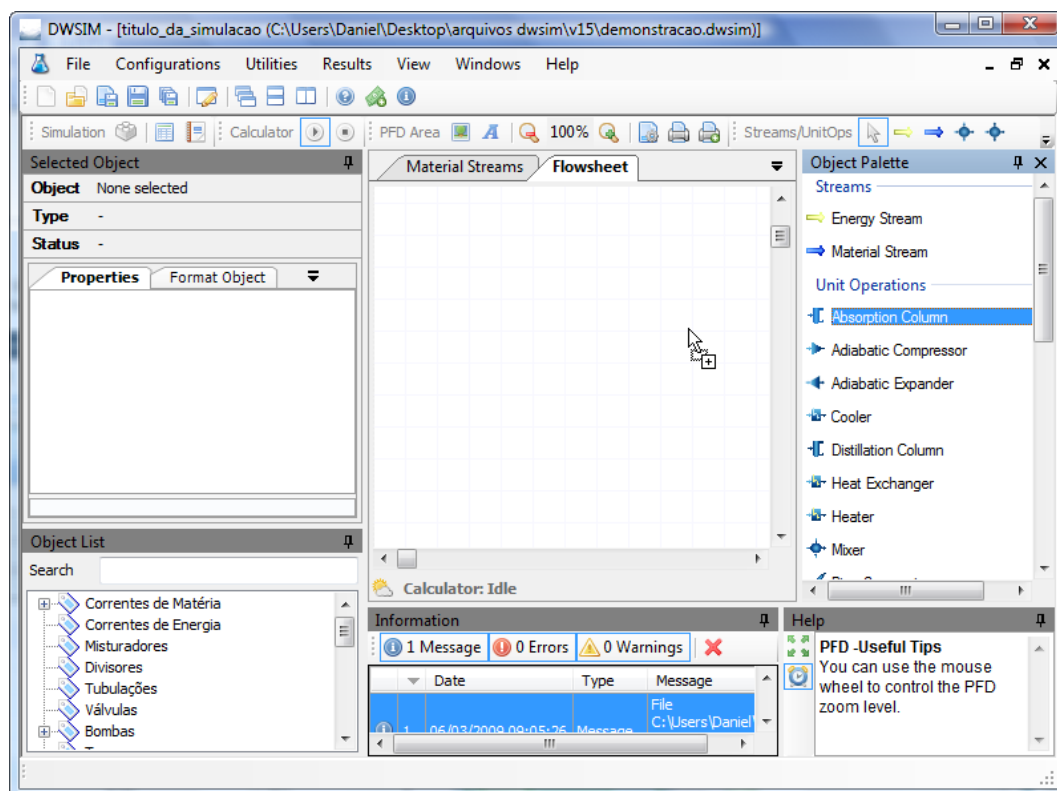


Figure 13: Dragging items from the Object palette window.

Figure 14 shows a material stream added to the flowsheet by one of the method described above. It can be observed that the stream is selected and that the "Selected Object" window is filled with the object's information.

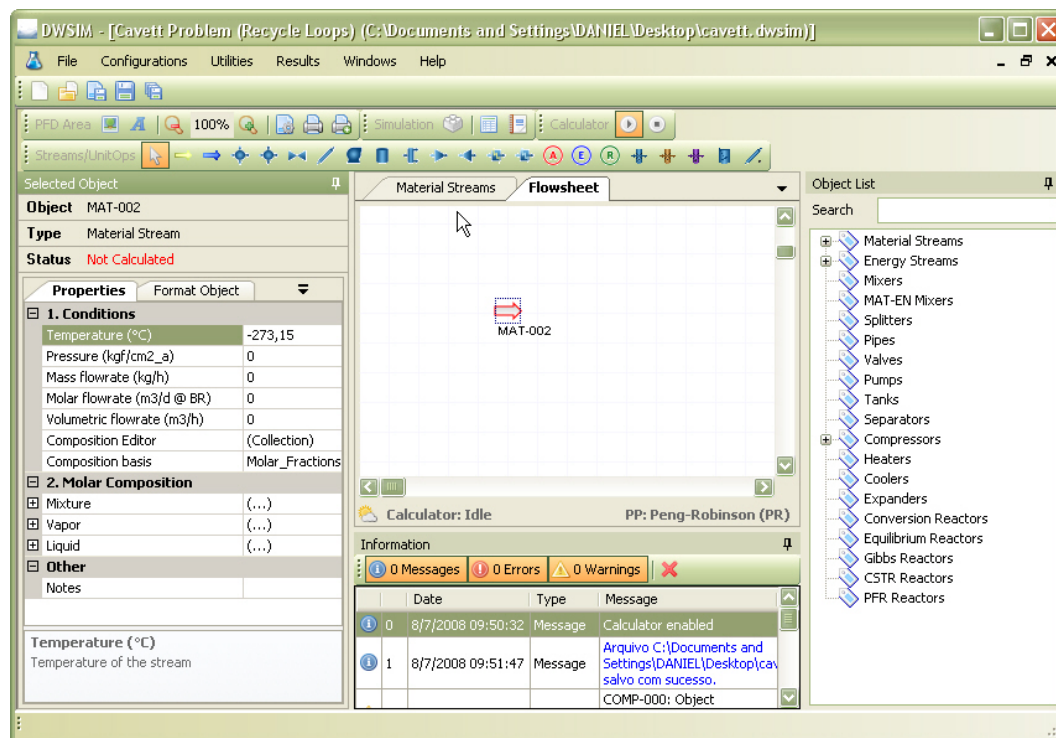


Figure 14: A material stream in the flowsheet.

Connecting objects The material streams represent mass flowing between unit operations. There are two different ways in which a material stream can be connected to a unit operation (or *vice-versa*):

- Through the context menu activated with a right mouse button click over the object (Figure 15);

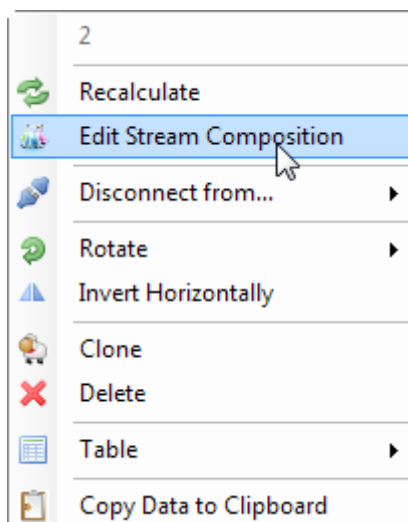


Figure 15: Selected object context menu.

- Through the unit operation property window - inlet/outlet/energy streams. It is possible to inform the name of a stream that doesn't exist (so it will be created and connected

to the unit automatically) or select a existing stream by using the menu activated with a mouse click in the button on the right of the property description line:

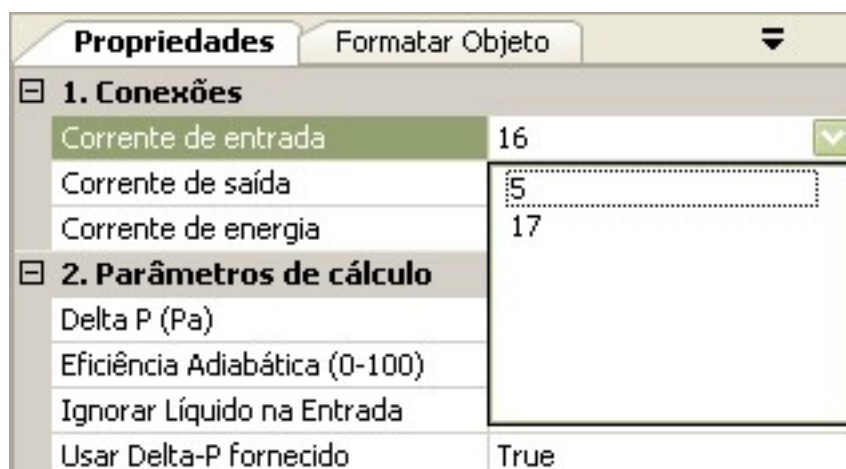


Figure 16: Stream selection menu.

A compression system with its connections is shown on Figure 17.

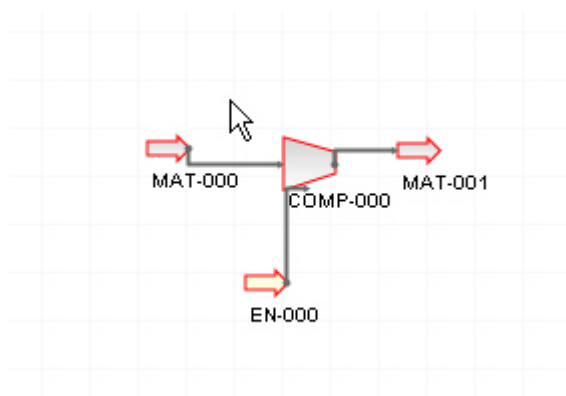


Figure 17: Compressor with all connections made.

Disconnecting objects Functions to disconnect objects can be found in the same place as the connecting ones.

Removing objects from the flowsheet The selected object can be removed from the flowsheet by pressing the DEL keyboard button or by using the context menu - "Delete" item (Figure 15).

3.3.2 Process data management

Entering process data The objects' process data (temperature, pressure, flow, composition and/or other parameters) can be entered in the "Selected Object" window (Figure 18). Properties that cannot be edited (read-only) are grayed-out.

Object	COMP-000
Type	Adiabatic Compressor
Status	Not Calculated
Properties Format Object	
1. Connections	
Input Stream	MAT-000
Output stream	MAT-001
Energy Stream	
2. Parameters of calculation	
Delta P (kgf/cm2)	0,0
Adiabatic Efficiency (0-100)	75
Ignore Liquid in the input stream	True
Using Delta-P provided	True
3. Results	
Delta T (°C.)	0,0
Energy needed (kW)	0,0
4. Miscellanea	
Error Message	
Other	
Energy Stream	

Figure 18: Viewing object properties in the "Selected Object" window.

Some properties can be edited directly in the area to the right of their identification, like a stream temperature (Figure 19). Other properties require an auxiliary window, like a stream composition (Figure 20), and others can be selected by using a drop-down menu (Figure 21). When it is necessary to open another window to edit a property, a button with "..." will be shown to the right of the property line - clicking on it shows the property editing window.

Temperature (°C)	26,85
------------------	-------

Figure 19: Direct editing of a property.

Composition Editor	(Collection)	...
--------------------	--------------	-----

Figure 20: Using an auxiliary window to edit a property value.

Composition basis	Molar_Fractions
2. Molar Composition	
Mixture	
Vapor	
Liquid	
3. Properties	
Vapor	

Figure 21: Selecting a value for the property in a drop-down menu.

If all object properties were correctly defined, it will be calculated by DWSIM and its flowsheet representation will have a blue border instead of a red one, indicating that the object was calculated successfully (Figure 22).

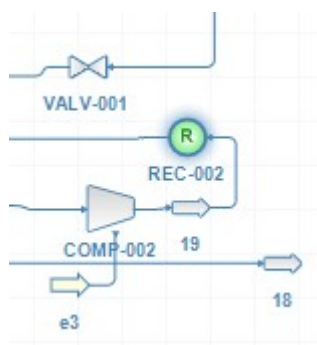




Figure 22: Calculated objects.

3.3.3 Simulation

DWSIM is a sequential modular process simulator, that is, all calculations are made in a per-module basis, according to the connections between the objects. The calculator checks if an object has all of its properties defined and, if yes, passes the data for the downstream object and calculates it, repeating the process in a loop until it reaches an object that doesn't have any of its downstream connections attached to any object. This way, the entire flowsheet can be calculated as many times as necessary without having to "tell" DWSIM which object must be calculated. In fact, this is done indirectly if the user define all the properties and make all connections between objects correctly.

DWSIM's calculation starts when the user edits a property which defines an object. For example, editing a stream mass flow when its temperature, pressure and composition are already well-defined activates DWSIM's calculator.

It is possible to control DWSIM's calculator by using its button bar (Figure 23). Clicking on the  button, the calculator is disabled. The  button enables it. DWSIM's calculator is enabled by default - if it is disabled, modifying of a property is accepted, but **does not** recalculate the object nor the ones that are downstream in the flowsheet.




From later 1.5 builds and up, DWSIM now includes three more buttons in the calculator control bar. The  button forces the recalculation of the entire flowsheet, while the  button stops the any ongoing calculation. The  button removes all items which may still be present in the calculator queue, waiting to be processed.




Figure 23: DWSIM's calculator control bar.

As DWSIM's calculator does its job, messages are added to the "Information" window. These messages tell the user if the object was calculated successfully or if there was an error while calculating it, among others (Figure 24).

		Date	Type	Message
	7	8/7/2008 11:21:53	Warning	COMP-000: No energy stream associated with the compressor.
	6	8/7/2008 11:13:59	Message	File C:\Documents and Settings\ DANIEL\Desktop loaded successfully.

Figure 24: A DWSIM's calculator message.



Remember that is possible to edit the simulation configuration options at any time by clicking in the  button or in the "Configurations" menu > "Configure simulation", in the DWSIM's button bar.

3.3.4 Results

Results can be viewed in reports, generated (Figures 25 and 26) for printing. Report data can also be saved to a XLS or Text file.

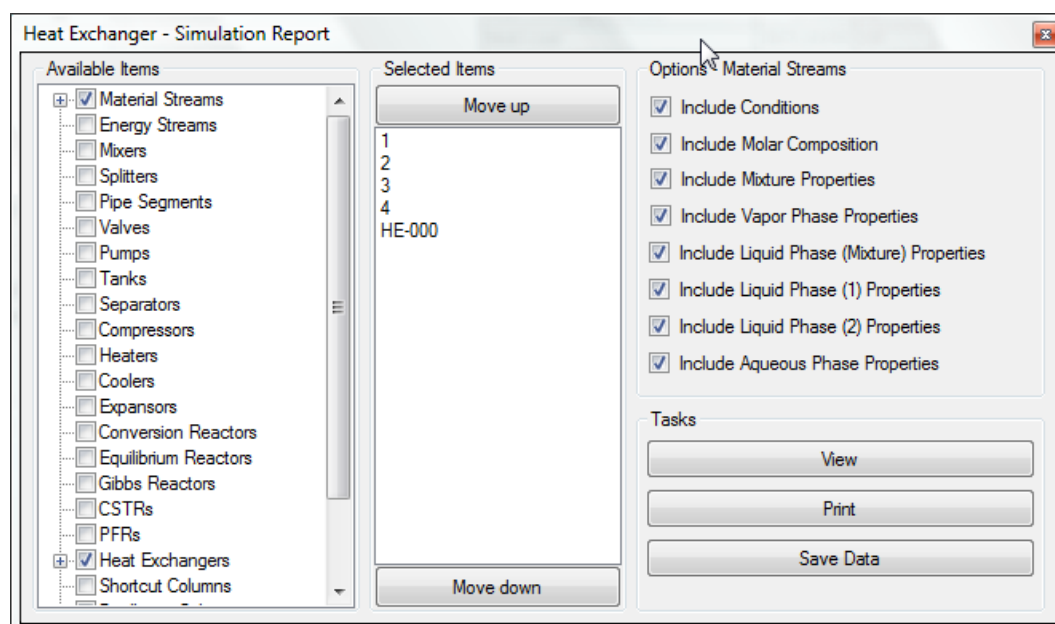


Figure 25: Results report configuration.

Relatório da Simulação
DWSIM v1.2

Detalhes
Título: Teste 1
Comentários: Simulação-teste para o Guia do Usuário do DWSIM

Corrente de Matéria: MAT-000

	Mistura	Vapor	Líquido
Definições			
Temperatura (K)	300,0	-	-
Pressão (Pa)	101325,0	-	-
Vazão mássica (kg/s)	25,0	25,0	0,0
Vazão molar (mol/s)	1084,29293	1084,29293	0,0
Vazão volumétrica (m3/s)	26,69078	26,69078	0,0
Composição em Frações Molares			
Metano (C1)	0,5	0,5	0
Etano (C2)	0,5	0,5	0
Propriedades			
Fração Molar (-)	0,0	1,0	0,0
Fração Mássica (-)	0,0	1,0	0,0
Entalpia Específica (kJ/kg)	2,02486	2,02486	0,0
Entropia Específica (kJ/(kg.K))	0,28737	0,28737	0,0
Massa Molar (kg/kmol)	23,0565	23,0565	0,0
Massa Específica (kg/m3)	0,93665	0,93665	0,0

Figure 26: Results report.

3.4 Sensitivity Analysis

You can use the Sensitivity Analysis Utility in order to study the influence of up to 2 variables into other dependent flowsheet variables. The changes in variables are defined by a value range and a number of equally spaced points within this range. For example, you can analyze the influence of temperature and pressure in the enthalpy of a mixture, from 200 to 400 K and from 100 to 1000 kPa, nine points for temperature and 5 points for pressure, totaling 45 points on which the enthalpy will be calculated at different temperatures and pressures. This also means that the flowsheet will be recalculated 45 times (!), so be careful with the number of points you choose as the calculation time can be prohibitive.

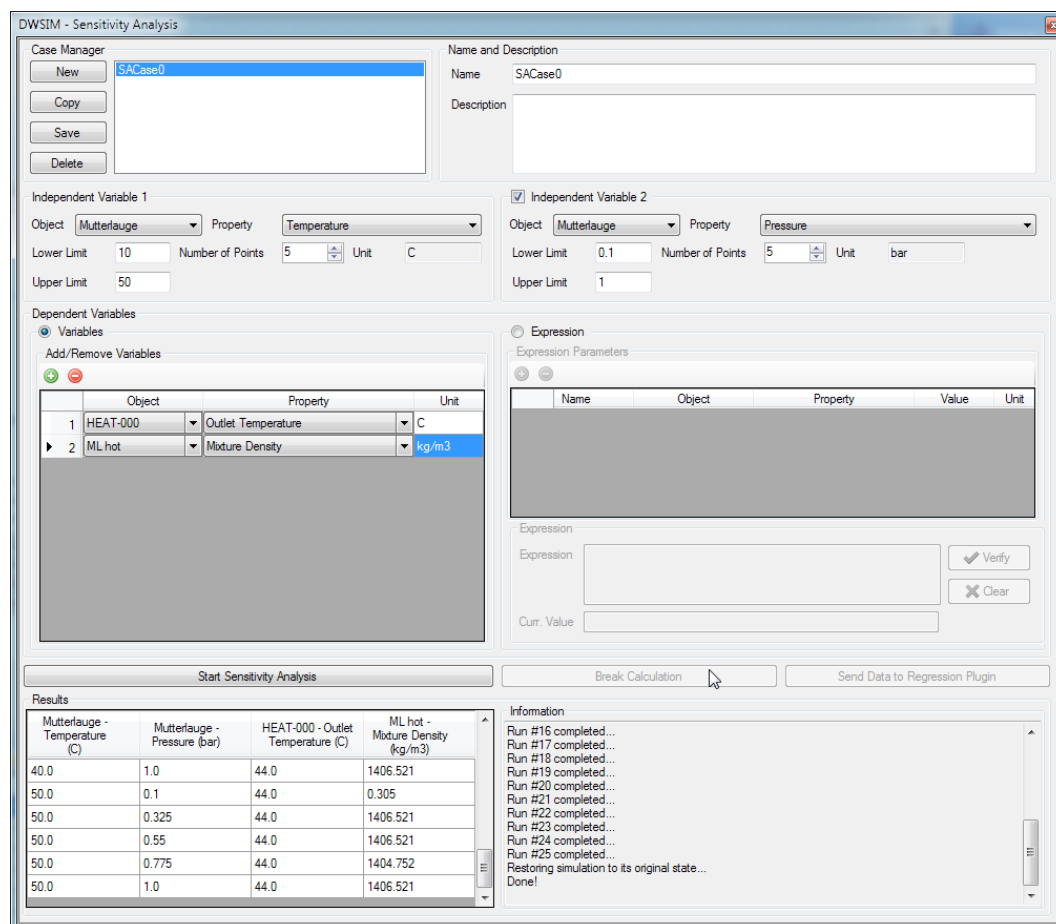


Figure 27: Sensitivity Analysis Utility (1).

The sensitivity analysis utility is based on case studies. In a single simulation one can define a number of cases, each one with its own variables, ranges and results. These cases will be saved together with the simulation, and cannot be exported to other ones. The results are shown in a table, so the data can be copied and pasted into another specialized data analysis software or sent directly to the data regression plugin.

3.5 Flowsheet Optimization

The new Optimizer in DWSIM handles single and multivariate optimization problems with or without bound constraints. The objective function can be either a variable in the flowsheet or an expression as a function of as many variables as you need.

The interface is very similar to Sensitivity Analysis's one. One can define a number of cases, each one with its own variables, ranges and results. These cases will be saved together with the current simulation, and cannot be exported to other simulations.

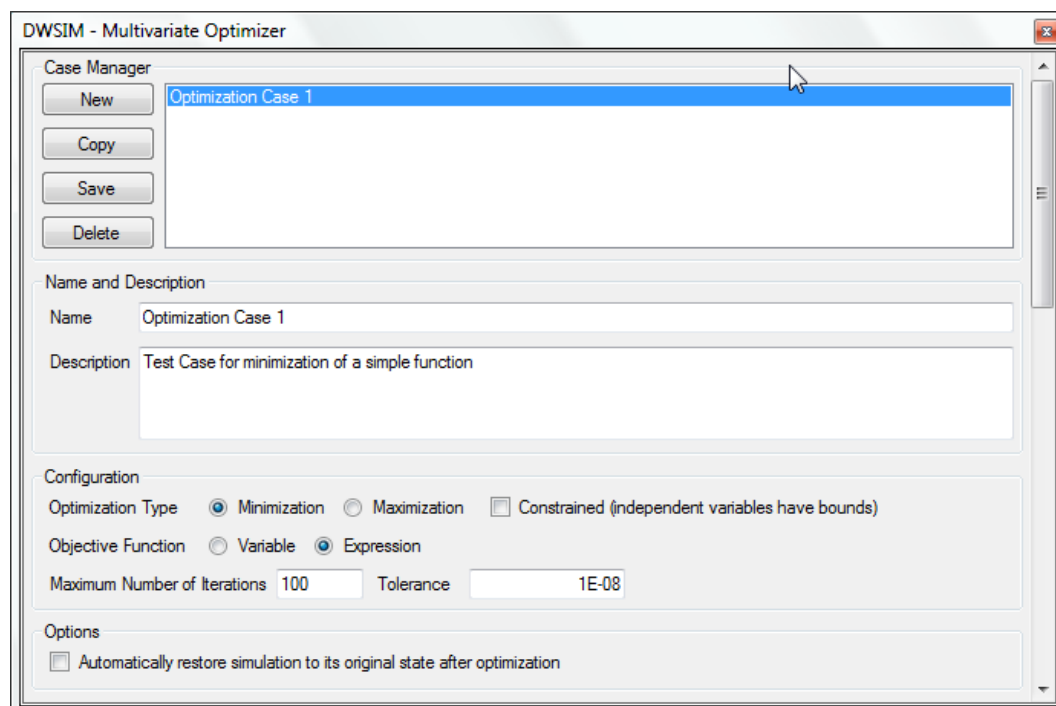


Figure 28: Multivariate Optimization Utility (1).

There are some options to choose from in DWSIM's Multivariate Optimizer. It is possible to select the type of the optimization (minimization or maximization of the objective function), choose if the independent variables will have lower and/or upper bounds and if the objective function will be a flowsheet variable or an expression based on flowsheet variables. One can also define a maximum number for the iterations and a tolerance for the variation of the calculated value for the objective function - if the variation is less than the defined value, the flowsheet is considered optimized and the process stops. There is also an option to choose if the flowsheet will be returned to its original state after optimization, so the results will be shown only in the current window, and the flowsheet initial configuration will remain intact.

In order to define variables to be used in the optimization process, a variable can be added by clicking on the "+" button. With the variable row added to the list, one chooses an object, then the desired property and the type of variable (IND for independent, AUX for auxiliary or DEP for dependent variables). If necessary, one can define a lower and/or upper limit for the IND variables, according to the current unit system. The variable name is the one which will be used in the expression.

DWSIM only considers bounds for independent variables. Also, if the objective function is a DEP variable, and you defined multiple DEP variables, only the first will be used. AUX variables are used in the context of an expression only. To remove a variable, a row must be selected by clicking at the row header before pressing the "-" button.

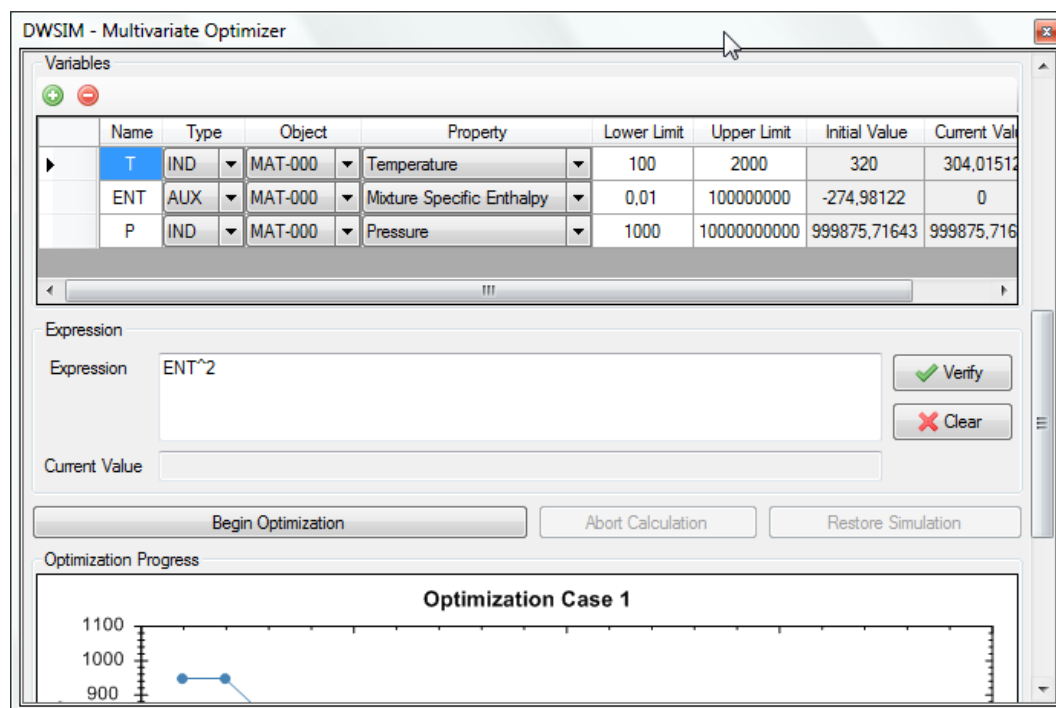


Figure 29: Multivariate Optimization Utility (2).

With all the variables defined and the case configured, the optimization can be carried out by clicking on the appropriate button - the button will become disabled. After some time, if the optimization converges, the button will become active again, indicating that the optimization process is over.

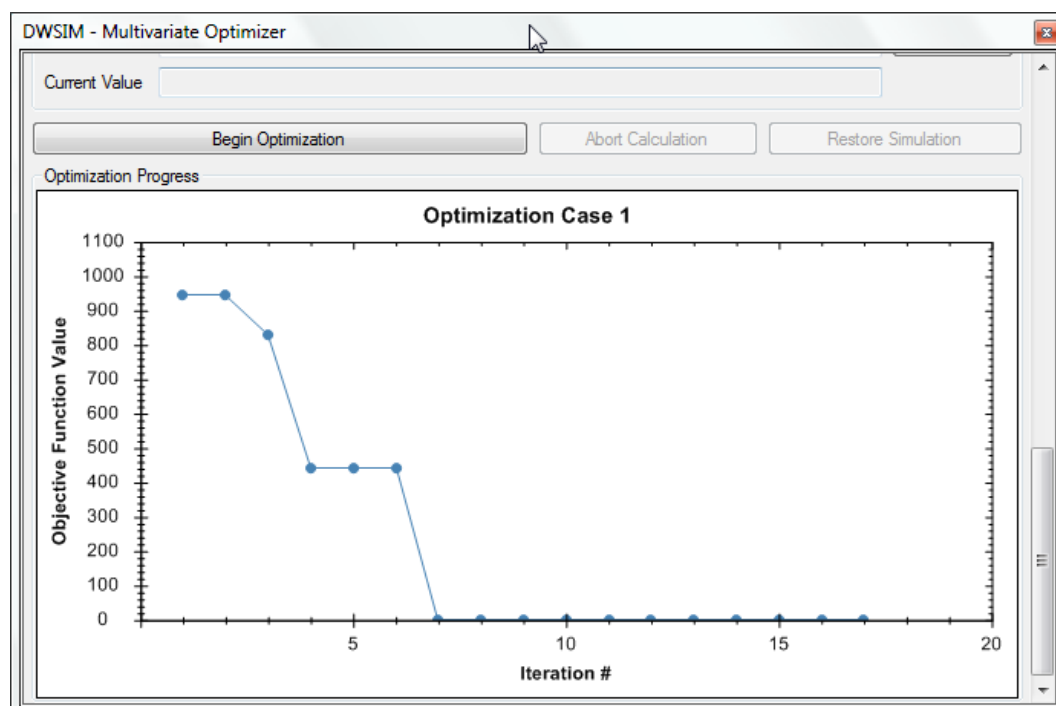


Figure 30: Multivariate Optimization Utility (3).

3.6 Utilities

DWSIM includes some utilities which provides the user with more information about the process being simulated.

→ **True Critical Point** - utility to calculate the true critical point of a mixture (Figure 31).

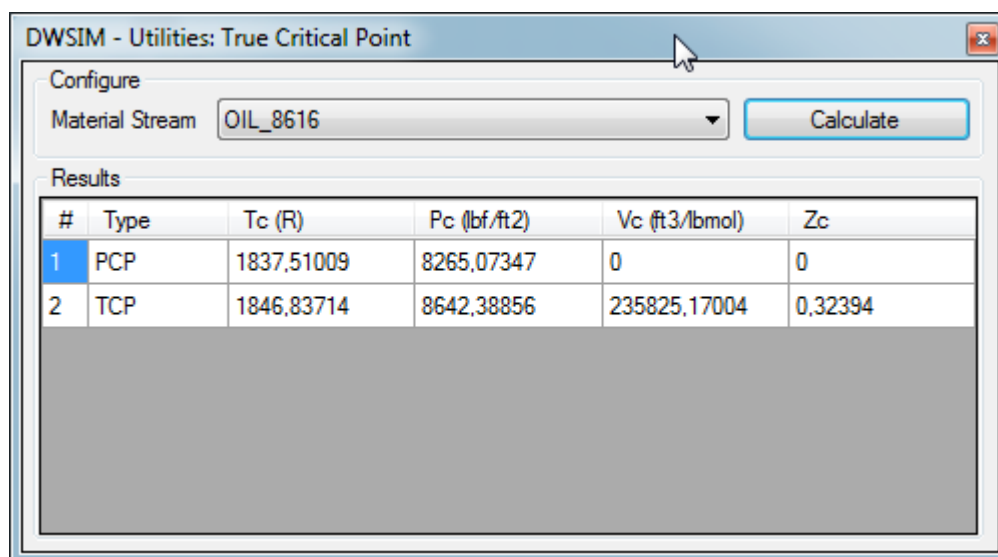


Figure 31: Utilities - True Critical Point.

→ **Hydrate Equilibrium/Dissociation Utility** - calculation of the equilibrium conditions for natural gas hydrates (Figure 32);

DWSIM - Utilities: Hydrate Dissociation Conditions

Configure

Material Stream: MAT-000

Model: van der Waals & Platteeuw (modified by Parrish & Prausnitz) (1972)

Calculate

Results

Equilibrium at stream conditions

Hydrate forms: No

Hydrate type: N/A

Equilibrium conditions at stream temperature

Pressure: 444,61554 kgf/cm2_a

Temperature: 26,85 °C

Equilibrium phases: Liquid (water), Gas and Hydrate (sl) Details

Equilibrium conditions at stream pressure

Pressure: 1,25862 kgf/cm2_a

Temperature: -2,27088 °C

Equilibrium phases: Solid (Ice), Gas and Hydrate (sl) Details

Figure 32: Utilities - Hydrate Calculations.

→ **Pure Component Properties** - pure component property viewing and editing (Figure 33);

DWSIM - Utilities: Pure Component Properties

View

Component: Toluene [Toluene] ☐ Enable Constant Property Editing [Restore Defaults](#)

Constants Molecular Ideal Gas Cp Enthalpy of Vaporization Vapor Pressure Liquid Viscosity Liquid Density Solid Density Cp Solid

Properties

Property	Value	Unit
Database	ChemSep	
Component Type	Normal	
ID	502	
CAS Number	108-88-3	
Molecular Weight	92.141	kg/kmol
Critical Temperature	591.75	K
Critical Pressure	4108000.0	Pa
Critical Volume	0.316	m ³ /kmol
Critical Compressibility	0.264	
Acentric Factor	0.264	
Ideal Gas Enthalpy of Formation at 25 °C	544.49159	kJ/kg
Ideal Gas Gibbs Energy of Formation at 25 °C	1326.22828	kJ/kg
Normal Boiling Point	383.79	K
Temperature of Fusion	178.18	K
Enthalpy of Fusion @ Tf	6.636	kJ/mol
Solid Density Temperature	0.0	K
Solid Density @ Ts	0.0	kg/m ³
Chao-Seader Acentric Factor	0.2591	-
Chao-Seader Solubility Parameter	0.00436	(cal/mL) ^{0.5}
Chao-Seader Liquid Molar Volume	106.8	mL/mol
Rackett Compressibility	0.2646	

Figure 33: Utilities - Pure Component Properties.

→ **Phase Envelope** - Material stream phase equilibria envelope calculation (Figure 34);

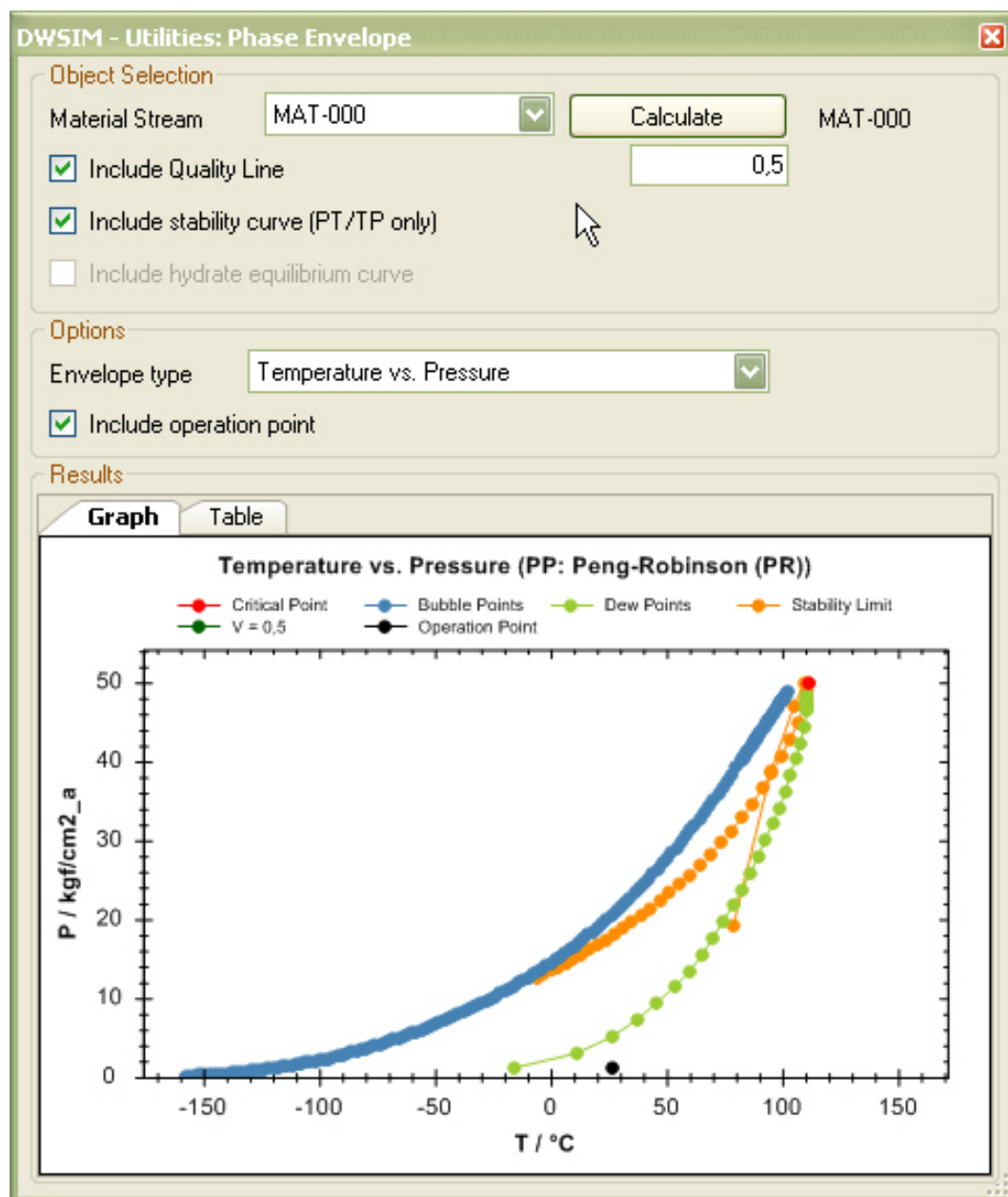


Figure 34: Utilities - Phase Envelope.

→ **Binary Envelope** - special envelopes for binary mixtures (Figure 35).

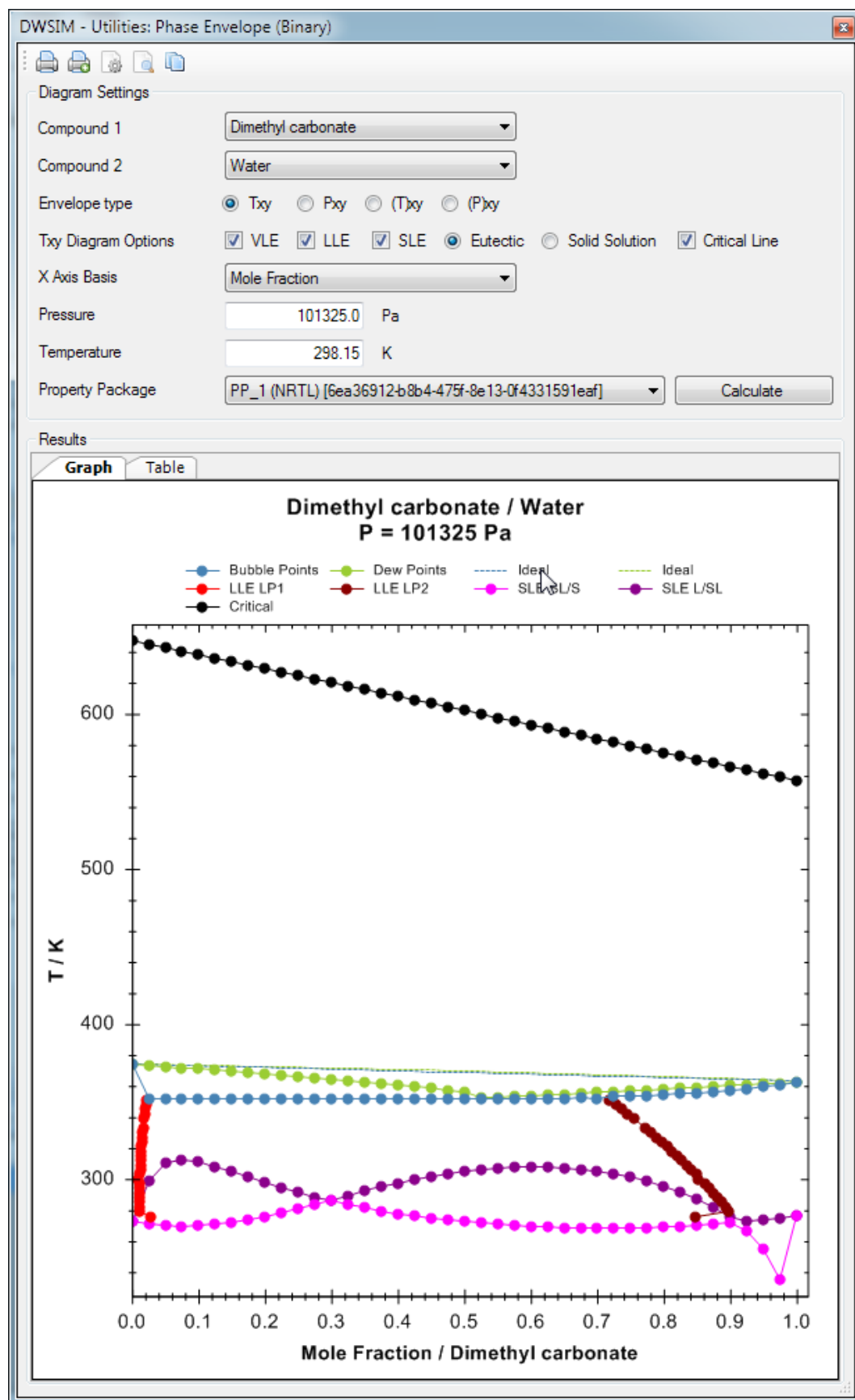
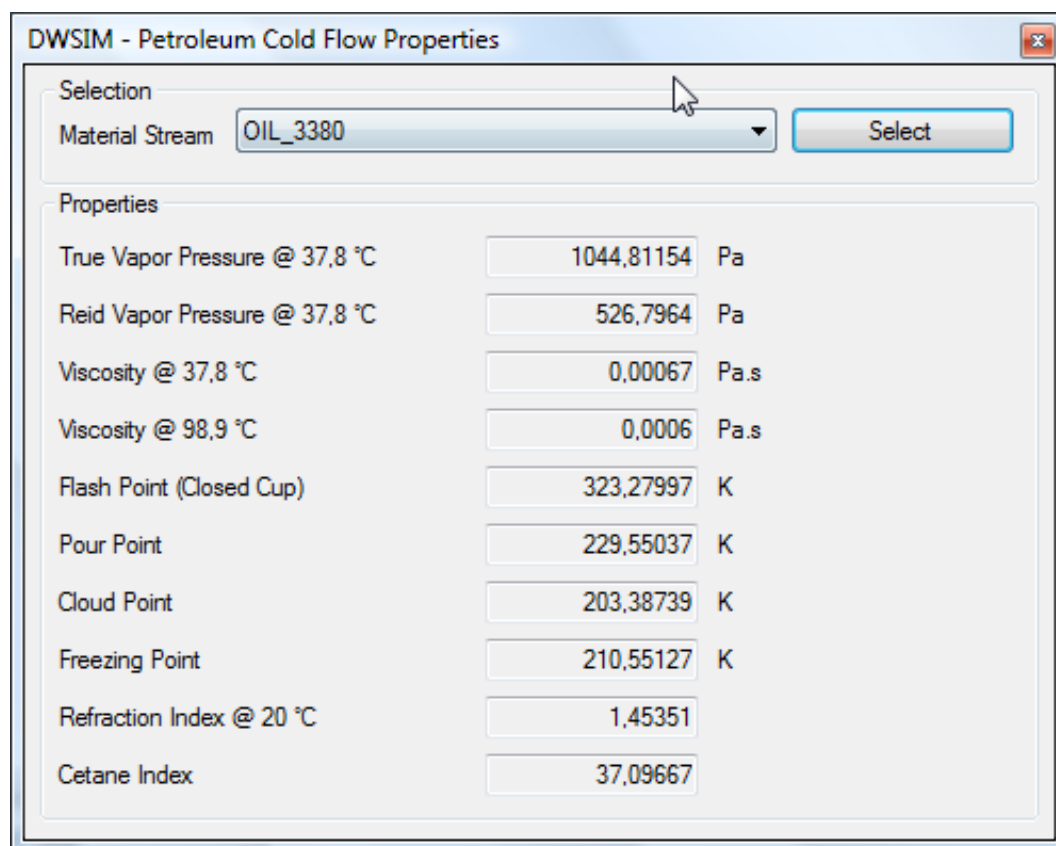


Figure 35: Utilities - Binary Envelope.

→ **Petroleum Cold Flow Properties** - special properties of petroleum fractions, like cetane index, flash point, refraction index, etc. (Figure 36).



DWSIM - Petroleum Cold Flow Properties		
Selection		
Material Stream	OIL_3380	Select
Properties		
True Vapor Pressure @ 37,8 °C	1044,81154	Pa
Reid Vapor Pressure @ 37,8 °C	526,7964	Pa
Viscosity @ 37,8 °C	0,00067	Pa.s
Viscosity @ 98,9 °C	0,0006	Pa.s
Flash Point (Closed Cup)	323,27997	K
Pour Point	229,55037	K
Cloud Point	203,38739	K
Freezing Point	210,55127	K
Refraction Index @ 20 °C	1,45351	
Cetane Index	37,09667	

Figure 36: Utilities - Petroleum Cold Flow Properties.

Utilities calculate their properties for one object only, which is selected inside their own windows. In the majority of cases, this object must be calculated in order to be available for selection in the utility window.



Please view DWSIM's Technical Manual for more details about the models and methods used by the Utilities.

3.7 Chemical Reactions

DWSIM classifies chemical reactions in three different types: Conversion, where the conversion of a reagent can be specified as a function of temperature; Equilibrium, where the reaction is characterized by an equilibrium constant K, and Kinetic, where the reaction is led by a velocity expression which is a function of concentration of reagents and/or products.



Please view DWSIM's *Technical Manual and Equipment and Utilities Guide* for more details about chemical reactions and reactors, respectively.

Chemical reactions in DWSIM are managed through the **Chemical Reactions Manager** (Simulation Settings > Thermodynamic and Reactions) (Figure 37):

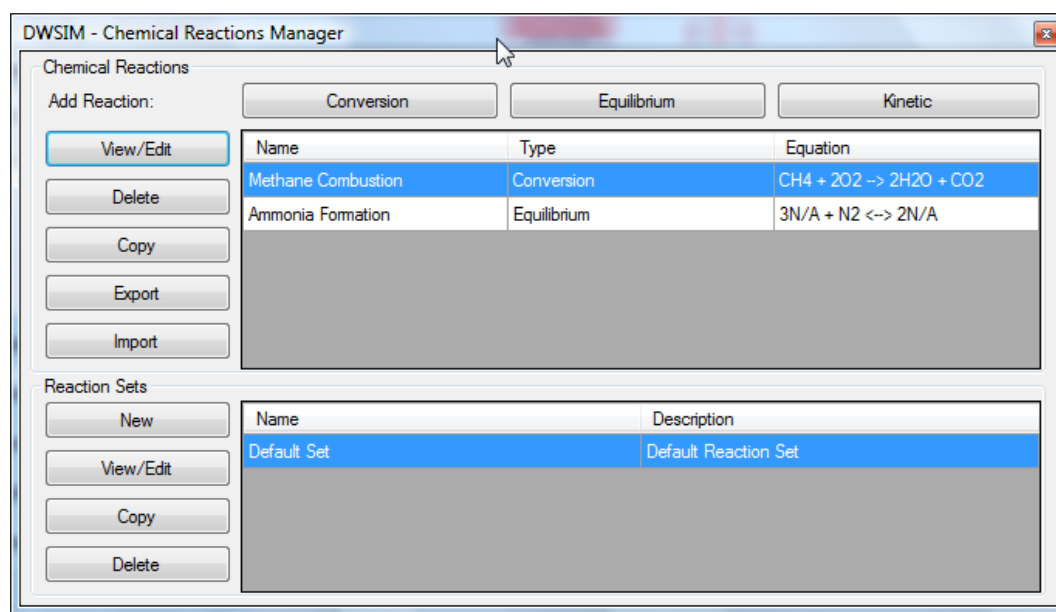


Figure 37: Chemical Reactions Manager.

The user can define various reactions which are grouped in *Reaction Sets*. These reaction sets list all chemical reactions, and the user must activate only those he wants to become available for one or more reactors (since the reactor's parameter is the **reaction set** and not the chemical reactions themselves). In the reaction set configuration window it is also possible to define the reaction ordering. Equal indexes define parallel reactions (Figure 38):

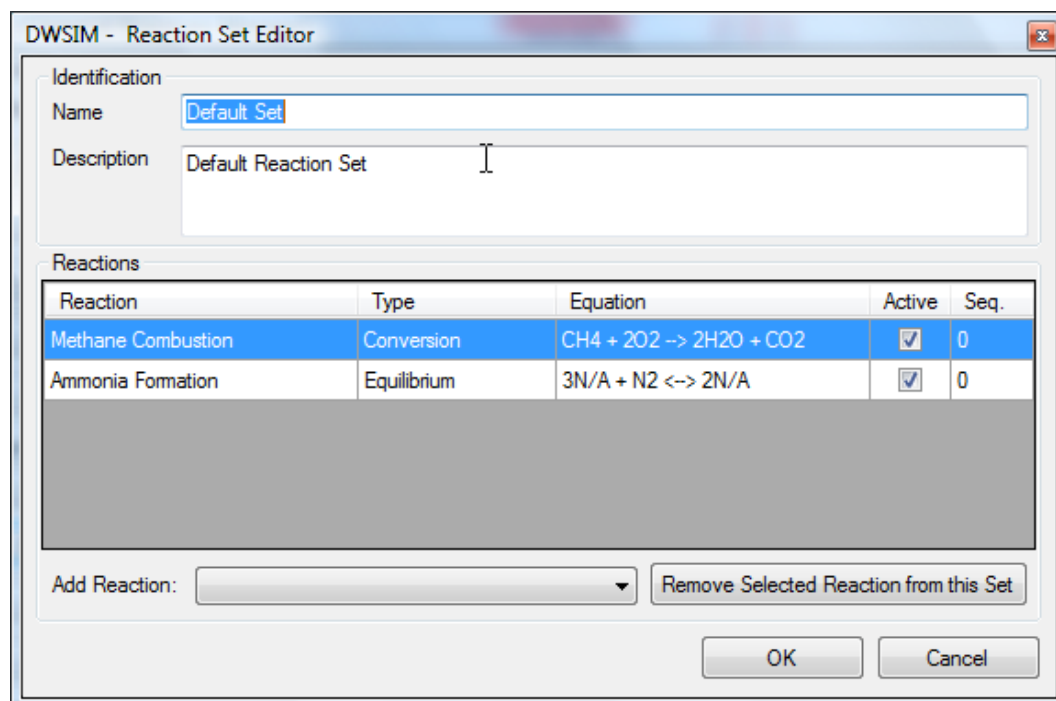


Figure 38: Reaction Set editor.

When the reactions and their respective reaction sets are correctly defined, the last will be available for selection in the property window of a reactor in the simulation. The reactor will then look for active reactions inside the selected set (Figure 39):

Object	RC-000									
Type	Reator de Conversão									
Status	Calculated									
<div> <div>Properties</div> <div>Format Object</div> <div></div> </div>										
<div> <div>1. Connections</div> <table> <tr><td>Input Stream</td><td>1</td></tr> <tr><td>Vapor outlet</td><td>2</td></tr> <tr><td>Liquid outlet</td><td>3</td></tr> <tr><td>Energy Stream</td><td>e1</td></tr> </table> </div>			Input Stream	1	Vapor outlet	2	Liquid outlet	3	Energy Stream	e1
Input Stream	1									
Vapor outlet	2									
Liquid outlet	3									
Energy Stream	e1									
<div> <div>2. Parameters of calculation</div> <table> <tr><td>Reaction Set</td><td>Default Set</td></tr> <tr><td>Operation Mode</td><td>Isothermic</td></tr> <tr><td>Pressure drop (Pa)</td><td>0,0</td></tr> </table> </div>			Reaction Set	Default Set	Operation Mode	Isothermic	Pressure drop (Pa)	0,0		
Reaction Set	Default Set									
Operation Mode	Isothermic									
Pressure drop (Pa)	0,0									
<div> <div>3. Results</div> <table> <tr><td>Delta T (K)</td><td>0,0</td></tr> <tr><td>Heat Load (kW)</td><td>-3841071,32356</td></tr> </table> </div>			Delta T (K)	0,0	Heat Load (kW)	-3841071,32356				
Delta T (K)	0,0									
Heat Load (kW)	-3841071,32356									
<div> <div>Reactions and Conversions (%)</div> <div>(...)</div> <table> <tr><td>Methane Combustion</td><td>90,3</td></tr> </table> </div>			Methane Combustion	90,3						
Methane Combustion	90,3									
<div> <div>Property Package</div> </div>										
<div> <div>Reactions and Conversions (%)</div> <div>Show active reactions and their conversions, in percent (%).</div> </div>										

Figure 39: Reaction set in a reactor's property window.

3.8 Characterization of Petroleum Fractions

DWSIM provides two tools for characterization of petroleum fractions ("Simulation Settings" > "Tools" > "Petroleum Characterization"). One of them characterizes C7+ fractions from bulk properties (Figure 40). The other characterizes the oil from an ASTM or TBP distillation curve (Figure 41).

In both tools, the characterization is done through the creation of various components with different boiling points (pseudocomponents) which together represent the assay as a whole.

- **Characterization from bulk properties** The method itself requires a minimum of information to generate the pseudocomponents, though the more data the user provides, the better will

be the results (Figure 40). It is recommended that the user provides the specific gravity of the C7+ fraction at least. Viscosity data is also very important.

DWSIM - Bulk C7+ Petroleum Characterization

General Options

Input Data

Molecular Weight (MW) kg/kmol

Specific Gravity (d60/60) 0,87 [adimensional]

Avg. Boiling Temperature K

Viscosity data (leave blank to calculate)

T1 37,78 °C Visc 1 cSt

T2 98,89 °C Visc 2 cSt

Pseudocomponents 10

Properties

Name	Molar Fraction	NBP (K)	SG	MW (kg/kmol)	Tc (K)	Pc (Pa)	Ac. Factor
PSE_6491_2	0,1	430,57251	0,77497	129,94632	618,25856	2530230,32513	0,37296
PSE_6491_3	0,1	500,9978	0,81593	176,79062	690,99271	2016624,06851	0,47662
PSE_6491_4	0,1	551,17542	0,84061	217,03795	740,01856	1724984,07188	0,55751
PSE_6491_5	0,1	597,69994	0,86098	260,64929	783,70248	1499466,04091	0,63883
PSE_6491_6	0,1	644,70208	0,87962	312,24068	826,31569	1307894,75544	0,72834
PSE_6491_7	0,1	695,01427	0,89786	377,99601	870,44868	1136179,01316	0,83402
PSE_6491_8	0,1	751,84282	0,91681	469,53874	918,71932	976137,35063	0,96845
PSE_6491_9	0,1	820,24094	0,93797	614,91426	975,0268	821876,09522	1,15726

Stream Name OIL_4565

Figure 40: C7+ petroleum fraction characterization utility.

- **Characterization from distillation curves** This tool gets data from an ASTM or TBP distillation curve to generate pseudocomponents. It is also possible to include viscosity, molecular weight and specific gravity curves to enhance the characterization.

The interface has a wizard-like style, with various customization options (Figure 41):

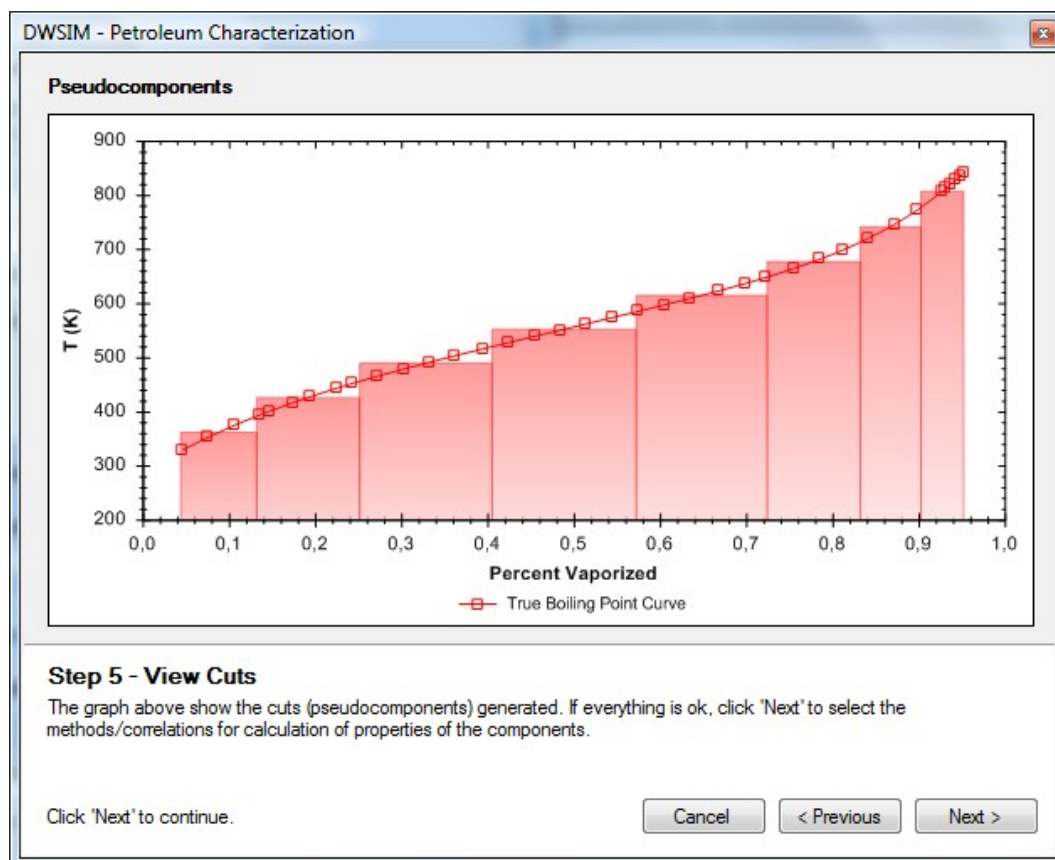


Figure 41: Characterizing petroleum from distillation curves.

After the pseudocomponents are created, a material stream with a defined composition is also created, which represents the characterized petroleum fraction.



The hypo and pseudocomponents are available for use only in the simulation in which they were generated, even if there is more than one opened simulation in DWSIM. Nevertheless, the user can export these components to a file and import them into another simulation.

4 Compound Creator

4.1 Component Databases

4.1.1 Databases

The components available for use in simulations are grouped in *databases*. DWSIM comes with one database with the most common compounds used in the petroleum industry plus some alcohols and inert gases. It is also possible to load the database from *ChemSep™ LITE*. If you installed ChemSep, DWSIM will try to load its database automatically.

Databases in DWSIM can be managed through a window which can be opened from the Main Menu > Settings > General Settings (Figure 42):

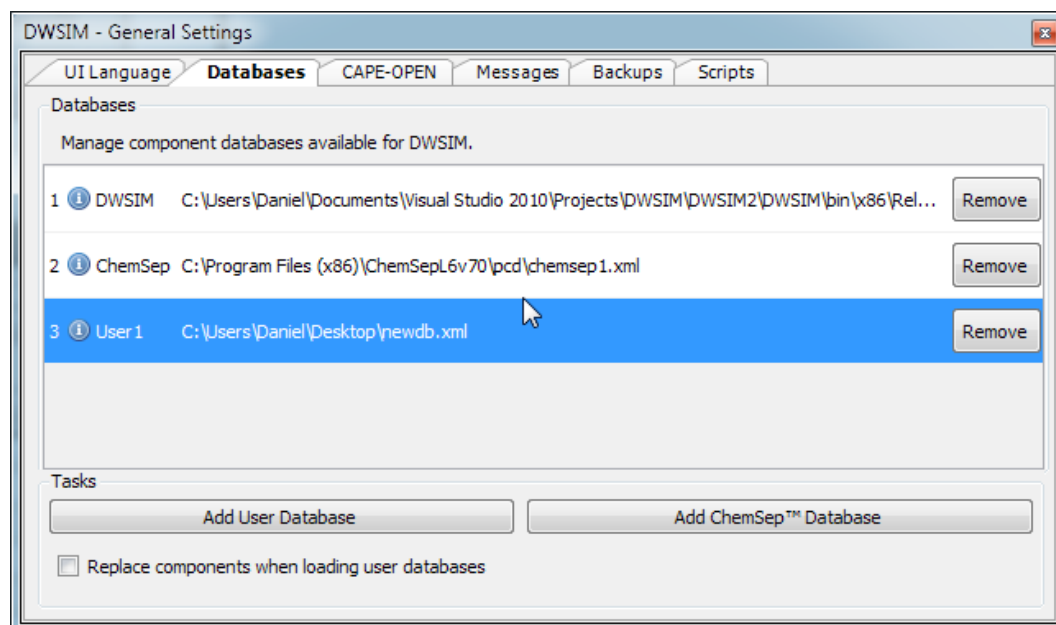


Figure 42: Database manager.

On this window the user can add and/or remove modified databases (created from the **Components** tab in the **Simulation Settings** window) and add the ChemSep™ database, if it has not been loaded automatically. The DWSIM database cannot be modified nor deleted.

User databases can be created and managed through the **Compound Creator Utility**, which unifies the Quick Component Creator and Hypothetical Component utilities into a single, easy-to-use tool.

4.2 About the Compound Creator Utility

The Compound Creator puts together the features found in the Hypothetical and Quick Compound Creator, allowing the user to save his compounds into a database that can be loaded later globally in DWSIM, that is, your compounds can be used in all simulations, not only in the one that they were created. The Compound Creator also allows you to save and load your compound creation study/case for later use.

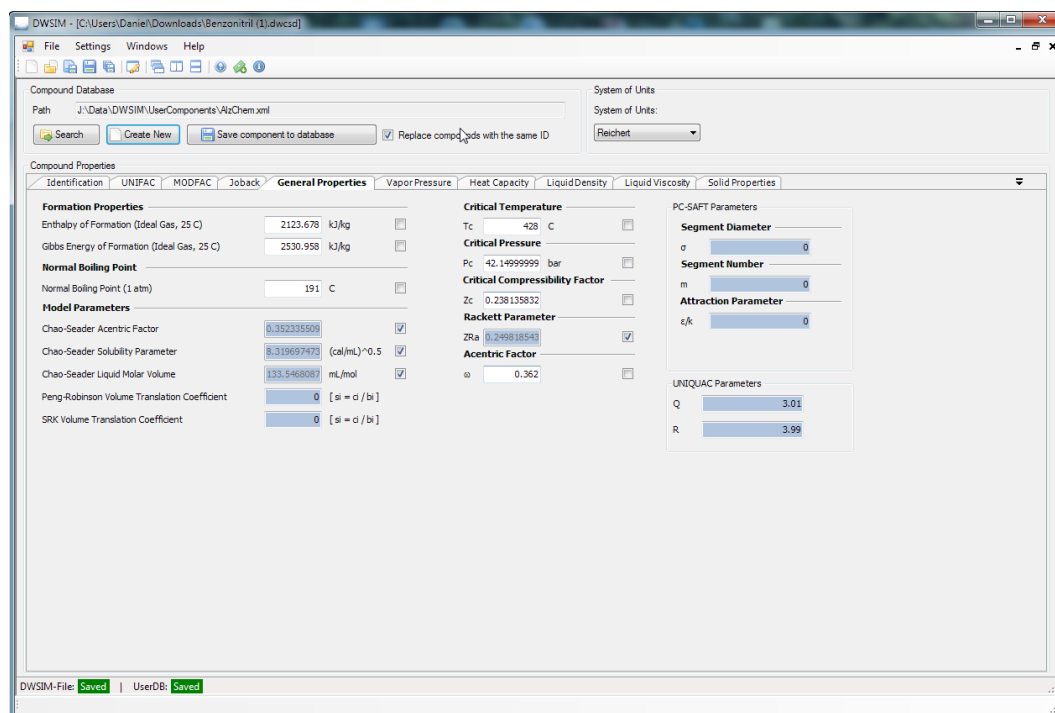


Figure 43: Compound Creator Utility.

5 Data Regression

DWSIM can regress experimental binary VLE/LLE/SLE data in order to calculate interaction parameters for a variety of thermodynamic models. This way you can calculate interaction parameters for compounds in DWSIM and ChemSep databases that do not have them or calculate parameters between known compounds and one that you just created using the Compound Creator utility.

5.1 About the Data Regression Utility

The Data Regression Utility supports regression of experimental binary data for determination of interaction parameters for the following models:

- PC-SAFT
- Peng-Robinson
- Peng-Robinson-Stryjek-Vera 2
- Soave-Redlich-Kwong
- UNIQUAC
- NRTL
- Lee-Kesler-Plöcker

The following data sets are supported:

- ➔ VLE Temperature and molar fractions (Txy)
- ➔ VLE Pressure and molar fractions (Pxy)
- ➔ VLE Temperature, Pressure and molar fractions (TPxy)
- ➔ LLE Temperature and molar fractions (Txx)
- ➔ LLE Pressure and molar fractions (Pxx)
- ➔ LLE Temperature, Pressure and molar fractions (TPxx)
- ➔ SLE Temperatures and mole fractions (TTx)

The Data Regression Utility also possesses some handy additional features like:

- ➔ Calculation of initial values for the binaries using UNIFAC/MODFAC structure information
- ➔ Calculation of missing experimental data using known models/binaries for determination of parameters for other models
- ➔ Optimization method selection
- ➔ Objective Function selection (Least Squares of temperature/pressure plus vapor fractions)

The Data Regression Utility also supports loading and saving of a regression study/case for later use.

Currently, there is no way to export the generated binaries for a simulation or a database - you'll have to do this manually.

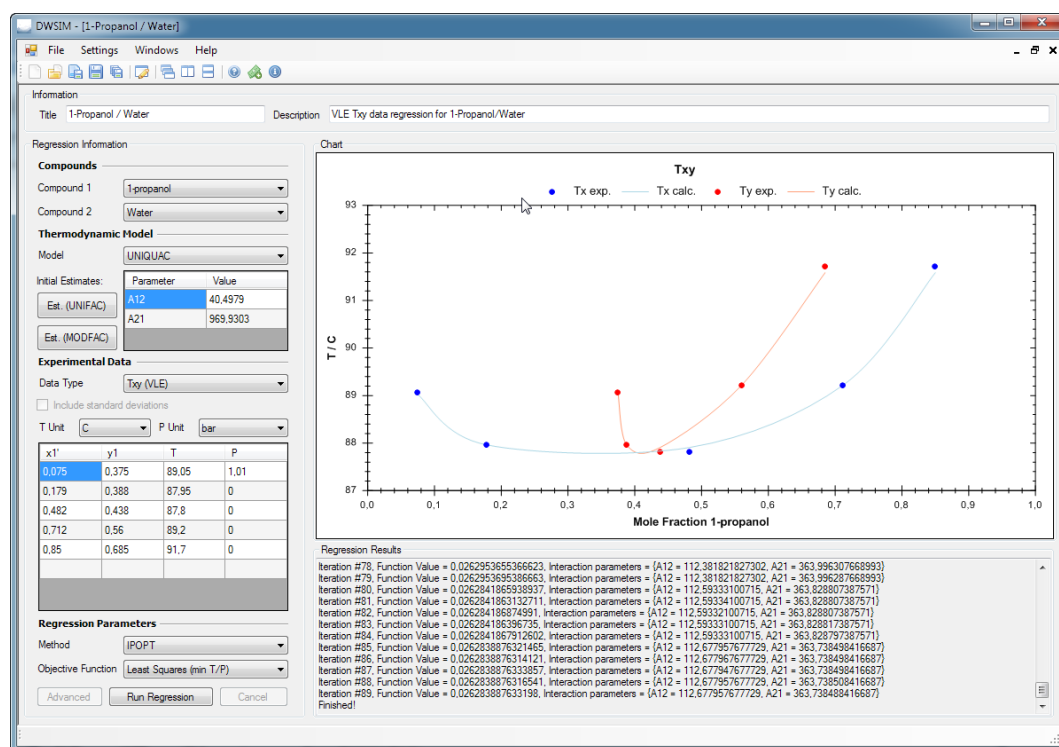


Figure 44: Data Regression Utility.