DWSIM - Process Simulation, Modeling and Optimization
User Guide

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Contact Information

DWSIM - Process Simulation, Modeling and Optimization

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Contents

List of Figures

1 Introduction

This document gives a detailed description about how to setup, run, modify and view results of a basic process simulation in DWSIM. The document is organized according to the sequence of execution of a 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 context-sensitive help available inside the application by through the 'F1' key.

Visit DWSIM's Wiki for more up-to-date information about DWSIM, including general usage tips and tricks.

2 Welcome screen

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

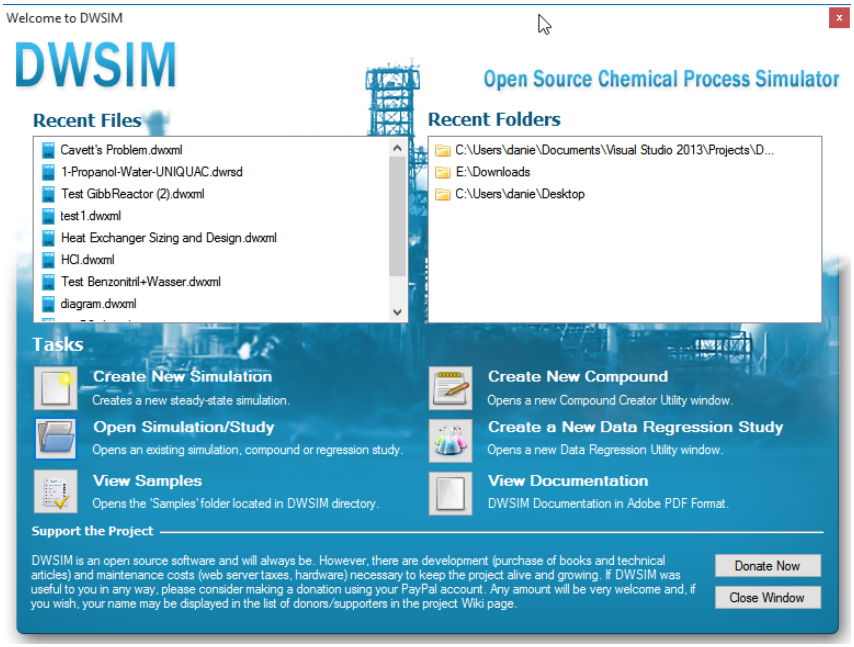


Figure 1: DWSIM's welcome screen.

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. The "Close Window" button closes the window and shows the main DWSIM interface.

In the main DWSIM window, the following items can be seen:

- ***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.;

> ***The menu bar is filled with other items if a simulation file is opened in DWSIM.***

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

There are various ways 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 tabbed window:

- ***Compounds*** - Add or remove compounds to/from the simulation and petroleum fractions (pseudocompounents) utilities.
- ***Basis*** - Property Package configuration and management of chemical reactions.
- ***Advanced Thermo*** - Phase equilibrium flash algorithm selection and other advanced thermodynamic model settings.
- ***Units System*** - Units system management.
- ***Miscelaneous*** - Simulation info (title, author and description), number formatting and password settings.

3.2 Configuration

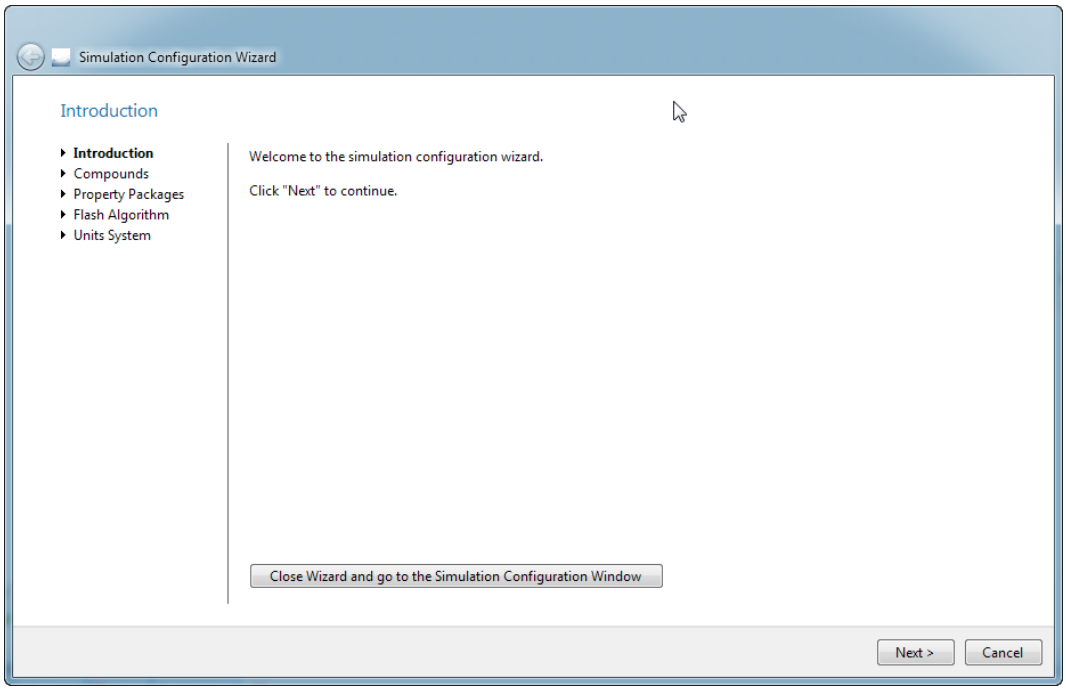


Figure 2: Simulation Configuration Wizard.

Starting from DWSIM 3.3, a new Simulation Configuration Wizard (Figure 2) is opened as soon as a new simulation is created, and will display the interfaces described in the following sections in a more streamlined way. The older simulation configuration window can be accessed anytime during the simulation or through a button located in the first page of the config wizard.

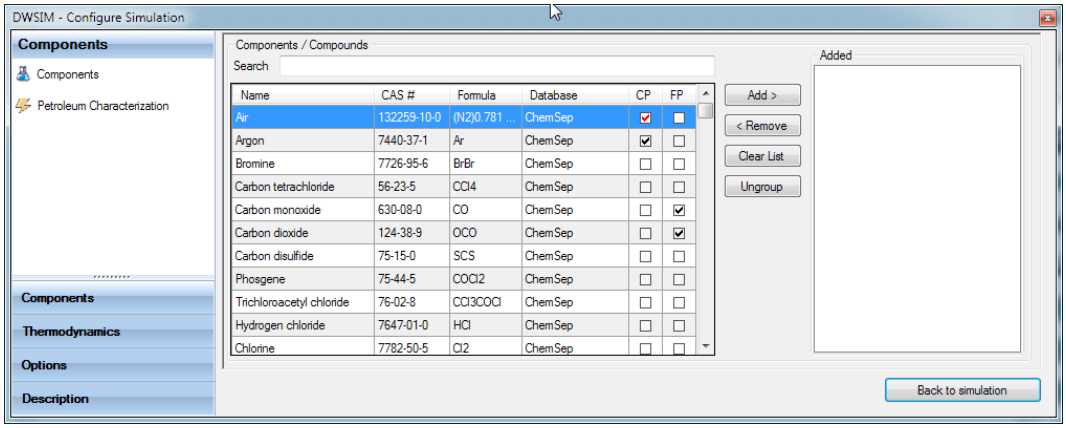


Figure 3: Simulation configuration window.

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 simulation configuration window can be accessed anytime when a simulation is opened in DWSIM. The changes made through it have immediate effect on the simulation.***

3.2.1 Components/Compounds

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

3.2.2 Basis

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. The figure 4 shows the interface for configuration of the property package.

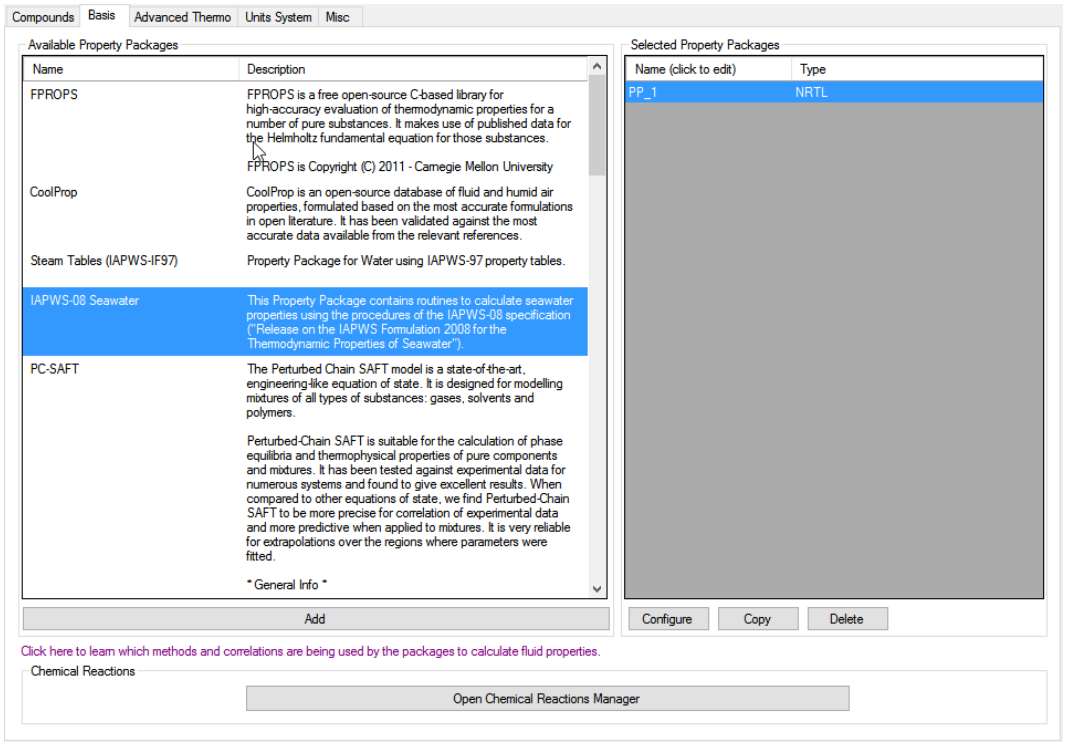


Figure 4: Property Package configuration interface.

3.2.3 Advanced Thermo

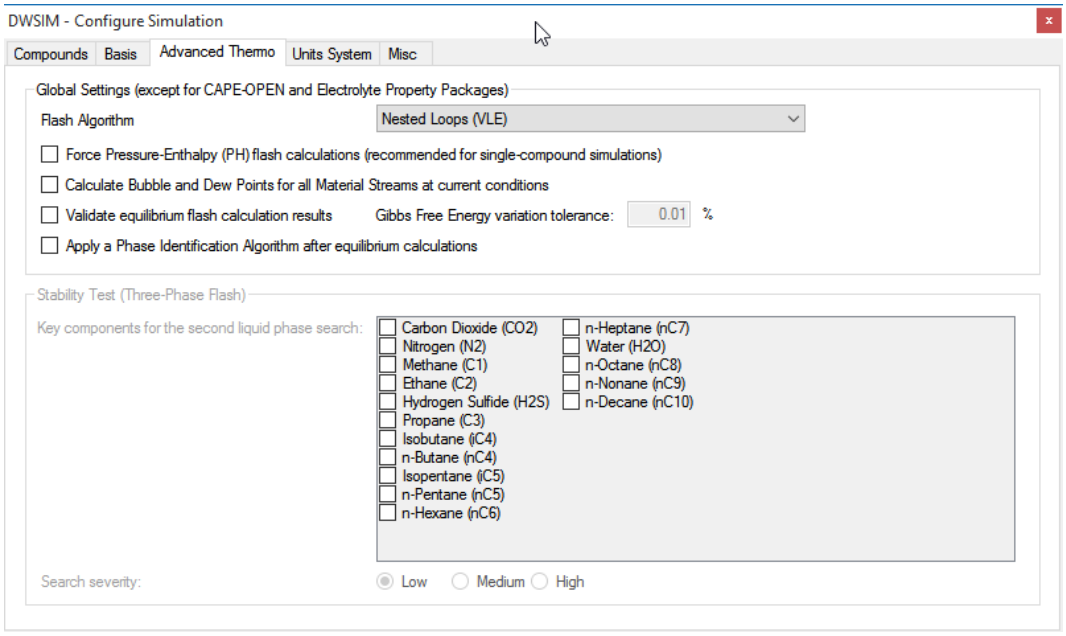


Figure 5: Property Package configuration interface.

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 (VLE):** recommended for the vast majority of VLE systems;
2. **Nested Loops (VLLE):** recommended for systems where the liquid phase may be unstable (will split in two liquid phases with different compositions);
3. **Inside-Out (VLE/VLLE):** 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);
4. **Gibbs Minimization (VLE/VLLE):** recommended for difficult chemical systems;
5. **Nested Loops for Eutectic Solid Systems (SLE-E):** Calculates Solid-Liquid Equilibria for eutectic systems considering the solid phase as being ideal.
6. **Nested Loops for Solid Solution Systems (SLE-SS):** Calculates Solid-Liquid Equilibria for solid solution systems considering the solid phase as being ideal.
7. **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.

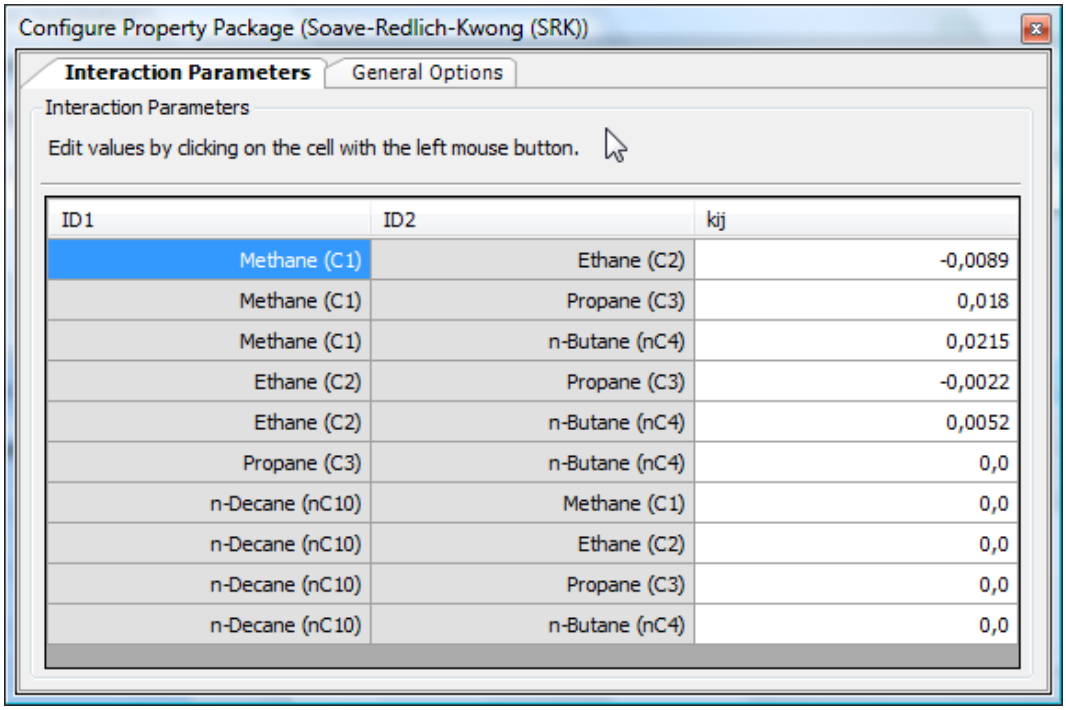
➙ *Stability Test*

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).



ID1	ID2	kij
Methane (C1)	Ethane (C2)	-0,0089
Methane (C1)	Propane (C3)	0,018
Methane (C1)	n-Butane (nC4)	0,0215
Ethane (C2)	Propane (C3)	-0,0022
Ethane (C2)	n-Butane (nC4)	0,0052
Propane (C3)	n-Butane (nC4)	0,0
n-Decane (nC10)	Methane (C1)	0,0
n-Decane (nC10)	Ethane (C2)	0,0
n-Decane (nC10)	Propane (C3)	0,0
n-Decane (nC10)	n-Butane (nC4)	0,0

Figure 6: Property package configuration window (1).

➙ *Enable Flash Algorithm Fast Mode*

Use this setting to define the calculation scheme for the current flash algorithm. Fast mode (setting equal to 1) is the default mode which has been used up to DWSIM 3.3. Try disabling this setting (set to 0) if your simulation is having trouble converging compressors, expanders and valves in extreme conditions (near to the critical point).

➙ *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).

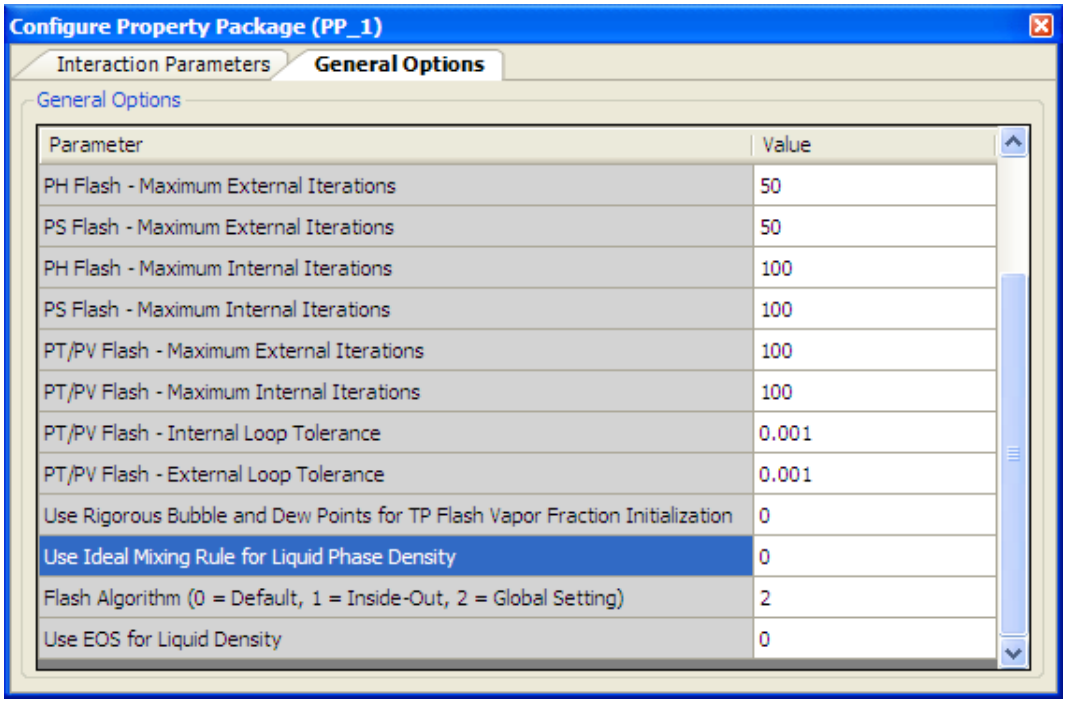


Figure 7: Property package configuration window for EOS-based models.

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 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.

➙ *Enthalpy/Entropy/Cp calculation method (Activity Coefficient Property Packages only)*

Defines the Enthalpy, Entropy and Heat Capacity calculation model (0 = Lee-Kesler, 1 = Ideal, 2 = Excess).

➙ *Ignore maximum salinity limit (IAPWS-08 Seawater Property Package only)*

Ignores the maximum supported salinity value (0.12 kg/kg) for calculations and doesn't display any warnings. Use 0 to disable, 1 to enable this option. If enabled, the calculated salinity will be send directly to the property calculation routines without further check. If disabled, the maximum value of 0.12 will be used if the calculated salinity is higher, and a warning message will be displayed in the flowsheet log window.

3.2.4 Units systems

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).

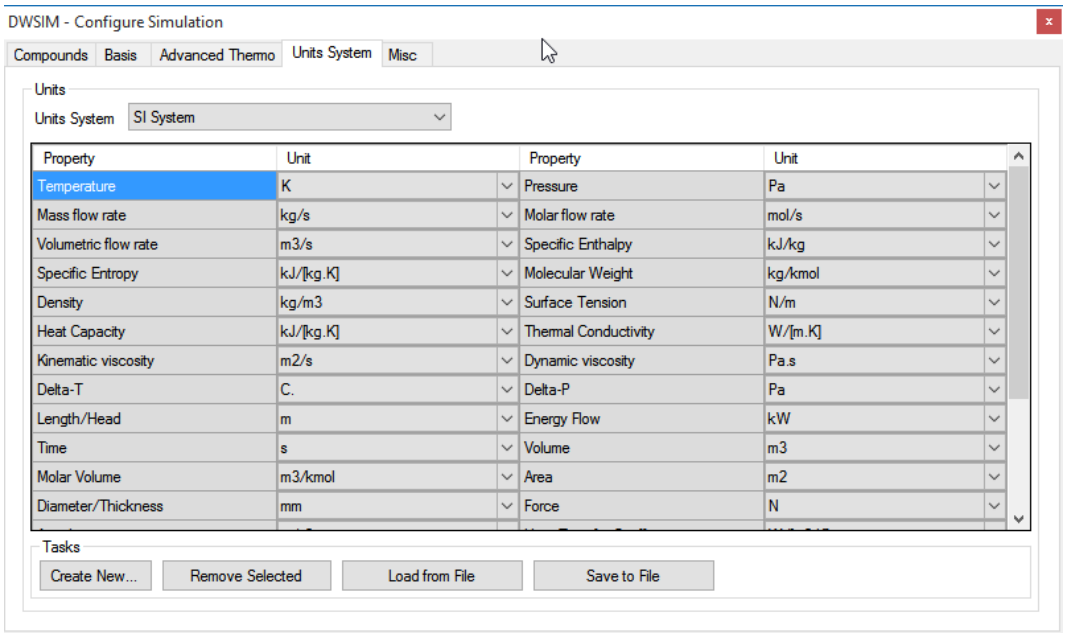


Figure 8: Units system configuration interface.

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.

3.2.5 Miscelaneous

In the "Misc" section it is possible to define the number formatting in the simulation (Figure 9). In the "Description" group box 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).

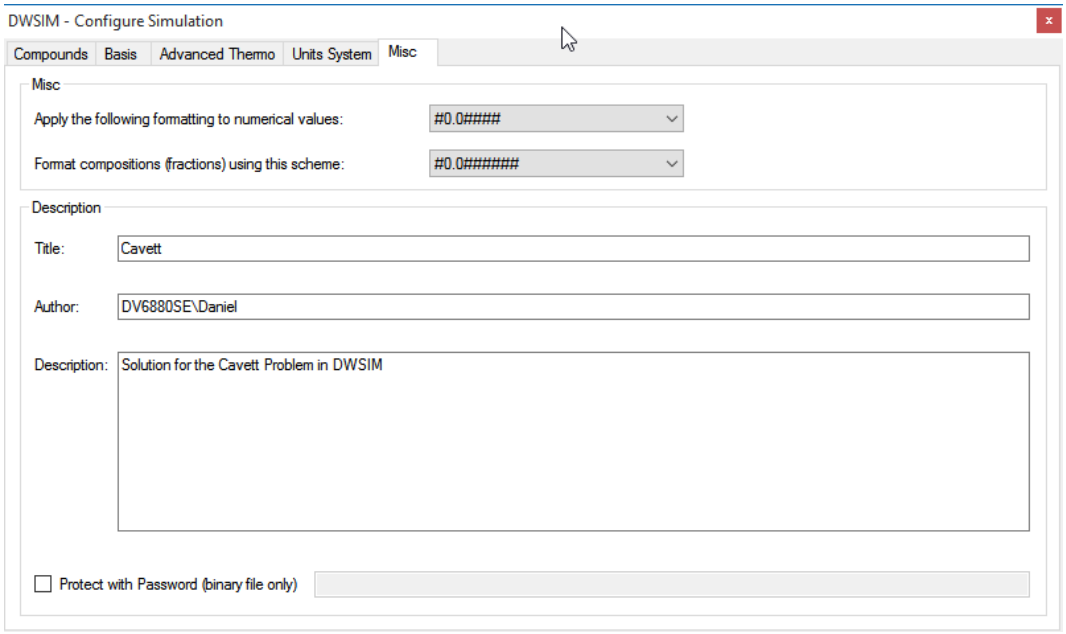


Figure 9: Misc settings interface.

3.3 Process modeling (Flowsheeting)

After configuring the simulation, the user is taken to the main simulation window (Figure 10). In this window we can highlight the following areas:

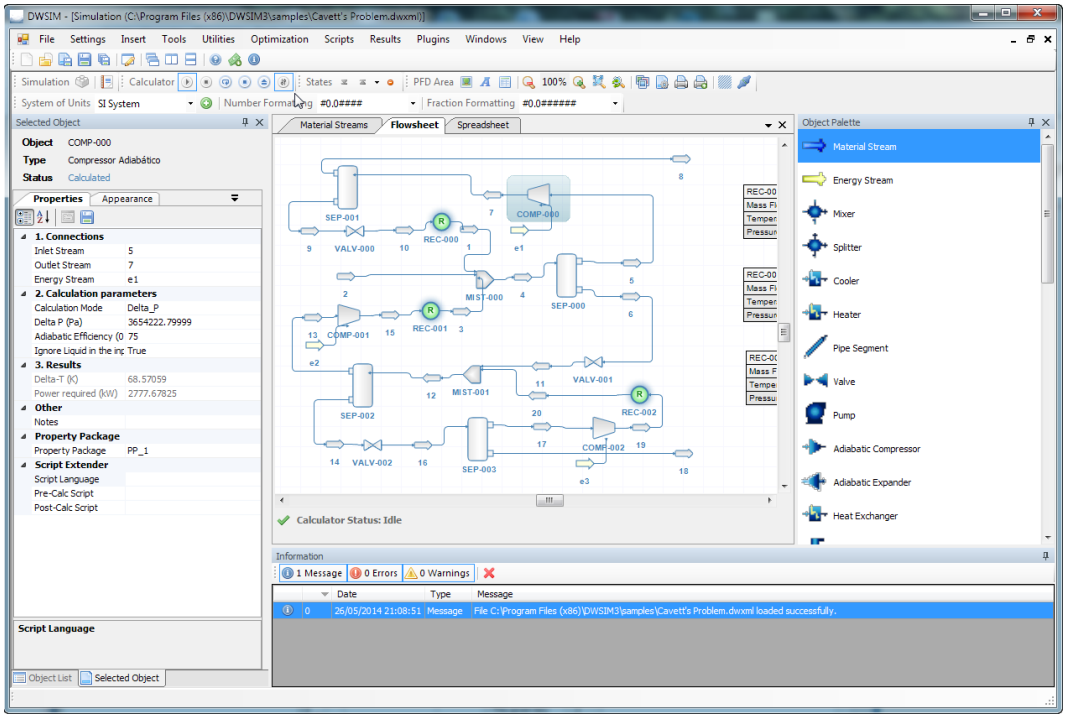


Figure 10: Simulation interface.

➙ ***Menu bars*** (left-right / up-down): simulation configuration, results viewer, image ant 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.

When running DWSIM on a Windows platform, 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 11).

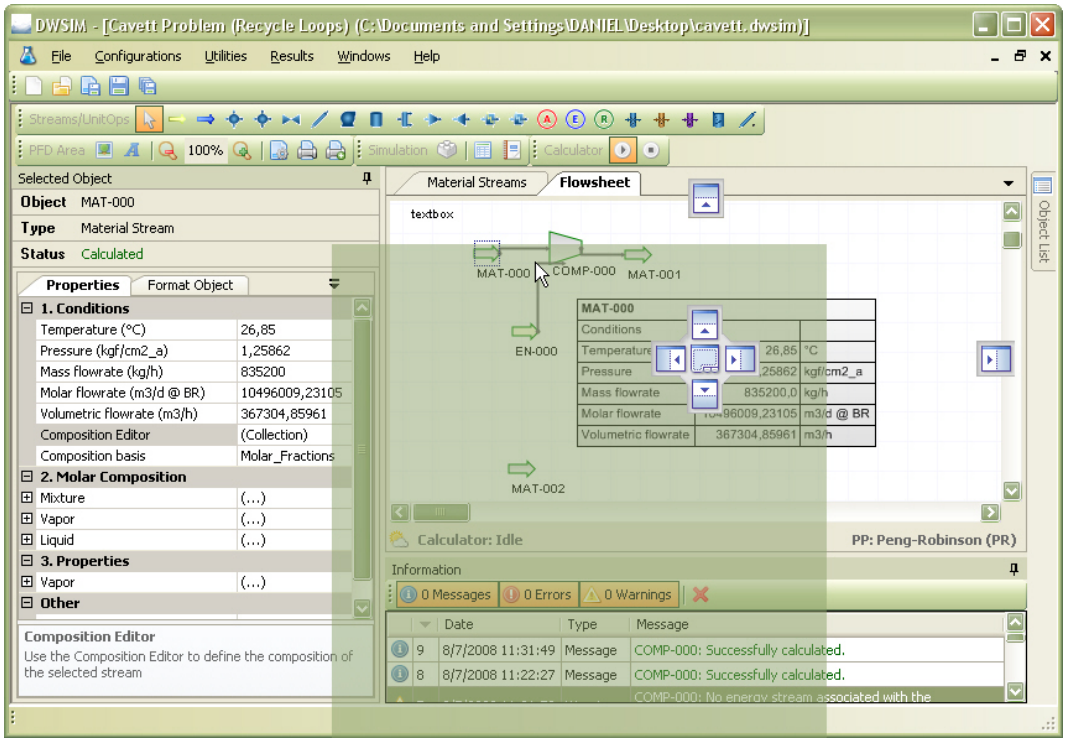


Figure 11: Window repositioning.

When running DWSIM on Mono, use the context menus (right-click with the mouse on the window caption bar) on each window to reposition/dock its contents.

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 reduces 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 shorcut 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.
- ***Spreadsheet Unit Operation:*** Unit Operation where the model is defined and calculated in Spreadsheet (XLS/XLSX/ODS) files.
- ***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 droping items from the **Object Palette** or by using the corresponding toolstrip menu items (**Insert** menu item).

To insert objects into the flowsheet by using the toolstrip 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 were you want to position the object.

To insert objects from the Object Palette, drag and drop the items into the PFD (Figure 12):

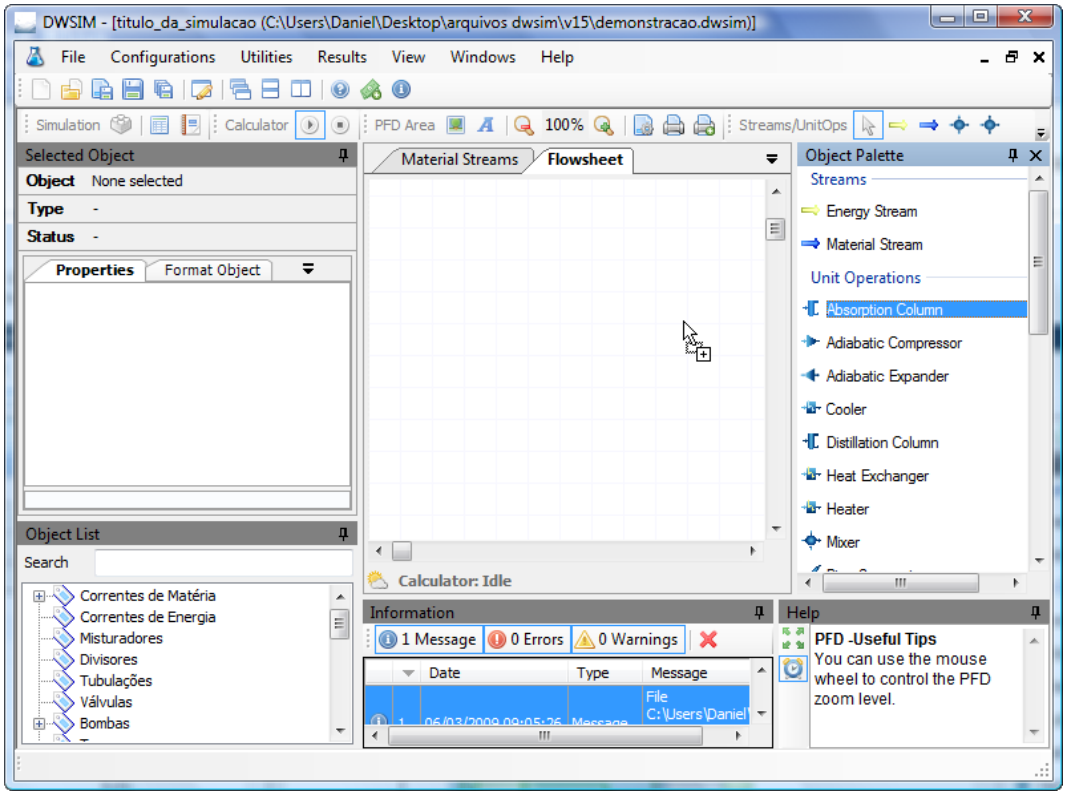


Figure 12: Dragging items from the Object palette window.

Figure 13 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.

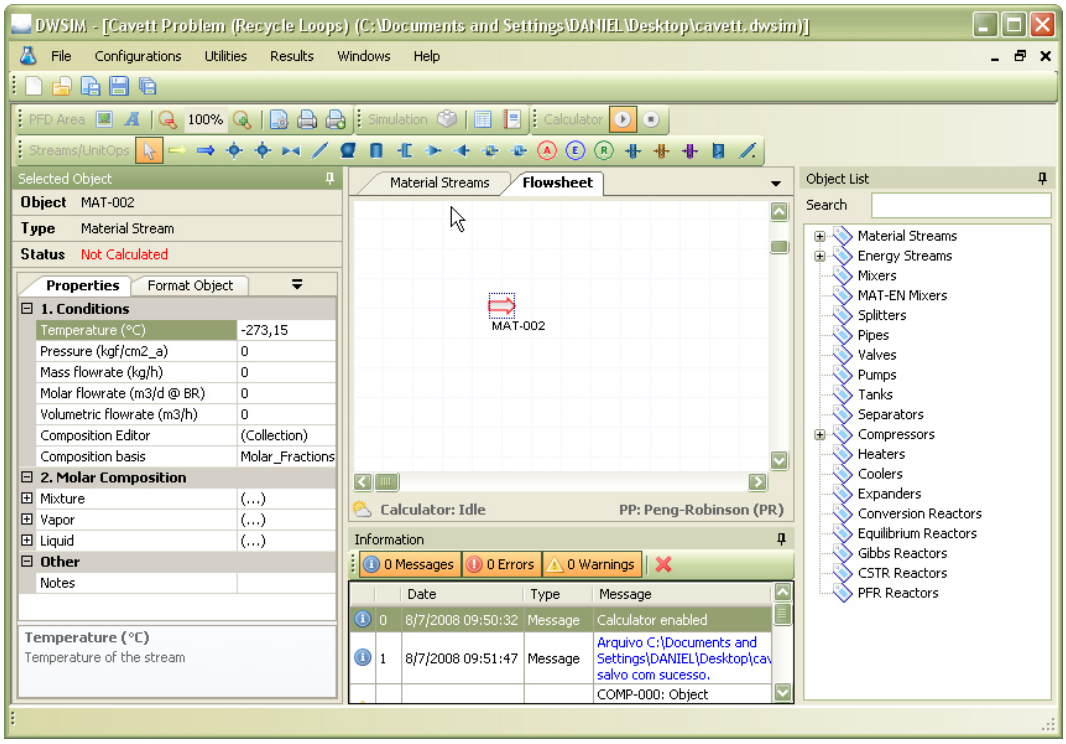


Figure 13: A material stream in the flowsheet.

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 14);

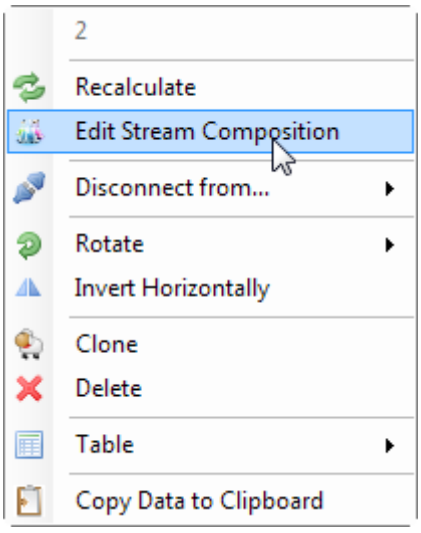


Figure 14: Selected object context menu.

- 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:

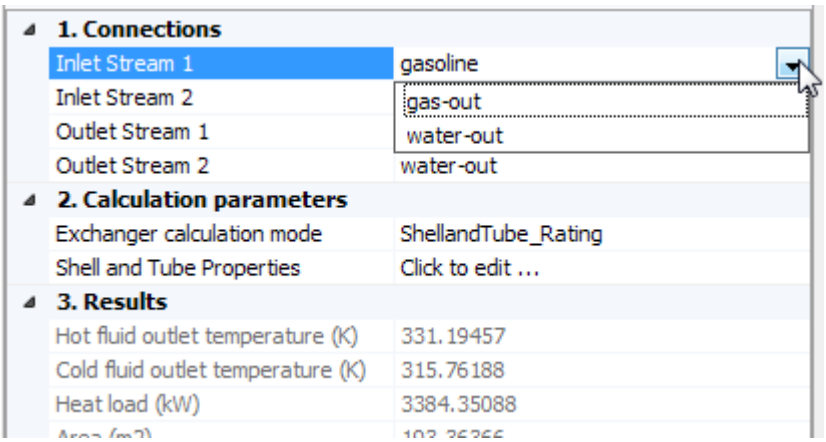


Figure 15: Stream selection menu.

A compression system with its connections is shown on Figure 16.

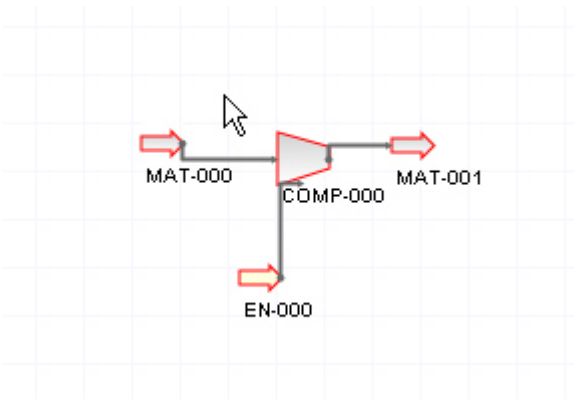


Figure 16: Compressor with all connections correctly configured.

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 14).

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 17). Properties that cannot be edited (read-only) are grayed-out.

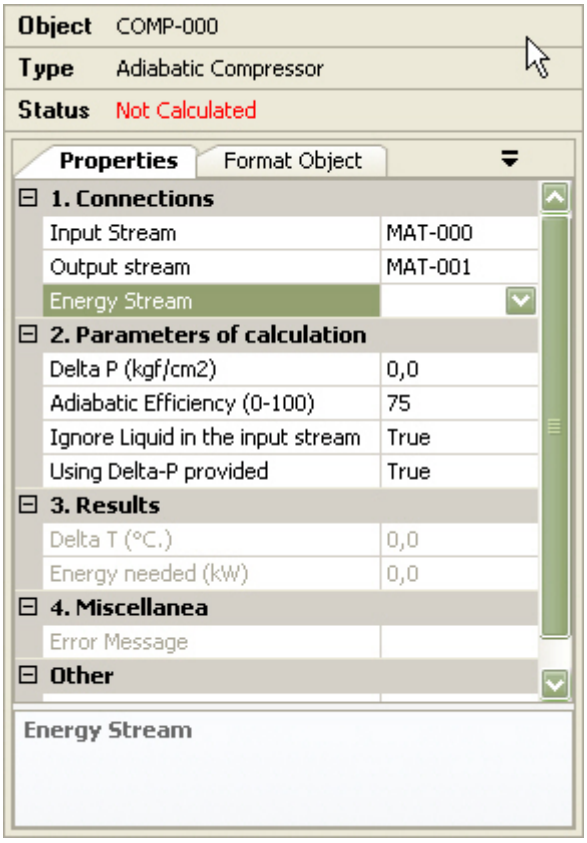


Figure 17: Viewing object properties in the "Selected Object" window.

Some properties can be edited directly in the area to the right of their identification, like a stream temperature (Figure 18). Other properties require an auxiliary window, like a stream composition (Figure 19), and others can be selected by using a *drop-down* menu (Figure 20). 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.

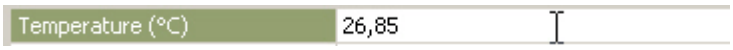


Figure 18: Direct editing of a property.

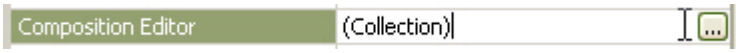


Figure 19: Using an auxiliary window to edit a property value.

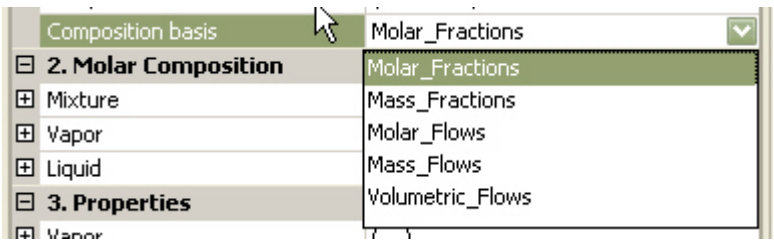


Figure 20: Selecting a value for the property in a drop-down menu.

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 21).

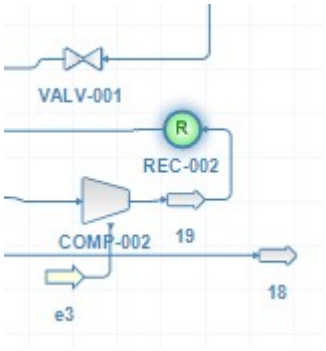


Figure 21: Calculated objects.

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 dowstream 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 22). 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 22: 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 23).

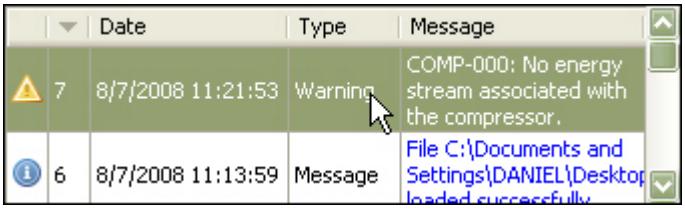


Figure 23: A DWSIM's calculator message.

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 24 and 25) for printing. Report data can also be saved to a XLS or Text file, or exported to XML.

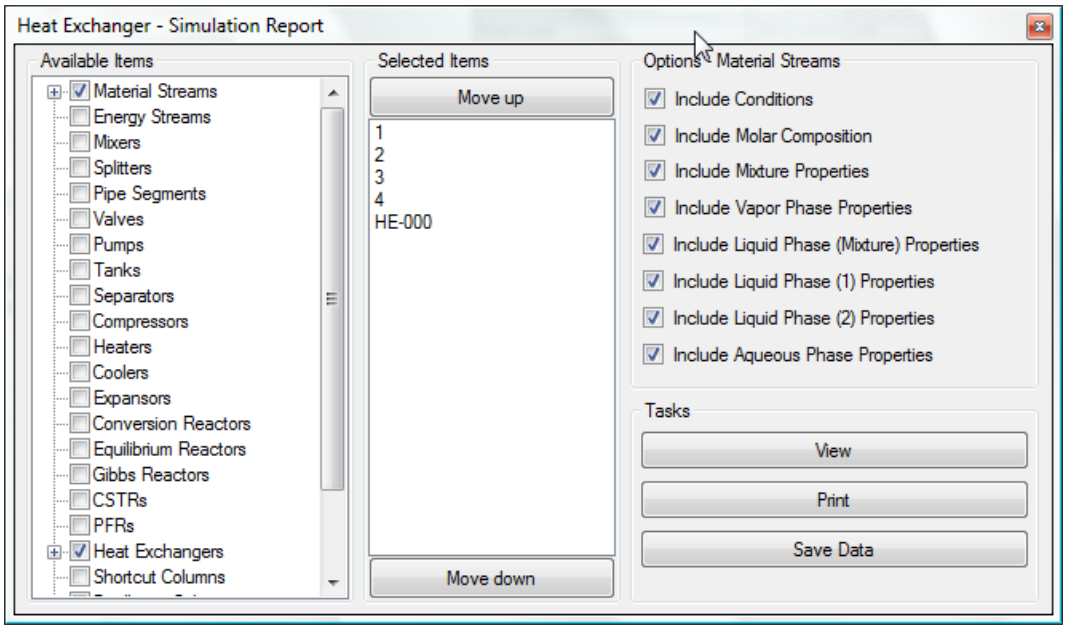


Figure 24: Results report configuration.

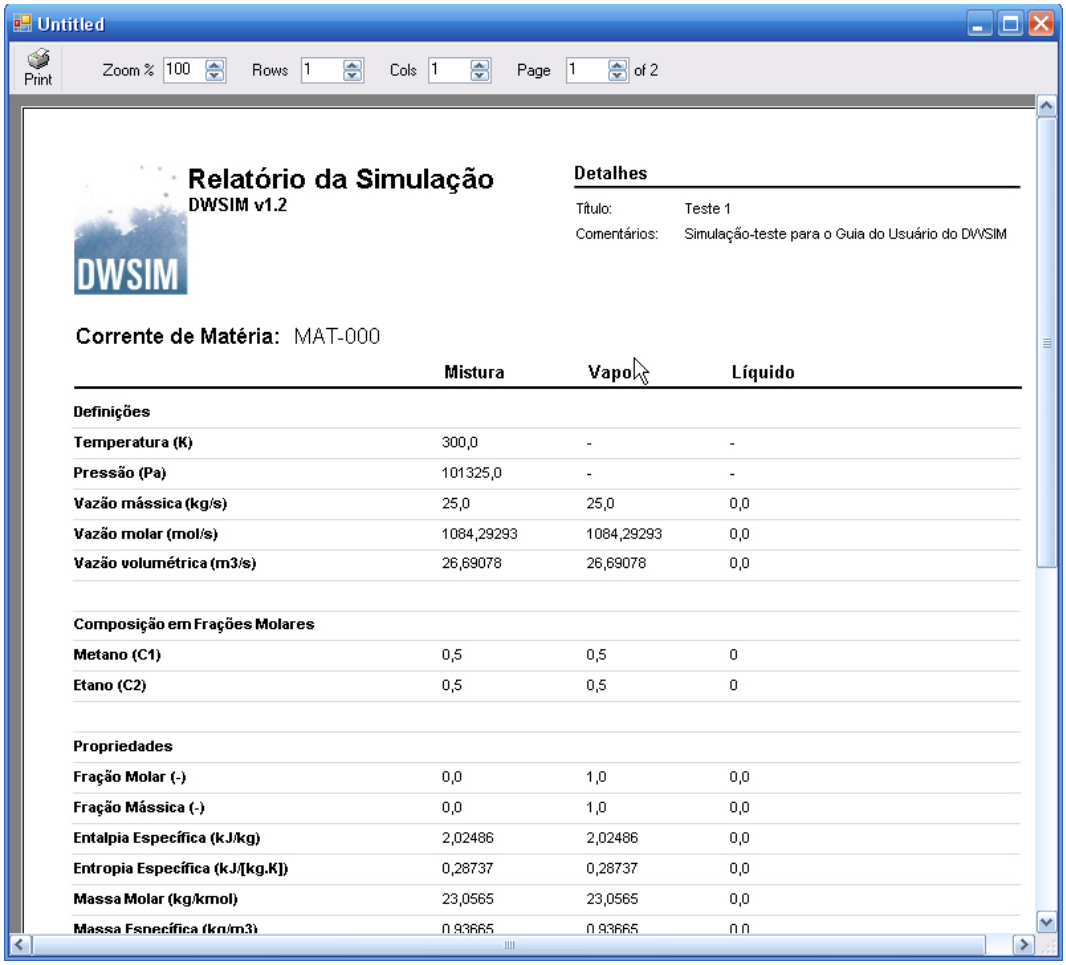


Figure 25: Results report.

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.

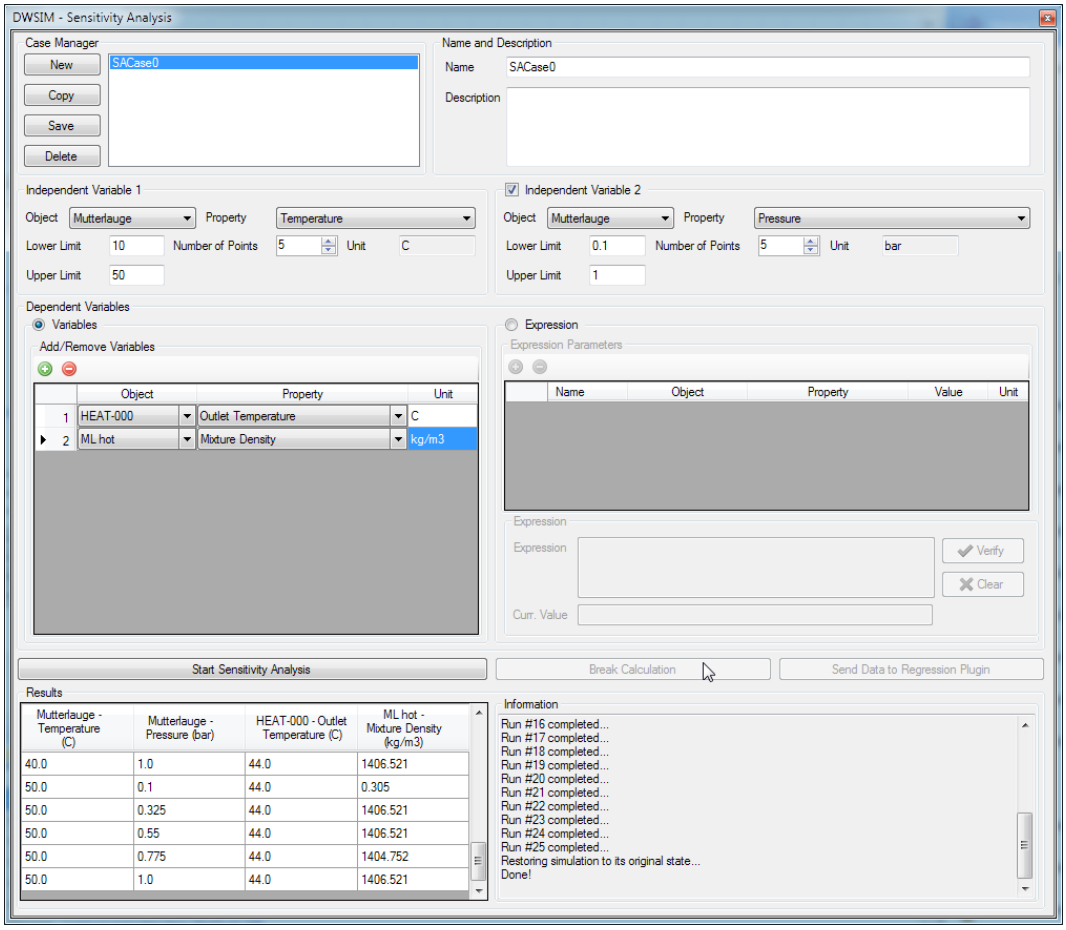


Figure 26: Sensitivity Analysis Utility (1).

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.

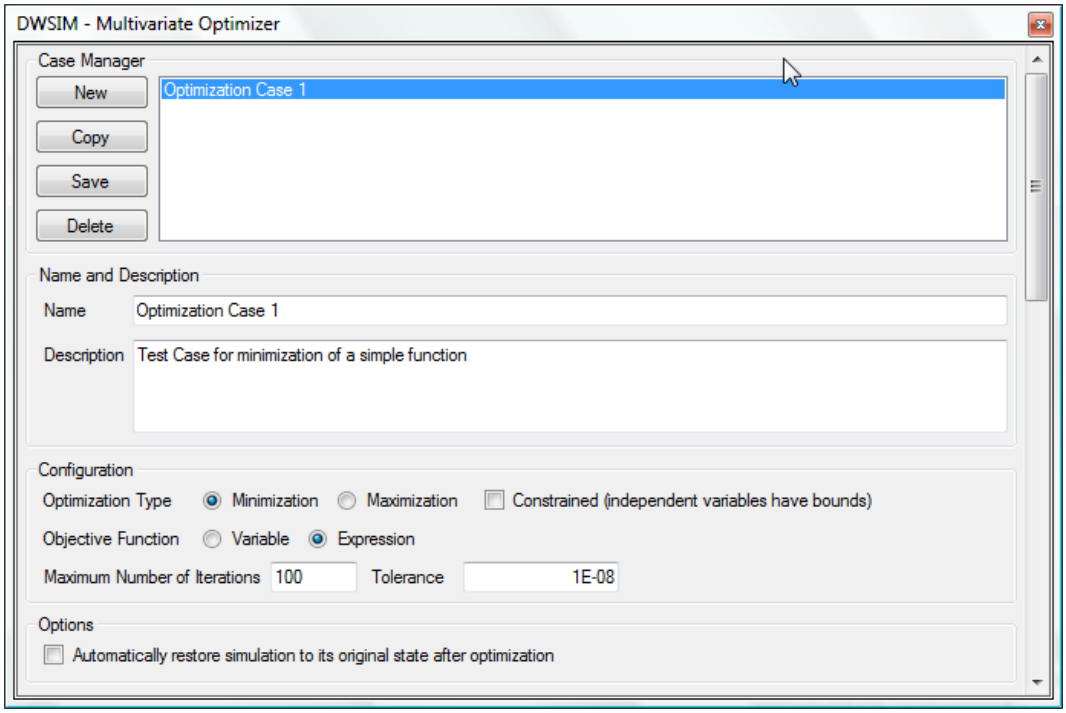


Figure 27: Multivariate Optimization Utility (1).

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 indendent 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.

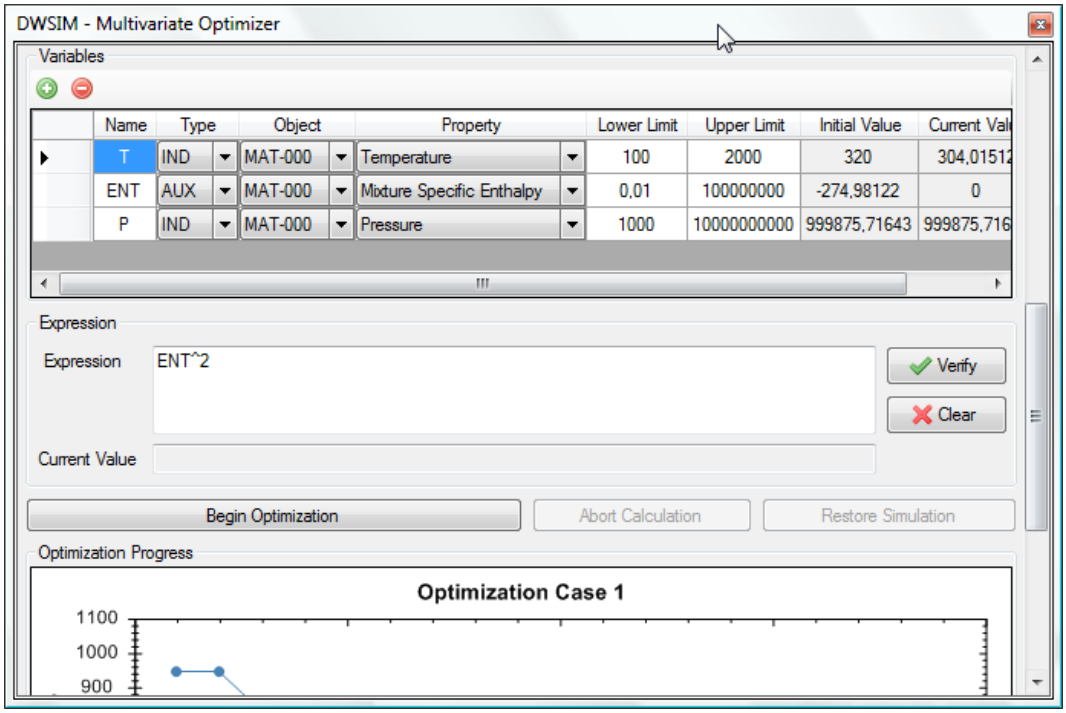


Figure 28: Multivariate Optimization Utility (2).

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 the optimization process is over.

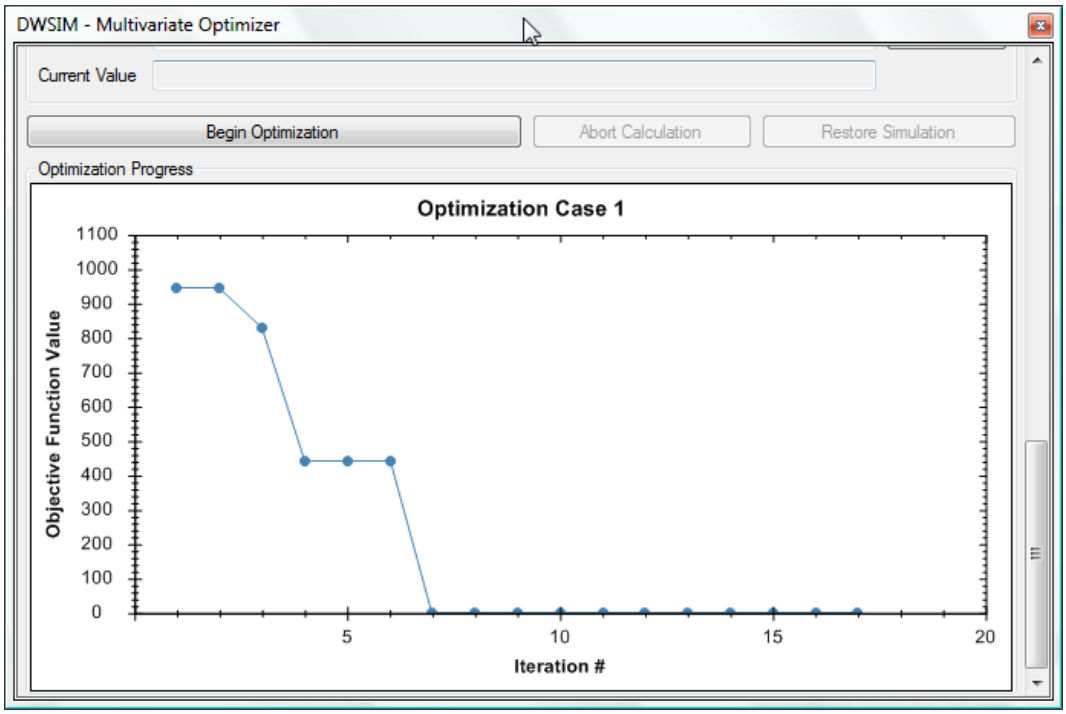


Figure 29: Multivariate Optimization Utility (3).

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 30).

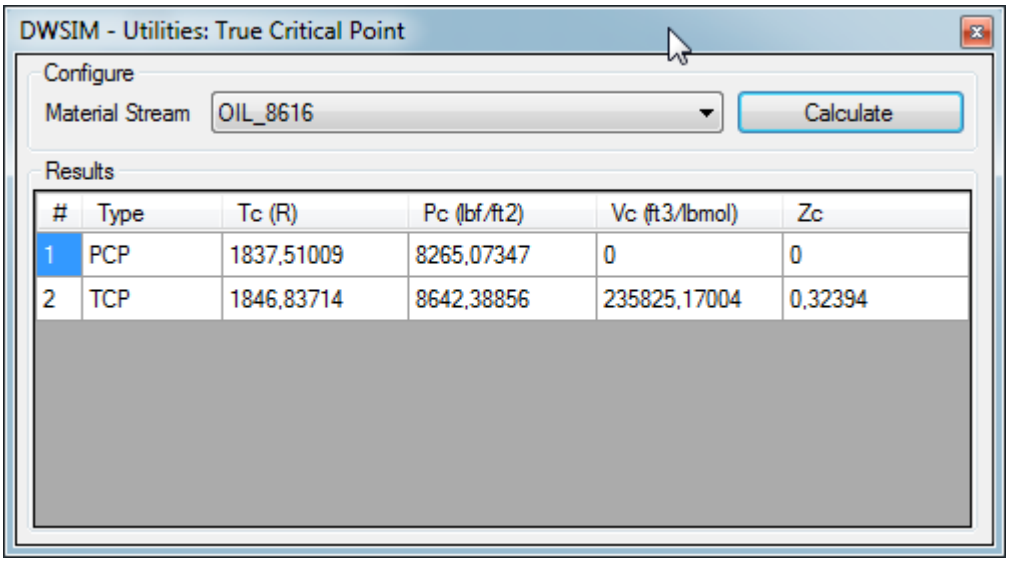


Figure 30: Utilities - True Critical Point.

- ***Hydrate Equilibrium/Dissociation Utility*** - calculation of the equilibrium conditions for natural gas hydrates (Figure 31);

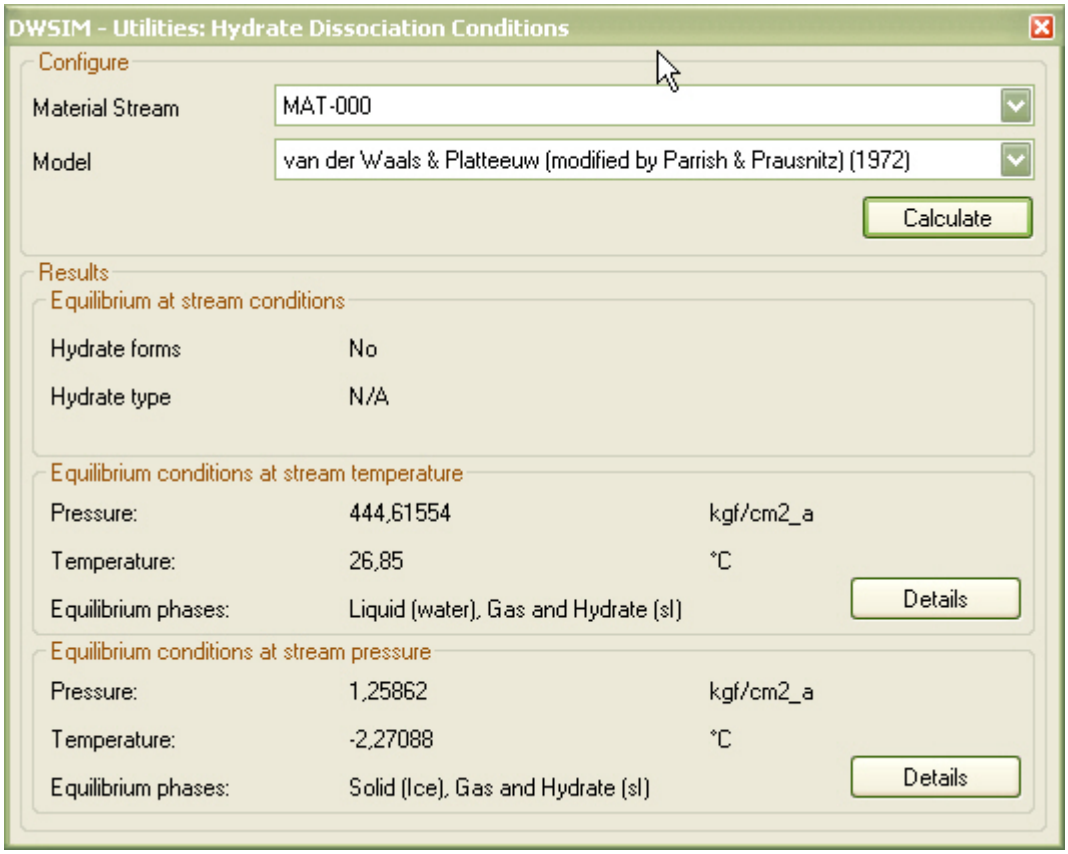


Figure 31: Utilities - Hydrate Calculations.

- ***Pure Component Properties*** - pure component property viewing and editing (Figure 32);

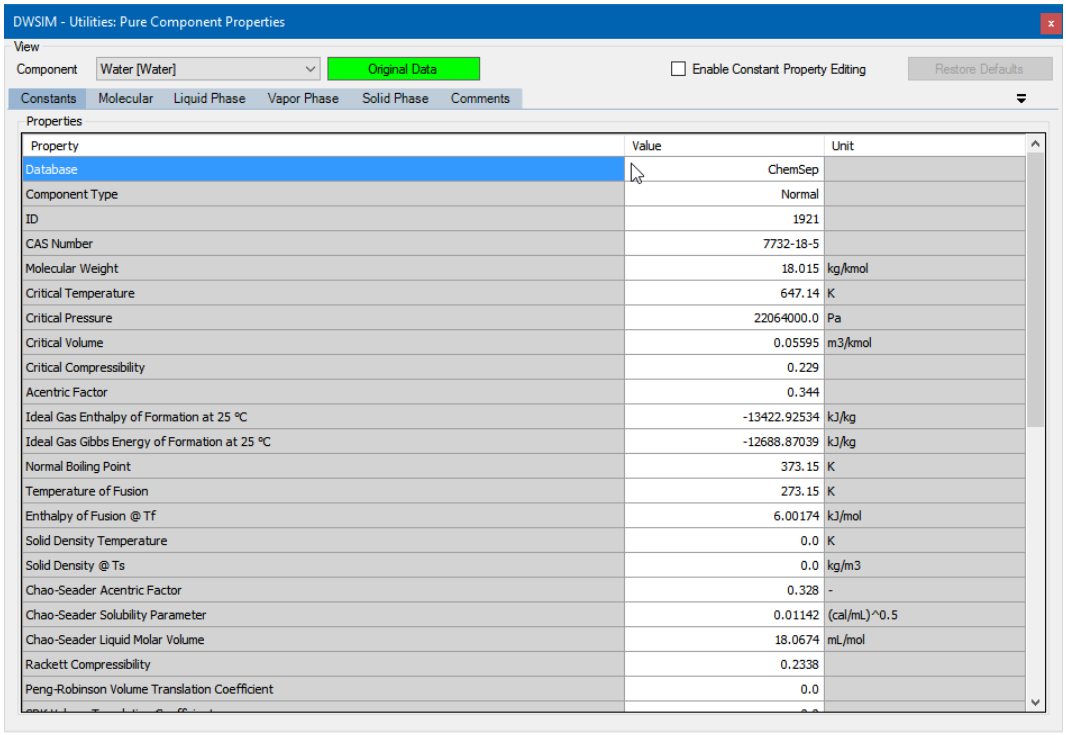


Figure 32: Utilities - Pure Component Properties.

➙ ***Phase Envelope*** - Material stream phase equilibria envelope calculation (Figure 33);

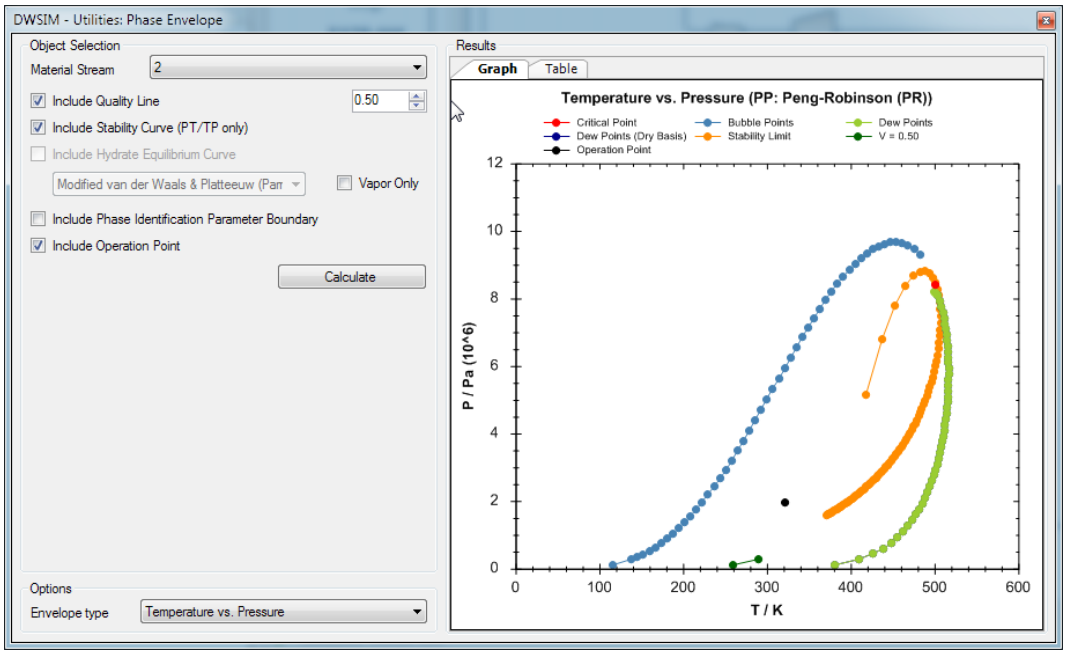


Figure 33: Utilities - Phase Envelope.

➙ ***Binary Envelope*** - special envelopes for binary mixtures (Figure 34).

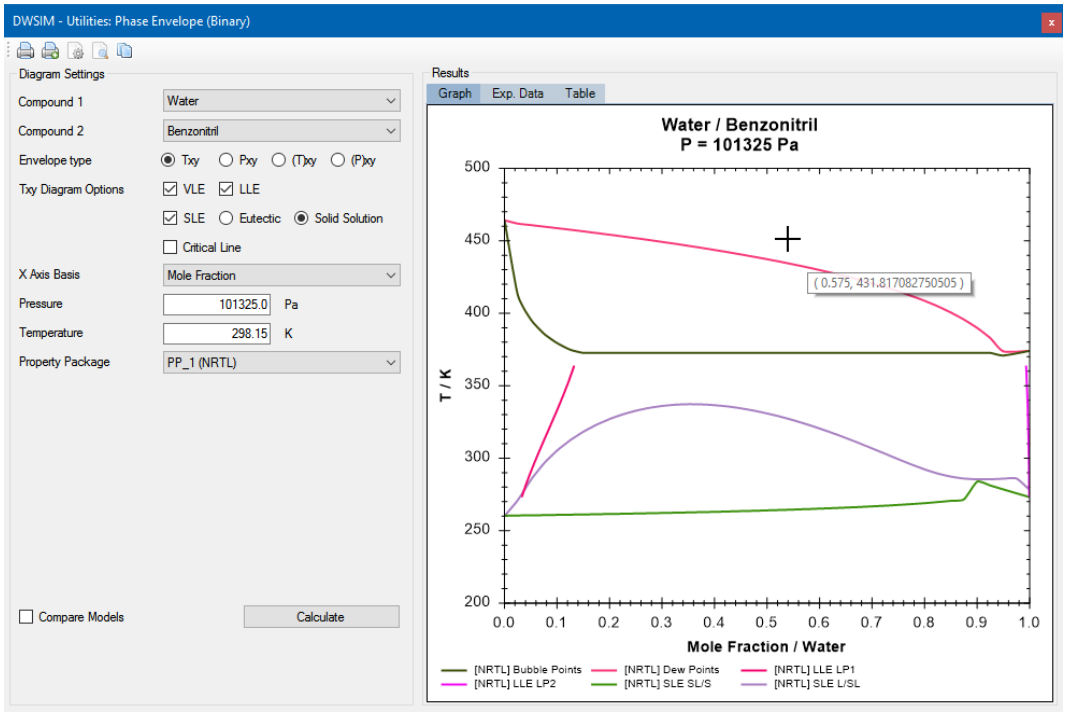


Figure 34: Utilities - Binary Envelope.

- ***Petroleum Cold Flow Properties*** - special properties of petroleum fractions, like cetane index, flash point, refraction index, etc. (Figure 35).

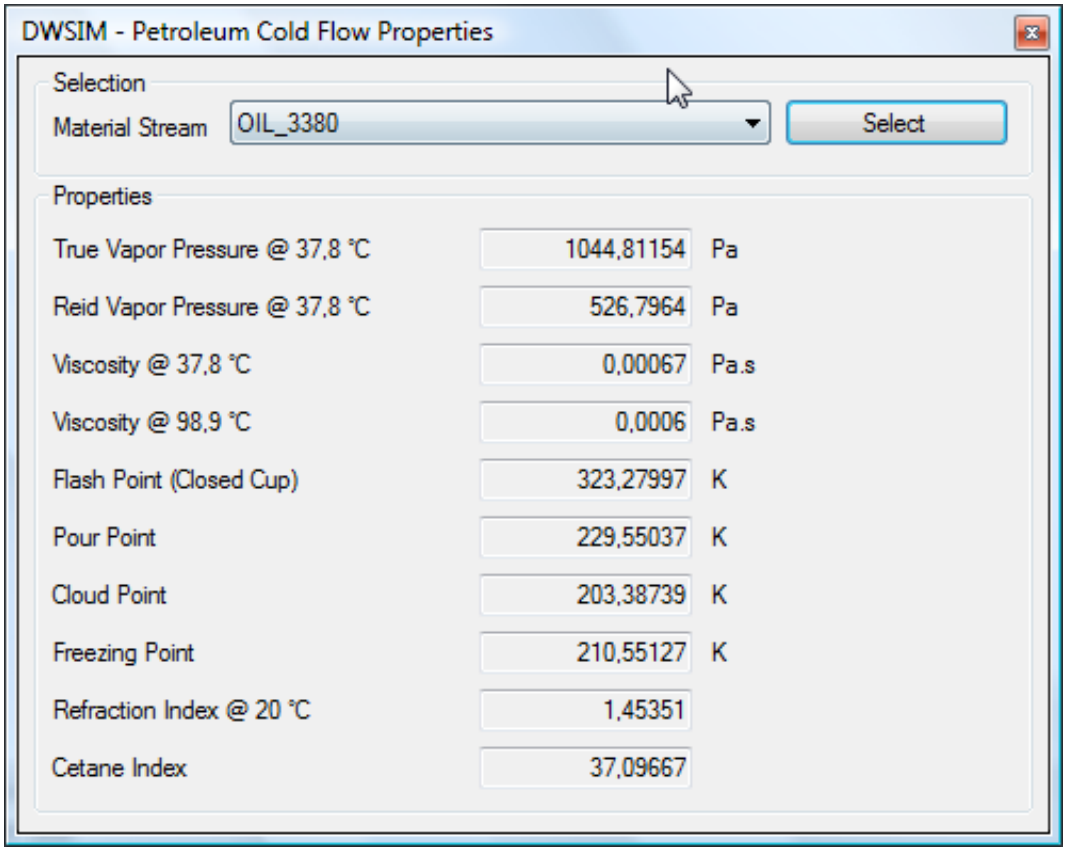


Figure 35: Utilities - Petroleum Cold Flow Properties.

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 36):

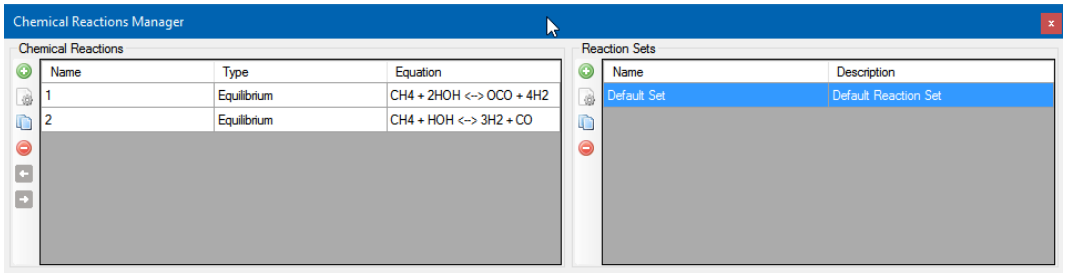


Figure 36: Chemical Reactions Manager.

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 37):

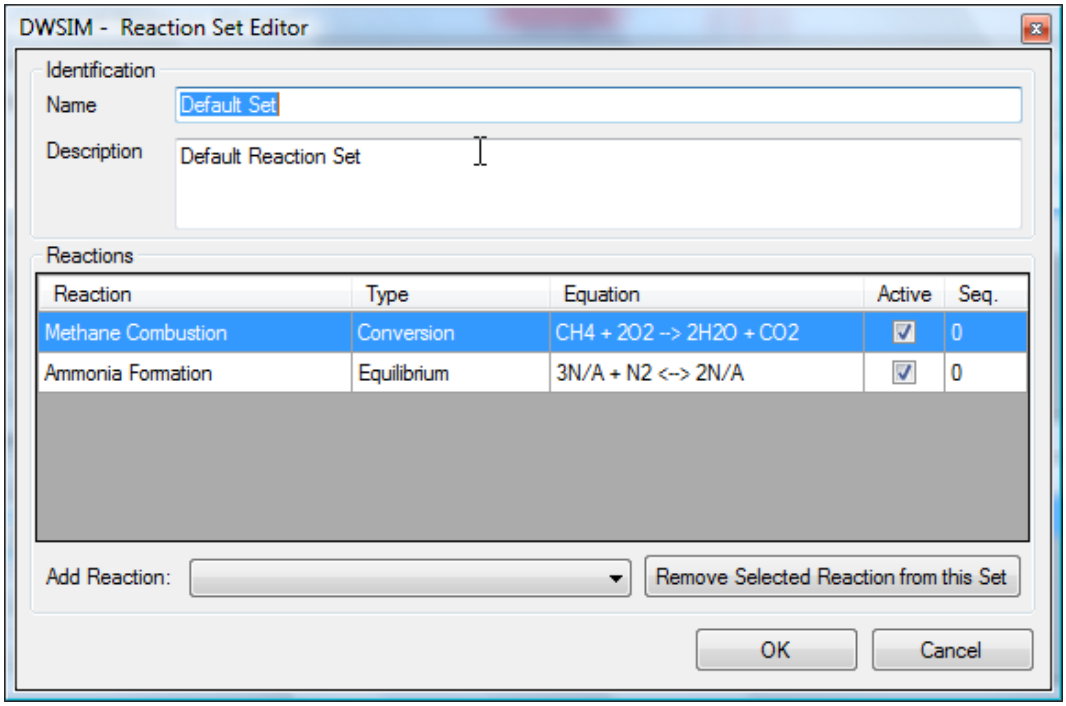


Figure 37: Reaction Set editor.

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 38):

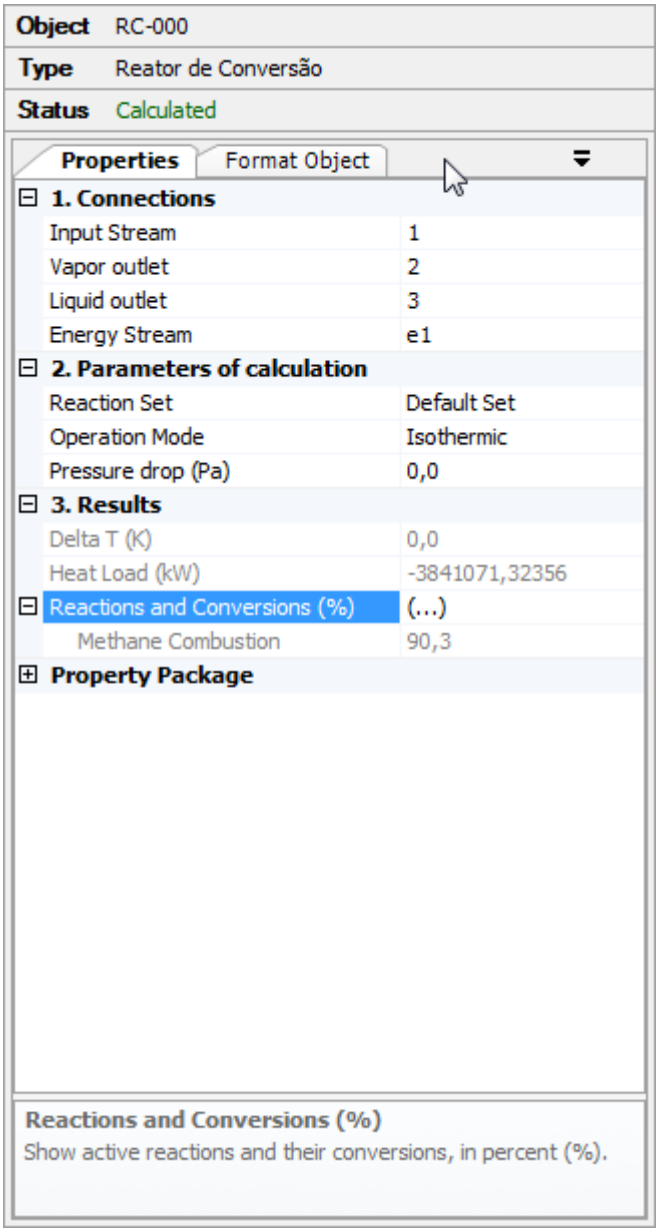


Figure 38: Reaction set in a reactor's property window.

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 39). The other characterizes the oil from an ASTM or TBP distillation curve (Figure 40).

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 39). It is recommended that the user provides the specific gravity of the C7+ fraction at least. Viscosity data is also very important.

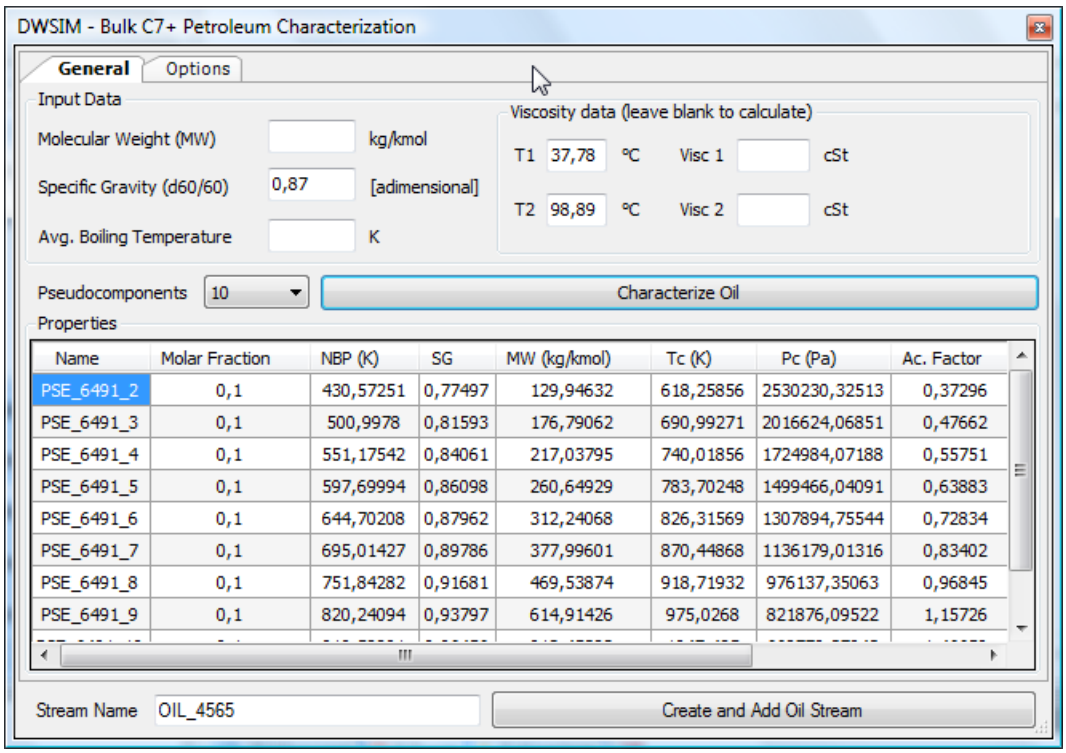


Figure 39: C7+ petroleum fraction characterization utility.

- ***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 40):

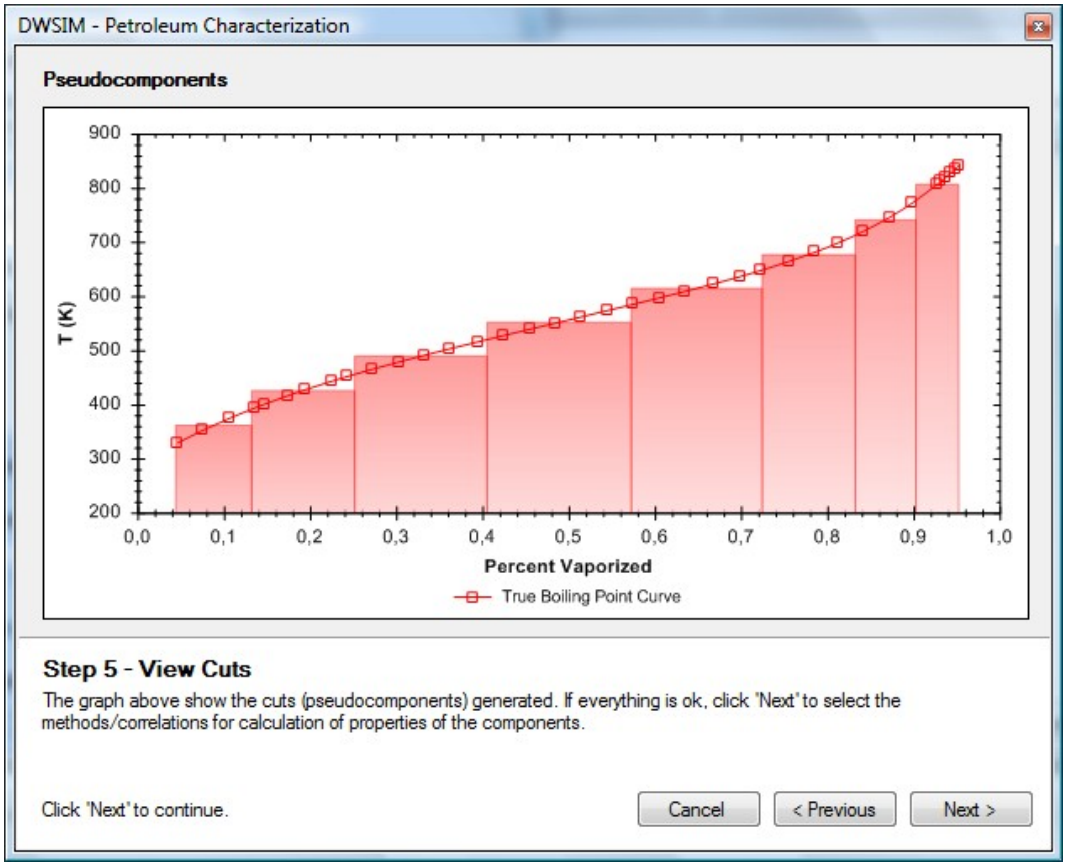


Figure 40: Characterizing petroleum from distillation curves.

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 41):

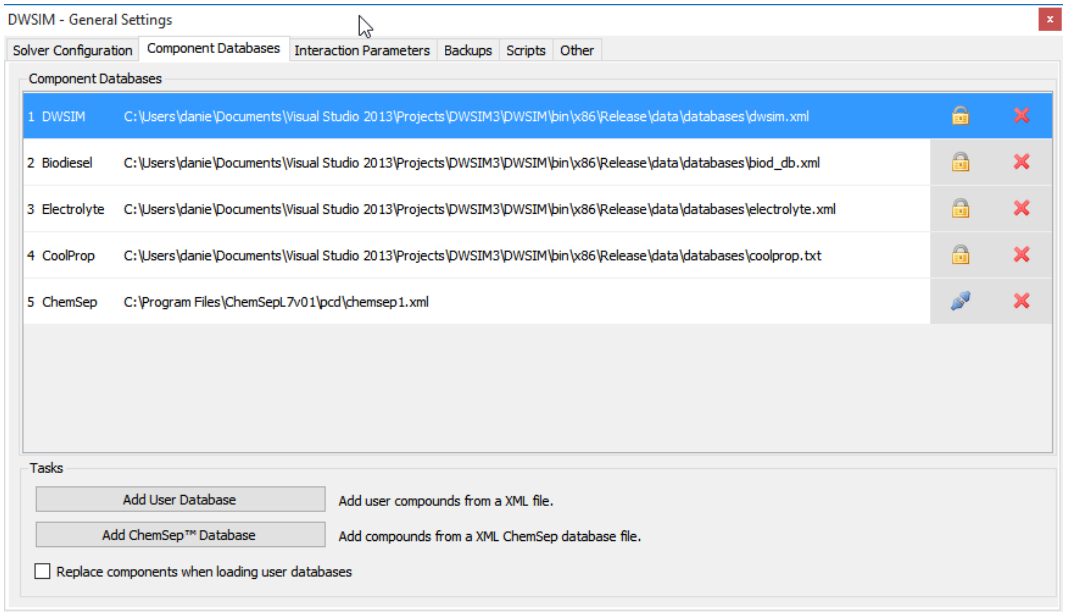


Figure 41: Database manager.

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.

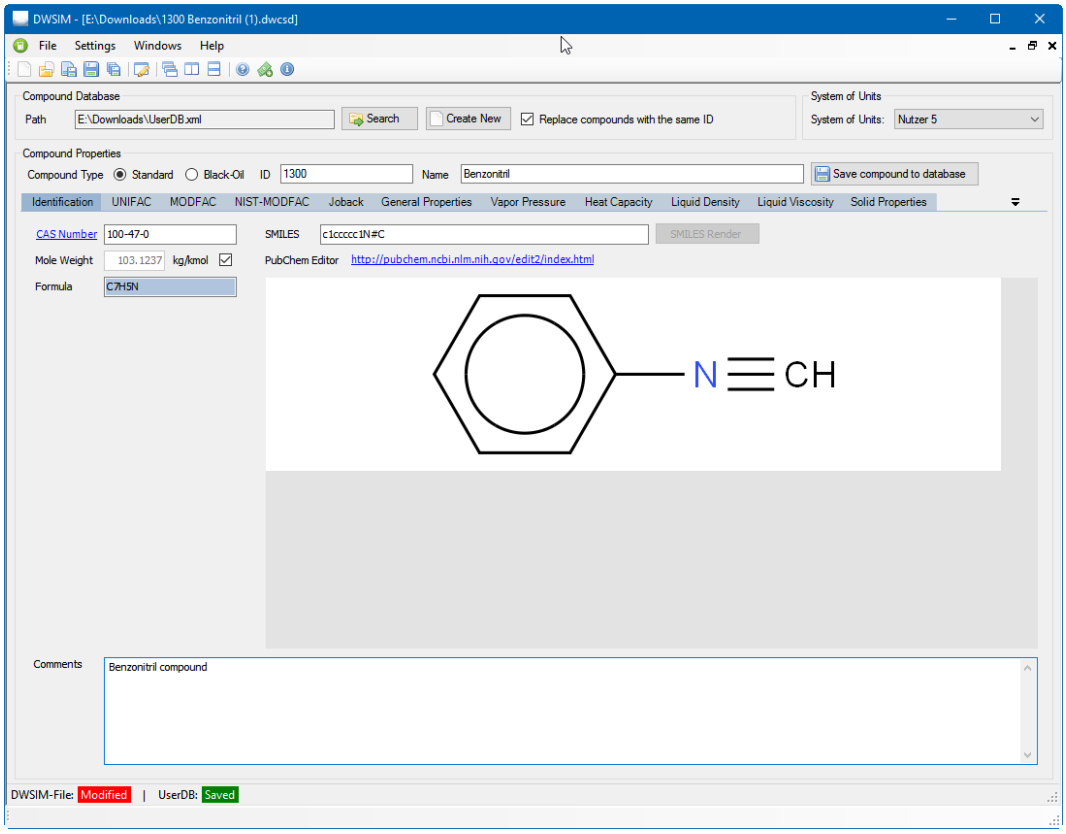


Figure 42: Compound Creator Utility.

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 aditional 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.

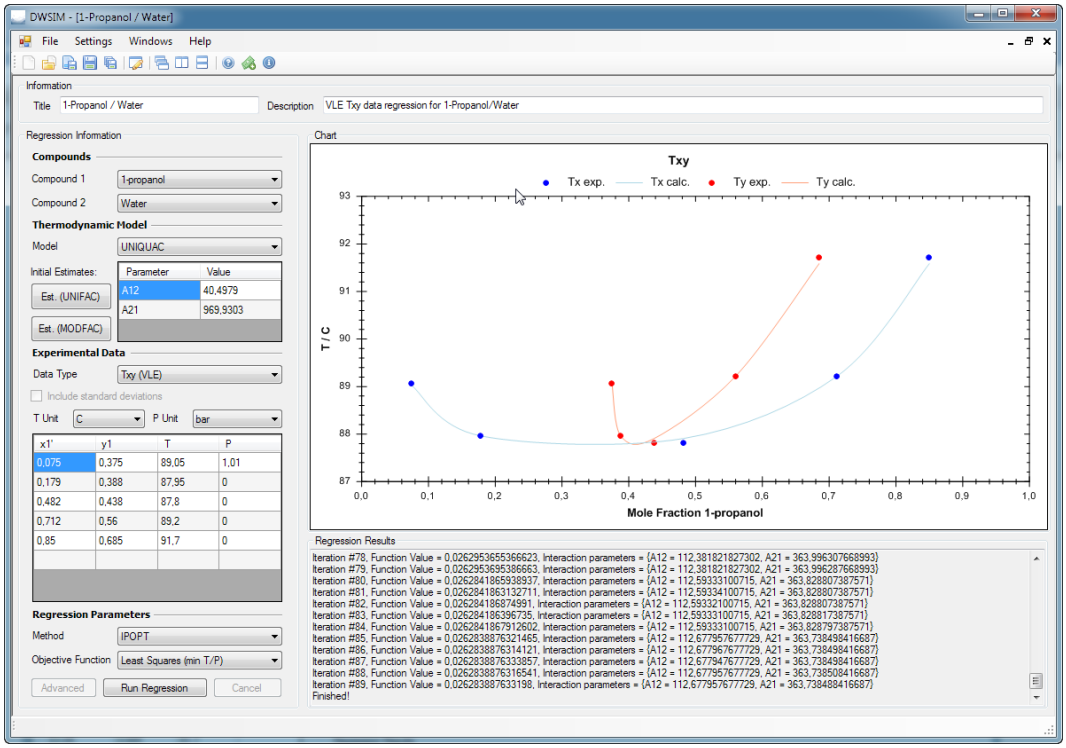


Figure 43: Data Regression Utility.