DWSIM - Process Simulation, Modeling and Optimization
User Guide

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Contact Information

DWSIM - Process Simulation, Modeling and Optimization

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1 Introduction

This *User Guide* was created with the purpose to provide information for DWSIM users about the utilization of the software with respect to the GUI, commands and functions available. The structure of the document is organized according to the sequence of execution of a simple simulation. Each step is explained with the help of images of the associated windows and descriptions for the functions and necessary commands.

For details about the models used for calculation of thermodynamic properties, please view the **Technical Manual**. Detailed description about the Unit Operations and Utilities can be found in the **Unit Operations and Utilities Guide**.

2 Welcome screen

When DWSIM is run for the first time, after the database is loaded, the following window appears (Figure 1):

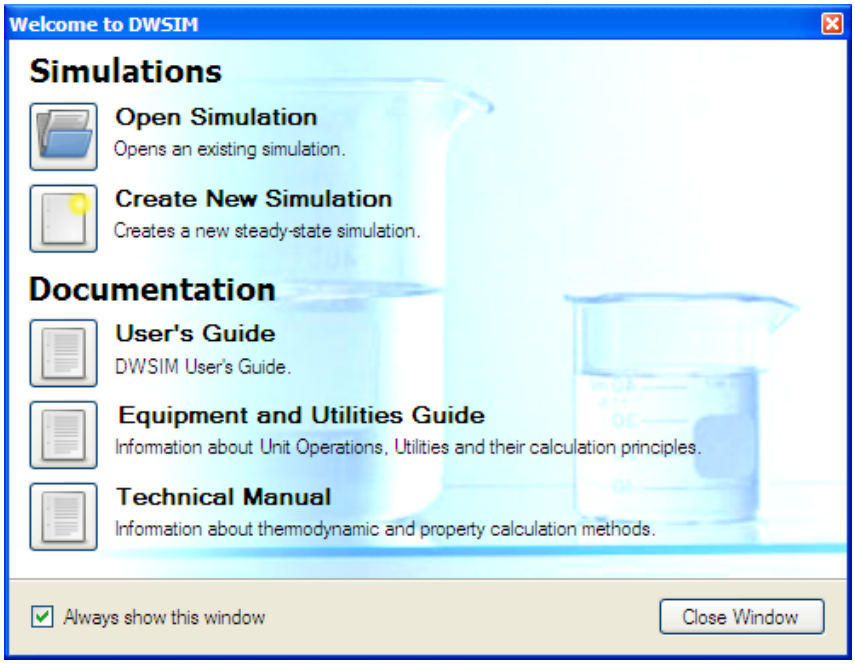


Figure 1: DWSIM's welcome screen.

The welcome screen provides the user with shortcuts to open existing simulations, create new ones and view the documentation. It is possible to view some usage tips in the bottom of the window. For this window do not open when DWSIM starts, the checkbox "Always show this window" must be unchecked. The "Close" button close this window and shows the main DWSIM interface:

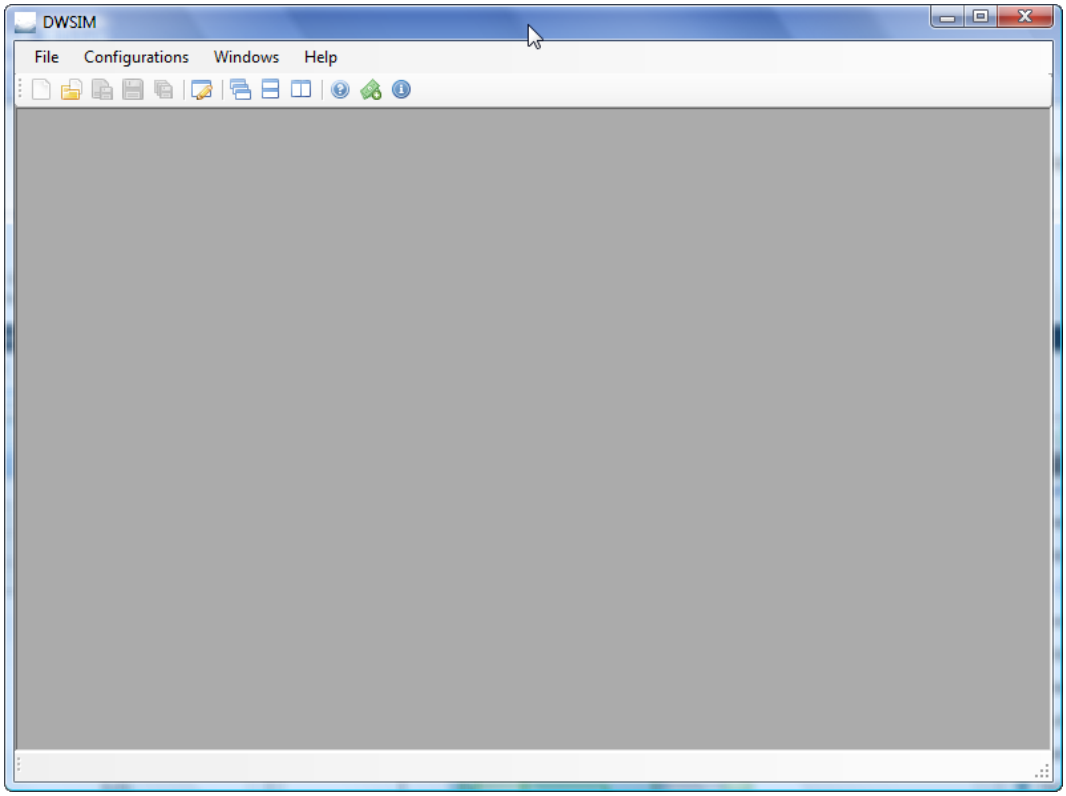


Figure 2: DWSIM's main window.

In the main DWSIM window (Figure 2), it's possible to view the following items:

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

> ***If there is an active simulation in DWSIM, the menu bar is filled with other specific items.***

- ***Button strip,*** to open, save and create new steady-state simulations.

There are various options to access the most commonly operations with simulation files - open, save and create. In the next sections you will be guided through some necessary steps to create and configure a steady-state simulation.

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*:

- ***Components*** - Contains sections for manage the components in the simulation.
- ***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

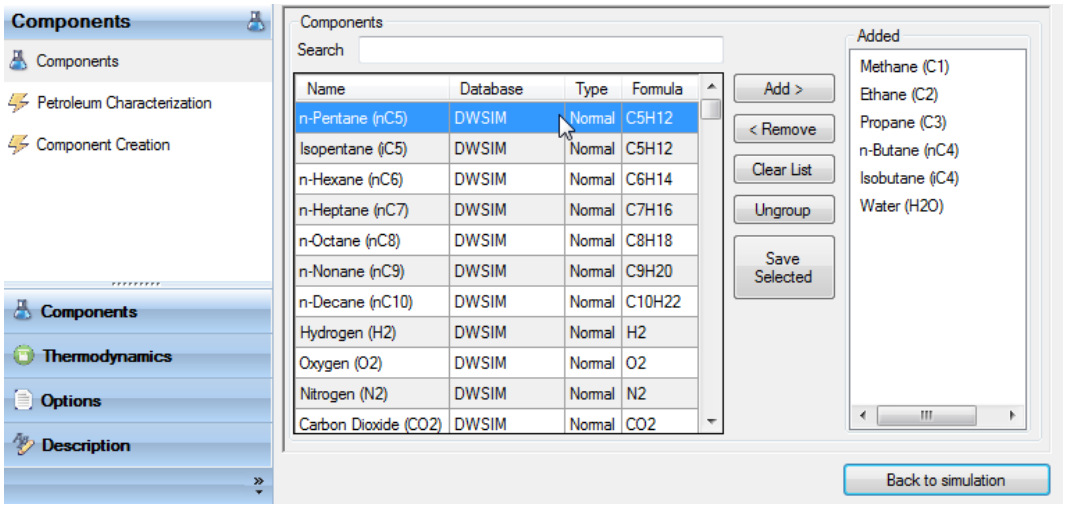


Figure 3: Simulation configuration window.

The simulation configuration window (Figure 3) is the interface where all the functions for configuration and personalization of a simulation in DWSIM are concentrated. In this window, the user can be manage the simulation components, the property package (thermodynamic package), 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. DWSIM shows a confirmation box when the user makes any change to important settings, like the property package selection.

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***. 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 **Hypothetical Creation Utility** 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 exclusion 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).

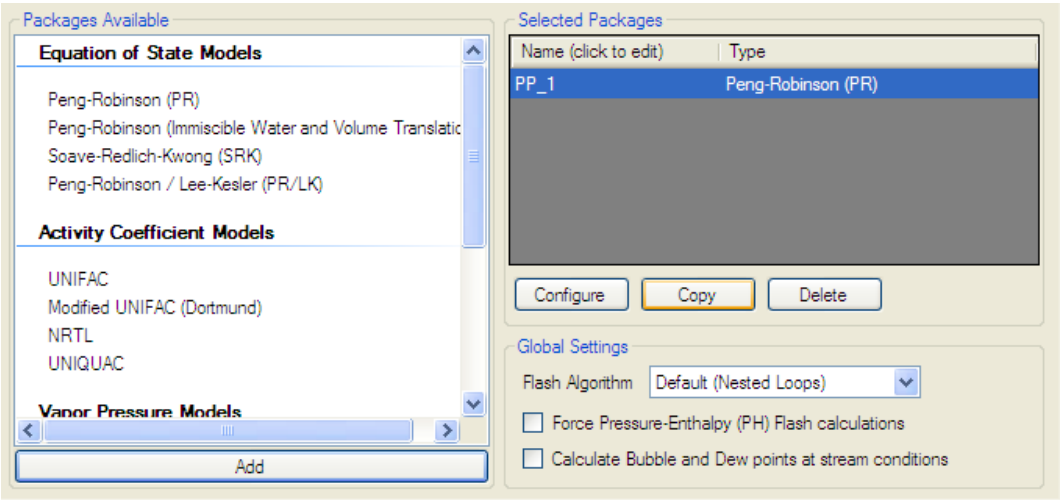


Figure 4: Property Package configuration interface.

Extra configuration options for EOS-based Property Packages You can define some options which will be used throughout all Property Packages, in all simulation objects. They are:

➙ *Flash Algorithm*

Select the flash algorithm to be used by DWSIM. You can choose between "Nested Loops" (default) and "Inside-Out". The latter is faster in most cases, specially if your simulation contains

many components. The first is more stable and should work on most cases, as it is being used since early DWSIM builds.

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

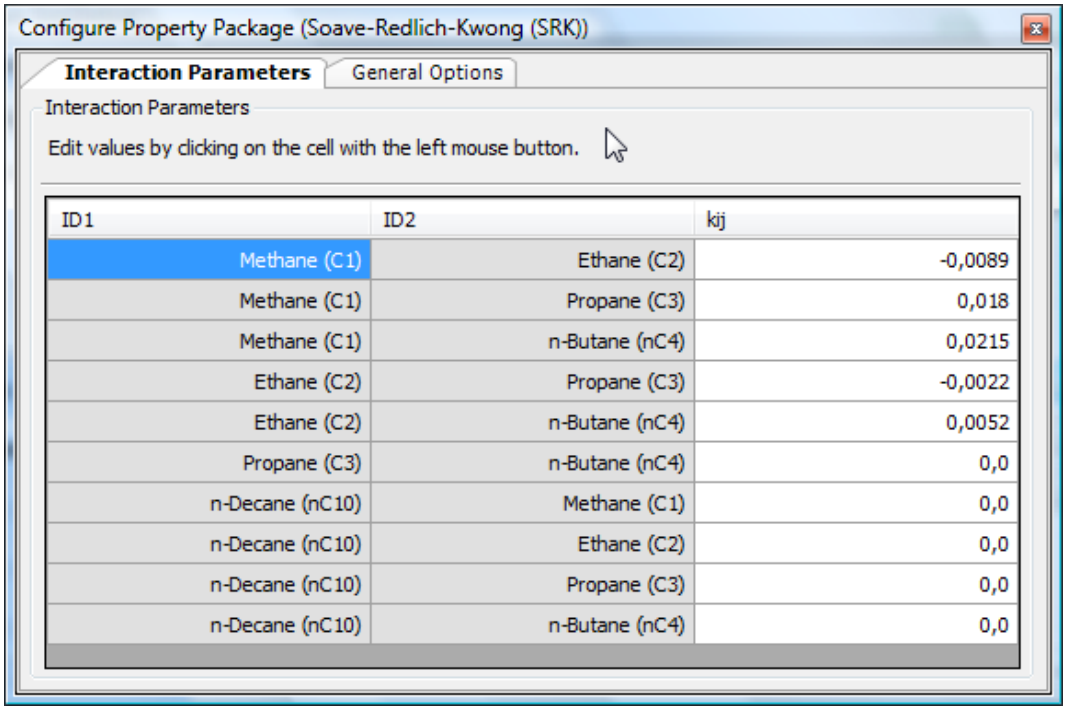
If you check the box, all requests by unit operations for PT Flashes will be replaced by PH ones. This option must be activated if you are working with only one component (steam simulation, for example), otherwise you won't have partial vaporization/liquefaction in valves, compressors and expanders,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

Multiple Property Packages Starting from DWSIM 1.5, the user can define more than one property package to be used in the simulation, which can be associated to each unit operation on a individual basis. Each property package has its own settings, independently of having two or more packages of the same type.

Property Package configuration If the selected property package has any editable property, the "Configure" button becomes activated and the user can click on it to show the property package configuration window. In the case of the SRK property package, the editable parameters are the binary interaction parameters (Figure 5) and some convergence/tolerance values for flash calculations (Figure 6).



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 5: 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).

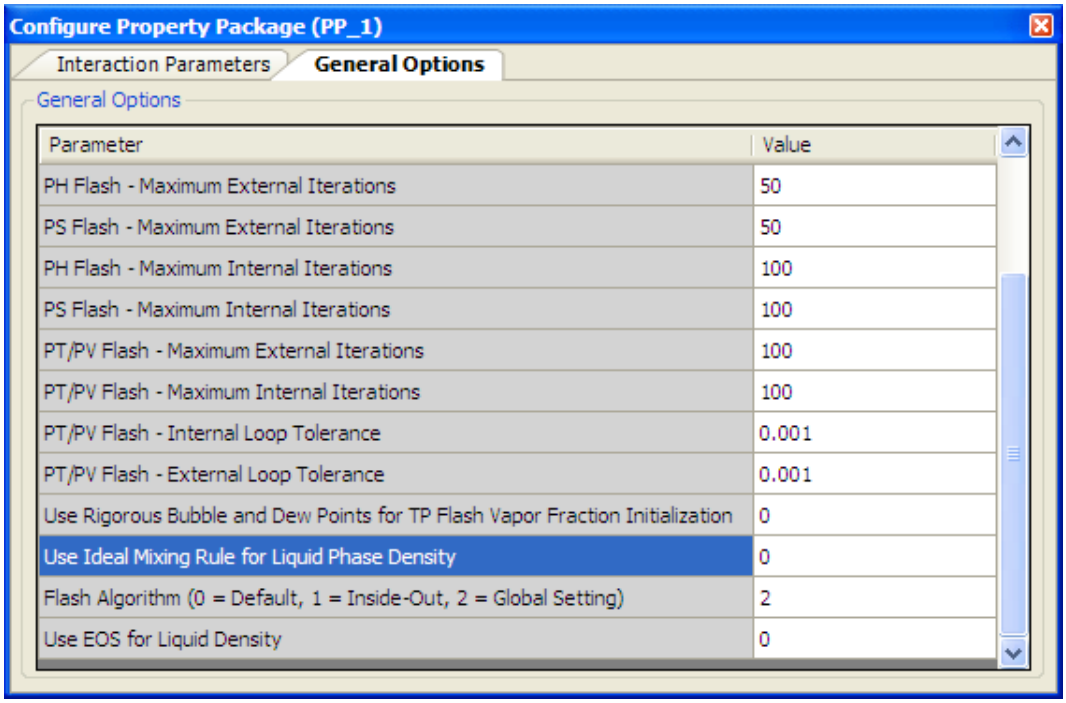


Figure 6: Property package configuration window for EOS-based models.

Extra configuration options for EOS-based Property Packages 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.

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 7).

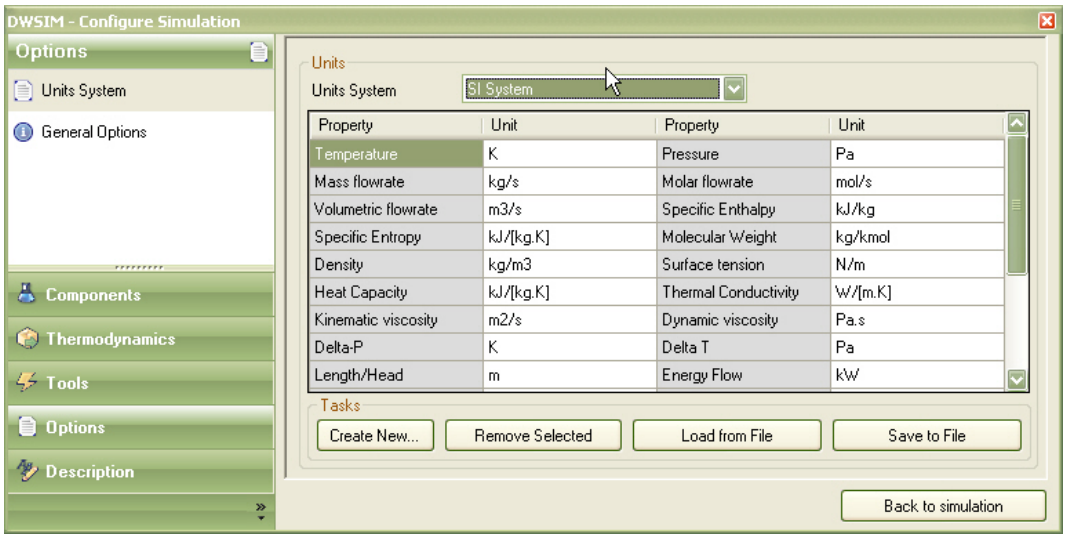


Figure 7: Units system configuration interface.

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 8).

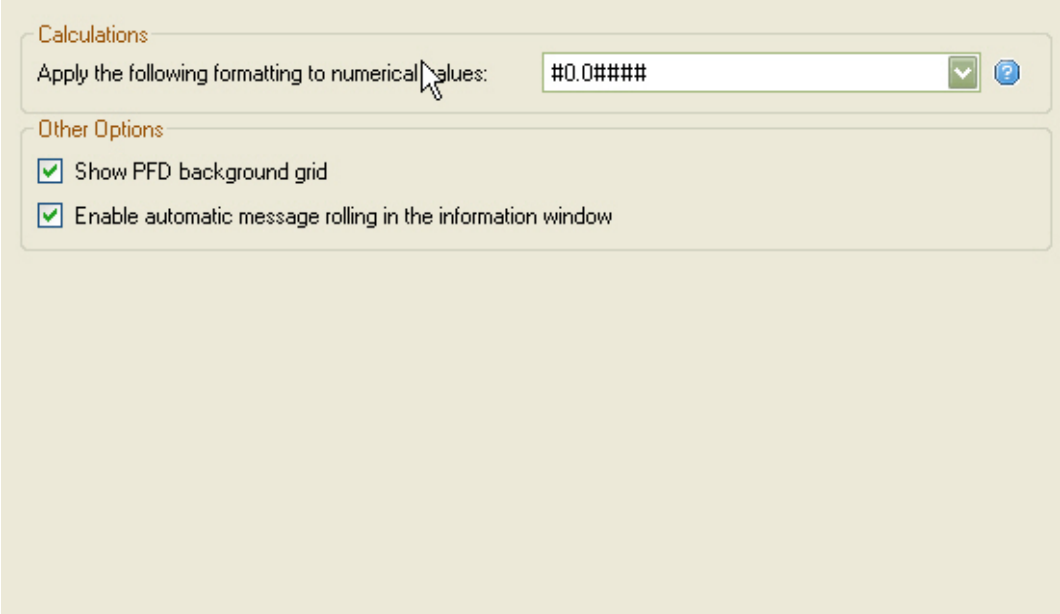


Figure 8: Number formatting selection interface.

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) (Figure 9).

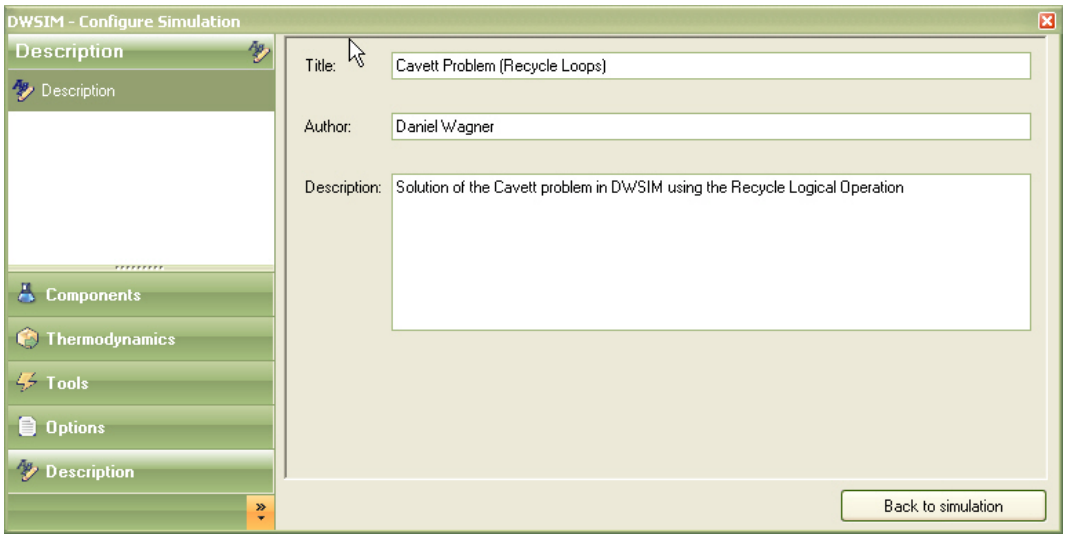


Figure 9: Simulation description editing interface.

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 10). In this window we can highlight the following areas:

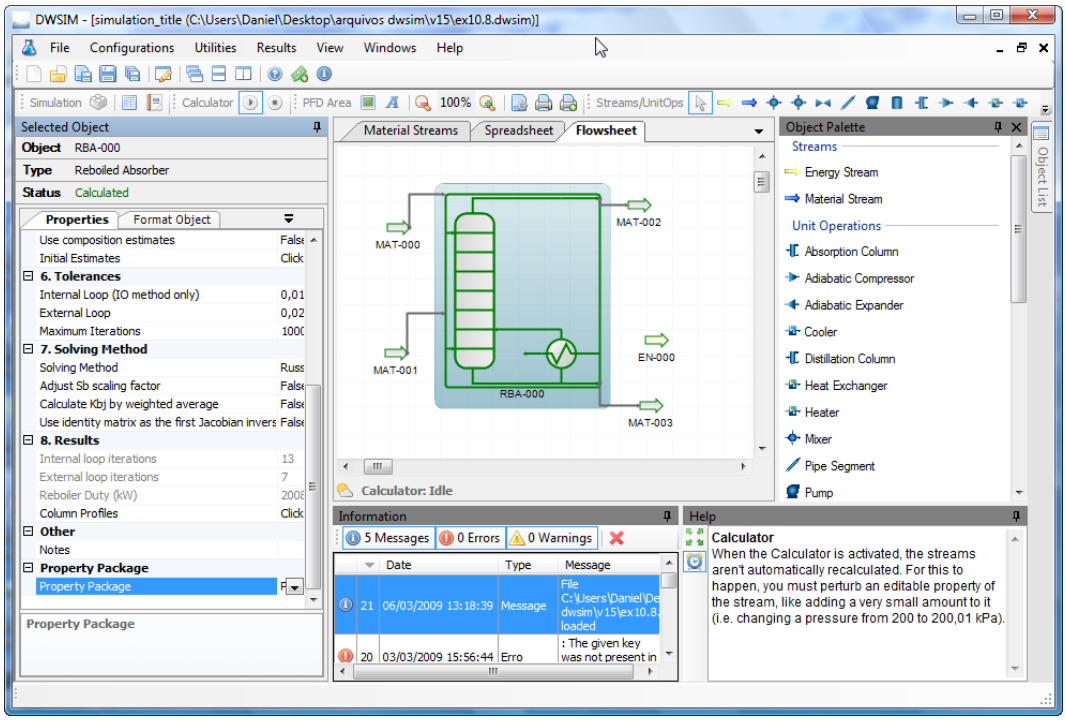


Figure 10: Simulation interface.

- ***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.

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).

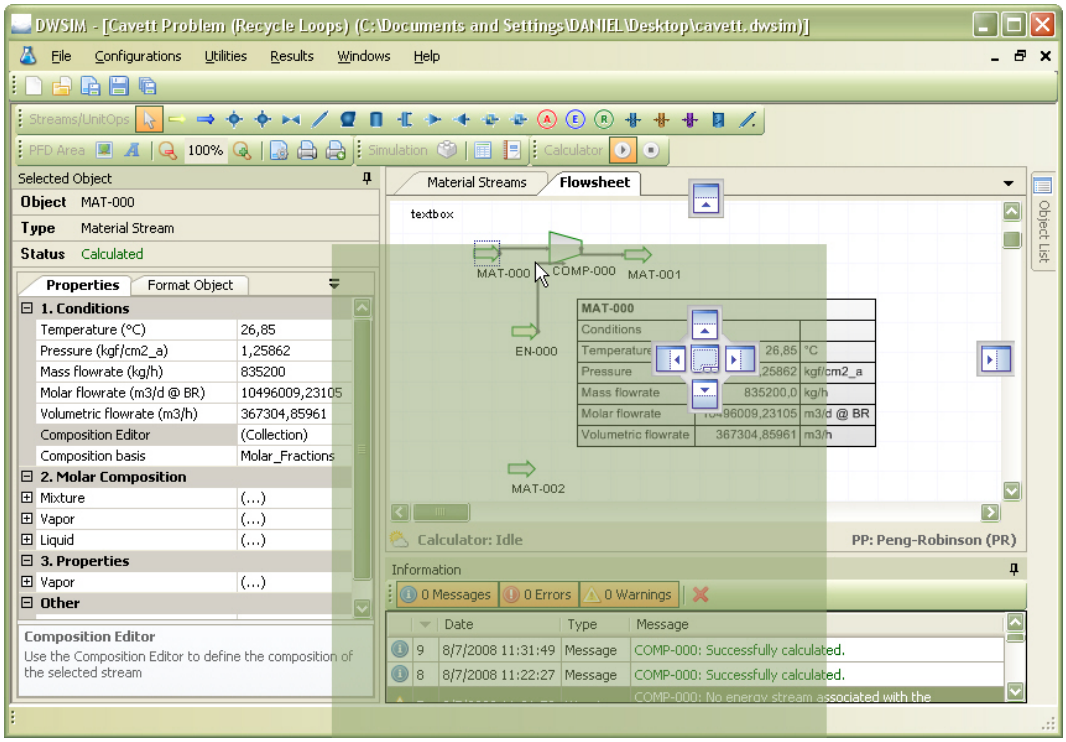


Figure 11: Window repositioning.

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.

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 through the object buttons bar (Figure 12), dragging and droping items from the **Object Palette** or by using keyboard shortcuts.

Figure 12: Object buttons bar.

To insert objects into the flowsheet by using the buttons bar, one must follow the sequence below:

1. With the left mouse button, one clicks in the desired object button;
2. With the left mouse button, the user clicks in the flowsheet area, at the point were he wants to add the object.

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

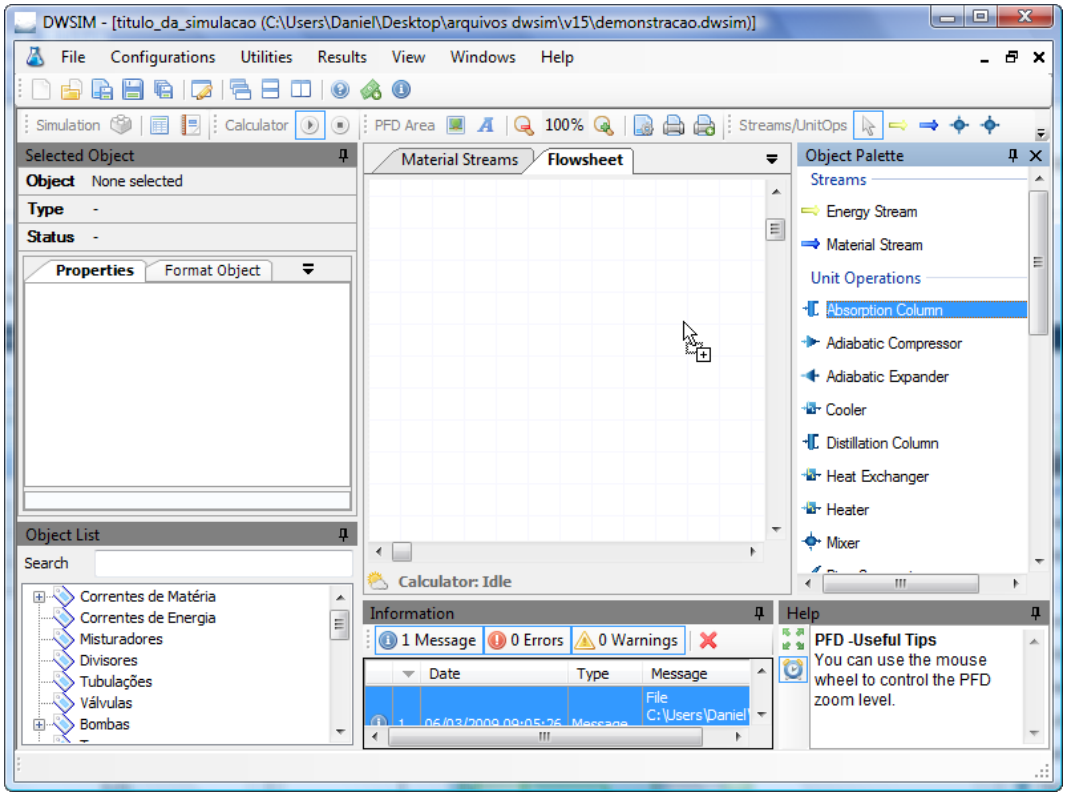


Figure 13: Dragging items from the Object palette window.

To insert objects into the flowsheet by using keyboard shortcuts, the following sequence should be observed:

1. With the flowsheet window in focus (activated), the user press the keyboard button combination corresponding to the desired object (see Figure 14 for an example) - the mouse cursor changes its shape to indicate that a keyboard shortcut was pressed;

2. The user clicks with the left mouse button in the flowsheet, at the point were he wants to add the object.

Figure 14: Viewing keyboard shortcuts to add objects.

Figure 15 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.

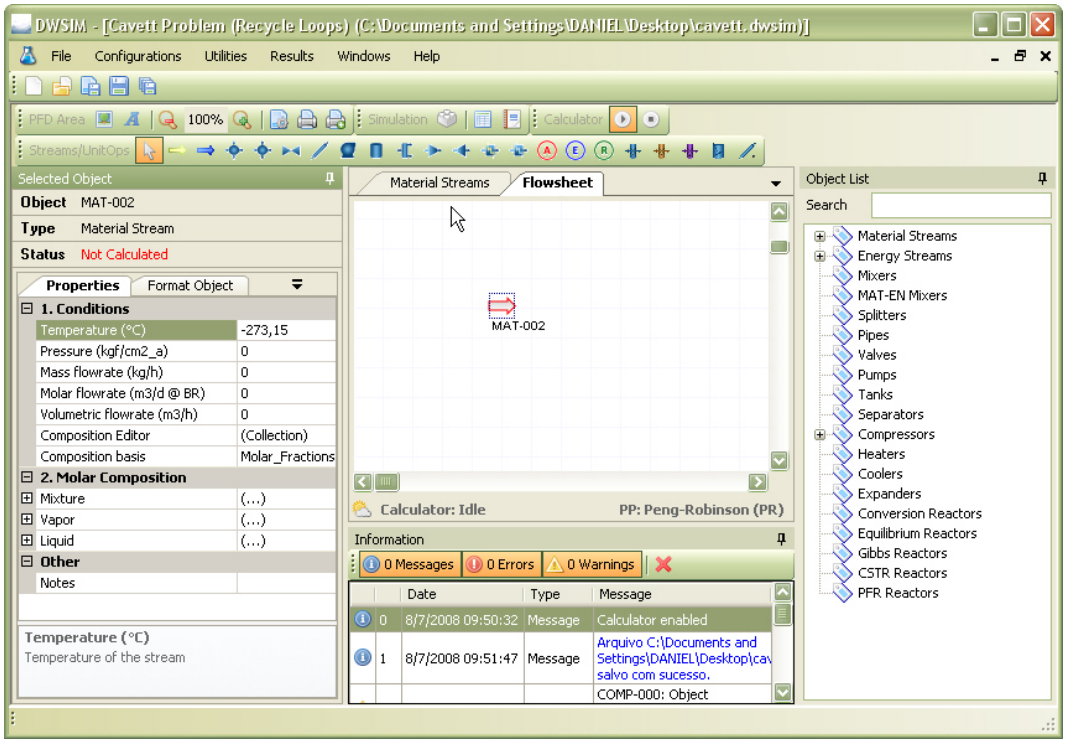


Figure 15: A material stream in the flowsheet.

Connecting objects The material streams work like a connection between unit operations. The same stream van represent, i.e., the vapor outlet from a separator vessel and the inlet of a compressor. There are two different ways in which a material stream can be connected to a unit op (or *vice-versa*):

- Through the context menu activated with a right mouse button click over the object (Figure 16);

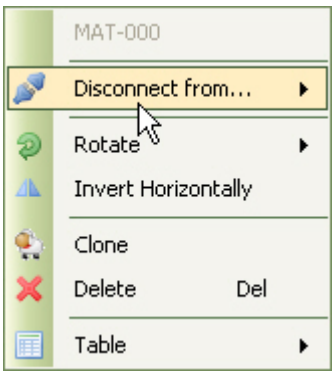


Figure 16: Selected object context menu.

- 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:

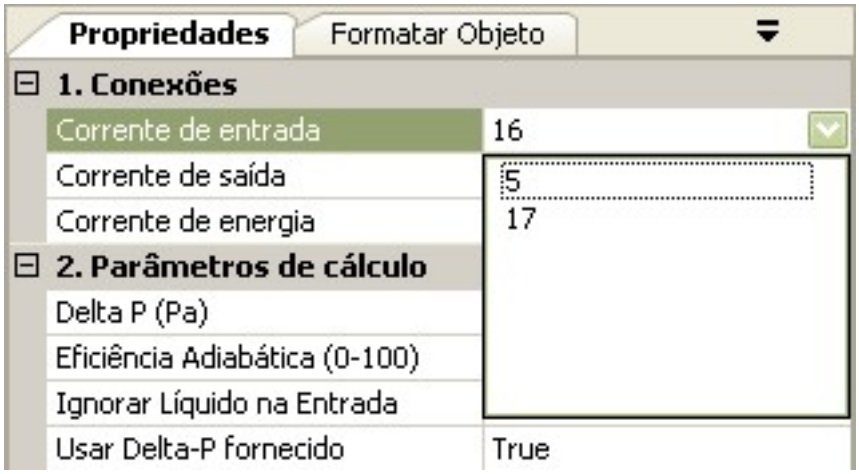


Figure 17: Stream selection menu.

A compression system with its connections is shown on Figure 18.

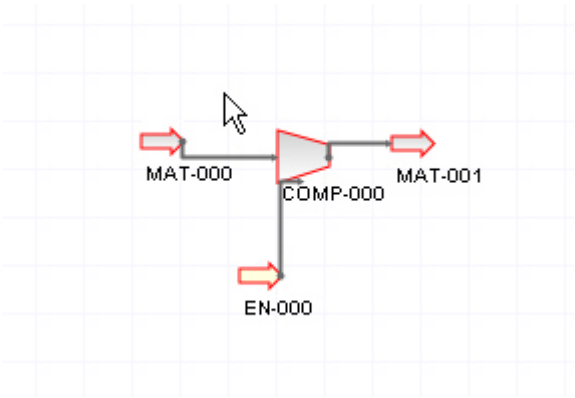


Figure 18: Compressor with all connections made.

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 16).

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 19). Properties that cannot be edited appear in gray.

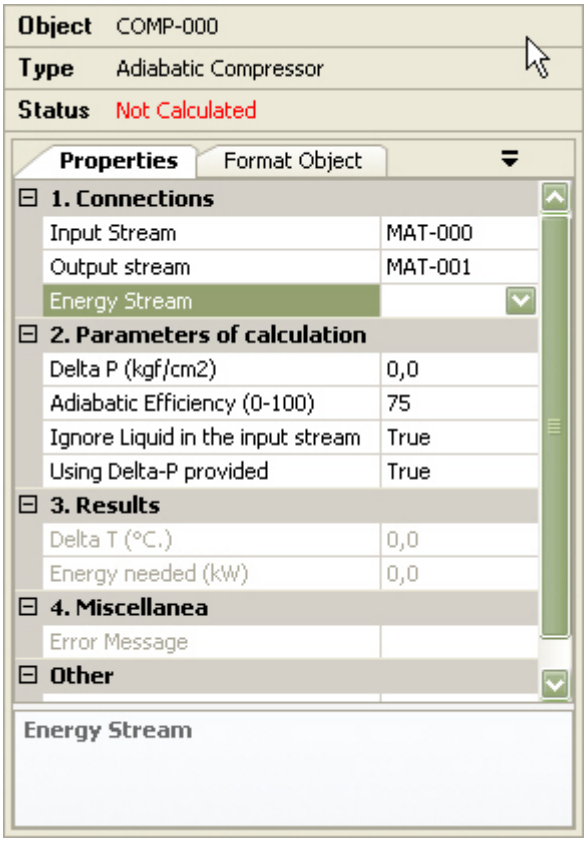


Figure 19: Viewing object properties in the "Selected Object" window.

Some properties can be edited directly in the area to the right of their identification, like a stream temperature (Figure 20). Other properties require the opening of an auxiliary window, like a stream composition (Figure 21), and others can be selected by using a *drop-down* menu (Figure 22). 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.

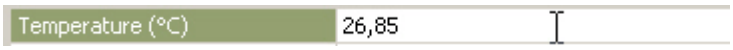


Figure 20: Direct editing of a property.

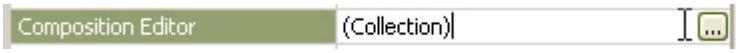


Figure 21: Using an auxiliary window to edit a property value.

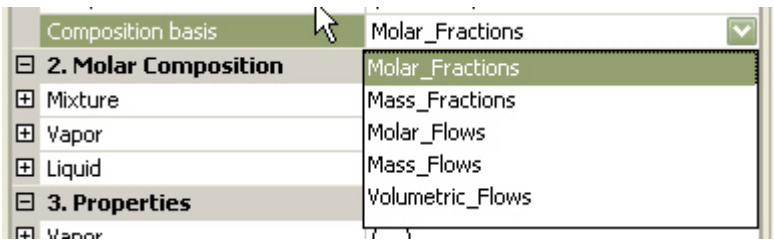


Figure 22: Selecting a value for the property in a drop-down menu.

If all object properties were correctly defined, it is calculated by DWSIM and its flowsheet representation will have a green border instead of a red one, indicating that the object was calculated successfully (Figure 23).

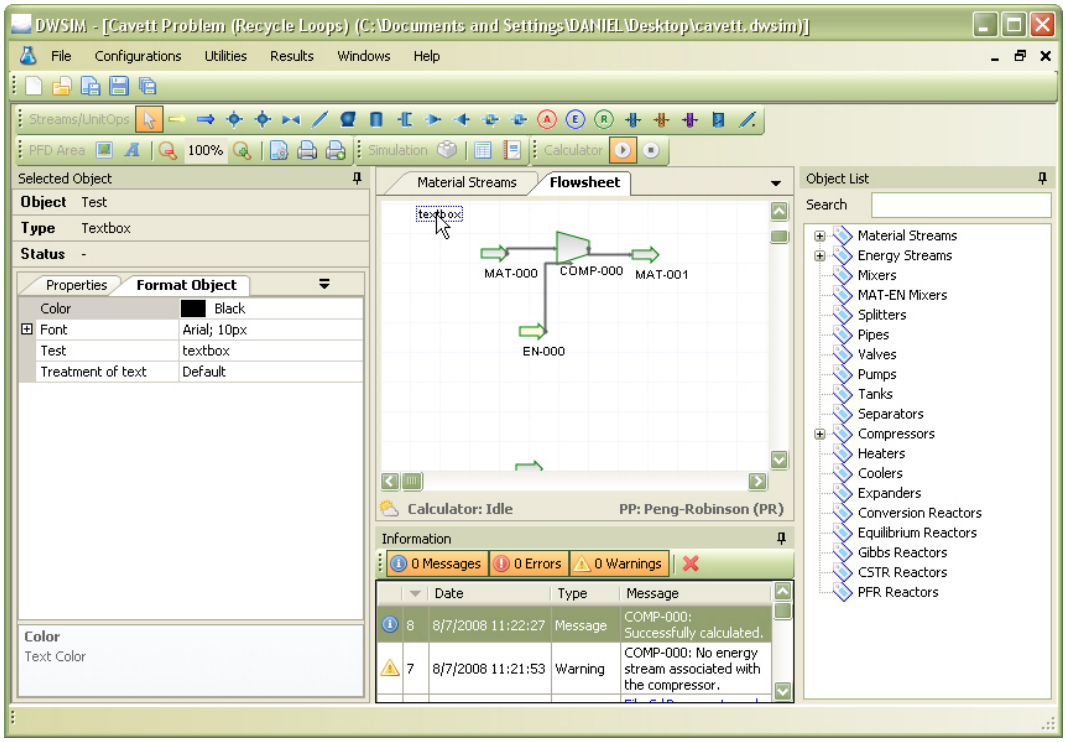


Figure 23: Calculated objects.

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. DWSIM's calculator verify if an object has its properties well-defined and, if positive, passes the data for the downstream object and calculate it, repeating the process in a loop until it reaches an object that is not downstream-connected to anyone. 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 24). 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 24: 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 25).

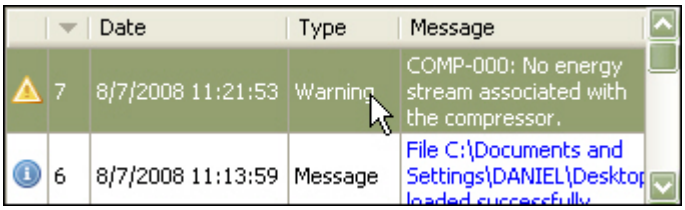
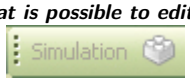


Figure 25: A DWSIM's calculator message.

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 26 and 27) for printing. Report data can also be saved to a XLS or Text file.

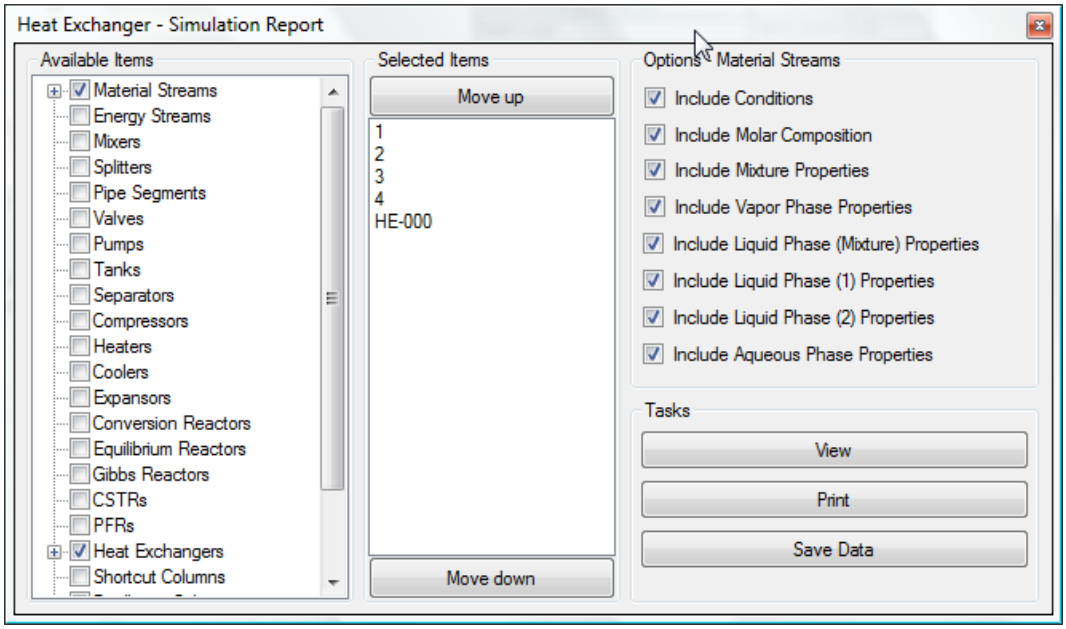


Figure 26: Results report configuration.

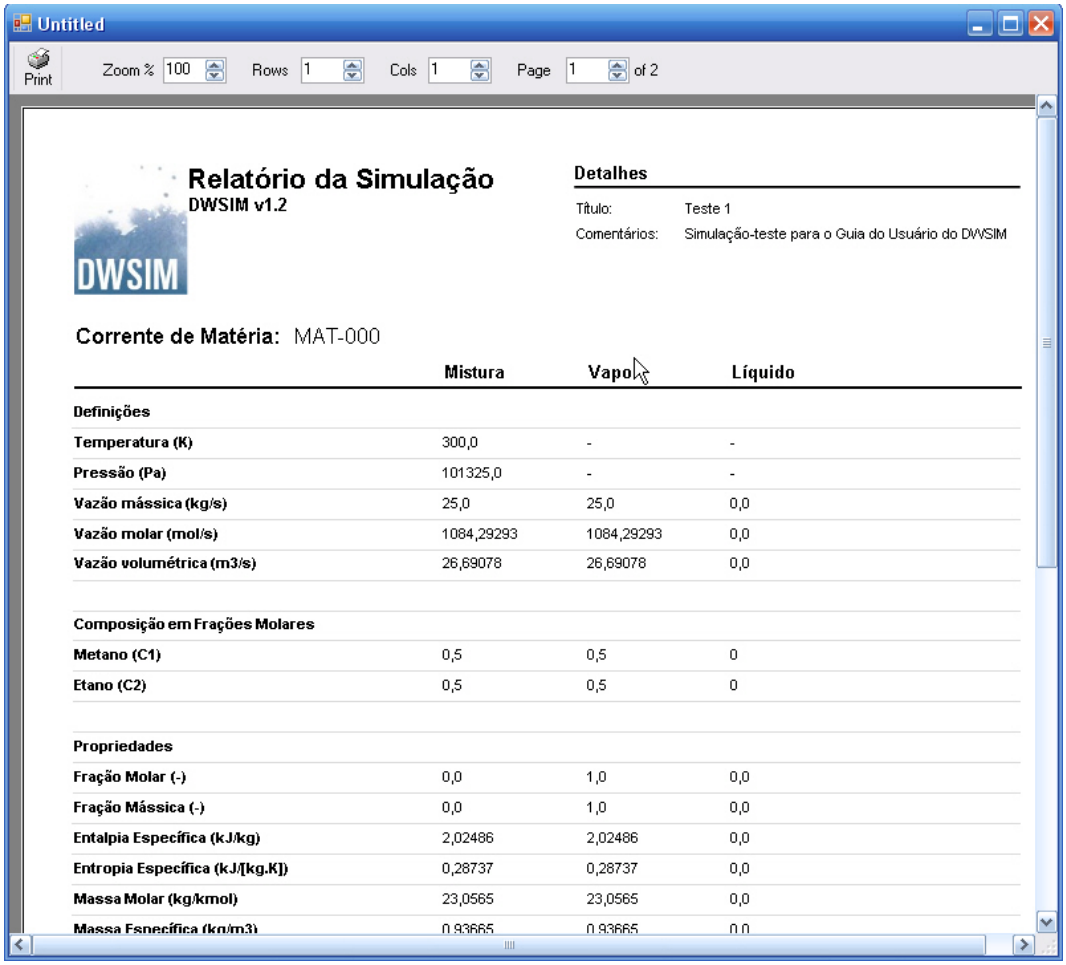


Figure 27: Results report.

3.4 Sensitivity Analysis

You can use the Sensitivity Analysis Utility in order to verify the influence of up to 2 variables into another third variable. 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, totalizing 45 points where the enthalpy will be calculated with differente values for the temperature and pressure. 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.

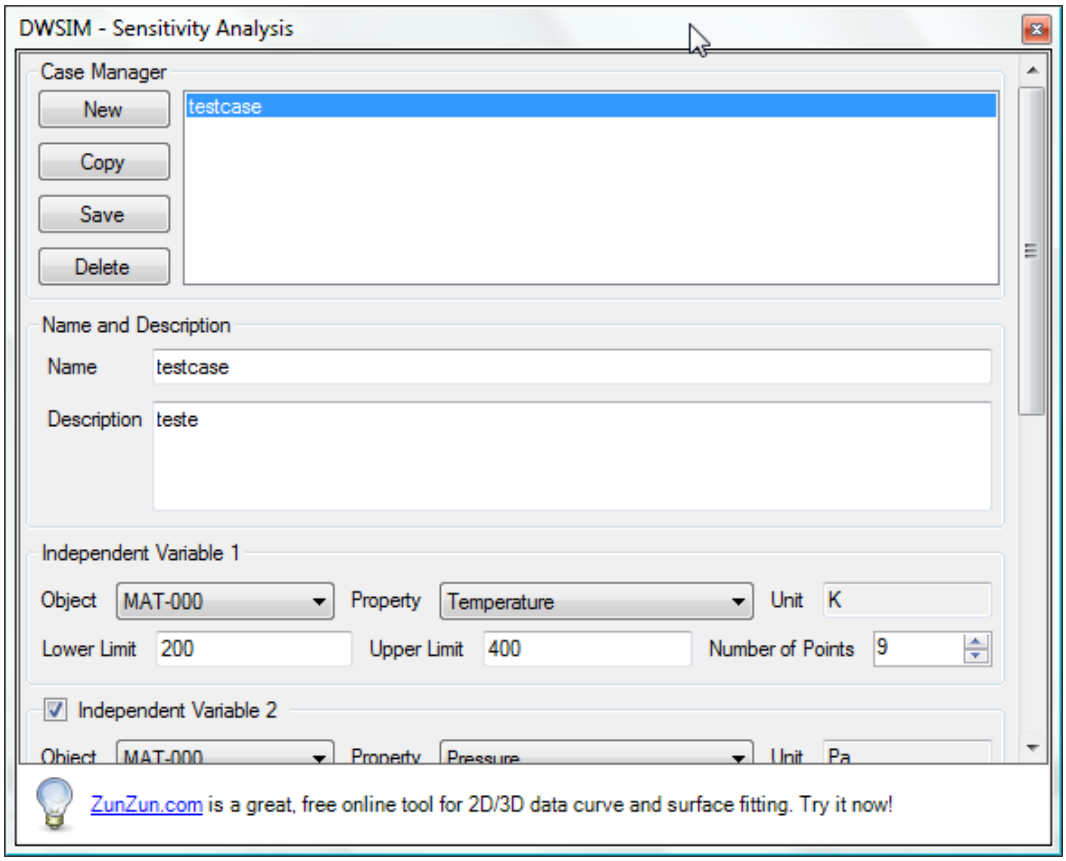


Figure 28: Sensitivity Analysis Utility (1).

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.

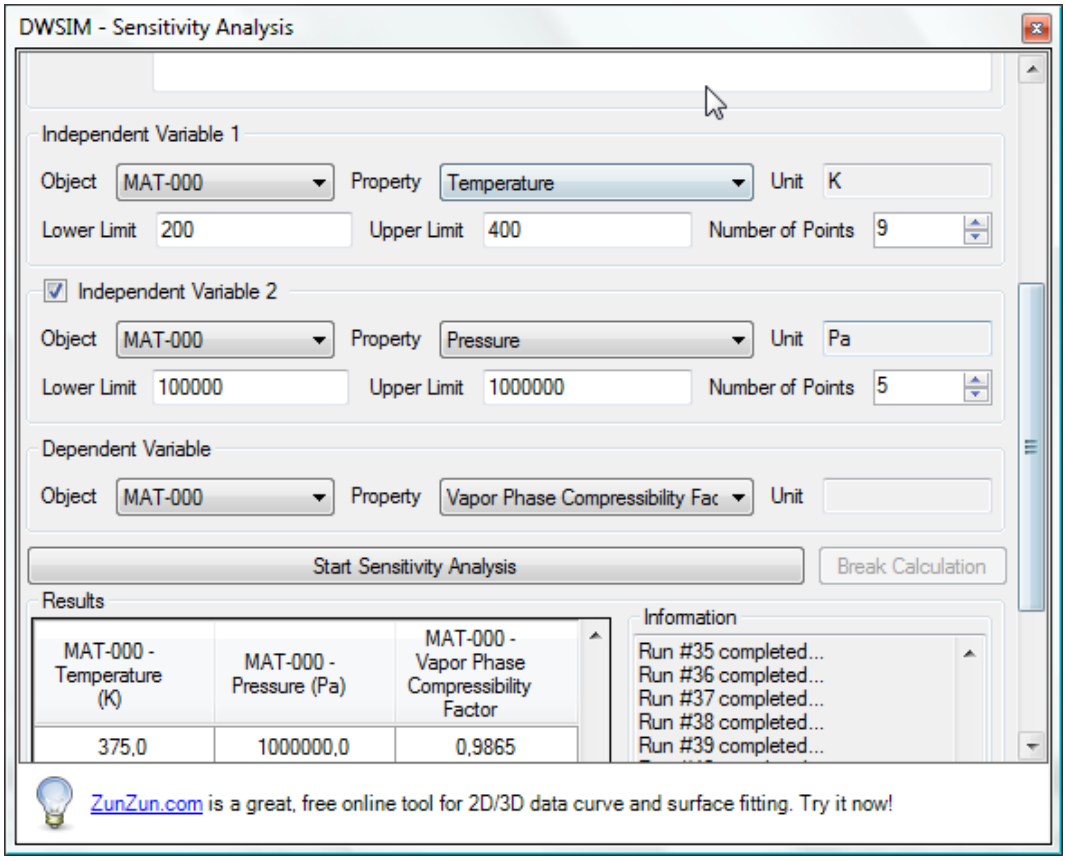


Figure 29: Sensitivity Analysis Utility (2).

The results are shown in a table, so the data can be copied and pasted into another specialized data analysis software.

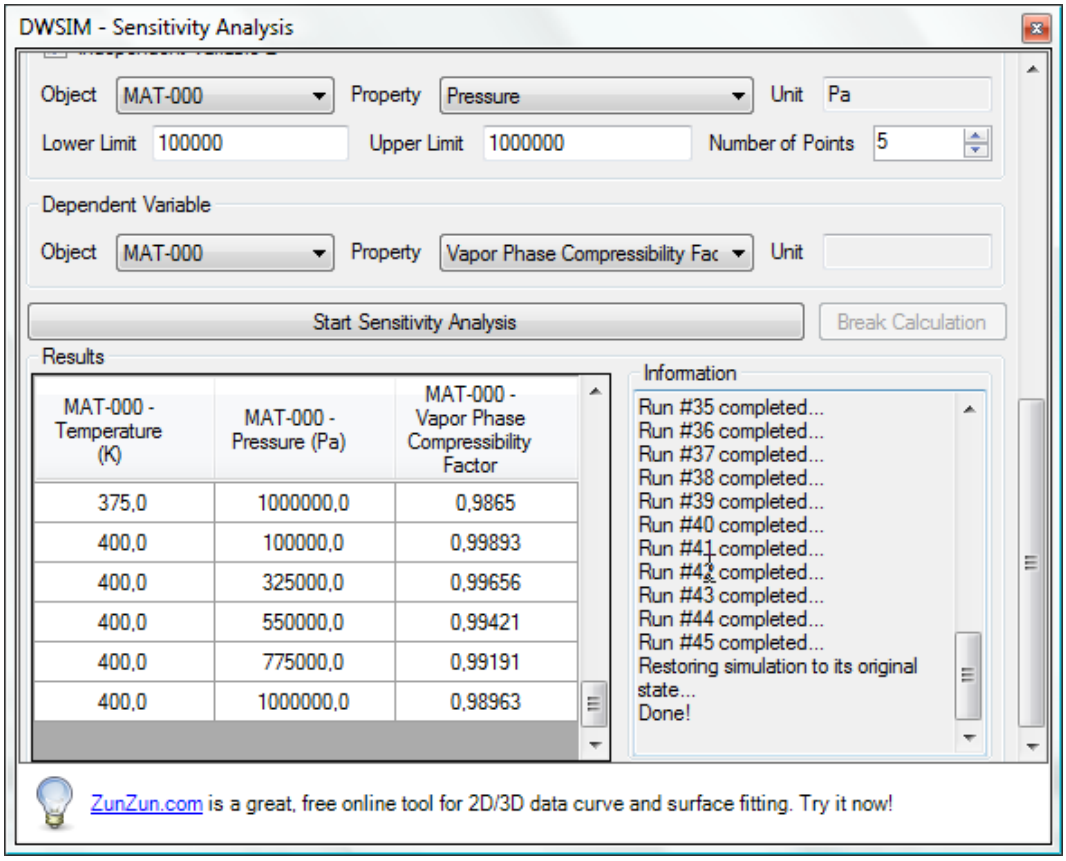


Figure 30: Sensitivity Analysis Utility (3).

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. Just like it happens to that utility, 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.

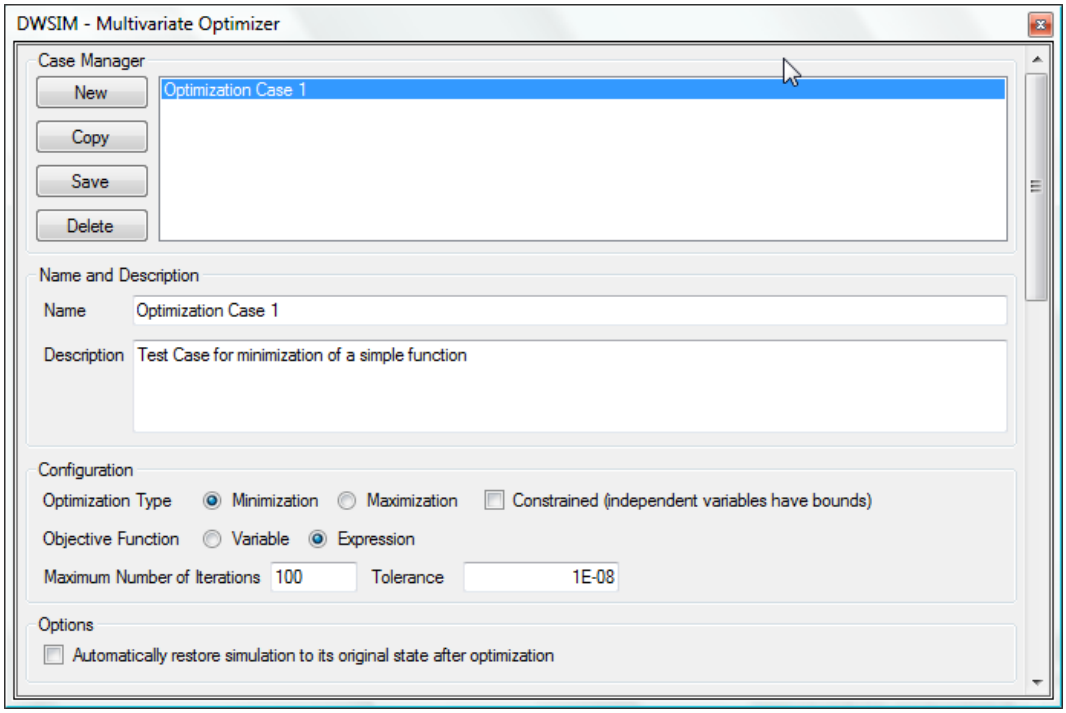


Figure 31: Multivariate Optimization Utility (1).

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 of 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 and considered in expressions only. To remove a variable, a row must be selected before pressing the "-" button.

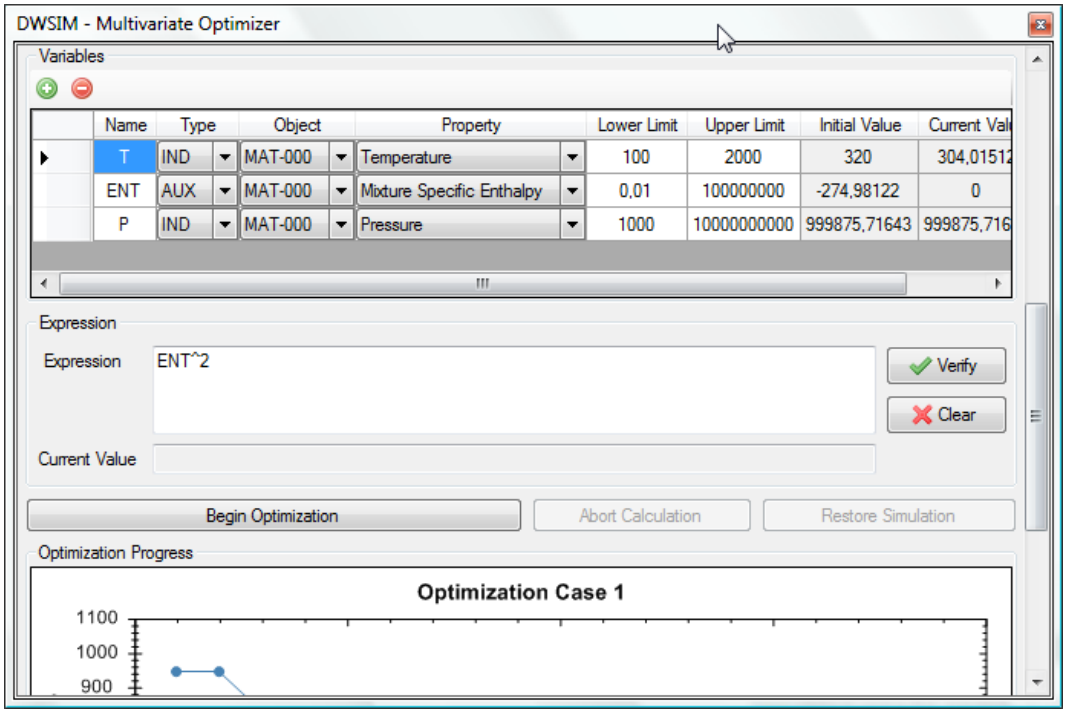


Figure 32: Multivariate Optimization Utility (2).

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 the the optimization process is over.

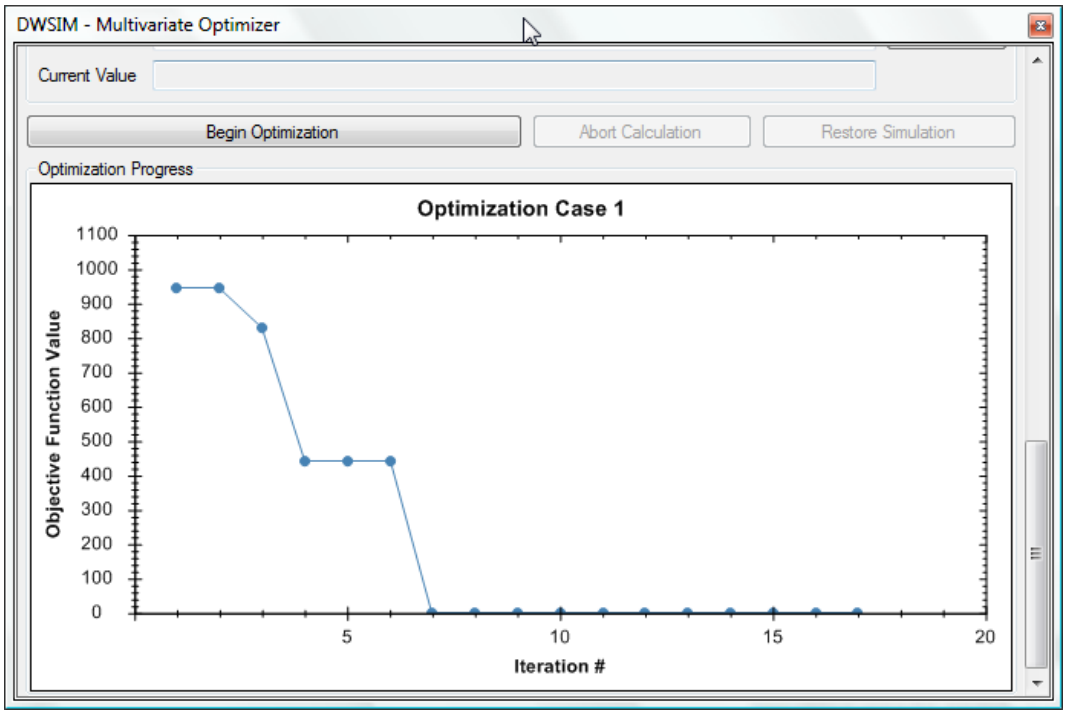


Figure 33: Multivariate Optimization Utility (3).

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 34). Uses the Peng-Robinson EOS;

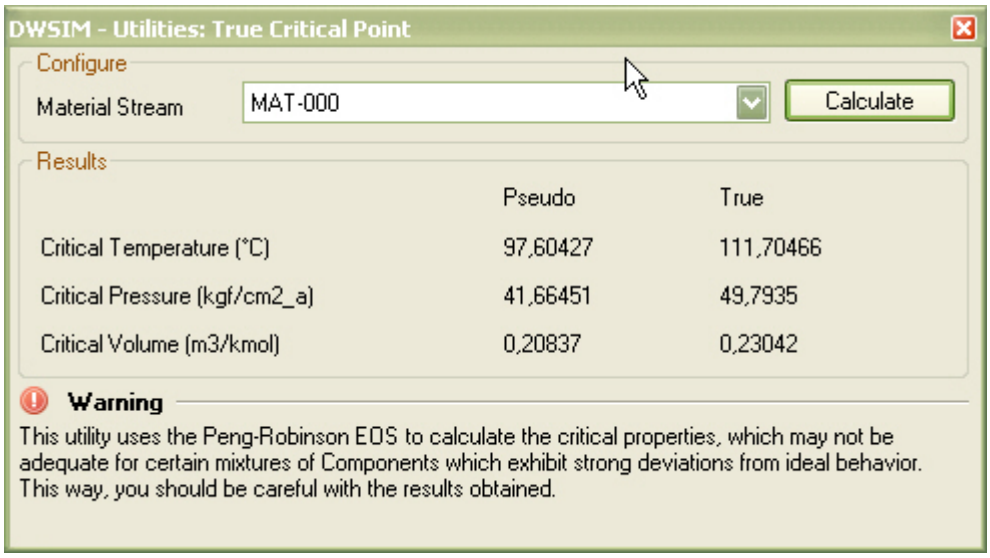


Figure 34: Utilities - True Critical Point.

- ***Hydrate Equilibrium/Dissociation Utility*** - calculation of the equilibrium conditions for natural gas hydrates (Figure 35);

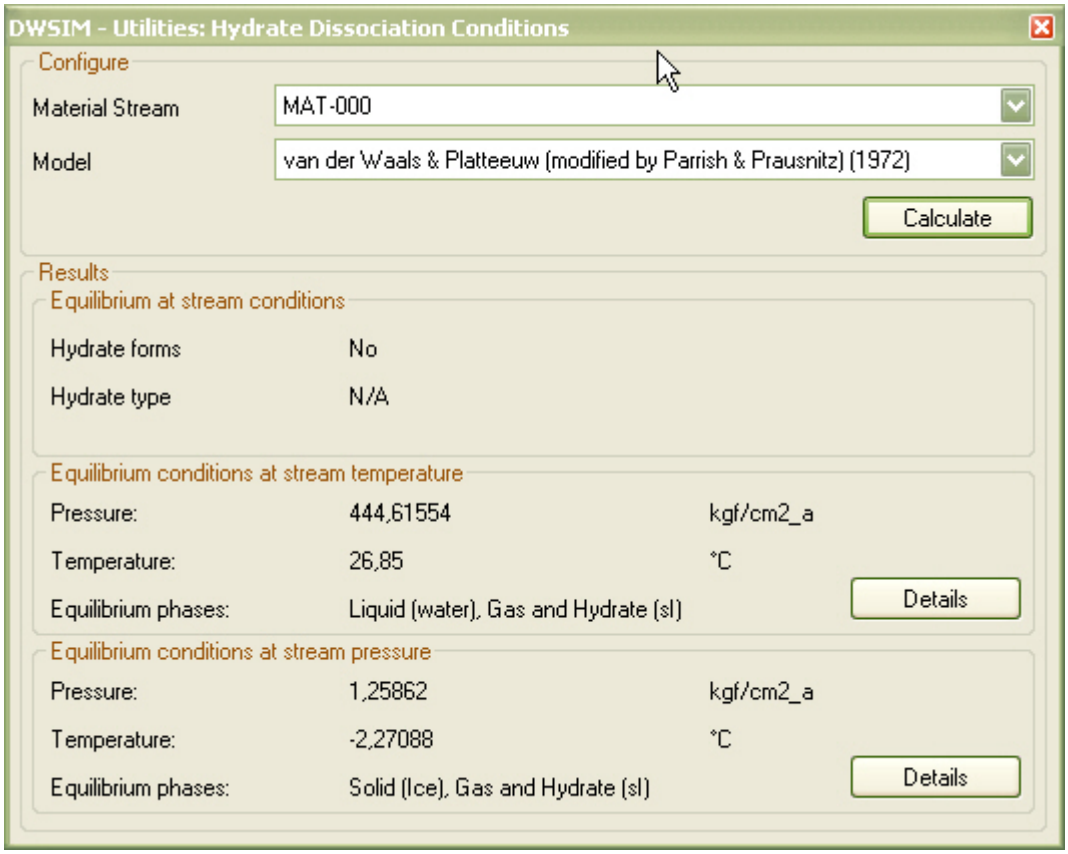


Figure 35: Utilities - Hydrate Calculations.

➙ ***Pure Component Properties*** - pure component property viewing (Figure 36);

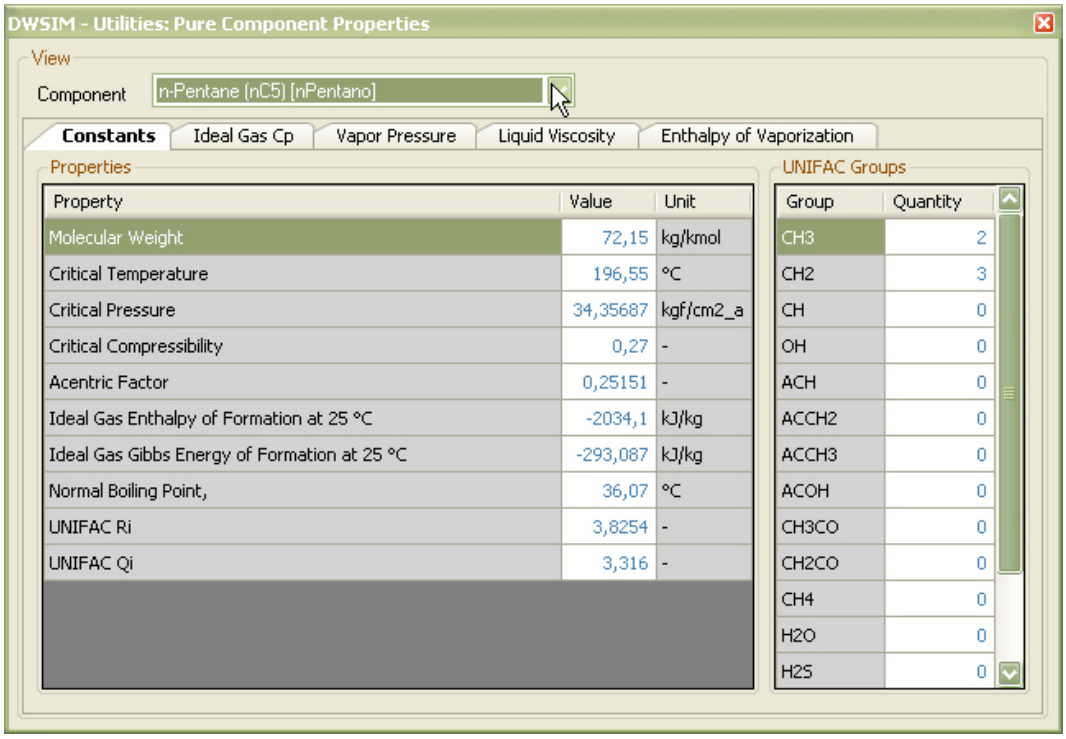


Figure 36: Utilities - Pure Component Properties.

➙ ***Phase Envelope*** - Material stream phase equilibria envelope calculation (Figure 37);

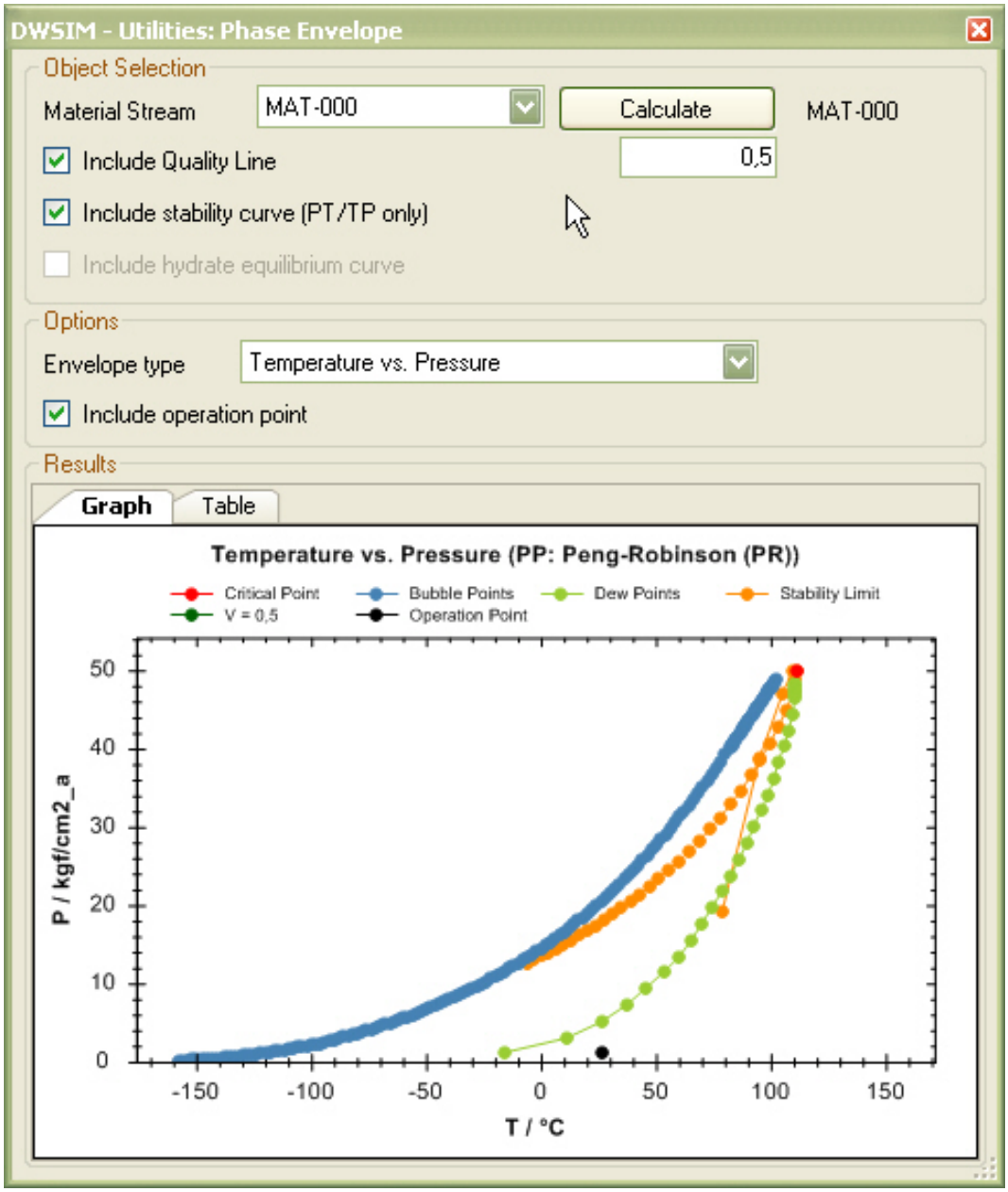


Figure 37: Utilities - Phase Envelope.

➙ ***Binary Envelope*** - special envelopes for binary mixtures (Figure 38).

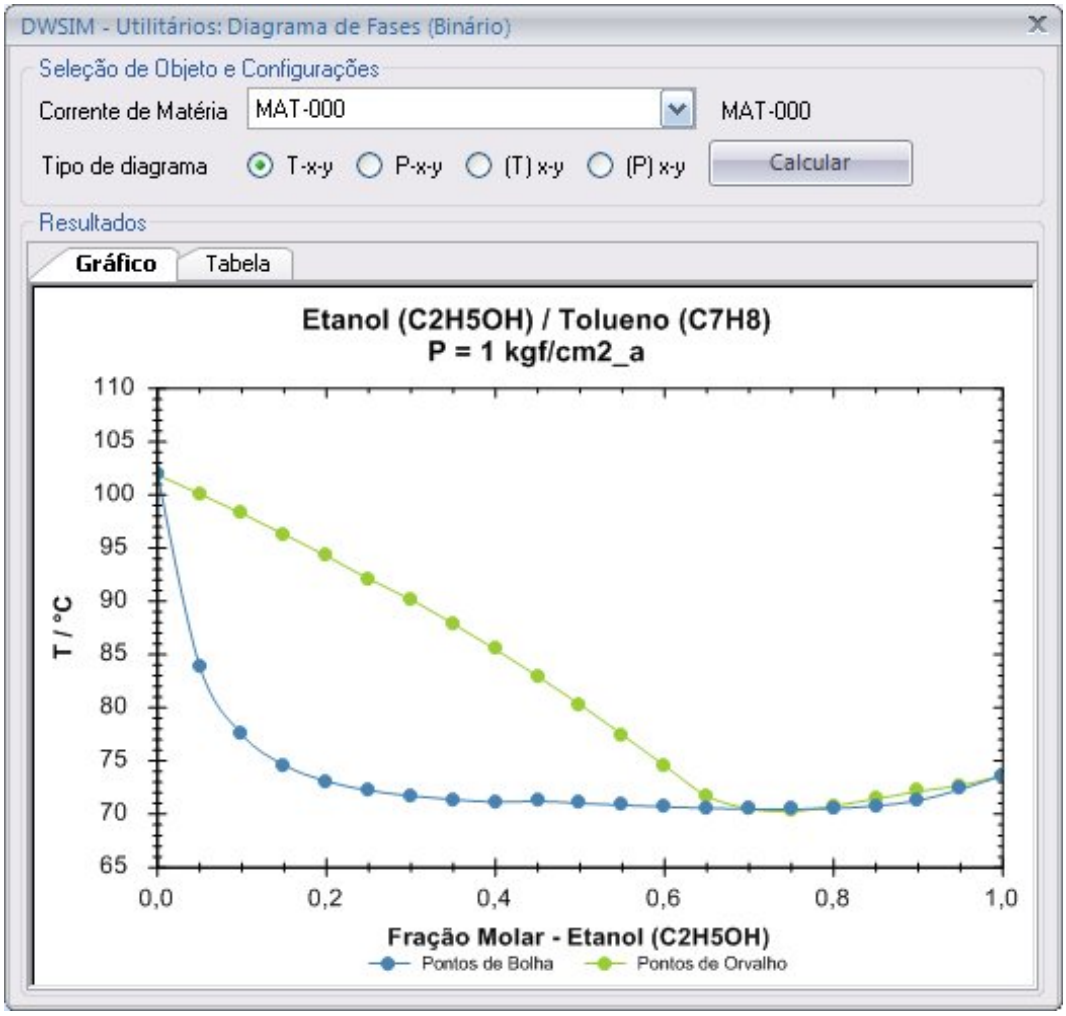


Figure 38: Utilities - Binary Envelope.

- ***Petroleum Cold Flow Properties*** - special properties of petroleum fractions, like cetane index, flash point, refraction index, etc. (Figure 39).

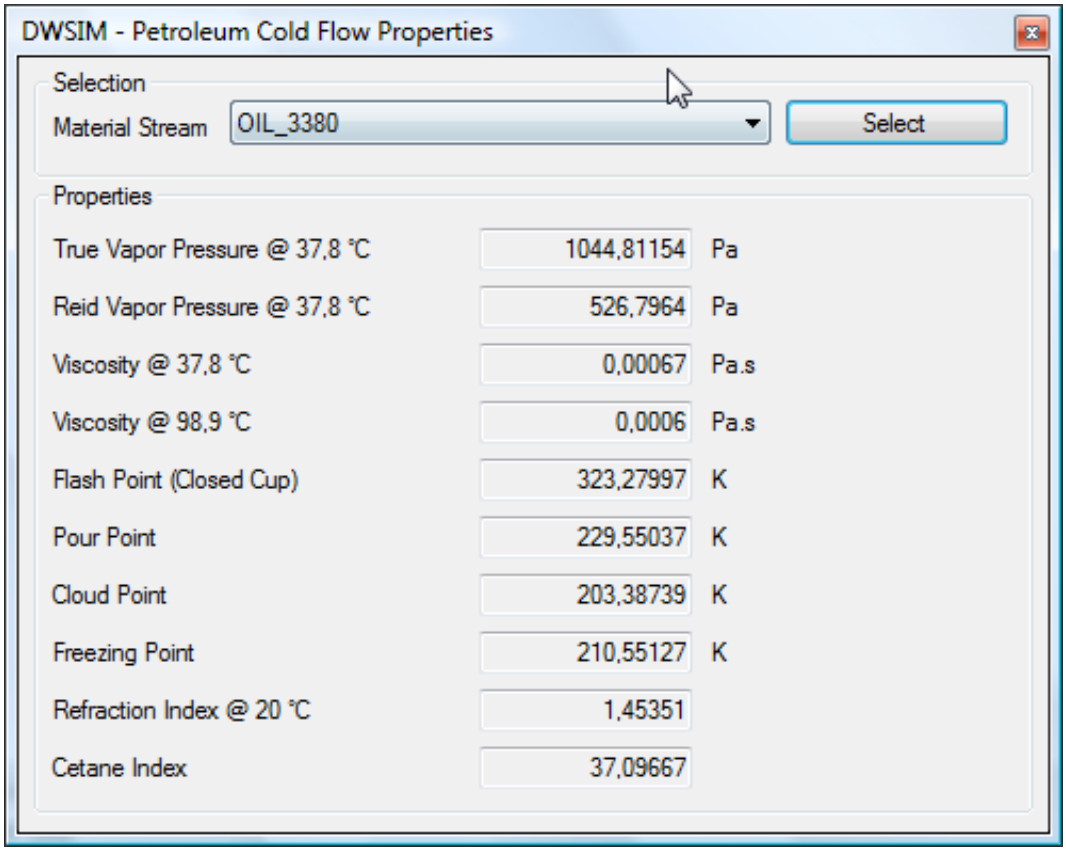


Figure 39: Utilities - Petroleum Cold Flow Properties.

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 40):

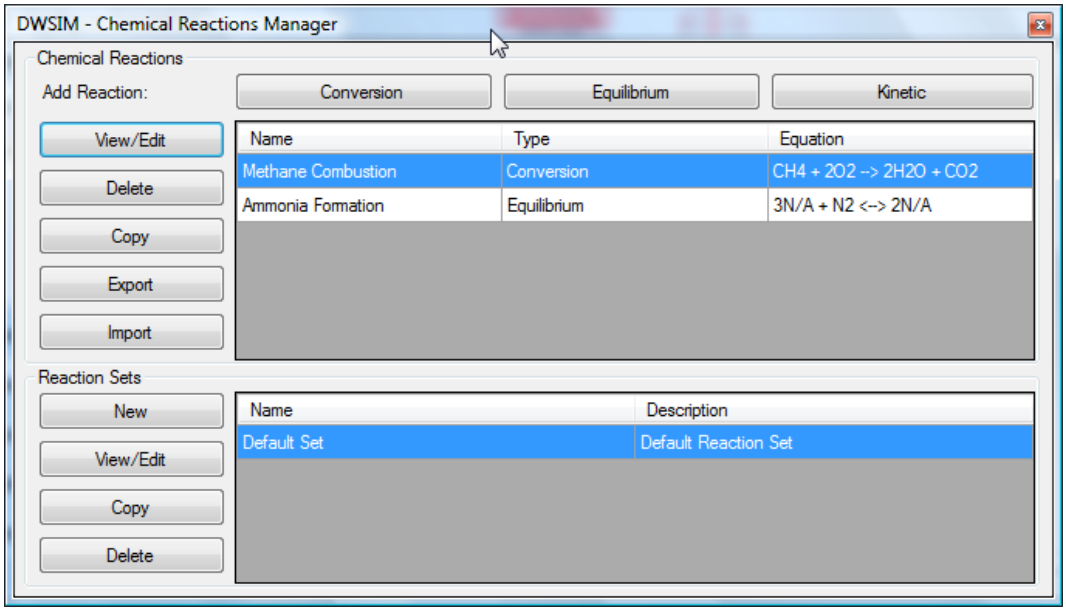


Figure 40: Chemical Reactions Manager.

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 41):

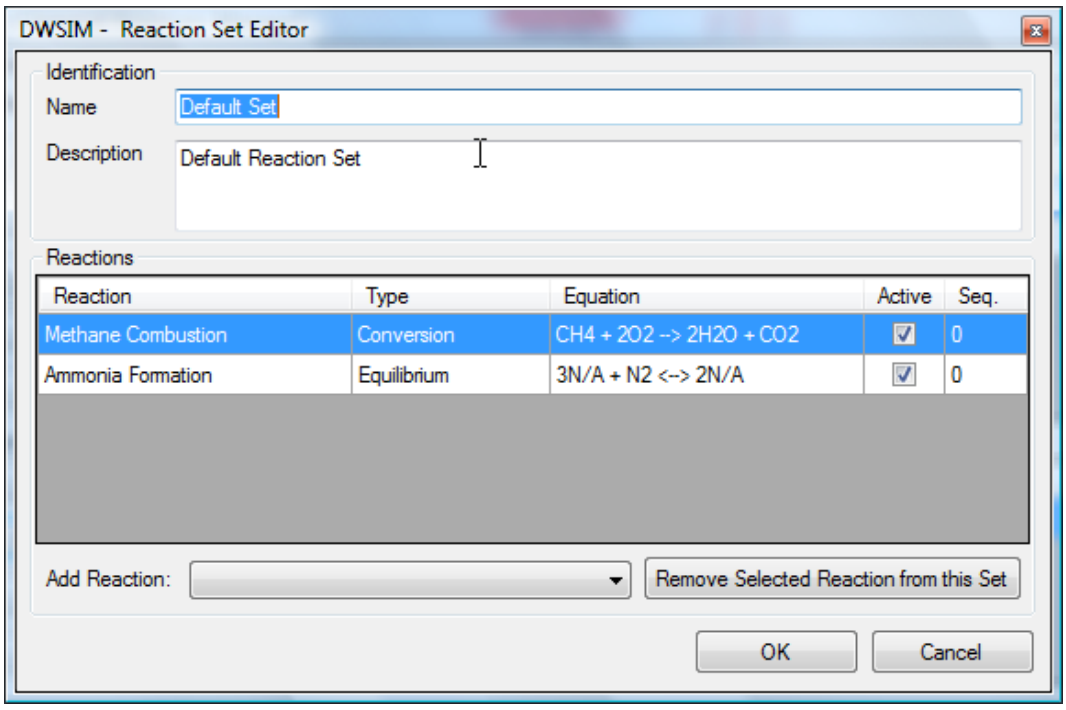


Figure 41: Reaction Set editor.

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 42):

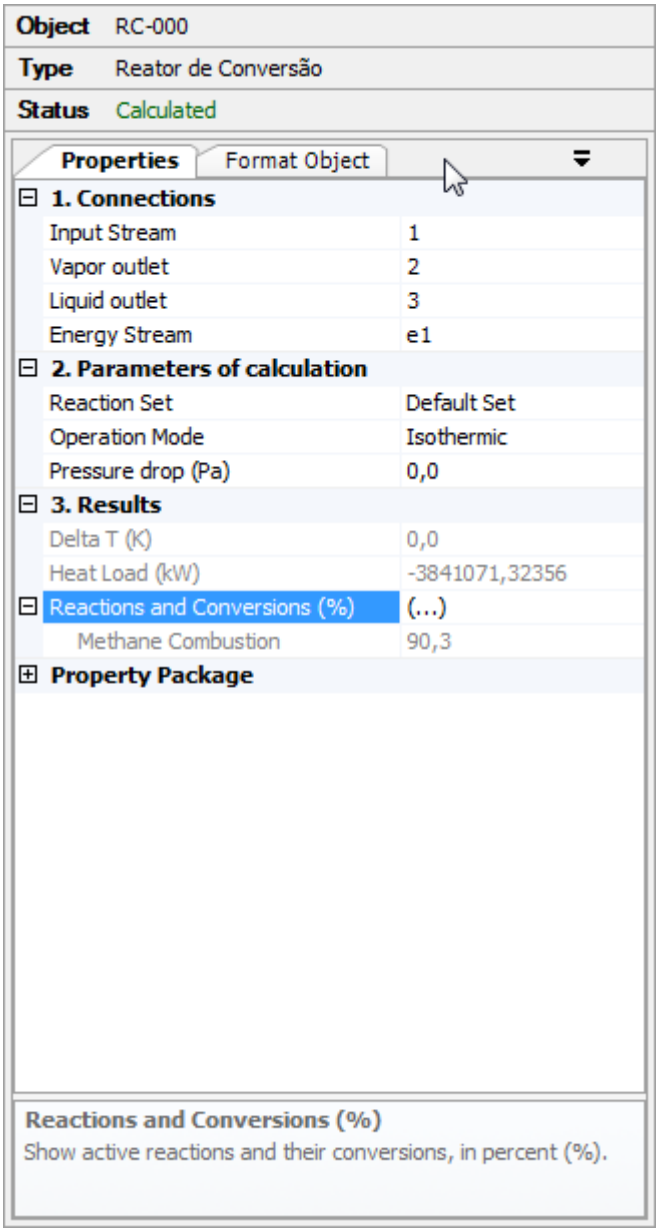


Figure 42: Reaction set in a reactor's property window.

3.8 Hypothetical Components and Characterization of Petroleum Fractions

3.8.1 Hypotheticals

Among the components present in the database, the user can add their own components through the **hypothetical creation tool**, which can be opened in the simulation configuration window (Figure 3), "Tools" tab, "Hypotheticals Creation" section. The interface for hypo creation is shown in Figure 43:

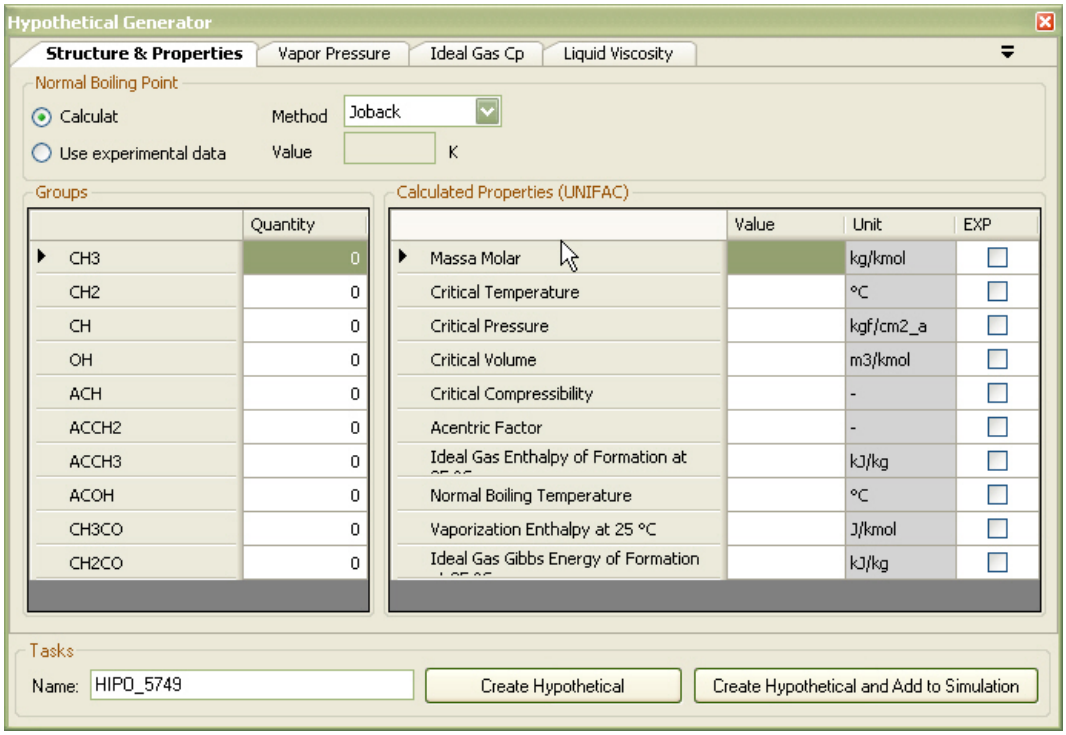


Figure 43: Hypotheticals Generator.

In order to create a hypo component, the user must, provide its UNIFAC structure. The UNIFAC structure is composed by groups which represent together the molecular structure of the component. As the user "builds" the component molecule, their properties are automatically calculated and shown in the corresponding table (Figure 44):

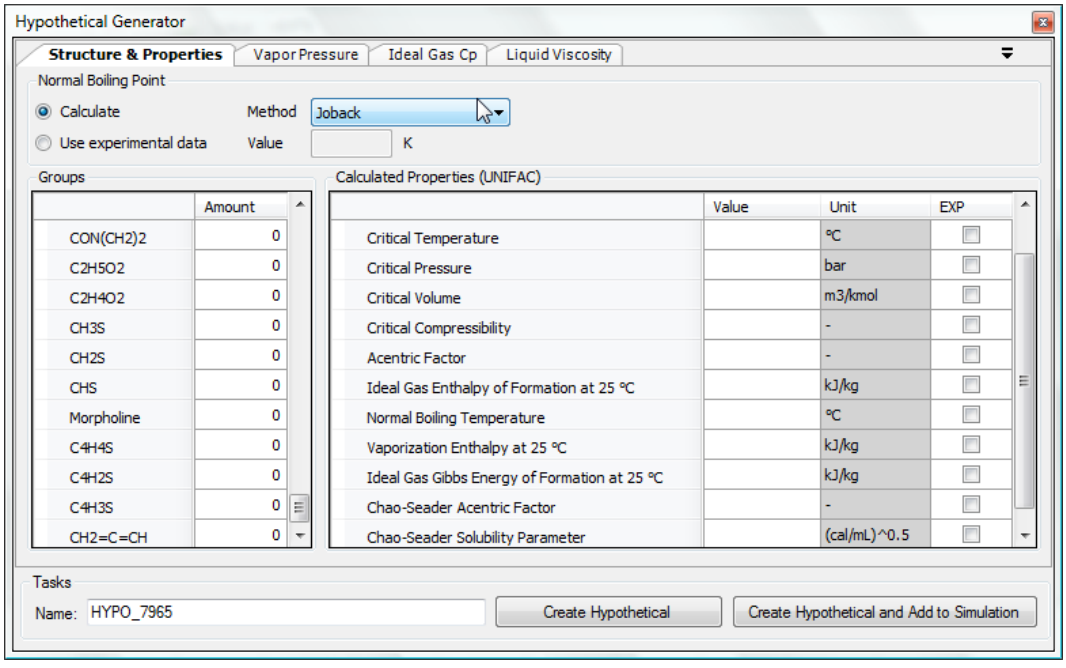


Figure 44: Hypo properties.

> ***It is highly recommended that the user provides a value for the Normal Boiling Point of the component, since this property is used as a parameter in the calculation of the other ones and has a significant impact on them.***

DWSIM includes methods and models for calculation of all the properties required in the simulation. However, the user can edit these properties and/or provide experimental data for the regression of the coefficients for vapor pressure, liquid viscosity and ideal gas heat capacity calculations. (Figure 45):

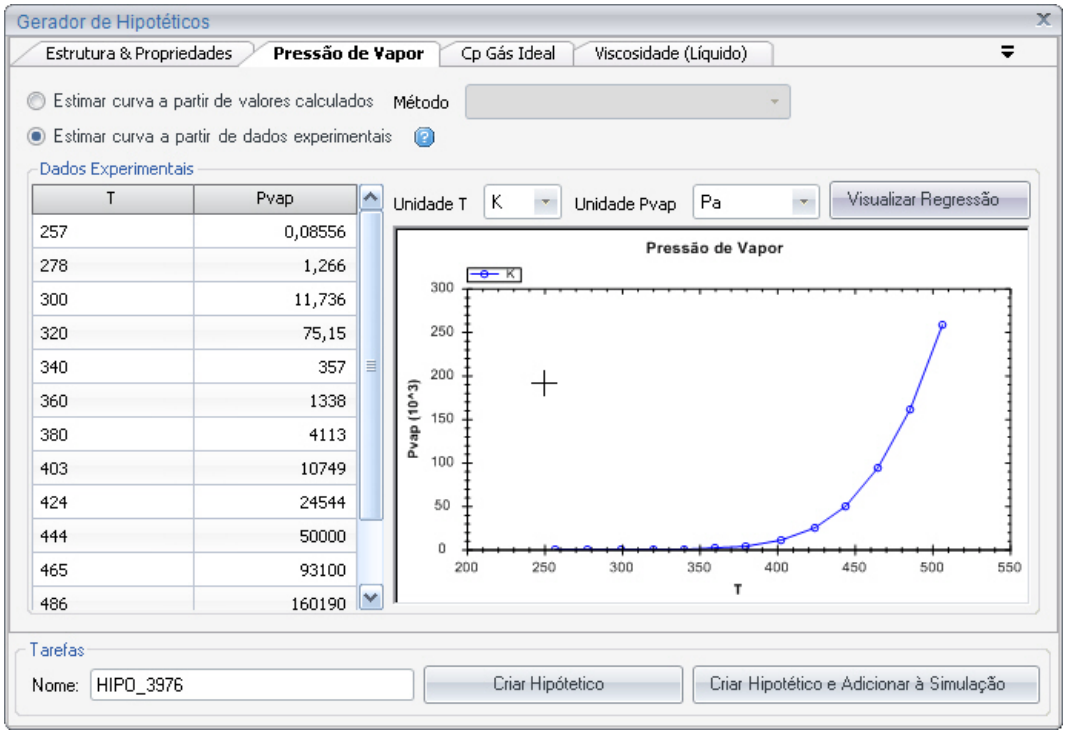


Figure 45: Entering data for regression of the parameters for vapor pressure calculation.

If the user is satisfied with the calculated or entered property values, the hypo component can then be added to the simulation. A checklist is shown to warn the user about the correctness of the calculated properties (Figure 46):

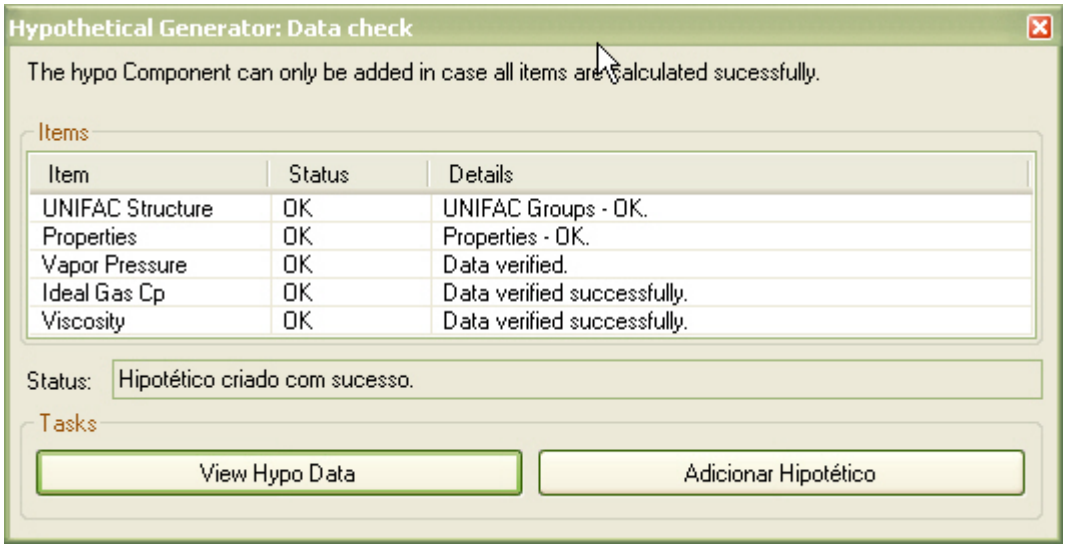


Figure 46: Hypo data verification.

At this point the user can view hypo data or add it to the simulation. After inclusion of the component in the simulation, it can be manipulated like any other component, and it will be already shown in the composition edit window for material streams.

3.8.2 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 47). The other characterizes the oil from an ASTM or TBP distillation curve (Figure 48).

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

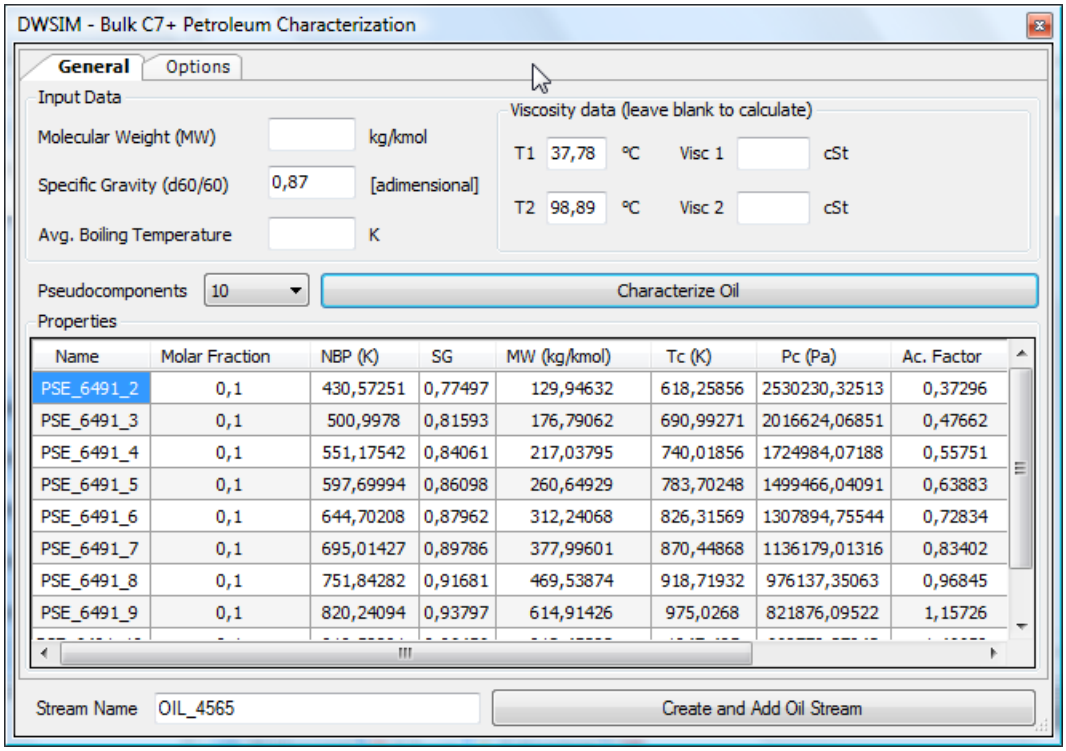


Figure 47: C7+ petroleum fraction characterization utility.

- ***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 48):

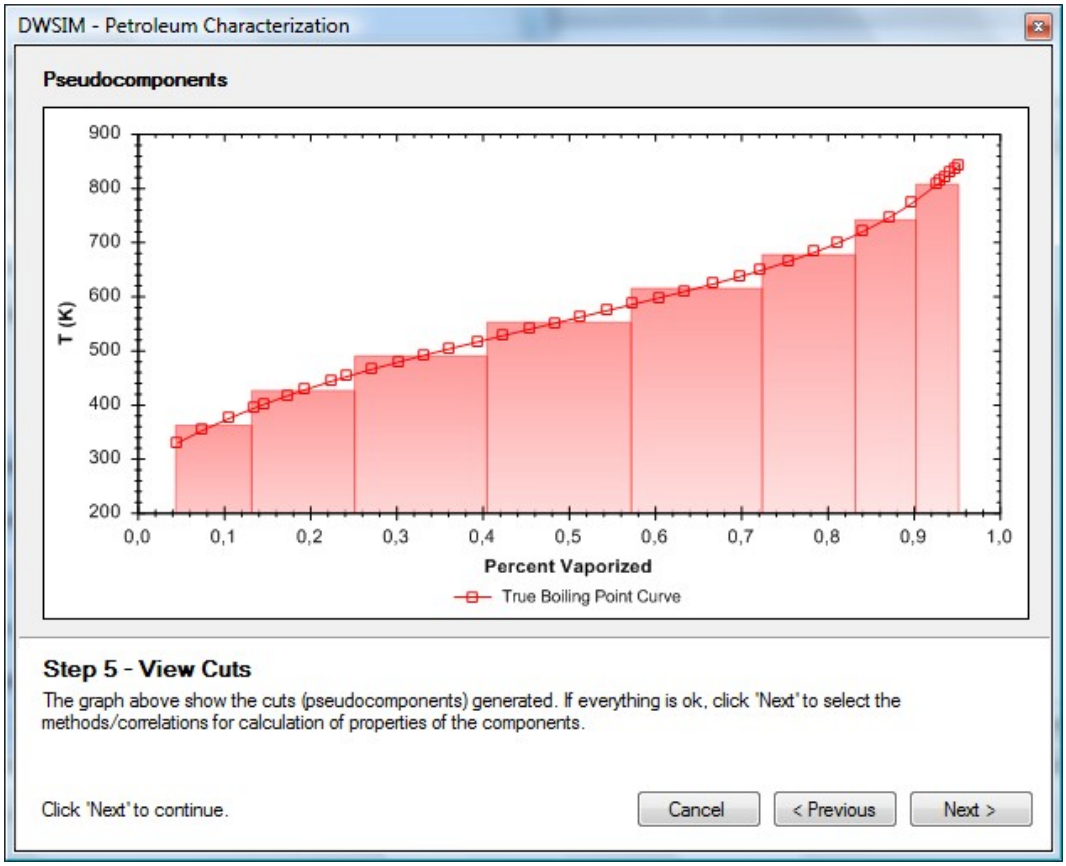


Figure 48: Characterizing petroleum from distillation curves.

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.***

3.9 Component Databases

3.9.1 Databases

The components available for use in simulations are grouped in *databases*. Two databases are installed together with DWSIM, one of them being the default database which is included with every public release. The second one is an adaptation of an excel databank available at the *Chemical Engineering Resources's page* (http://www.cheresources.com), which contais more than 400 components, although some of them are not usable because they are missing critical data (like acentric factors, liquid viscosity data, etc.), but there are means to include these missing data through tools present in DWSIM.

It is also possible to load the database from *ChemSep™ LITE 6.2* (http://www.chemsep.com), a free version of a powerful standalone, CAPE-OPEN compliant

Column Simulator. The ChemSep™ database is one of the most complete in the market.

Databases in DWSIM can be managed from the Mais Menu > Configurations > General Settings (Figure 49):

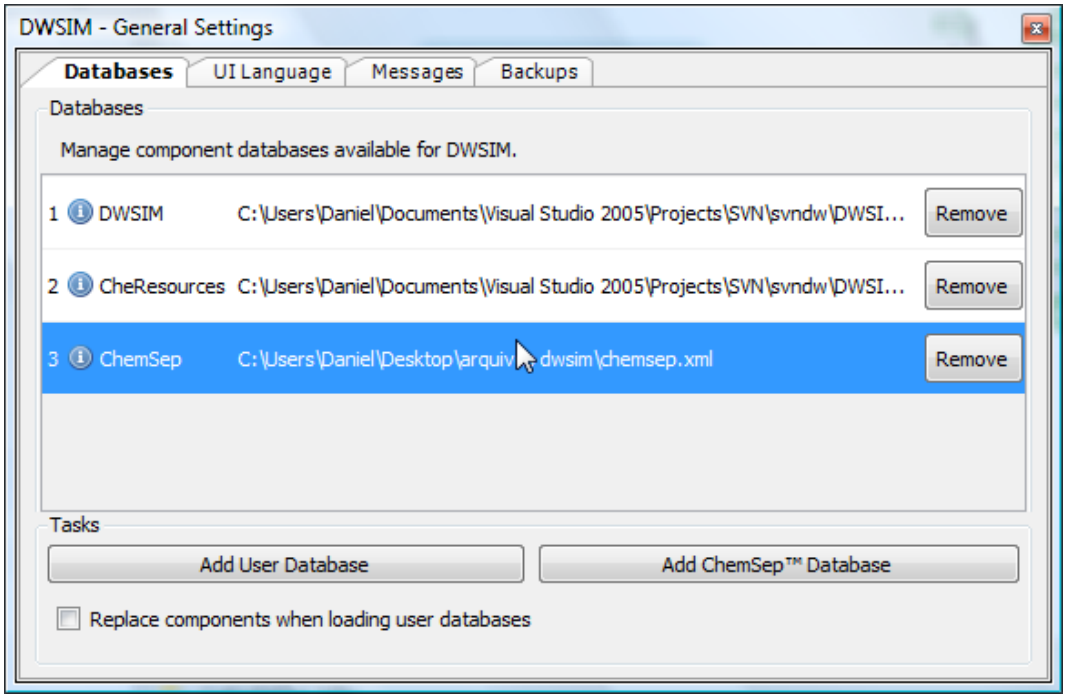


Figure 49: Database manager.

At 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. The two default databases cannot be modified nor deleted.

Changes in this window take effect only after DWSIM is restarted.

3.9.2 Managing Components

From DWSIM version 1.5 and up, some flexibility was added for the management of available components in a simulation. In addition to having the ability to load other databases, the user can save components of all types to a file - and not only hypotheticals or pseudocomponents, modify their properties and load them again into the simulation. The user can also insert its own components, using a friendly tool for insertion of the necessary properties for the component to be available in the simulation.

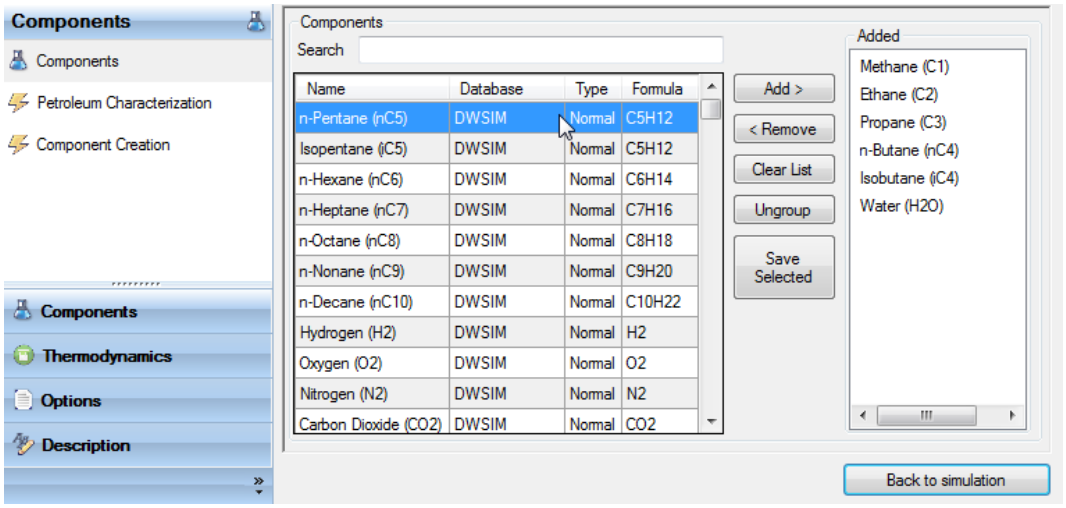


Figure 50: Selecting components from the list.

Exporting components to a XML file Select the components you wish to export using the cursor and click on the "Save Selected (XML)" button (Figure 50).

Attention: this selection is done by selecting the lines on the list using either the mouse (clicking on a item and dragging the cursor with the left button pressed) or the keyboard (SHIFT + down/up arrow).

To import/insert these components again into another simulation, use the *Database Manager* in the **General Settings** window.

Adding user components User components can be added by opening the tool to add components ("Add Component" button) and providing the necessary data (Figure 51):

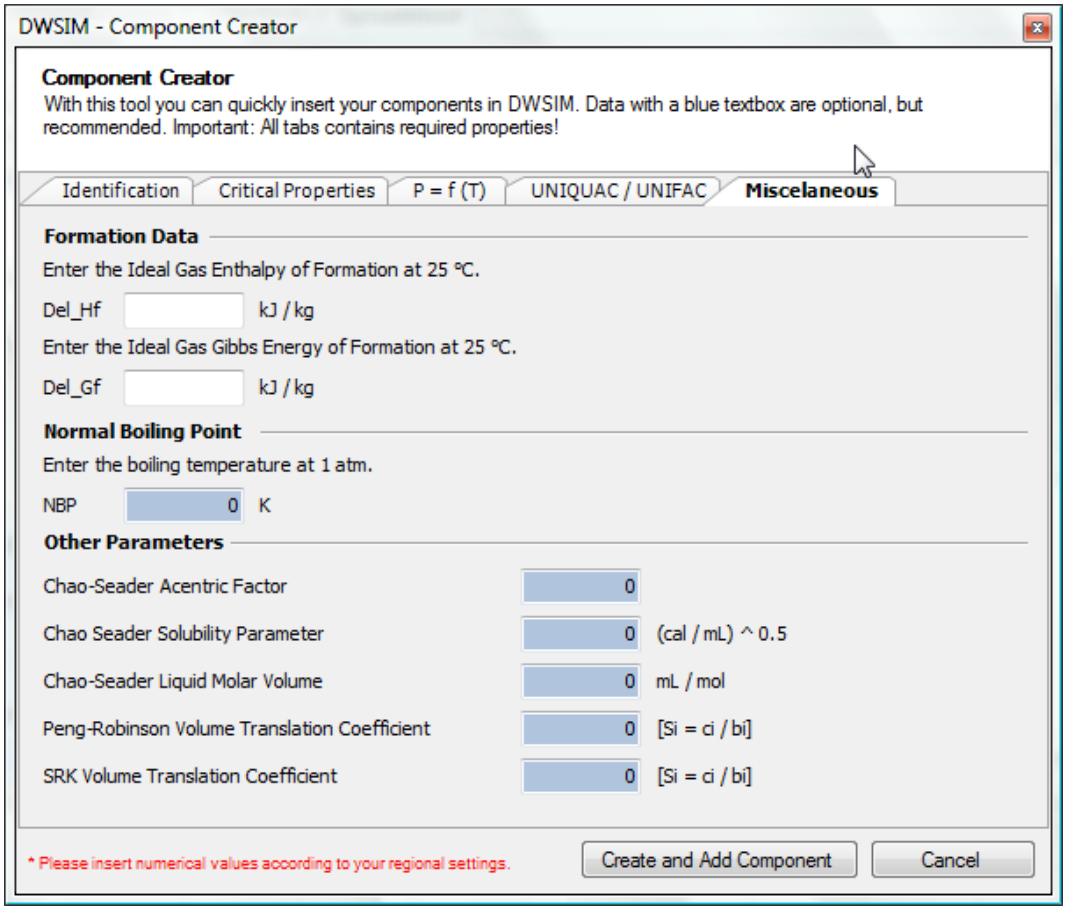


Figure 51: Utility for adding user components.