DWSIM - Process Simulation, Modeling and Optimization
Unit Operations and Utilities Guide

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Contact Information

DWSIM - Process Simulation, Modeling and Optimization

Author: Daniel Medeiros

Website: http://dwsim.inforside.com.br / http://www.sourceforge.net/projects/dwsim

E-mail: danielwag@gmail.com

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1 Introduction

This guide describes the calculation principles of the unit operation models in DWSIM. For details about the thermodynamic and property calculation models, please read the **Technical Manual**. Guidelines about software usage and interface navigation can be found in DWSIM's **User Guide**.

2 Simulation Objects

2.1 Streams

2.1.1 Material Stream

The Material Stream is used to represent matter which enters and leaves the limits of the simulation, passing through the unit operations.

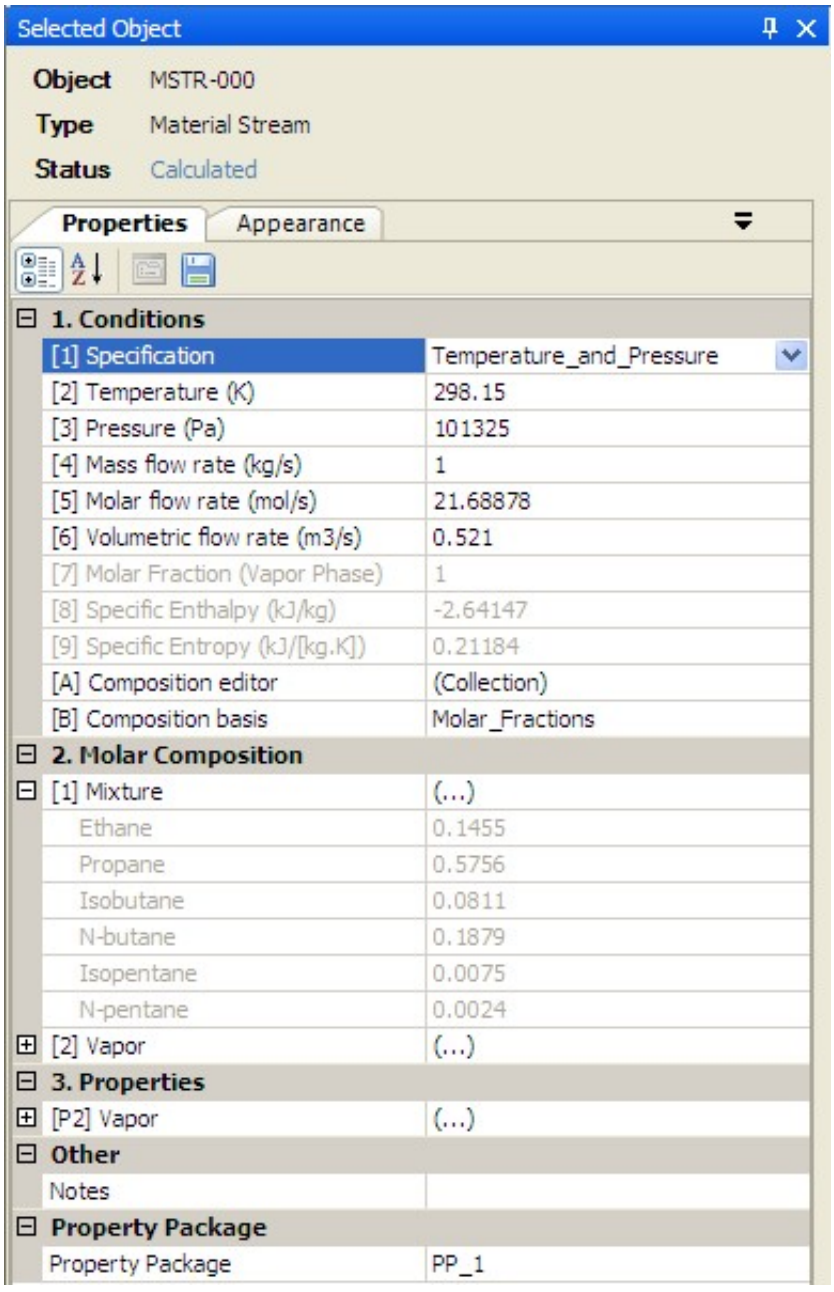


Figure 1: Material Stream properties.

Input Parameters

➙ Specification:

- Temperature and Pressure
- Pressure and Enthalpy
- Pressure and Entropy
- Pressure and Vapor Fraction
- Temperature and Vapor Fraction

The above selection dictates which variables should be defined in order to DWSIM calculate the others.

- Temperature: stream temperature;
- Pressure: stream pressure;
- Specific Enthalpy: stream's specific enthalpy;
- Specific Entropy: stream's specific entropy;
- Molar Fraction (Vapor Phase): the vapor phase mole fraction of the stream;
- Composition: the stream composition can be entered on Mole/Mass Fraction/Flow, Standard Liquid Volumetric Fraction, Molality or Molarity basis (Figure 2).

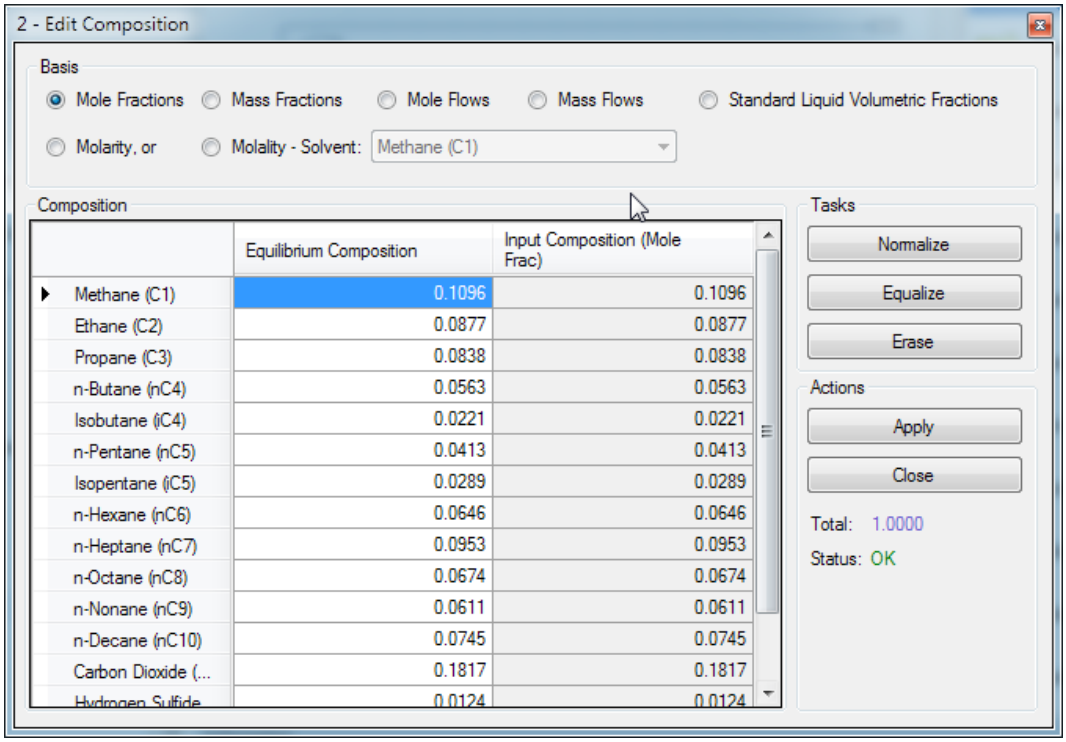


Figure 2: Material Stream composition editor.

If the simulation contains electrolytes and an Electrolyte Property Package is associated with the current Material Stream, the equilibrium composition may be different from the input composition. The Input Composition column will always show Mole Fraction values only.

For the mole/mass fraction basis options, the user must enter the composition in such a way that the amounts sum up to 1. **Regardless of the input basis option, new values are saved only when the "Apply" button is pressed**.

Molarity and Molality input composition options only make sense in the context of an electrolyte simulation. In this case, the solute amounts should be entered in **moles** and the solvent amount in **L** (molarity) or **kg** (molality).

- Flow: one of the three types of flow (mass, molar or volumetric) must be given - the other two are calculated in the case of temperature and pressure are already defined.

The material stream composition can only be edited if the stream is not connected to any unit op upstream, that is, if it doesn't work as an output of any operation. If that is the case, the stream configures itself as "read-only" and the user will not be able to edit any of its properties directly.

Calculation Method When the four properties described above are defined, the material stream is calculated and its properties are shown in the same window. The calculation sequence for the material stream is the following:

1. A flash calculation is done to know the component distribution between phases;
2. Properties of each phase are calculated individually;
3. Finally, the mixture properties are calculated.

In the first step, a TP Flash is done by default, but it can be replaced by a PH flash if the user defines this option in the simulation configuration window. When in "read-only" mode, the stream properties are calculated according to parameters given by the upstream unit operation (in the majority of cases, a TP flash is done as well).

Output parameters Component distribution between phases and phase properties: specific enthalpy, specific entropy, molecular weight, density, volumetric flow rate @ T and P, phase molar and mass fraction, compressibility factor Z, constant-pressure heat capacity (Cp), Cp/Cv, thermal conductivity, surface tension (liquid phase only) and kinematic and dynamic viscosity. Mixture properties: specific enthalpy and entropy, molecular weight, density and thermal conductivity. If the global setting "Calculate bubble and dew points at stream conditions" is activated, these are also shown in the "Mixture" properties section.

2.1.2 Energy Stream

The energy stream is used to represent energy entering and leaving the limits of the simulation, used by the unit operations, either to represent loss, demand or power generation. As we are dealing with steady-state simulations, one defines the energy stream in terms of power (energy by unit of time) and not energy itself (Figure 3).

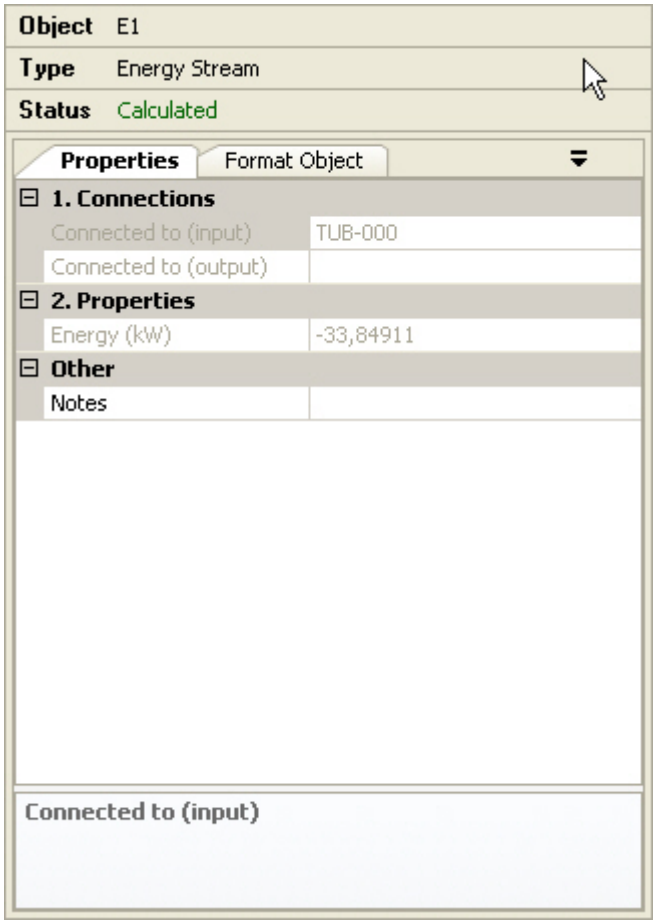


Figure 3: Energy Stream properties.

Input Parameters

- Energy: Energy by unit of time (power) which is represented by the stream;

Output Parameters There are no output parameters for this object.

2.2 Unit Operations

2.2.1 Mixer

The Mixer is used to mix up to six material streams into one, while executing all the mass and energy balances (Figure 4).

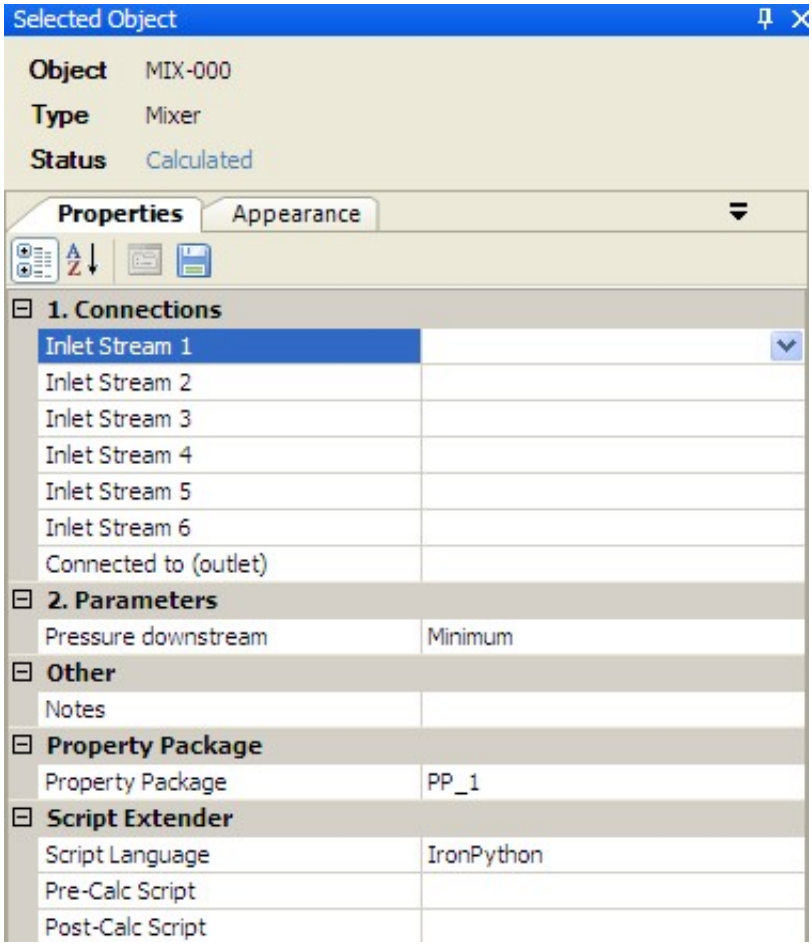


Figure 4: Mixer properties.

Input Parameters

- Downstream pressure: defines how the downstream pressure must be calculated from the pressure of the streams connected to the mixer inlets.

Calculation Method The mixer does the mass balance in the equipment and determines the mass flow and the composition of the outlet stream. Pressure is calculated according to the parameter defined by the user. Temperature is calculated by doing a PH Flash in the outlet stream, with the enthalpy calculated from the inlet streams (energy balance).

Output Parameters There are no output parameters for this object.

2.2.2 Splitter

The splitter is a mass balance unit operation - divides a material stream into two or three other streams (Figure 5).

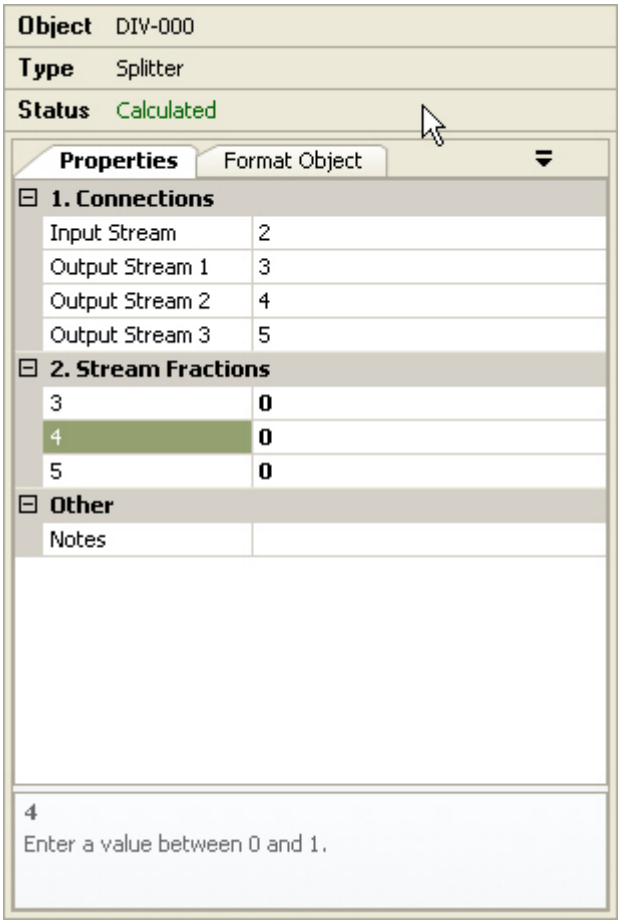


Figure 5: Splitter properties.

Input Parameters

- Stream fractions: this property defines the mass flow fraction to be passed to each outlet stream in the splitter. Each fraction must have a value between 0 and 1 and the total sum must not be bigger than 1.

Output Parameters There are no output parameters for this object.

2.2.3 Separator Vessel

The separator vessel (also known as *flash drum*) (Figure 6) is used to separate liquid phases from vapor in a mixed material stream.

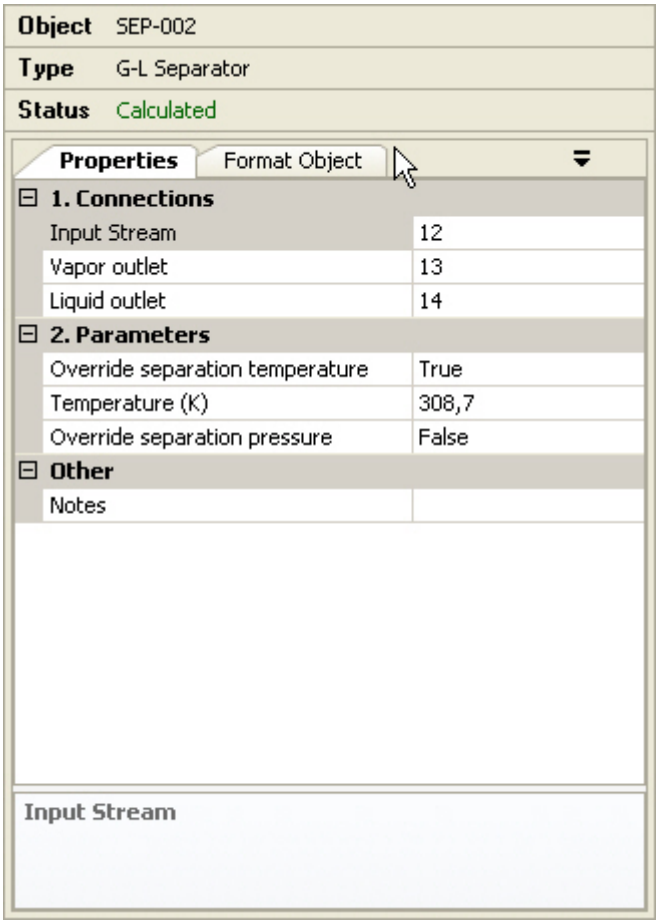


Figure 6: Separator Vessel properties.

Input Parameters

- Override separation temperature and pressure: these properties define if the flash calculation will be done with the temperature and pressure of the inlet stream or the ones defined by the user.

> ***The utilization of different temperatures and pressures from the inlet stream unbalance the simulation in terms of energy.***

Calculation Method The separator vessel just divides the inlet stream phases into two or three distinct streams. If the user defines values for the separation temperature and/or pressure, a TP Flash is done in the new conditions before the distribution of phases through the outlet streams.

Output Parameters There are no output parameters for this object.

2.2.4 Tank

In the current version of DWSIM, the Tank works like a fixed pressure drop for the process (Figure 7).

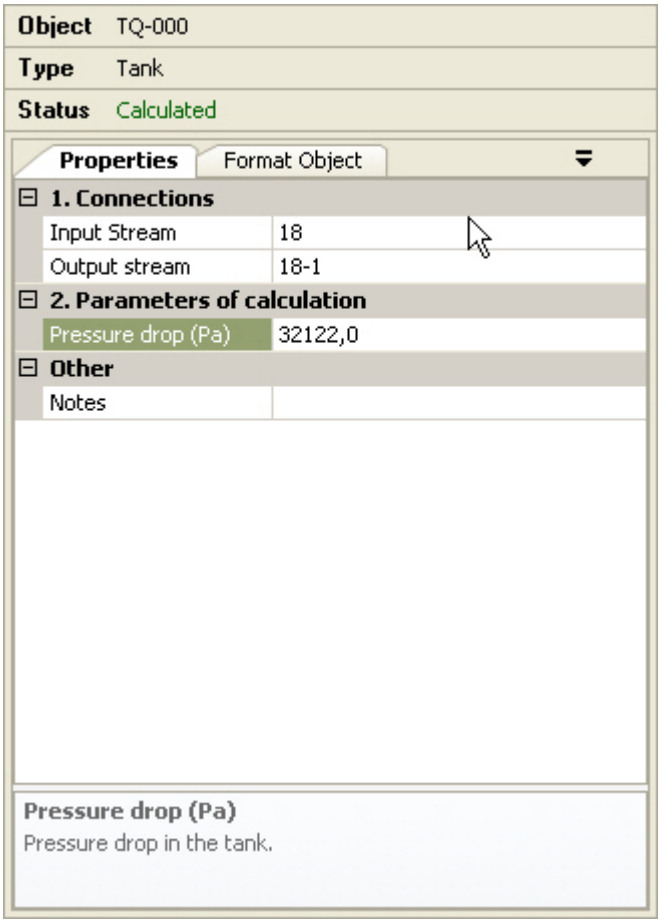


Figure 7: Tank properties.

Input Parameters

- Pressure drop: pressure difference between the outlet and inlet streams.

Calculation Method The outlet stream pressure is calculated from the inlet pressure and the pressure drop given. The temperature remains the same. A TP Flash is done to calculate the properties of the outlet stream.

Output Parameters There are no output parameters for this object.

2.2.5 Pipe Segment

The Pipe Segment unit operation (Figure 8) can be used to simulate fluid flow process in a pipe. Two of the most used correlations for the calculation of pressure drop are available in DWSIM. Temperature can be rigorously calculated considering the influence of the environment.

With the help of the Recycle Logical Operation, the user can build large water distribution systems, as an example.

The pipe segment is divided in sections, which can be straight tubes, valves, curves, etc. Each section is subdivided in small sections for calculation purposes, as defined by the user.

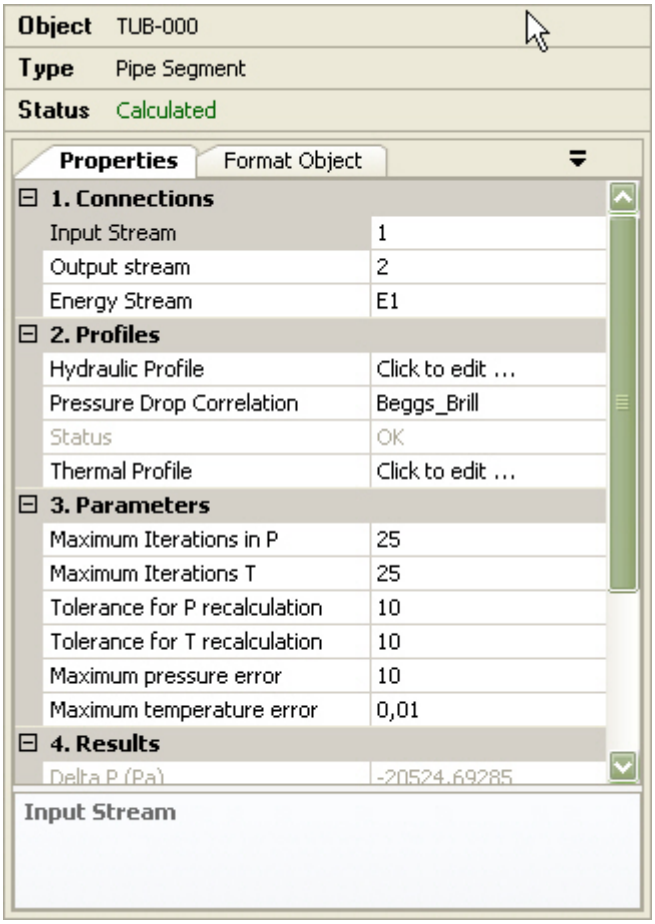


Figure 8: Pipe Segment properties.

Input Parameters

- Hydraulic profile: clicking on the ellipsis button opens the pipe hydraulic profile editor (Figure 9). In the hydraulic profile editor, the user adds sections, define their type and in how many increments it will be divided during the calculations, the pipe material, length, elevation and internal and external diameters. Each change can be saved by clicking in the "Apply" button.

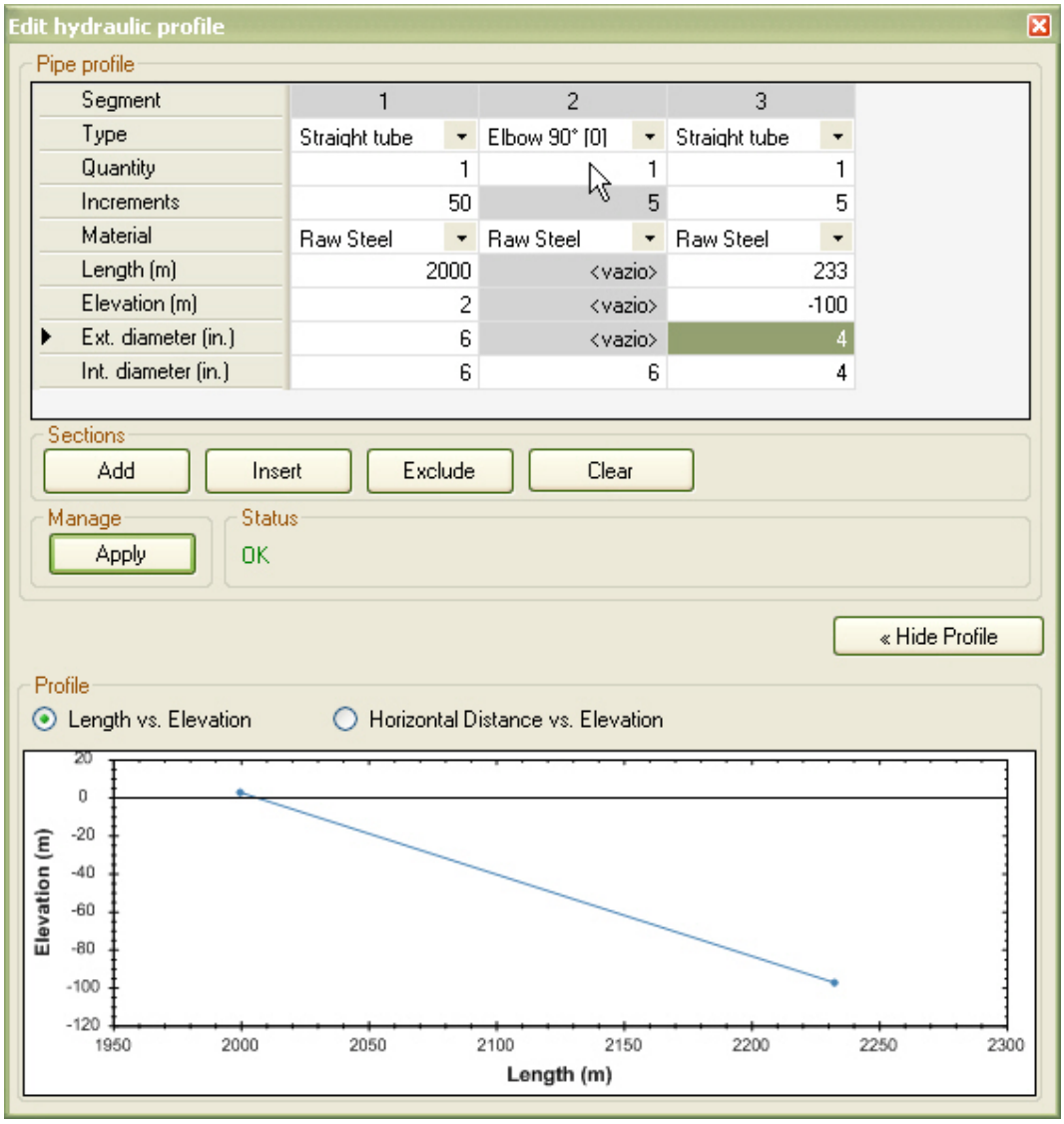


Figure 9: Pipe hydraulic profile editor.

- Pressure drop correlation: select the model to be used for the pressure drop calculation in the pipe segment.
- Thermal profile: clicking on the ellipsis button opens the pipe thermal profile editor (Figure 10). In the thermal profile editor it is possible to define how the temperature profile in the pipe should be calculated. The configurations in this window are valid for the **entire** pipe segment. Changes are saved automatically.

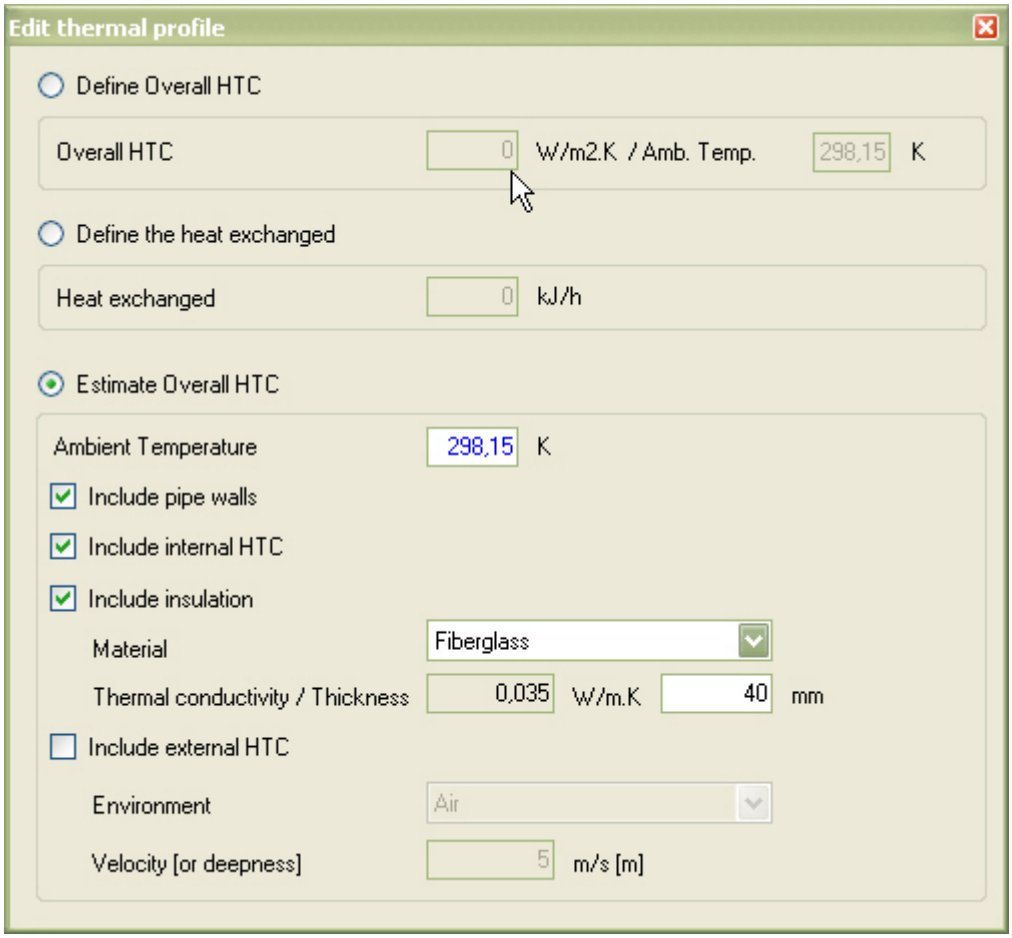


Figure 10: Pipe thermal profile editor.

Calculation Method The pipe segment is calculated based on incremental mass and energy balances. The complete algorithm consists in three nested loops. The external loop iterates on the sections (increments), the middle loop iterates on the temperature and the internal loop calculates the pressure. The pressure and temperature are calculated as follows:

1. The inlet temperature and pressure are used to estimate the increment outlet pressure and temperature.
2. Fluid properties are calculated based in a arithmetic mean of inlet and outlet conditions.
3. The calculated properties and the inlet pressure are used to calculate the pressure drop. With it, the outlet pressure is calculated.
4. The calculated and estimated pressure are compared, and if their difference exceeds the tolerance, a new outlet pressure is estimated, and the steps 2 and 3 are repeated.
5. Once the internal loop has converged, the outlet temperature is calculated. If the global heat transfer coefficient (U) was given, the outlet temperature is calculated from the following equation:

$$Q = UA\Delta T_{ml} \tag{2.1}$$

where: Q = heat transferred, A = heat transfer area (external surface) and ΔT_{ml} = logarithmic mean temperature difference.

6. The calculated temperature is compared to the estimated one, and if their difference exceeds the specified tolerance, a new temperature is estimated and new properties are calculated (return to step 2).

7. When both pressure and temperature converges, the results are passed to the next increment, where calculation restarts.

Output Parameters

- Delta-T: temperature variation in the pipe segment.
- Delta-P: pressure variation in the pipe segment.
- Heat exchanged: amount of heat exchanged with the environment, or lost by friction in the pipe walls.
- Results (table): results are show section by section in a table.
- Results (graph): a graph shows the temperature, pressure, liquid holdup, velocity and heat exchanged profiles.

2.2.6 Valve

The 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 (Figure 11).

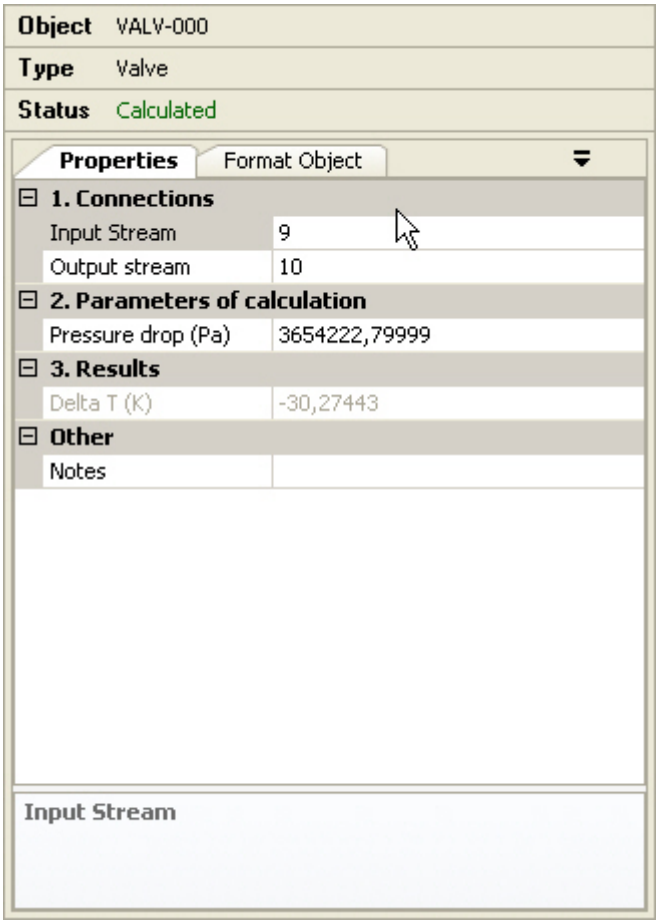


Figure 11: Valve properties.

Input Parameters

- Pressure drop: pressure difference between the outlet and inlet streams.

Calculation Method The outlet stream pressure is calculated from the inlet pressure and the pressure drop. The outlet stream temperature is found by doing a PH Flash. This way, in the majority of cases, the outlet temperature will be less than or equal to the inlet one.

Output Parameters

- Delta-T: temperature drop observed in the valve expansion process.

2.2.7 Pump

The pump is 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 (Figure 12).

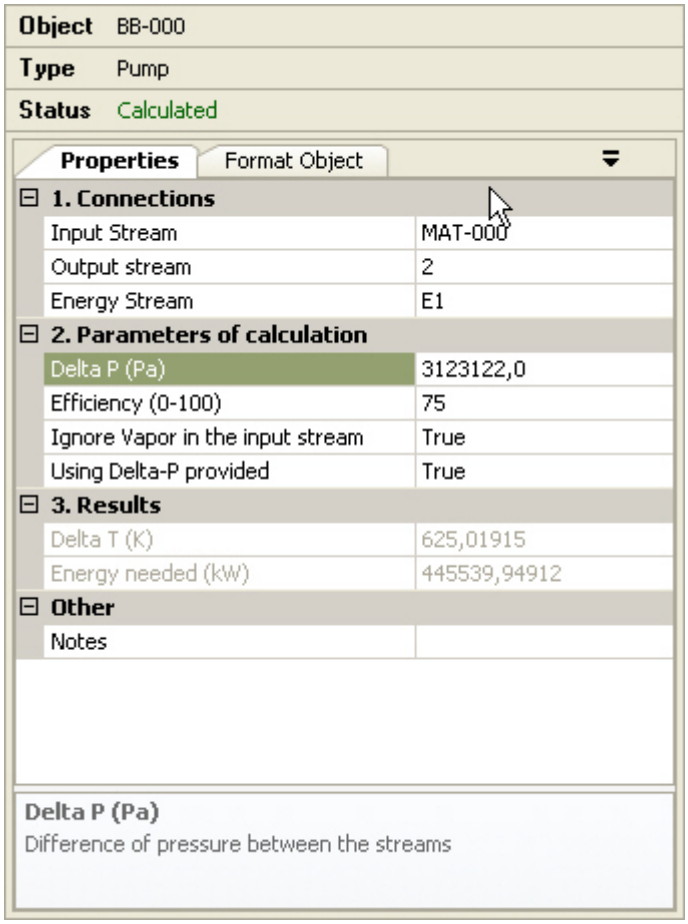


Figure 12: Pump properties.

Input Parameters

- Delta-P: pressure rise in the pump.
- Efficiency: pump adiabatic efficiency;
- Ignore vapor in the inlet stream: defines if the calculator should ignore any vapor in the inlet stream;
- Use the provided Delta-P: defines if the pressure of the outlet stream will be calculated by the user-defined Delta-P or the energy stream connected to the pump.

Calculation Method The calculation method for the pump is different for the two cases (when the provided delta-p or the potency of the energy stream is used). In the first method, we have the following sequence:

- Outlet stream enthalpy:

$$H_2 = H_1 + \frac{\Delta P}{\rho}, \tag{2.2}$$

- Pump discharge pressure:

$$P_2 = P_1 + \Delta P \tag{2.3}$$

➙ Pump required power:

$$Pot = \frac{W\,(H_2 - H_1)}{\eta}, \tag{2.4}$$

where:

Pot	pump power
W	mass flow
H_2	outlet stream specific enthalpy
H_1	inlet stream specific enthalpy
η	pump efficiency

➙ Outlet temperature: PH Flash (with P2 and H2).

In the second case (calculated outlet pressure), we have the following sequence:

➙ Outlet stream enthalpy:

$$H_2 = H_1 + \frac{Pot\,\eta}{W}, \tag{2.5}$$

➙ ΔP:

$$\Delta P = \rho(H_2 - H_1), \tag{2.6}$$

➙ Discharge pressure:

$$P_2 = P_1 + \Delta P \tag{2.7}$$

➙ Outlet temperature: PH Flash.

Outlet Parameters

➙ Delta-T: temperature variation in the pumping process.

➙ Power required: power required by the pump.

2.2.8 Compressor

The compressor is 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 (Figure 13).

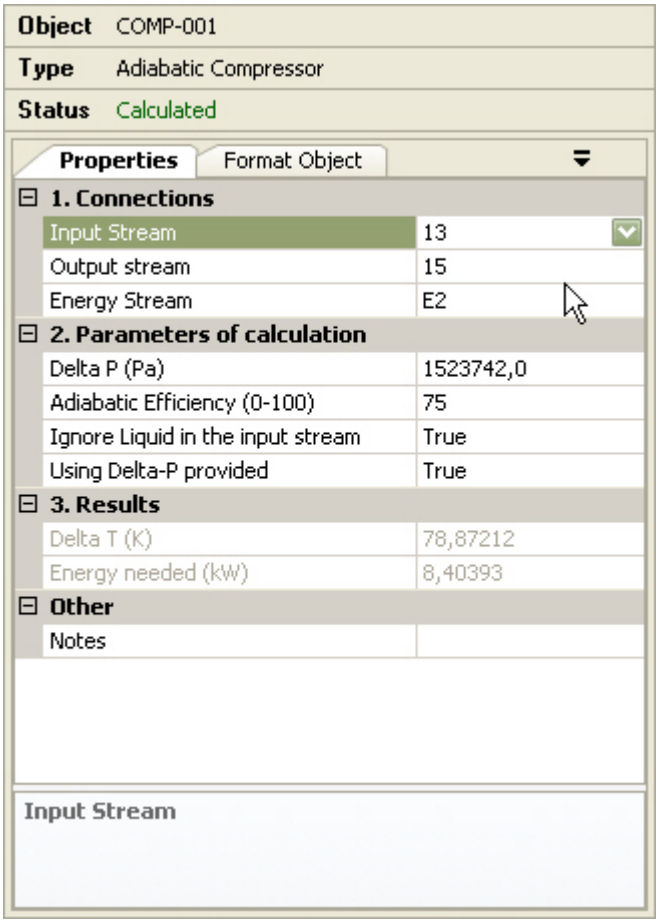


Figure 13: Compressor properties.

Input Parameters

- Delta-P: pressure rise in the compressor.
- Efficiency: compressor adiabatic efficiency;
- Ignore liquid in the inlet stream: defines if the calculator should ignore any liquid in the inlet stream;
- Use the provided Delta-P: defines if the pressure of the outlet stream will be calculated by the user-defined Delta-P or the energy stream connected to the compressor.

Calculation Method The compressor calculation is different for the two cases (when the provided delta-p or the potency of the energy stream is used). In the first method, we have the following sequence:

- Outlet pressure calculation:

$$P_2 = P_1 + \Delta P \tag{2.8}$$

➙ Outlet enthalpy: A PS Flash (Pressure-Entropy) is done to obtain the ideal process enthalpy change. The outlet real enthalpy is then calculated by:

$$H_2 = H_1 + \frac{\Delta H_{id}}{\eta W}, \tag{2.9}$$

➙ Power required by the compressor:

$$Pot = \frac{W\left(H_{2_{id}} - H_1\right)}{\eta}, \tag{2.10}$$

➙ Outlet temperature: PH Flash with P_2 and H_2.

In the second case (calculated outlet pressure), we have the following sequence:

➙ Discharge pressure:

$$P_2 = P_1 \left[1 + \frac{Pot}{\eta W}\frac{k-1}{k}\frac{MM}{8.314 T_1}\right]^{[k/(k-1)]}, \tag{2.11}$$

where:

P_2	outlet stream pressure
P_1	inlet stream pressure
Pot	compressor power
W	mass flow
η	compressor adiabatic efficiency
k	adiabatic coefficient (Cp_{gi}/Cv_{gi})
MM	gas molecular weight
T_1	inlet stream temperature

➙ Outlet enthalpy: A PS Flash (Pressure-Entropy) is done to obtain the ideal process enthalpy change. The outlet real enthalpy is then calculated by:

$$H_2 = H_1 + \frac{\Delta H_{id}}{\eta W}, \tag{2.12}$$

➙ Outlet temperature: PH Flash with P_2 and H_2.

Output Parameters

➙ Delta-T: temperature change in the compression process.

➙ Power required: power required by the compressor.

2.2.9 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(Figure 14).

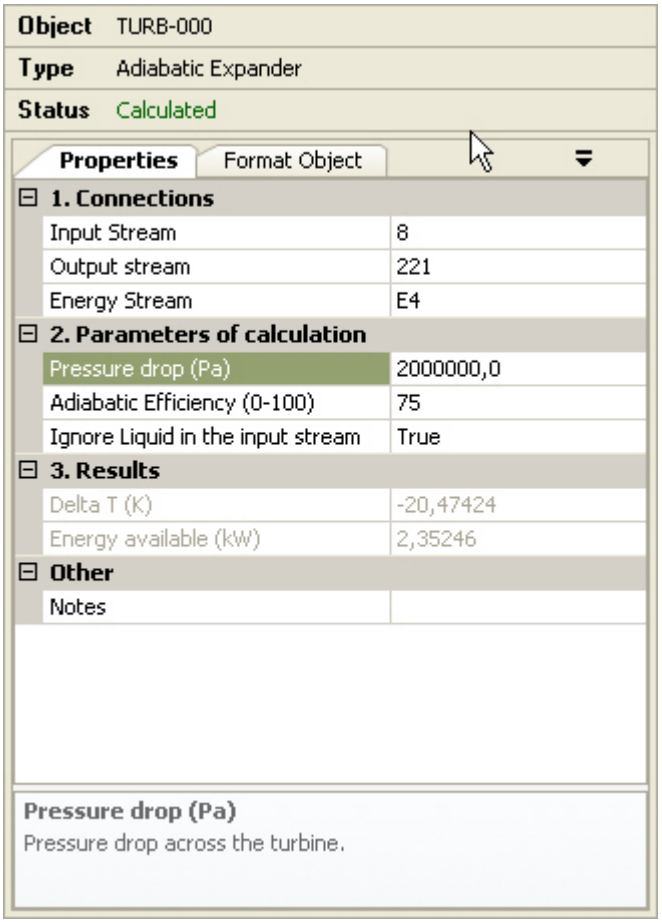


Figure 14: Expander Properties.

Input Parameters

- Delta-P: pressure drop in the expander.
- Efficiency: expander adiabatic efficiency;
- Ignore liquid in the inlet stream: defines if the calculator should ignore any liquid in the inlet stream;

Calculation Method

- Discharge pressure calculation:

$$P_2 = P_1 - \Delta P \tag{2.13}$$

- Outlet enthalpy: A PS Flash (Pressure-Entropy) is done to obtain the ideal process enthalpy change. The outlet real enthalpy is then calculated by:

$$H_2 = H_1 + \frac{\Delta H_{id}}{\eta W}, \tag{2.14}$$

- Power generated by the expander:

$$Pot = \frac{W\left(H_{2_{id}} - H_1\right)}{\eta}, \tag{2.15}$$

- Outlet temperature: PH Flash with P_2 and H_2.

Output Parameters

- Delta-T: temperature change in the compression process.
- Power generated: power generated by the expander.

2.2.10 Heater

The heater simulates a stream heating process (Figure 15).

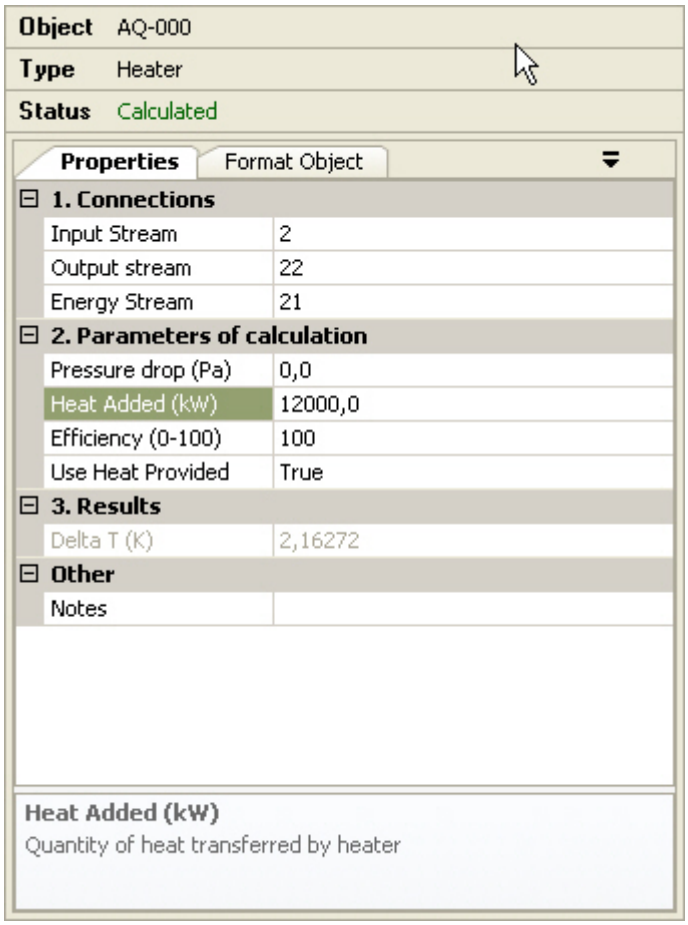


Figure 15: Heater properties.

Input Parameters

- Pressure drop: pressure drop in the heater.
- Heat added: amount of heat added in the heater.
- Efficiency: heater efficiency.
- Use heat provided: defines if the heat added is determined by the value informed by the user or by the energy stream connected to the heater.

Calculation Method The outlet stream temperature is calculated by doing a PH Flash, were the outlet stream enthalpy is calculated by a energy balance in the heater.

Output Parameters

- Delta-T: temperature rise observed in the heating process.

2.2.11 Cooler

The cooler simulates a stream cooling process(Figure 16).

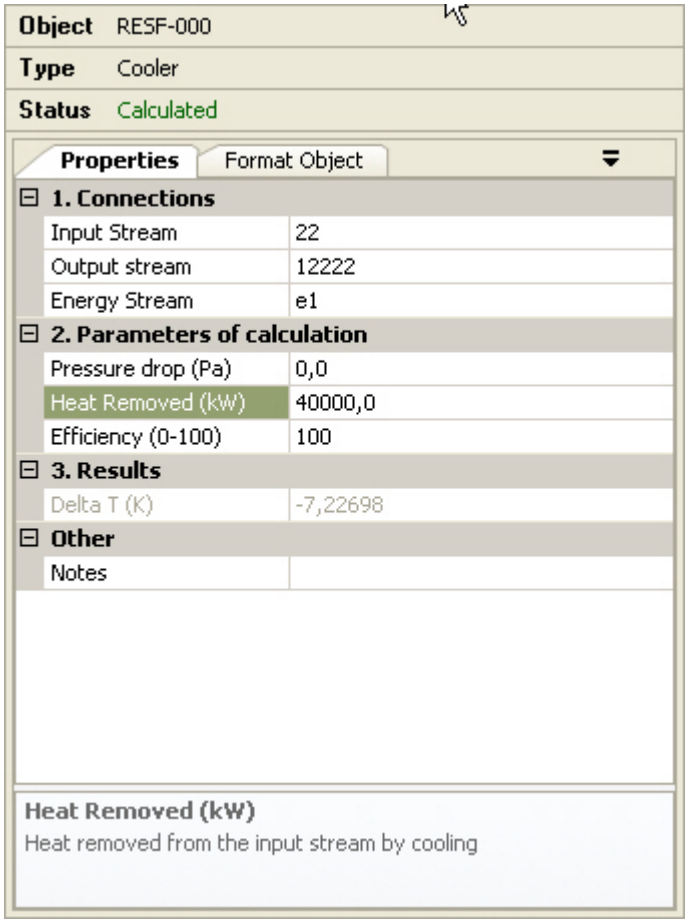


Figure 16: Cooler properties.

Input Parameters

- Pressure drop: pressure drop in the cooler.
- Heat removed: amount of heat removed by the cooler.
- Efficiency: cooler efficiency.

Calculation Method The outlet stream temperature is calculated by doing a PH Flash, were the outlet stream enthalpy is calculated by a energy balance in the cooler.

Output Parameters

- Delta-T: temperature drop observed in the cooling process.

2.2.12 Shortcut Column

The shortcut column is used to calculate the minimum reflux and distribution of products in a distillation column by the method of Fenske-Underwood-Gilliland [1]. The column should have a single feed stage, two products (top and bottom), condenser (partial or total) and reboiler. The results are the minimum reflux, thermal loads and temperature of the condenser and reboiler for a fixed reflux ratio, in addition to determining the optimum feed stage and the minimum number of stages.

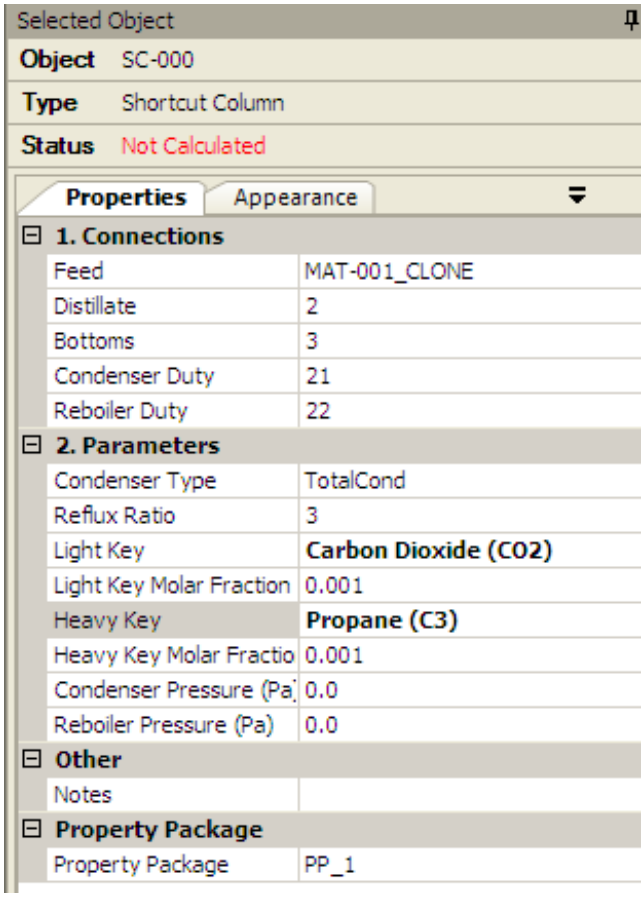


Figure 17: Shortcut Column Properties..

Input Parameters

- Connections: feed, product, top, bottom and heat loads (condenser / reboiler).
- Type of condenser: partial or total.
- Reflux Ratio: ratio between the flow of liquid that returns from the condenser to the column and the one that leaves the condenser as the top product.
- Light Key: component used as a reference so that the lighter ones are present only in the top product.
- Heavy Key: component used as a reference so that the heavier ones are present only in the product of fund.
- Condenser pressure: pressure of the condenser.
- Reboiler pressure: pressure of the reboiler.

Output Parameters

- Minimum reflux: reflux ratio of minimum to ensure the separation specified.
- Minimum number of stages: the minimum number of training which ensures the separation specified.
- Optimal feed stage: the feed stage that minimizes the thermal load of the reboiler.
- Liquid / Vapor flows: internal flows in sections of rectification and stripping of the column.
- Thermal loads: thermal loads of condenser and reboiler.

2.2.13 Rigorous Column (Distillation / Absorption)

The rigorous column is an unit operation that represents the fractionating towers, where components in a mixture are separated in various equilibrium stages (or not). It is called *rigorous* because of the thermodynamic models used in the solution of the mass and energy balances throughout the column.

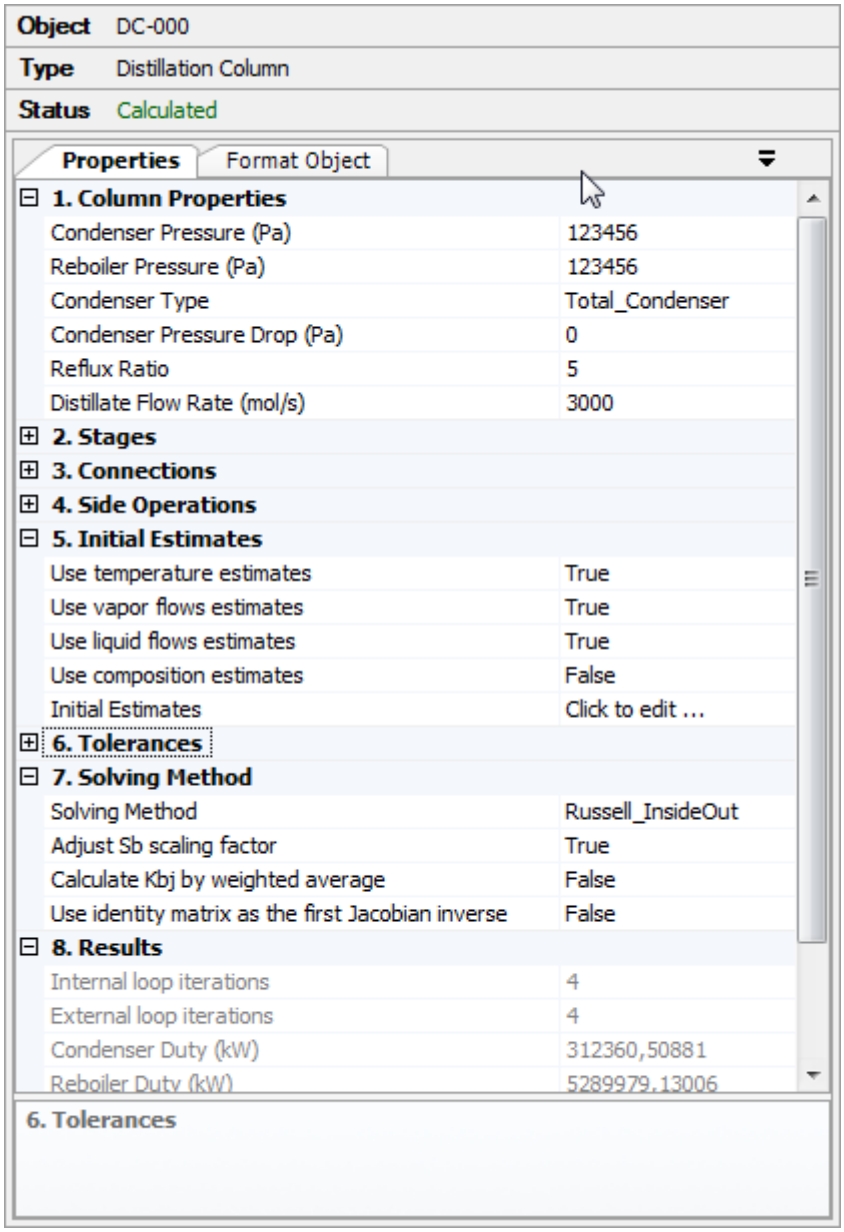


Figure 18: Distillation Column Properties.

In DWSIM, four types of rigorous columns are available: **Distillation Column**, **Absorption Column**, **Refluxed Absorber** and **Reboiled Absorber**. All of them share the same basic interface, with the following characteristics:

- Supports multiple feed streams
- Supports multiple side draws
- Supports energy streams representing heat exchangers on each stage
- Definition of pressure and efficiency by stage

Solving methods In the current version of DWSIM, three methods are available to solve the mass and energy balances in a column. They are:

- Bubble-Point method of Wang and Henke (distillation column only) [2]
- *Sum-Rates* method of Burningham and Otto (absorption column only)[2]
- Russell's *Inside-Out* method (all column types)[2]
- Simultaneous Correction method of Naphtali and Sandholm (all column types)[2]

Configuration options The following table describes the configuration options for each solving method.

Results After the solution of mass and energy balances for the entire column, the output streams are calculated and the following results are shown in the properties window of the column:

- Heat exchanged in the condenser (where applicable)
- Heat exchanged in the reboiler (where applicable)
- Temperature profiles and flow of liquid / vapor entering at each stage
- Distribution profiles of components on each stage

2.2.14 Heat Exchanger

DWSIM has a model for the countercurrent, two-stream heat exchanger which supports phase change and multiple phases in a stream.

Input Parameters The heat exchanger in DWSIM has five calculation modes:

1. Calculate hot fluid outlet temperature: you must provide the cold fluid outlet temperature and the exchange area to calculate the hot fluid temperature.
2. Calculate cold fluid outlet temperature: in this mode, DWSIM needs the hot fluid outlet temperature and the exchange area to calculate the cold fluid temperature.
3. Calculate both temperatures: in this mode, DWSIM needs the exchange area and the heat exchanged to calculate both temperatures.
4. Calculate area: in this mode you must provide the HTC and both temperatures to calculate the exchange area.
5. Rate a Shell and Tube exchanger: in this mode you must provide the exchanger geometry and DWSIM will calculate output temperatures, pressure drop on the shell and tubes, overall HTC, LMTD, and exchange area. This calculation mode uses a simplified version of Tinker's method [3] for Shell and Tube exchanger calculations.

You can provide the pressure drop for both fluids in the exchanger for modes 1 to 4 only.

Method	Parameter	Options	Default Value	Description
BP	Stop at iteration number	0 to 1000 (-1 to disable)	-1 (disabled)	You can use this option to generate initial estimates for the IO and SC methods.
IO/SC	Step for numerical derivatives	1E-3 to 1E-12	1E-5	Controls the value of change in variables in order to calculate the numerical derivatives.
IO/SC	Maximum variable change factor	>1	10	Limits the changes in variables so the maximum variable change will be (newvalue/oldvalue) = factor.
IO	Adjust Sb scaling factor	True/False	False	Use the Sb scaling factor to adjust the initial material balance estimation. Helps to stabilize the algorithm when poor initial estimates are used.
IO	Calculate Kbj by weighted average	True/False	False	Calculates the Kb (reference K) factor for each stage by using the weighted average method as suggested by Russell. If this option is set to false, the highest K-value is used for the relative volatility calculation for each component on each stage.
IO	Use identity matrix as the first jacobian inverse	True/False	False	If True, tells DWSIM to use an identity matrix as the first estimate of the Jacobian inverse, which by its turn is used to update each independent variable. If set to False, the first Jacobian is calculated using numerical derivatives.
IO	Use damping factor	True/False	True	Set this option to True to use a damping factor, which helps to minimize the error on each inner loop iteration.
SC/IO	Use Newton's method to update variables	True/False	False	The variables are normally updated by Broyden's method, but setting this option to True helps to stabilize the algorithm on hard-to-converge situations.
SC/IO	Store and reuse jacobian matrix	True/False	True	This option is useful when the column must be solved multiple times without significant changes in variables, i. e. when using recycled streams as column feeds.
SC	Damping factor	0 to 2	0.5	Set the damping factor which limits the changes to variables as predicted by the Newton (or Broyden) step.
SC	Maximum allowed stage temperature change	> 0	10 K	Sets the maximum allowable stage temperature change between iterations. Changes higher than this value will not be considered.

Table 1: Column solving methods' configuration parameters.

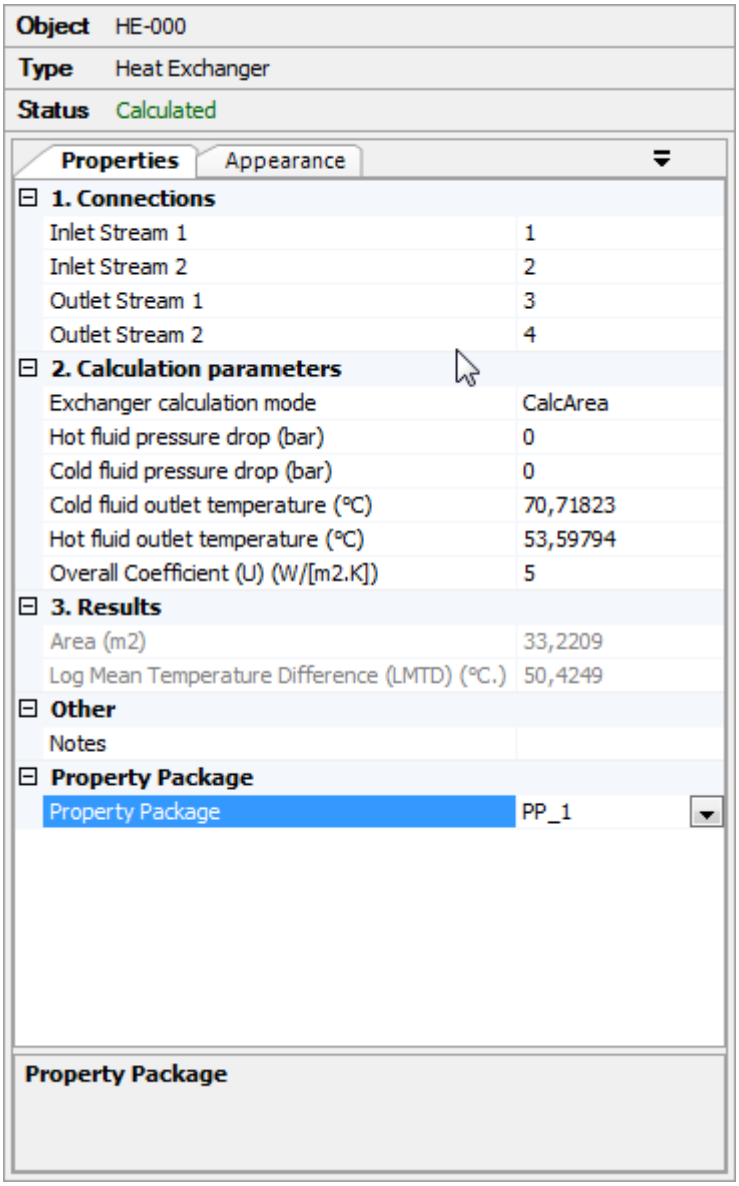


Figure 19: Heat Exchanger properties.

Calculation Mode The heat exchanger in DWSIM is calculated using the simple convection heat equation:

$$Q = UA\Delta T_{ml}, \tag{2.16}$$

where: Q = heat transferred, A = heat transfer area (external surface) and ΔT_{ml} = Logarithmic Mean Temperature Difference (LMTD). We also remember that:

$$Q = m\Delta H, \tag{2.17}$$

where: Q = heat transferred from/to the fluid and ΔH = outlet-inlet enthalpy difference.

The calculation procedure depends on the mode selected:

1. Calculate hot fluid outlet temperature: HTC (Heat Transfer Coefficient), hot fluid outlet temperature, heat load and LMTD.
2. Calculate cold fluid outlet temperature: HTC, cold fluid outlet temperature, heat load and LMTD.
3. Calculate both temperatures: HTC, cold and hot fluid outlet temperatures and LMTD.
4. Calculate area: exchange area and LMTD.
5. Rate Shell and Tube exchanger: exchanger geometry information.

Results The results given by the heat exchanger after calculation depends on the mode selected:

1. Calculate hot fluid outlet temperature: overall HTC, hot fluid outlet temperature, heat load and LMTD.
2. Calculate cold fluid outlet temperature: overall HTC, cold fluid outlet temperature, heat load and LMTD.
3. Calculate both temperatures: overall HTC, cold and hot fluid outlet temperatures and LMTD.
4. Calculate area: exchange area and LMTD.
5. Rate Shell and Tube exchanger: area, LMTD, LMTD correction factor (F), overall HTC, hot fluid outlet temperature, cold fluid outlet temperature, hot fluid pressure drop (shell/tubes only), cold fluid pressure drop (shell/tubes only).

2.2.15 Component Separator

The Component Separator is a mass balance unit operation. The components are separated between two streams, specified as fractions or absolute flow rates. The energy balance is then calculated after the separation.

Input Parameters

- Specified stream: sets the stream to which the separation specifications will be applied. "0" corresponds to the Outlet stream 1 (overhead) and "1" corresponds to the Outlet stream 2 (bottoms).

Results

- Energy imbalance: Difference between enthalpy of outlet and inlet streams. in some cases it can be interpreted as the energy necessary to do the separation.

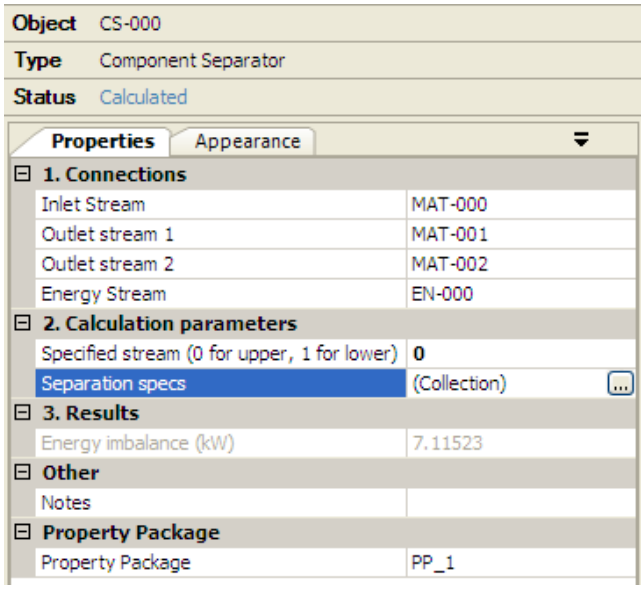


Figure 20: Component Separator properties.

2.2.16 Orifice Plate

This model corresponds to the ISO 5167 specification for Orifice Plates, and can be used to measure flow rates if used in conjunction with the Adjust logical operation (change flow rates until specified pressure drop matches the calculated one).

Input Parameters

- Pressure tappings: select the option which corresponds to the arrangement of the tappings for pressure reading.
- Orifice diameter: inner diameter of the plate.
- Beta (d/D): ratio between plate's inner and outer diameters.
- Correction factor: multiplier for the mass flow rate used in the calculation of the pressure drop across the orifice. Default is 1.

Results

- Orifice pressure drop: Pressure drop across the orifice. This is the value that is read through the tappings.
- Overall pressure drop: Pressure drop after recovery. This values should always be less or equal to the orifice pressure drop.
- Delta T: temperature drop across the orifice, considering that the process is an adiabatic expansion.

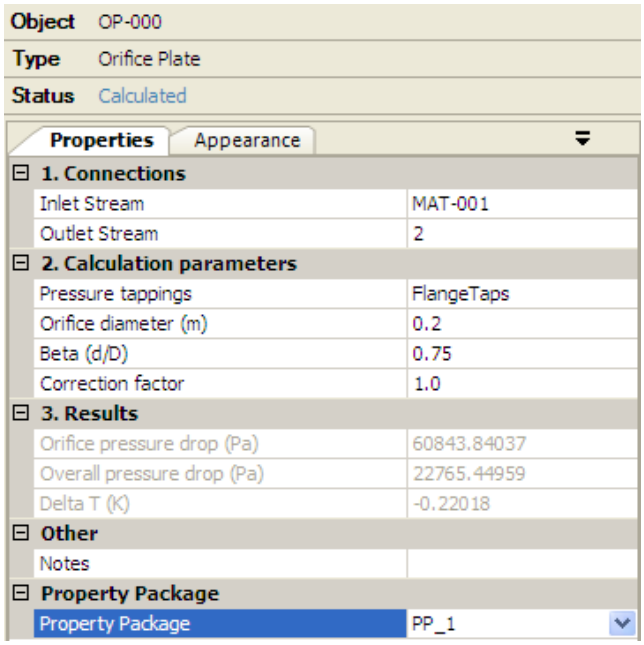


Figure 21: Component Separator properties.

2.2.17 Custom Unit Operation

This Unit Operation lets you run scripts as the main calculation routine (inside the Calculate() procedure which is called by the calculator for all flowsheet simulation objects). There are up to six streams available for the UO, three as input and three as output.

Supported Languages are IronPython, IronRuby, VBScript and JScript. You can use some predefined reference variables inside your script, defined as shortcuts to the most common objects:

ims1 Input Material Stream in slot 1 (MaterialStream class instance)

ims2 Input Material Stream in slot 2 (MaterialStream class instance)

ims3 Input Material Stream in slot 3 (MaterialStream class instance)

oms1 Output Material Stream in slot 1 (MaterialStream class instance)

oms2 Output Material Stream in slot 2 (MaterialStream class instance)

oms3 Output Material Stream in slot 3 (MaterialStream class instance)

Me Reference variable to the Custom UO object instance (CustomUO UnitOperation class)

Flowsheet Reference variable to the active flowsheet object (FormChild class)

Solver Flowsheet solver class instance, used to send commands to the calculator (COMSolver class)

For scripting documentation, including tutorials and samples, view the **DWSIM Scripting Documentation, DWSIM Source Code Guide** and the **DWSIM Class Documentation** (separate documents).

2.2.18 Solids Separator

The solids separator (Figure 22) is used to separate solids from a liquid phase in a mixed material stream.

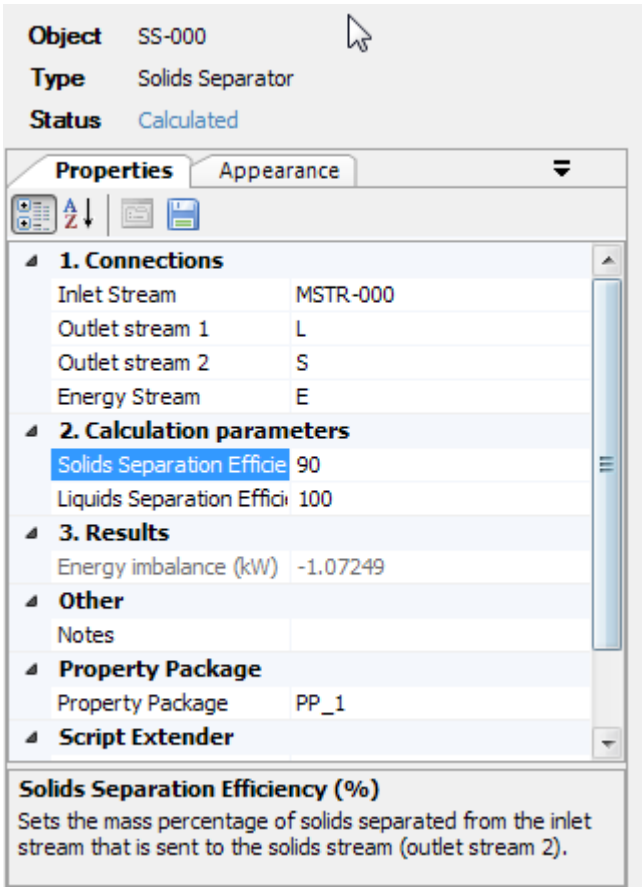


Figure 22: Solids Separator properties.

Input Parameters

- Solids Separation Efficiency: defines the amount of solids in the liquid stream. 100% efficiency means no solids in the liquid stream.
- Liquids Separation Efficiency: defines the amount of liquid in the solids stream. 100% efficiency means no liquid in the solids stream.

Calculation Method The solids separator does a mass balance and splits the inlet stream phases into two distinct streams.

2.2.19 Continuous Cake Filter

In a continuous filter, the feed, filtrate and cake move at steady constant rates. It is evident that the process consists of several steps in series - cake formation, washing, drying and discharging - and that each step involves progressive and continual change in conditions. The pressure drop across the filter during cake formation is, however, held constant.

Calculation Method For a continuous cake filter, the equation that relates the filter characteristics with the rate of solids production is [4]

$$\frac{\dot{m}_c}{A_T} = \frac{\left[2c\alpha\triangle Pfn/\mu + (nR_m)^2\right]^{0,5} - nR_m}{\alpha}, \tag{2.18}$$

where:

$\dot{m}_c$ rate of solids production, kg/s

A_T total filter area, m^2

ΔP total pressure drop, Pa

f fraction of filter area available for cake formation

c solids concentration in the solids stream

α specific cake resistance, m/kg

R_m filter medium resistance, m^{-1}

n drum speed, s^{-1}

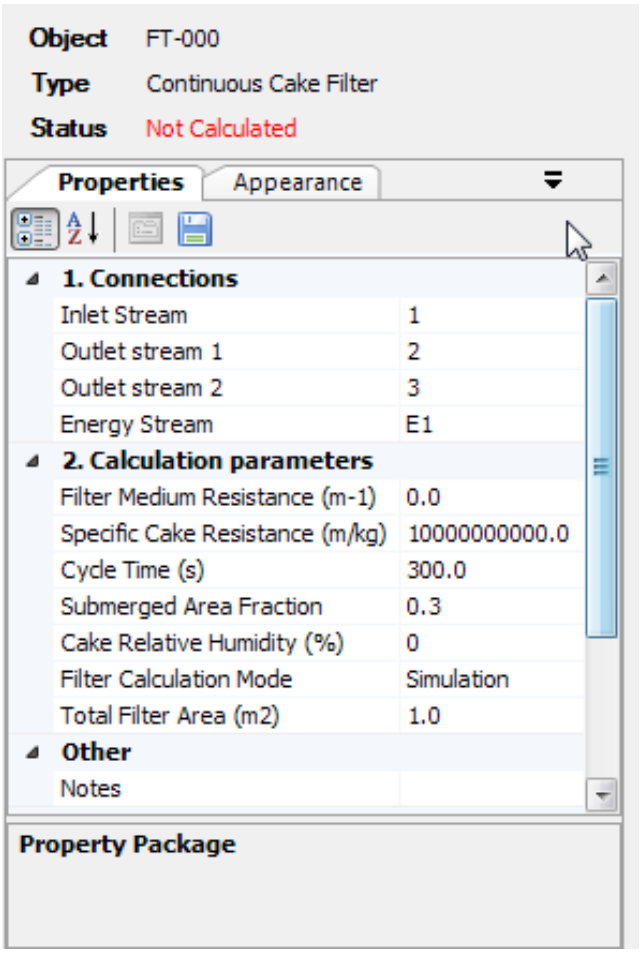


Figure 23: Continuous Cake Filter Properties.

Input and Output Parameters

- Filter Medium Resistance: filter medium flow resistance;
- Specific Cake Resistance: specific cake flow resistance;
- Cycle Time: filter cycle time.
- Cake Relative Humidity: filter cake moisture in % wet basis;
- Filter Calculation Mode: Design or Simulation. If ***Design*** is selected, DWSIM will calculate the filter area given the total pressure drop. If ***Simulation*** is selected, it will do the opposite;
- Total Filter Area: filter area measured perpendicularly to the direction of flow;
- Pressure Drop: total pressure drop across the filter (cake + medium).

2.3 Reactors

The reactors in DWSIM are specialized modules that solve a particular set of reactions in sequence or in parallel.

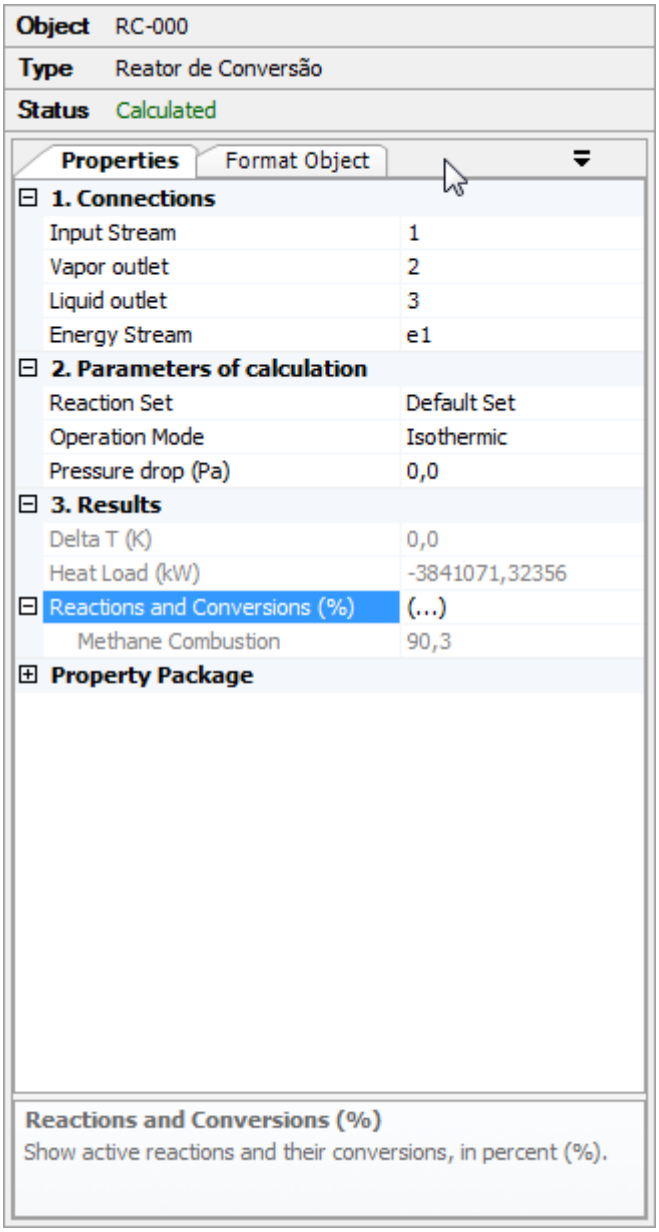


Figure 24: Conversion Reactor properties.

Input Parameters All reactors share the same basic interface. Should be set the input and output streams, energy streams that represent the heat exchanged with the environment, the reaction set to be used, the mode of operation (isothermal or adiabatic) and the pressure drop through the reactor. For the PFR and CSTR, it is also necessary to inform the volume of the reaction medium.

Output Parameters As results, are shown the conversions of the components involved in the reactions, the variation in temperature and the heat exchanged in the reactor. For the PFR are also shown the profiles of concentration of reactants and products (Figure 25) along the longitudinal axis of the reactor (assuming the concentration does not vary radially).

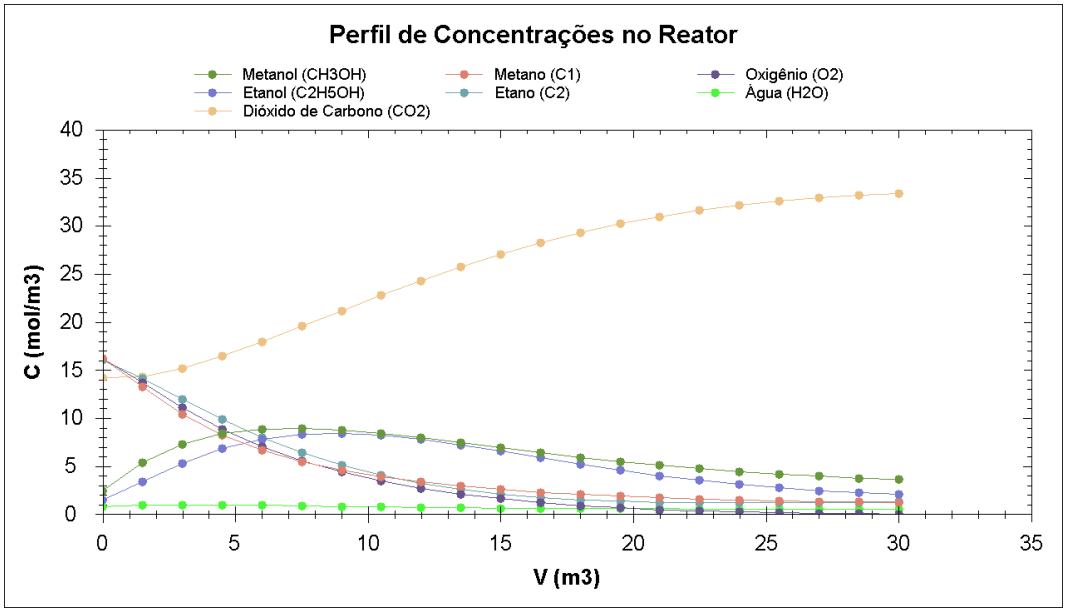


Figure 25: PFR concentration profile.

The following points should be observed when using reactors in DWSIM:

- Only the active and compatible reactions in the selected reaction set are considered.
- The index of each reaction defines the solving method: equal indices represent reactions in parallel, while different indexes define sequential reactions.

Method of calculation The **Conversion Reactor** is solved by simple energy and mass balances, calculating the reaction heat by considering the variation in the amount of the base component. The **PFR** and **CSTR** are solved by a numerical method for systems of ordinary differential equations (ODEs). **Equilibrium** and **Gibbs** Reactors are solved by using the procedure described by Michelsen in [**?**].

2.4 Logical Operations

2.4.1 Recycle

The Recycle operation (Figure 26) is composed by a block in the flowsheet which does convergence verifications in systems were downstream material connects somewhere upstream in the diagram. With this tool it is possible to build complex flowsheets, with many recycles, and solve them in an efficient way by using the acceleration methods presents in this logical operation.

There are two acceleration methods available: Wegstein and Dominant Eigenvalue. The Wegstein method must be used when there isn't a significant interaction between convergent variables, in the contrary the other method can be used. The successive substitution method is slow, but convergence is guaranteed.

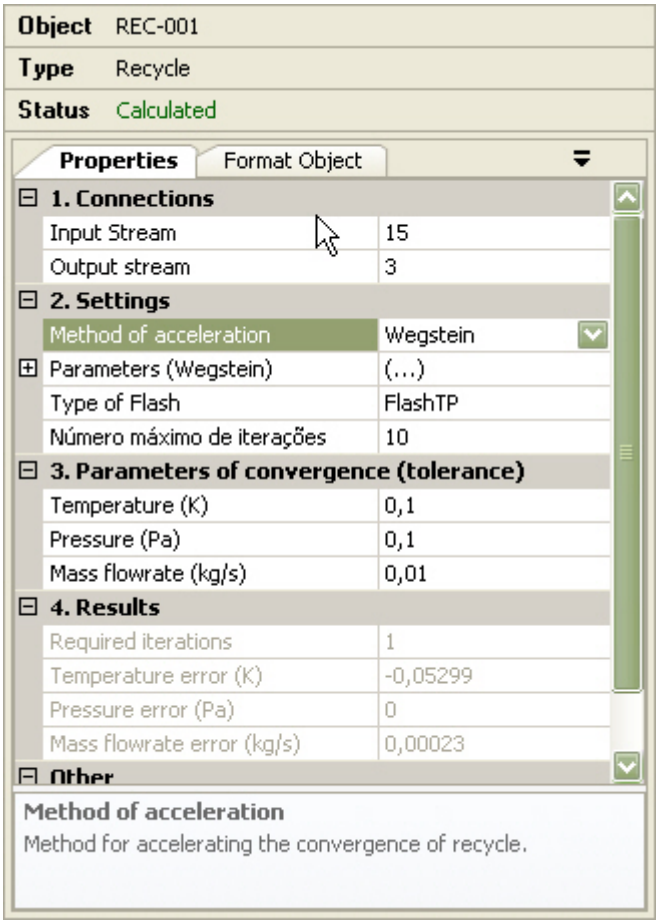


Figure 26: Recycle Properties.

The Wegstein method requires some parameters which can be edited by the user. The dominant eigenvalue does not require any additional parameter. The user can define convergence parameters for temperature, pressure and mass flow in the recycle, that is, the minimum acceptable values for the difference in these values between the inlet and outlet streams, which, rigorously, must be identical. The smaller these values are, the more time is used by the calculator in order to converge the recycle.

As a result, the actual error values are shown, together with the necessary convergence iteration steps.

2.4.2 Energy Recycle

The Energy Recycle logical operation works the same way as the normal Recycle, except that it is aimed at Energy Streams. Here, instead of defining convergence parameters for temperature, pressure and flow rate, you'll define the convergence error for the energy only.

2.4.3 Adjust

The Adjust (Figure 27) is a logical operation which changes the value of a variable in a stream in order to attain a specification which can be a user-defined value or the value of other variable, in other stream. The adjust operation is very useful when there is a specification which cannot

be accomplished directly, imposing the necessity of doing a trial and error calculation. If this is the case, the Adjust does everything automatically.

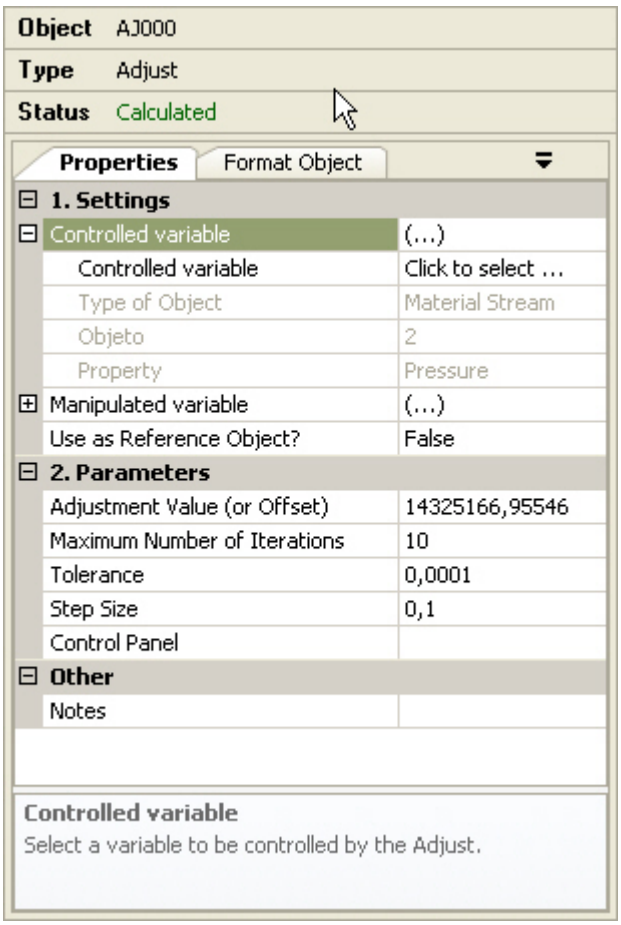


Figure 27: Adjust properties.

The user selects the controlled (specified) variable and the manipulated one. Then he defines the parameters:

- Adjust value (or offset): desired value for the variable or the value to be added or subtracted from the referenced variable.
- Maximum iterations: maximum number of iterations to be executed by the adjust;

In the Adjust Control Panel (Figure 28), the user controls the operation convergence. Two convergence methods are available.

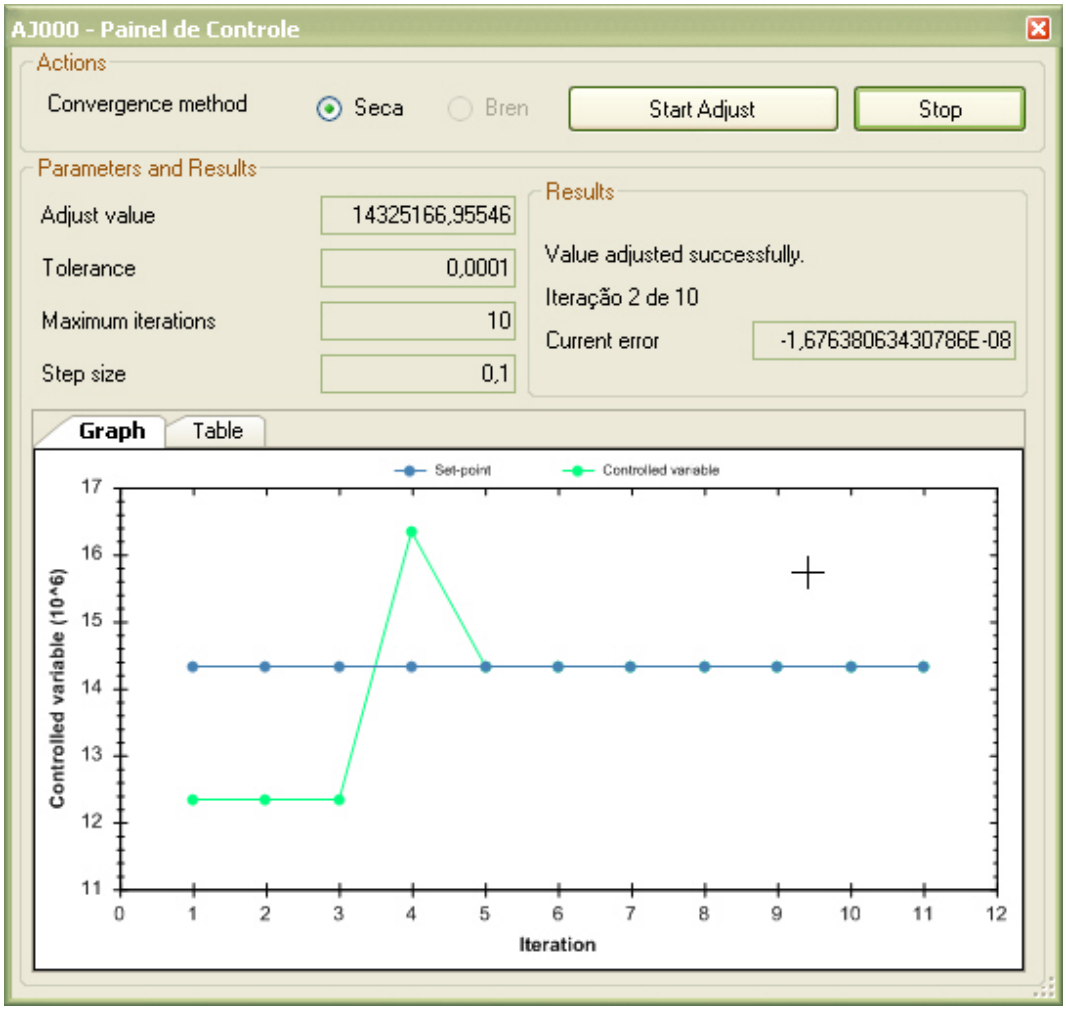


Figure 28: Adjust Control Panel.

2.4.4 Specification

The Specification Logical Operation (Figure 29) is used to make a variable assume a value which is function of other variable, from other object. In opposition to the Adjust Op, the Spec is calculated automatically if the source variable is modified during the flowsheet calculation. In order for the calculator do not make any repeated calculation in the target object, one can define the "Calculate target object?" as *False*.

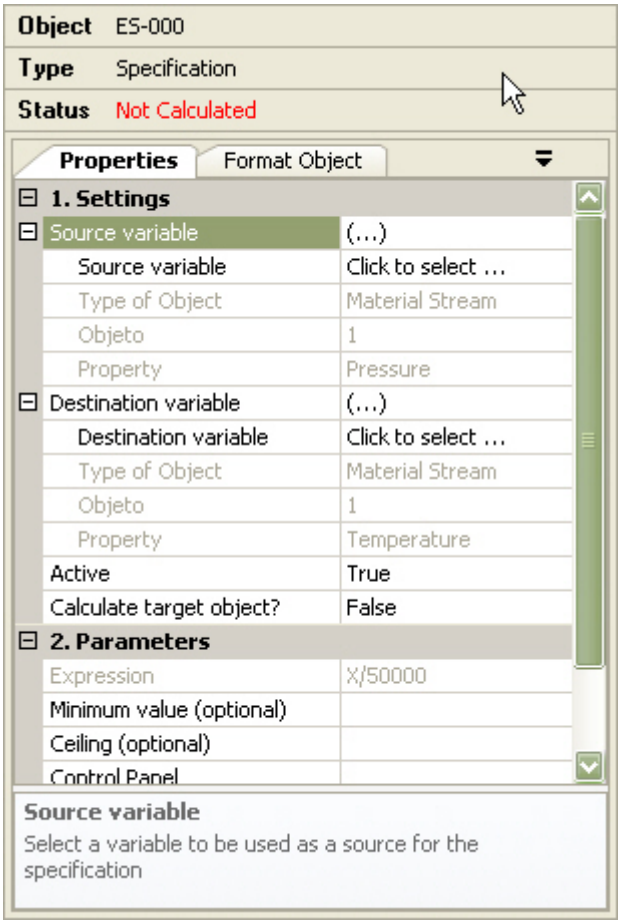


Figure 29: Specification properties.

In the Specification Control panel, the user can define the relation between the variables by writing a function as complex as necessary (Figure 30). The user can click on the "Evaluate Expression" to check if the expression is valid.

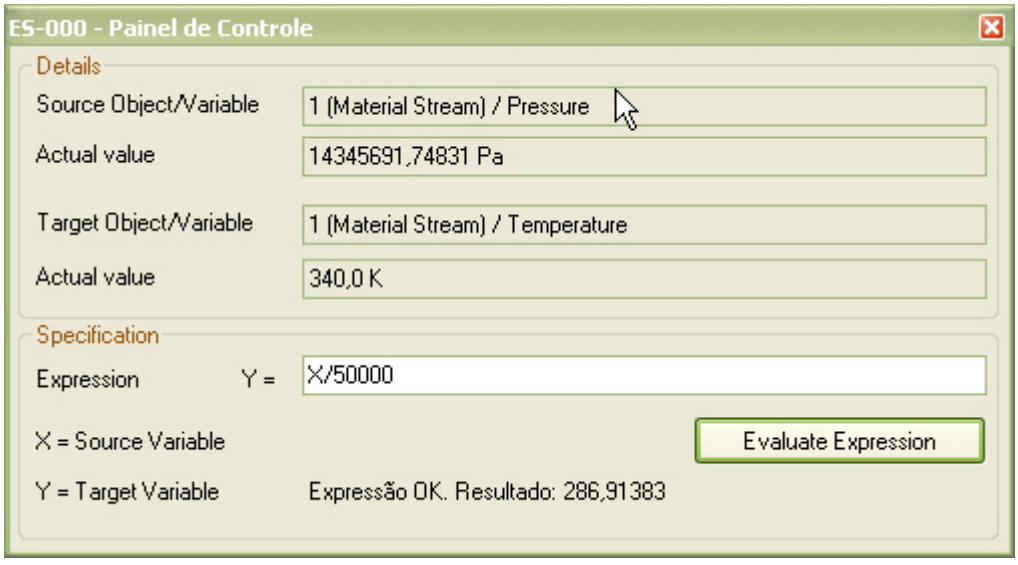


Figure 30: Specification Control Panel.

3 Utilities

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

In version 1.3 the following utilities are available: True Critical Point, Hydrate Dissociation Utility, Pure Component Properties and Phase/Binary Envelope.

3.1 True Critical Point

In DWSIM an utility is present which calculates a stream's mixture true critical point (Figure 31). The *Peng-Robinson* and *Soave-Redlich-Kwong* EOSes are used in the calculations, depending on the Property Package which is associated with the selected stream.

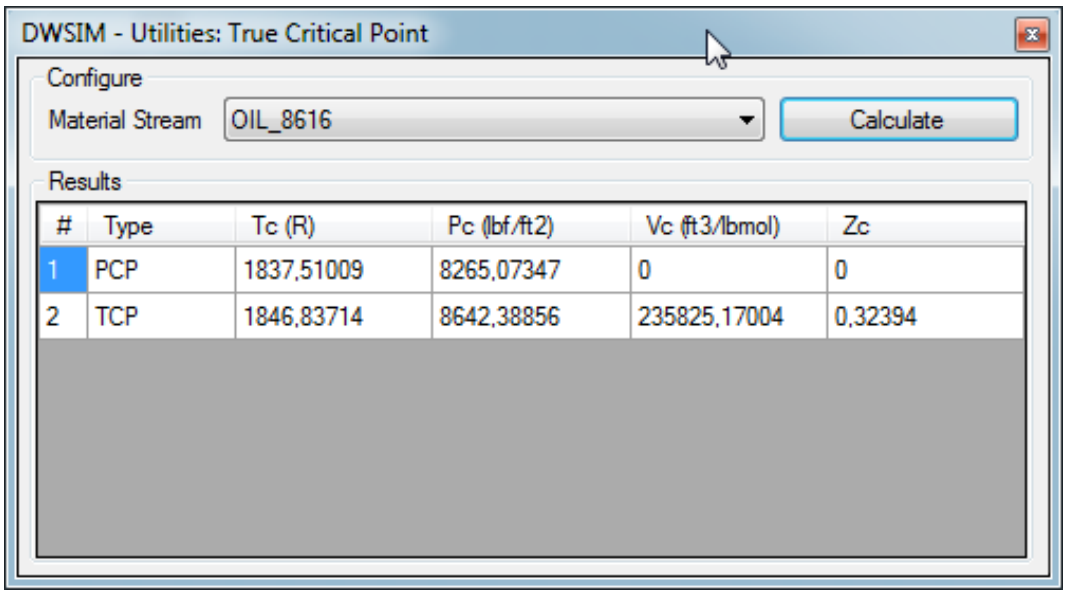


Figure 31: True Critical Point utility.

3.2 Hydrate Dissociation Utility

The Hydrate Dissociation Utility calculates the pressure and temperature conditions where hydrate formation can occur. The models implemented in DWSIM for hydrate calculations are based on the thermodynamic fundamental principles and in equations of state. These models can, therefore, be used in extreme operation conditions with a higher safety degree than the empirical table/graph-based methods.

View DWSIM's Technical Manual for more information about the models used in this utility.

The requirements for using this utility are:

- Water must be present in the stream (even in a infinitesimal amount);
- At least one of the hydrate formers must be present (i.e., methane, ethane, propane, butane, etc.).

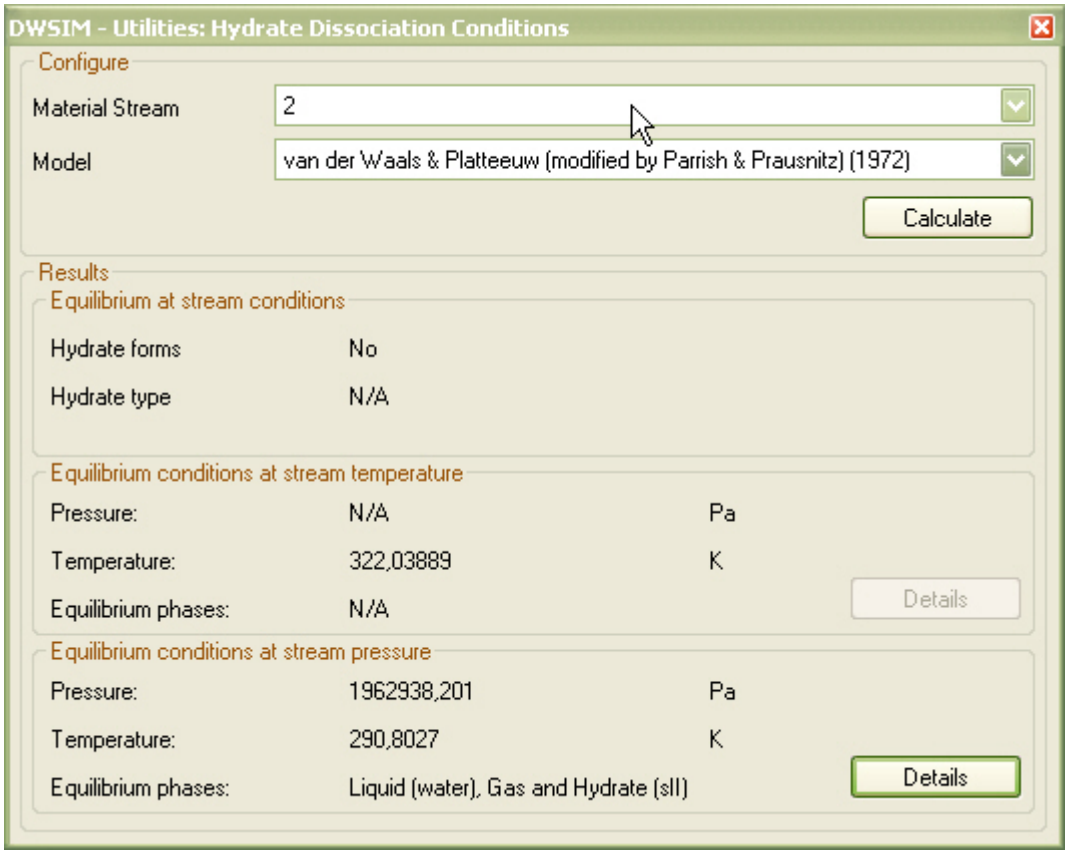
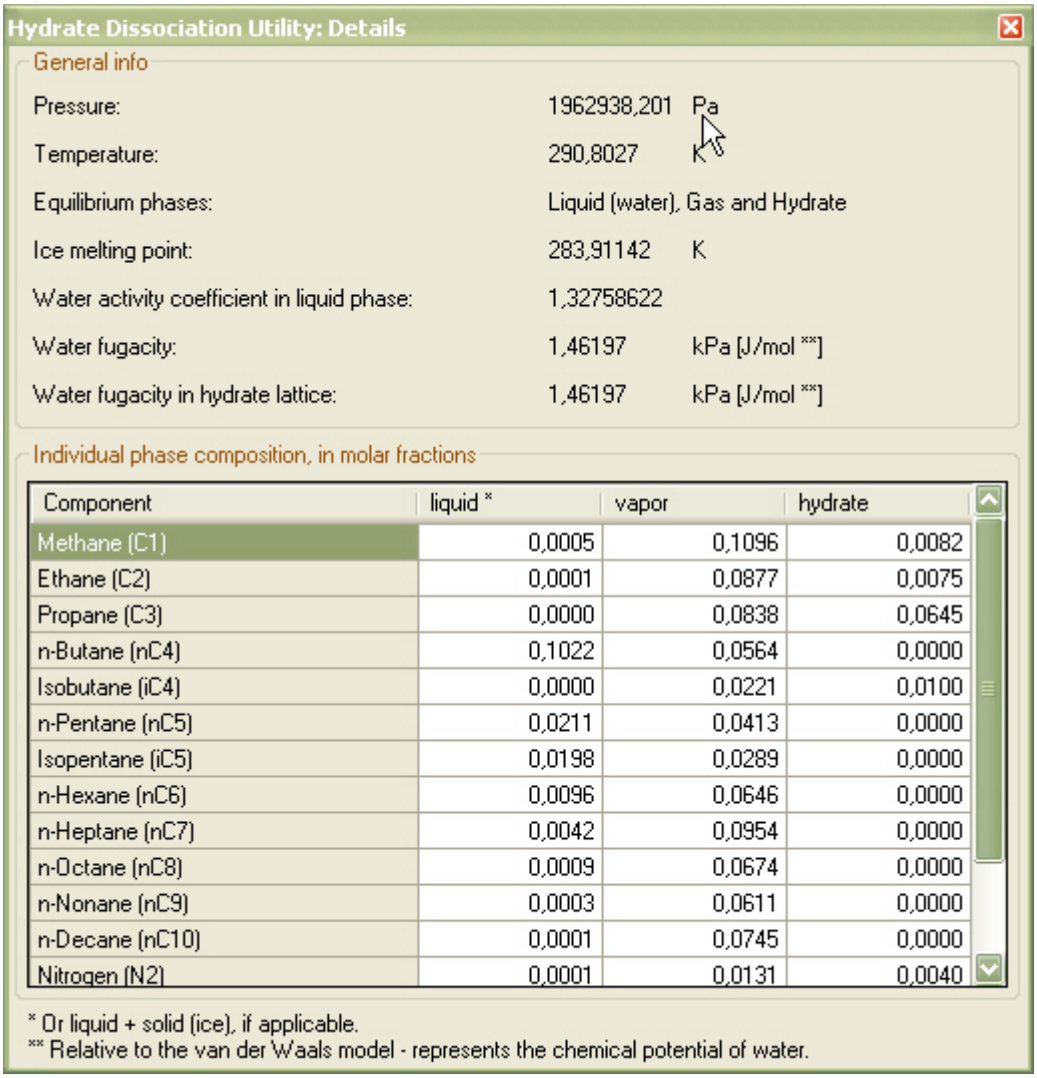


Figure 32: Hydrate calculation interface.

The composition of equilibrium phases and other information can be viewed by clicking in the "Details" button (Figure 33):



Component	liquid *	vapor	hydrate
Methane (C1)	0,0005	0,1096	0,0082
Ethane (C2)	0,0001	0,0877	0,0075
Propane (C3)	0,0000	0,0838	0,0645
n-Butane (nC4)	0,1022	0,0564	0,0000
Isobutane (iC4)	0,0000	0,0221	0,0100
n-Pentane (nC5)	0,0211	0,0413	0,0000
Isopentane (iC5)	0,0198	0,0289	0,0000
n-Hexane (nC6)	0,0096	0,0646	0,0000
n-Heptane (nC7)	0,0042	0,0954	0,0000
n-Octane (nC8)	0,0009	0,0674	0,0000
n-Nonane (nC9)	0,0003	0,0611	0,0000
n-Decane (nC10)	0,0001	0,0745	0,0000
Nitrogen (N2)	0,0001	0,0131	0,0040

Figure 33: Hydrate equilibrium phase compositions.

3.3 Pure Component Properties

The Pure Component Properties utility is used to view and edit pure component constants, view molecular properties and general temperature dependent properties like ideal gas Cp, vapor pressure, liquid viscosity and vaporization enthalpy (Figure 34).

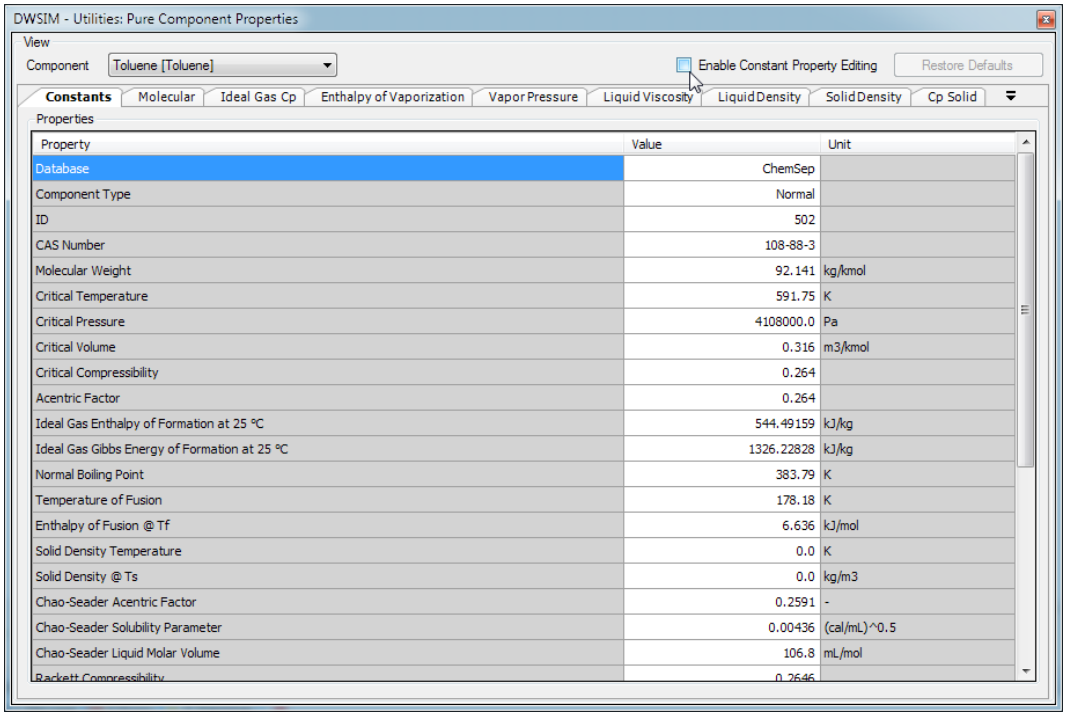


Figure 34: Pure Component Properties utility.

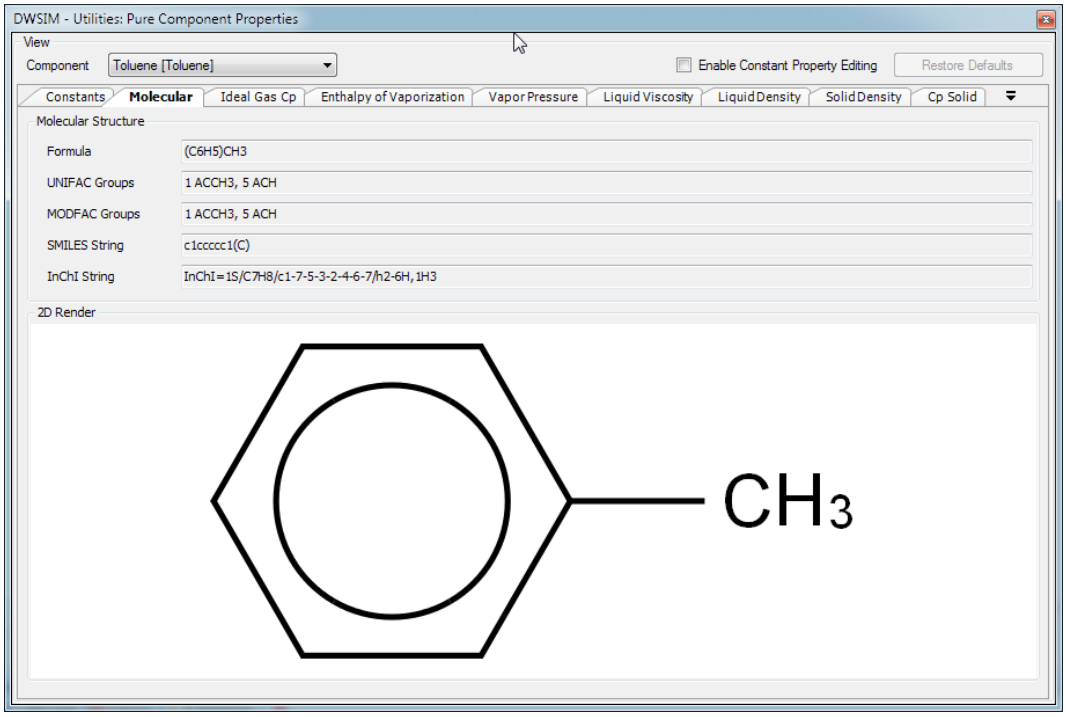
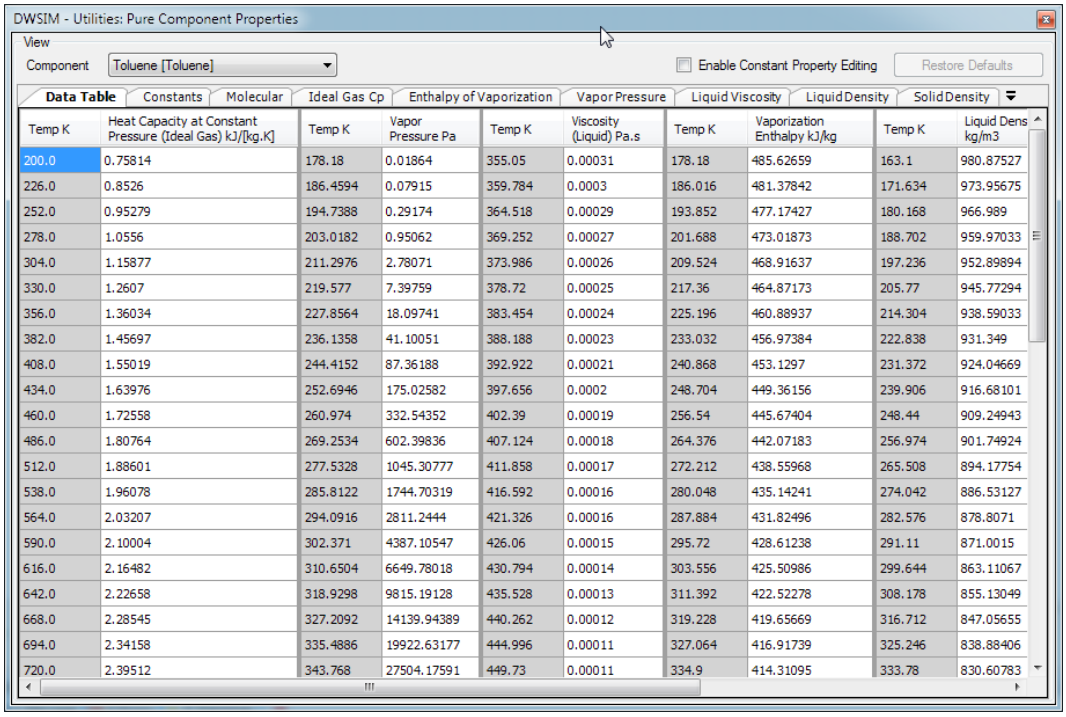


Figure 35: Pure Component Properties utility (2).



Temp K	Heat Capacity at Constant Pressure (Ideal Gas) kJ/[kg.K]	Temp K	Vapor Pressure Pa	Temp K	Viscosity (Liquid) Pa.s	Temp K	Vaporization Enthalpy kJ/kg	Temp K	Liquid Dens kg/m3
200.0	0.75814	178.18	0.01864	355.05	0.00031	178.18	485.62659	163.1	980.87527
226.0	0.8526	186.4594	0.07915	359.784	0.0003	186.016	481.37842	171.634	973.95675
252.0	0.95279	194.7388	0.29174	364.518	0.00029	193.852	477.17427	180.168	966.989
278.0	1.0556	203.0182	0.95062	369.252	0.00027	201.688	473.01873	188.702	959.97033
304.0	1.15877	211.2976	2.78071	373.986	0.00026	209.524	468.91637	197.236	952.89894
330.0	1.2607	219.577	7.39759	378.72	0.00025	217.36	464.87173	205.77	945.77294
356.0	1.36034	227.8564	18.09741	383.454	0.00024	225.196	460.88937	214.304	938.59033
382.0	1.45697	236.1358	41.10051	388.188	0.00023	233.032	456.97384	222.838	931.349
408.0	1.55019	244.4152	87.36188	392.922	0.00021	240.868	453.1297	231.372	924.04669
434.0	1.63976	252.6946	175.02582	397.656	0.0002	248.704	449.36156	239.906	916.68101
460.0	1.72558	260.974	332.54352	402.39	0.00019	256.54	445.67404	248.44	909.24943
486.0	1.80764	269.2534	602.39836	407.124	0.00018	264.376	442.07183	256.974	901.74924
512.0	1.88601	277.5328	1045.30777	411.858	0.00017	272.212	438.55968	265.508	894.17754
538.0	1.96078	285.8122	1744.70319	416.592	0.00016	280.048	435.14241	274.042	886.53127
564.0	2.03207	294.0916	2811.2444	421.326	0.00016	287.884	431.82496	282.576	878.8071
590.0	2.10004	302.371	4387.10547	426.06	0.00015	295.72	428.61238	291.11	871.0015
616.0	2.16482	310.6504	6649.78018	430.794	0.00014	303.556	425.50986	299.644	863.11067
642.0	2.22658	318.9298	9815.19128	435.528	0.00013	311.392	422.52278	308.178	855.13049
668.0	2.28545	327.2092	14139.94389	440.262	0.00012	319.228	419.65669	316.712	847.05655
694.0	2.34158	335.4886	19922.63177	444.996	0.00011	327.064	416.91739	325.246	838.88406
720.0	2.39512	343.768	27504.17591	449.73	0.00011	334.9	414.31095	333.78	830.60783

Figure 36: Pure Component Properties utility (3).

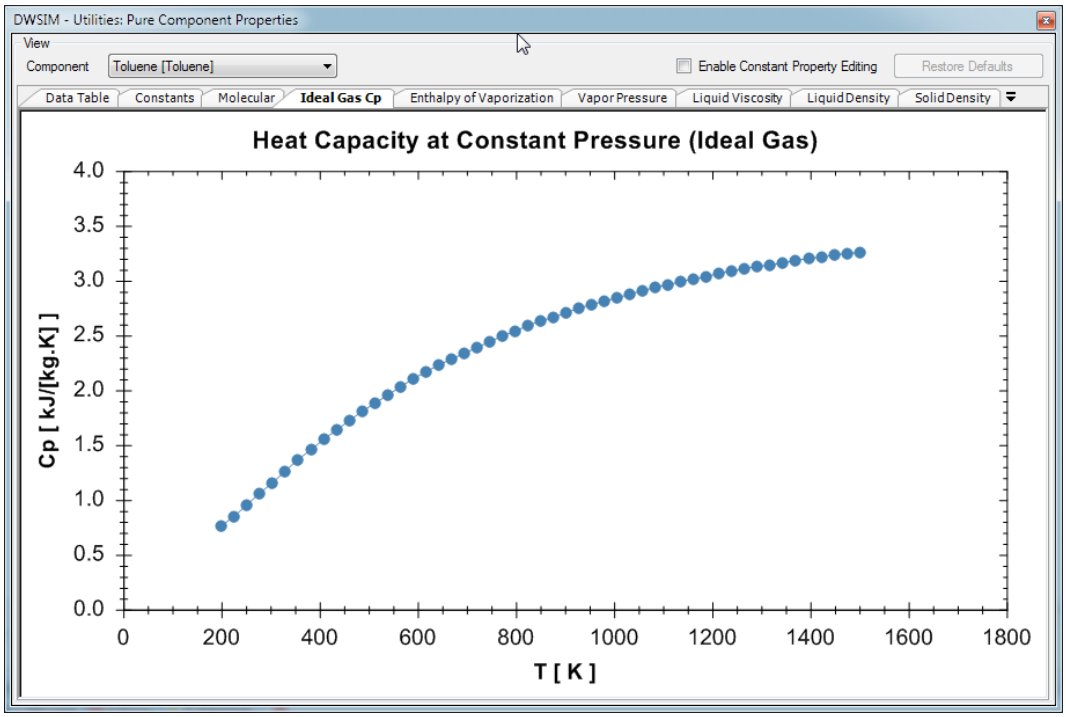


Figure 37: Pure Component Properties utility (4).

3.4 Phase Envelope

The Phase Envelope utility (Figure 39) allows the visualization of the existing relations between thermodynamic properties of a mixture of components in a material stream. The following phase

envelopes can be generated in DWSIM: Pressure-Temperature, Pressure-Enthalpy, Pressure-Entropy, Pressure-Volume, Temperature-Pressure, Temperature-Enthalpy, Temperature-Entropy, Temperature-Volume, Volume-Pressure, Volume-Temperature, Volume-Enthalpy and Volume-Entropy.

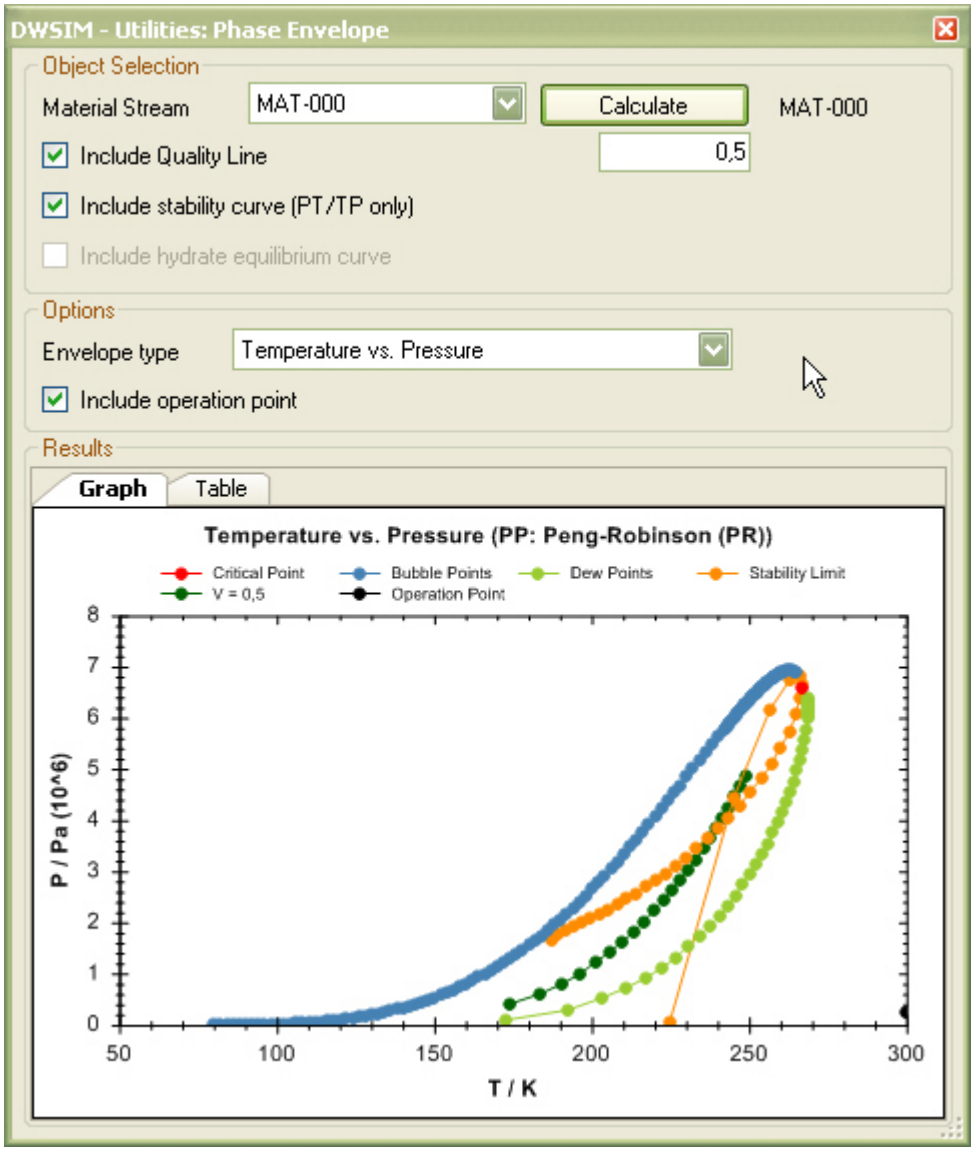


Figure 38: Phase Envelope utility.

It is possible to include quality and thermodynamic stability curves in the TP/PT diagrams. The stability limit curve refers to the limiting region where one can have a superheated liquid or a subcooled vapor. For all diagrams is also possible to include the operation point.

The stability curve can only be calculated by PR and SRK EOSes.

3.5 Binary Envelope

The Binary Envelope utility is a specialized phase envelope builder for viewing specific two-component diagrams (T-x-y, P-x-y, etc.). For the T-x-y diagram type, different equilibrium lines can be calculated, depending on Property Package and Flash Algorithm selections.

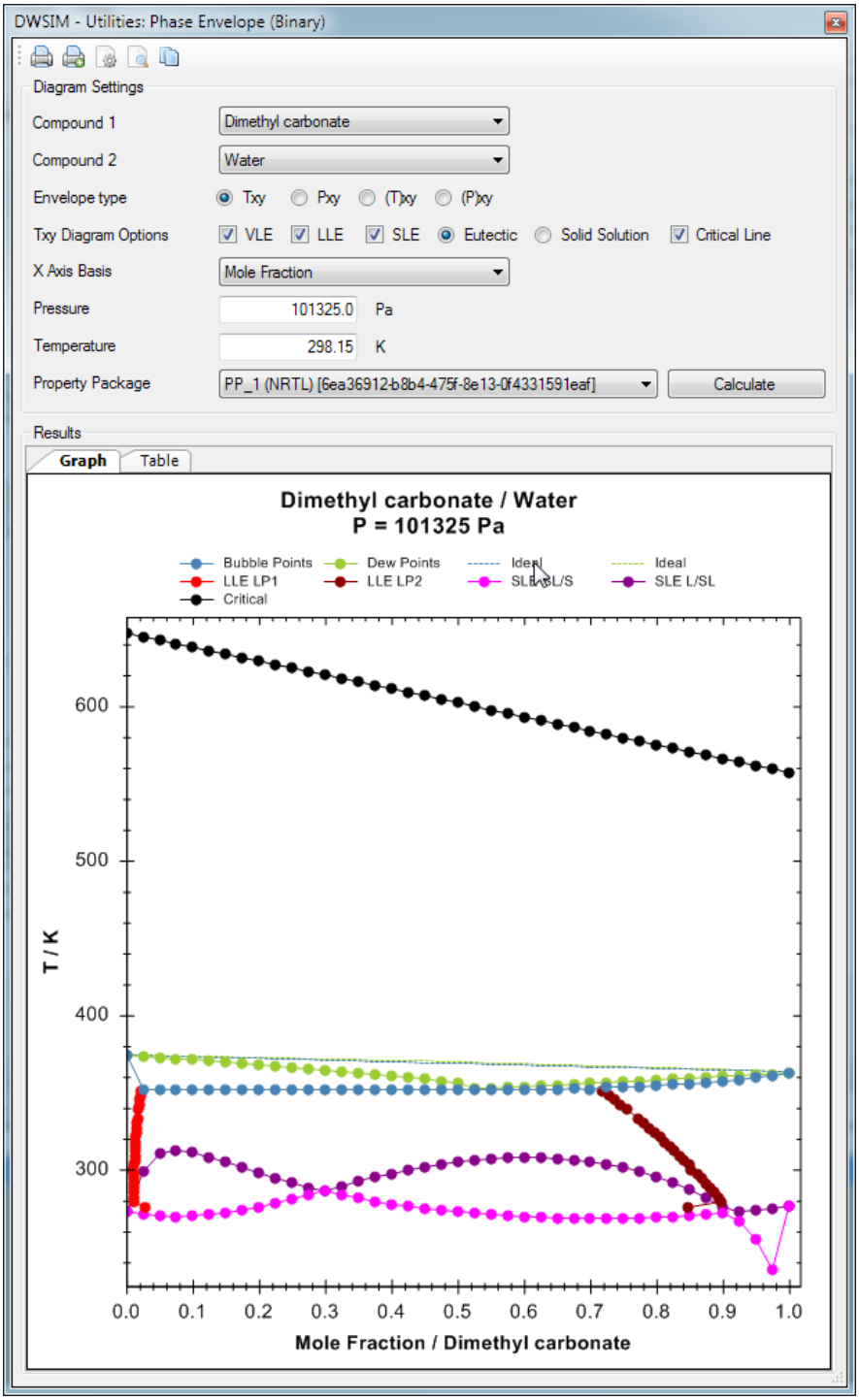


Figure 39: Binary Envelope utility.

3.6 Petroleum Cold Flow Properties

The utility for calculation of petroleum cold flow properties can be used to predict important fluid properties for the petroleum industry, like flash point, Reid vapor pressure, Cetane index, etc. (Figure 40).

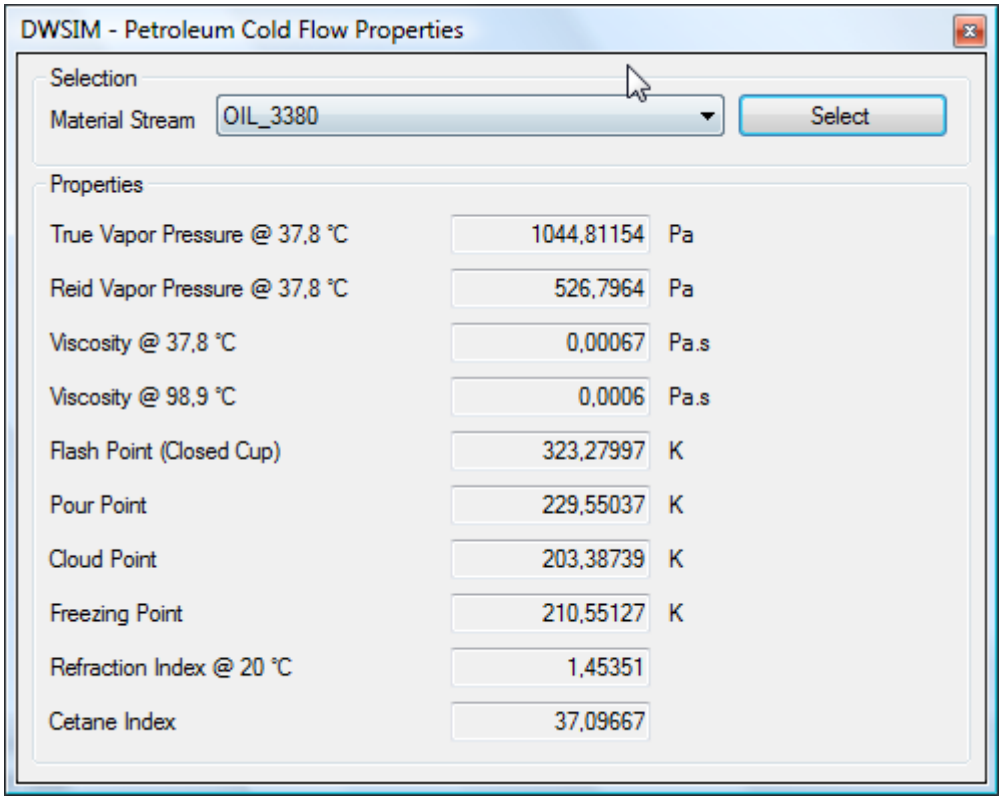


Figure 40: Cold Flow Properties interface.

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