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

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1 Introduction

This guide describes the calculation principles of the unit operations in DWSIM and their properties. For details about the models behind the simulation, please view 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.

Object	MAT-000	
Type	Material Stream	
Status	Calculated	

Properties		Format Object
<div> <div>1. Conditions</div> <div> <div>Temperature (K)</div> <div>300</div> </div> <div> <div>Pressure (Pa)</div> <div>234567</div> </div> <div> <div>Mass flowrate (kg/s)</div> <div>232</div> </div> <div> <div>Molar flowrate (mol/s)</div> <div>10062,23841</div> </div> <div> <div>Volumetric flowrate (m3/s)</div> <div>106,99389</div> </div> <div> <div>Composition Editor</div> <div>(Collection)</div> </div> <div> <div>Composition basis</div> <div>Molar_Fractions</div> </div> </div>		
<div> <div>2. Molar Composition</div> <div> <div>Mixture</div> <div>(...)</div> </div> <div> <div>Vapor</div> <div>(...)</div> </div> <div> <div>Liquid</div> <div>(...)</div> </div> </div>		
<div> <div>3. Properties</div> <div> <div>Vapor</div> <div>(...)</div> <div> <div>Specific Enthalpy (kJ/kg)</div> <div>-0,0208</div> </div> <div> <div>Specific Entropy (kJ/[kg.K])</div> <div>-0,01562</div> </div> <div> <div>Molecular Weight (kg/kmol)</div> <div>23,0565</div> </div> <div> <div>Density (kg/m3)</div> <div>2,16835</div> </div> <div> <div>Flowrate @ T, P (m3/s)</div> <div>106,99389</div> </div> <div> <div>Mass flowrate (kg/s)</div> <div>232</div> </div> <div> <div>Phase molar fraction</div> <div>1</div> </div> <div> <div>Phase mass fraction</div> <div>1</div> </div> <div> <div>Z</div> <div>0,98884</div> </div> <div> <div>Cp (kJ/[kg.K])</div> <div>1,95097</div> </div> <div> <div>Cp/Cv</div> <div>1,24304</div> </div> <div> <div>Thermal Conductivity (W/[m.K])</div> <div>0,02963</div> </div> <div> <div>Kinematic viscosity (m2/s)</div> <div>0</div> </div> <div> <div>Dynamic viscosity (Pa.s)</div> <div>1E-05</div> </div> </div> </div>		

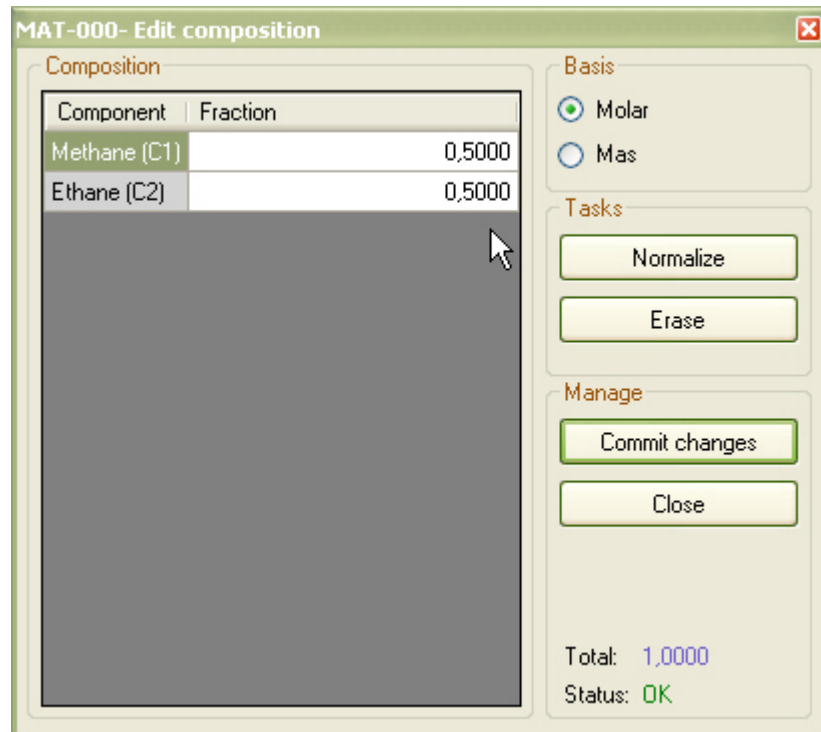
Vapor
Vapor Phase Properties

Figure 1: Material Stream properties.

Input Parameters

→ Temperature: stream temperature;

- Pressure: stream pressure;
- Composition: the stream composition must be given in molar or mass basis (Figure 2).



The image shows a software window titled "MAT-000- Edit composition". It contains a table for composition data and several control buttons on the right.

Component	Fraction
Methane (C1)	0,5000
Ethane (C2)	0,5000

On the right side of the window, there are three sections:

- Basis:** Two radio buttons, "Molar" (selected) and "Mas".
- Tasks:** Two buttons, "Normalize" and "Erase".
- Manage:** Two buttons, "Commit changes" and "Close".

At the bottom right, the following text is displayed:

Total: 1,0000
Status: OK

Figure 2: Material Stream composition editor.

In the composition editor, the user must enter the composition in such a way that the total sum be equal to 1. **The new values are saved only when the "Save Changes" button is pressed.**

- 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 up 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 (C_p), C_p/C_v , 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).

Object E1	
Type	Energy Stream
Status	Calculated
<div> <div>Properties</div> <div>Format Object</div> <div></div> </div>	
<div> <div>1. Connections</div> <div> <div>Connected to (input)</div> <div>TUB-000</div> </div> <div> <div>Connected to (output)</div> <div></div> </div> </div>	
<div> <div>2. Properties</div> <div> <div>Energy (kW)</div> <div>-33,84911</div> </div> </div>	
<div> <div>Other</div> <div> <div>Notes</div> <div></div> </div> </div>	
<div> <div>Connected to (input)</div> <div></div> </div>	

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 three material streams into one, while executing all the mass and energy balances(Figure 4).

Object MIST-000	
Type Mixer	
Status Calculated	
Properties Format Object	
<input checked="" type="checkbox"/> 1. Connections	
Input Stream 1	1
Input Stream 2	2
Input Stream 3	3
Connected to (output)	4
<input checked="" type="checkbox"/> 2. Parameters	
Pressure downstream	Mínimo
<input checked="" type="checkbox"/> Other	
Notes	
Input Stream 1	

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).

Object DIV-000									
Type Splitter									
Status Calculated									
<div> <div>Properties</div> <div>Format Object</div> <div>▼</div> </div>									
<div> <div>1. Connections</div> <table border="1"> <tr> <td>Input Stream</td> <td>2</td> </tr> <tr> <td>Output Stream 1</td> <td>3</td> </tr> <tr> <td>Output Stream 2</td> <td>4</td> </tr> <tr> <td>Output Stream 3</td> <td>5</td> </tr> </table> </div>		Input Stream	2	Output Stream 1	3	Output Stream 2	4	Output Stream 3	5
Input Stream	2								
Output Stream 1	3								
Output Stream 2	4								
Output Stream 3	5								
<div> <div>2. Stream Fractions</div> <table border="1"> <tr> <td>3</td> <td>0</td> </tr> <tr> <td>4</td> <td>0</td> </tr> <tr> <td>5</td> <td>0</td> </tr> </table> </div>		3	0	4	0	5	0		
3	0								
4	0								
5	0								
<div> <div>Other</div> <table border="1"> <tr> <td>Notes</td> <td></td> </tr> </table> </div>		Notes							
Notes									
<div> <div>4</div> <div>Enter a value between 0 and 1.</div> </div>									

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.

Object SEP-002							
Type G-L Separator							
Status Calculated							
<div> <div>Properties</div> <div>Format Object</div> </div>							
<div> <div>1. Connections</div> <table> <tr> <td>Input Stream</td> <td>12</td> </tr> <tr> <td>Vapor outlet</td> <td>13</td> </tr> <tr> <td>Liquid outlet</td> <td>14</td> </tr> </table> </div>		Input Stream	12	Vapor outlet	13	Liquid outlet	14
Input Stream	12						
Vapor outlet	13						
Liquid outlet	14						
<div> <div>2. Parameters</div> <table> <tr> <td>Override separation temperature</td> <td>True</td> </tr> <tr> <td>Temperature (K)</td> <td>308,7</td> </tr> <tr> <td>Override separation pressure</td> <td>False</td> </tr> </table> </div>		Override separation temperature	True	Temperature (K)	308,7	Override separation pressure	False
Override separation temperature	True						
Temperature (K)	308,7						
Override separation pressure	False						
<div> <div>Other</div> <table> <tr> <td>Notes</td> <td></td> </tr> </table> </div>		Notes					
Notes							
<div>Input Stream</div>							

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).

Object TQ-000					
Type Tank					
Status Calculated					
<div> <div>Properties</div> <div>Format Object</div> <div>▼</div> </div>					
<div> <div>1. Connections</div> <table border="1"> <tr> <td>Input Stream</td> <td>18</td> </tr> <tr> <td>Output stream</td> <td>18-1</td> </tr> </table> </div>		Input Stream	18	Output stream	18-1
Input Stream	18				
Output stream	18-1				
<div> <div>2. Parameters of calculation</div> <table border="1"> <tr> <td>Pressure drop (Pa)</td> <td>32122,0</td> </tr> </table> </div>		Pressure drop (Pa)	32122,0		
Pressure drop (Pa)	32122,0				
<div> <div>Other</div> <table border="1"> <tr> <td>Notes</td> <td></td> </tr> </table> </div>		Notes			
Notes					
<div> <div>Pressure drop (Pa)</div> <div>Pressure drop in the tank.</div> </div>					

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.

Object TUB-000	
Type	Pipe Segment
Status	Calculated
Properties Format Object	
1. Connections	
Input Stream	1
Output stream	2
Energy Stream	E1
2. Profiles	
Hydraulic Profile	Click to edit ...
Pressure Drop Correlation	Beggs_Brill
Status	OK
Thermal Profile	Click to edit ...
3. Parameters	
Maximum Iterations in P	25
Maximum Iterations T	25
Tolerance for P recalculation	10
Tolerance for T recalculation	10
Maximum pressure error	10
Maximum temperature error	0,01
4. Results	
Delta P (Pa)	-20524.69285
Input Stream	

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.

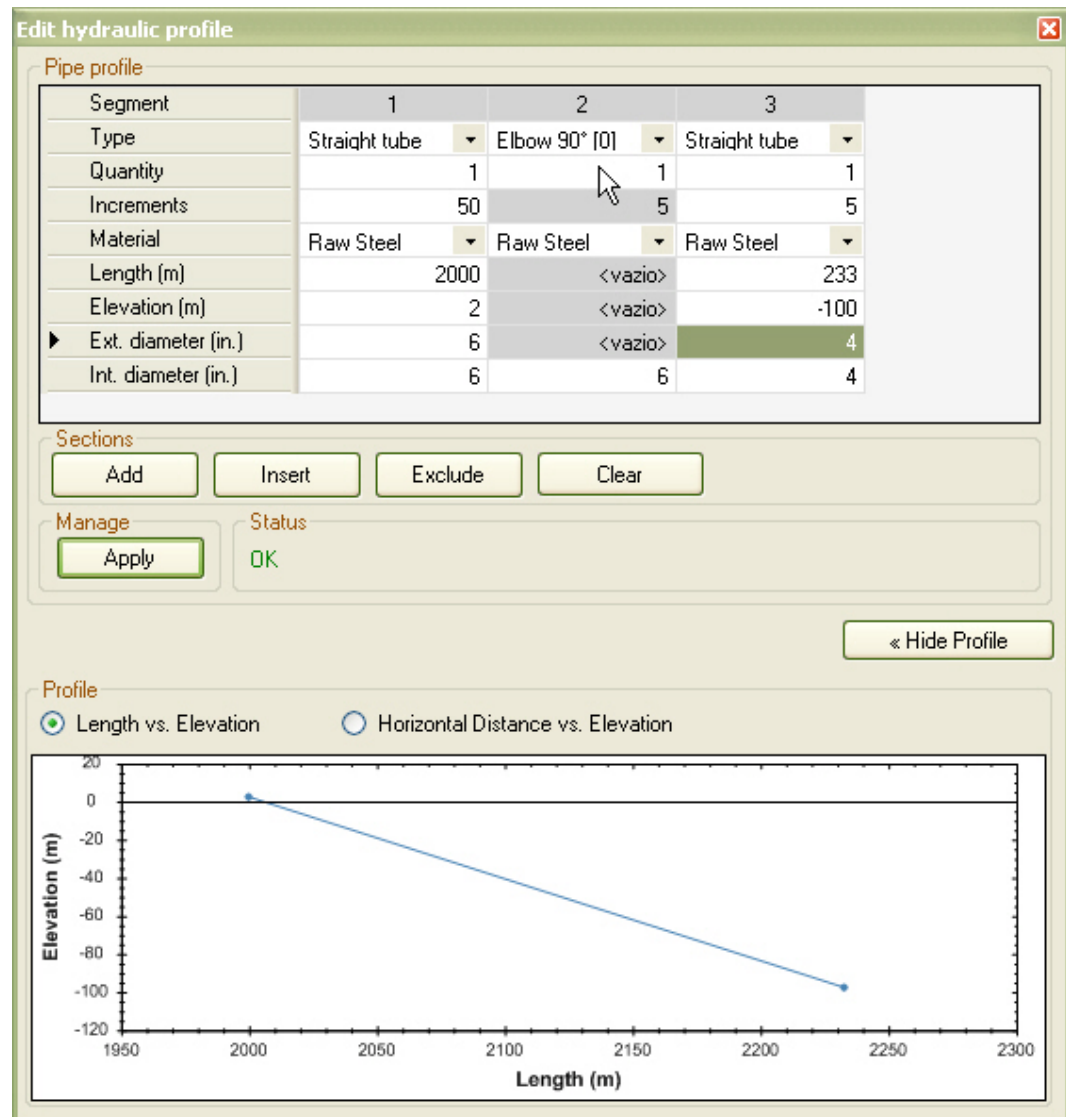


Figure 9: Pipe hydraulic profile editor.

- 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.

Edit thermal profile

☐ Define Overall HTC

Overall HTC W/m2.K / Amb. Temp. K

☐ Define the heat exchanged

Heat exchanged kJ/h

☒ Estimate Overall HTC

Ambient Temperature K

☒ Include pipe walls

☒ Include internal HTC

☒ Include insulation

Material

Thermal conductivity / Thickness W/m.K mm

☐ Include external HTC

Environment

Velocity [or deepness] m/s [m]

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:

$$Q = UA\Delta T_{ml} \quad (2.1)$$

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).

Object	VALV-000
Type	Valve
Status	Calculated
<div> <div>Properties</div> <div>Format Object</div> <div></div> </div>	
<div> <div>1. Connections</div> <div> <div>Input Stream</div> <div>9</div> </div> <div> <div>Output stream</div> <div>10</div> </div> </div>	
<div> <div>2. Parameters of calculation</div> <div> <div>Pressure drop (Pa)</div> <div>3654222,79999</div> </div> </div>	
<div> <div>3. Results</div> <div> <div>Delta T (K)</div> <div>-30,27443</div> </div> </div>	
<div> <div>Other</div> <div> <div>Notes</div> <div></div> </div> </div>	
<div>Input Stream</div>	

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).

Object	BB-000									
Type	Pump									
Status	Calculated									
<div> <div>Properties</div> <div>Format Object</div> <div></div> </div>										
<div> <div>1. Connections</div> <table border="1"> <tr> <td>Input Stream</td> <td>MAT-000</td> </tr> <tr> <td>Output stream</td> <td>2</td> </tr> <tr> <td>Energy Stream</td> <td>E1</td> </tr> </table> </div>			Input Stream	MAT-000	Output stream	2	Energy Stream	E1		
Input Stream	MAT-000									
Output stream	2									
Energy Stream	E1									
<div> <div>2. Parameters of calculation</div> <table border="1"> <tr> <td>Delta P (Pa)</td> <td>3123122,0</td> </tr> <tr> <td>Efficiency (0-100)</td> <td>75</td> </tr> <tr> <td>Ignore Vapor in the input stream</td> <td>True</td> </tr> <tr> <td>Using Delta-P provided</td> <td>True</td> </tr> </table> </div>			Delta P (Pa)	3123122,0	Efficiency (0-100)	75	Ignore Vapor in the input stream	True	Using Delta-P provided	True
Delta P (Pa)	3123122,0									
Efficiency (0-100)	75									
Ignore Vapor in the input stream	True									
Using Delta-P provided	True									
<div> <div>3. Results</div> <table border="1"> <tr> <td>Delta T (K)</td> <td>625,01915</td> </tr> <tr> <td>Energy needed (kW)</td> <td>445539,94912</td> </tr> </table> </div>			Delta T (K)	625,01915	Energy needed (kW)	445539,94912				
Delta T (K)	625,01915									
Energy needed (kW)	445539,94912									
<div> <div>Other</div> <table border="1"> <tr> <td>Notes</td> <td></td> </tr> </table> </div>			Notes							
Notes										
<div> <div>Delta P (Pa)</div> <div>Difference of pressure between the streams</div> </div>										

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:

$$H_2 = H_1 + \frac{\Delta P}{\rho}, \quad (2.2)$$

- Pump discharge pressure:

$$P_2 = P_1 + \Delta P \quad (2.3)$$

→ Pump required power:

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

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:

$$H_2 = H_1 + \frac{Pot \eta}{W}, \quad (2.5)$$

→ ΔP :

$$\Delta P = \rho(H_2 - H_1), \quad (2.6)$$

→ Discharge pressure:

$$P_2 = P_1 + \Delta P \quad (2.7)$$

→ 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).

Object COMP-001										
Type Adiabatic Compressor										
Status Calculated										
<div> <div>Properties</div> <div>Format Object</div> <div></div> </div>										
<div> <div>1. Connections</div> <table> <tr> <td>Input Stream</td> <td>13</td> <td>▼</td> </tr> <tr> <td>Output stream</td> <td>15</td> <td></td> </tr> <tr> <td>Energy Stream</td> <td>E2</td> <td></td> </tr> </table> </div>		Input Stream	13	▼	Output stream	15		Energy Stream	E2	
Input Stream	13	▼								
Output stream	15									
Energy Stream	E2									
<div> <div>2. Parameters of calculation</div> <table> <tr> <td>Delta P (Pa)</td> <td>1523742,0</td> </tr> <tr> <td>Adiabatic Efficiency (0-100)</td> <td>75</td> </tr> <tr> <td>Ignore Liquid in the input stream</td> <td>True</td> </tr> <tr> <td>Using Delta-P provided</td> <td>True</td> </tr> </table> </div>		Delta P (Pa)	1523742,0	Adiabatic Efficiency (0-100)	75	Ignore Liquid in the input stream	True	Using Delta-P provided	True	
Delta P (Pa)	1523742,0									
Adiabatic Efficiency (0-100)	75									
Ignore Liquid in the input stream	True									
Using Delta-P provided	True									
<div> <div>3. Results</div> <table> <tr> <td>Delta T (K)</td> <td>78,87212</td> </tr> <tr> <td>Energy needed (kW)</td> <td>8,40393</td> </tr> </table> </div>		Delta T (K)	78,87212	Energy needed (kW)	8,40393					
Delta T (K)	78,87212									
Energy needed (kW)	8,40393									
<div> <div>Other</div> <table> <tr> <td>Notes</td> <td></td> </tr> </table> </div>		Notes								
Notes										
<div>Input Stream</div>										

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:

$$P_2 = P_1 + \Delta P \quad (2.8)$$

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

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

- Power required by the compressor:

$$Pot = \frac{W (H_{2id} - H_1)}{\eta}, \quad (2.10)$$

- Outlet temperature: PH Flash with P_2 and H_2 .

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

- Discharge pressure:

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

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:

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

- 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).

Object TURB-000	
Type Adiabatic Expander	
Status Calculated	
<div> <div>Properties</div> <div>Format Object</div> <div></div> </div>	
1. Connections	
Input Stream	8
Output stream	221
Energy Stream	E4
2. Parameters of calculation	
Pressure drop (Pa)	2000000,0
Adiabatic Efficiency (0-100)	75
Ignore Liquid in the input stream	True
3. Results	
Delta T (K)	-20,47424
Energy available (kW)	2,35246
Other	
Notes	
<div> <div>Pressure drop (Pa)</div> <div>Pressure drop across the turbine.</div> </div>	

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:

$$P_2 = P_1 - \Delta P \quad (2.13)$$

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

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

→ Power generated by the expander:

$$Pot = \frac{W (H_{2id} - H_1)}{\eta}, \quad (2.15)$$

→ 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).

Object	AQ-000									
Type	Heater									
Status	Calculated									
<div> <div>Properties</div> <div>Format Object</div> <div></div> </div>										
<div> <div>1. Connections</div> <table> <tr> <td>Input Stream</td> <td>2</td> </tr> <tr> <td>Output stream</td> <td>22</td> </tr> <tr> <td>Energy Stream</td> <td>21</td> </tr> </table> </div>			Input Stream	2	Output stream	22	Energy Stream	21		
Input Stream	2									
Output stream	22									
Energy Stream	21									
<div> <div>2. Parameters of calculation</div> <table> <tr> <td>Pressure drop (Pa)</td> <td>0,0</td> </tr> <tr> <td>Heat Added (kW)</td> <td>12000,0</td> </tr> <tr> <td>Efficiency (0-100)</td> <td>100</td> </tr> <tr> <td>Use Heat Provided</td> <td>True</td> </tr> </table> </div>			Pressure drop (Pa)	0,0	Heat Added (kW)	12000,0	Efficiency (0-100)	100	Use Heat Provided	True
Pressure drop (Pa)	0,0									
Heat Added (kW)	12000,0									
Efficiency (0-100)	100									
Use Heat Provided	True									
<div> <div>3. Results</div> <table> <tr> <td>Delta T (K)</td> <td>2,16272</td> </tr> </table> </div>			Delta T (K)	2,16272						
Delta T (K)	2,16272									
<div> <div>Other</div> <table> <tr> <td>Notes</td> <td></td> </tr> </table> </div>			Notes							
Notes										
<div> <div>Heat Added (kW)</div> <div>Quantity of heat transferred by heater</div> </div>										

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, where 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).

Object	RESF-000						
Type	Cooler						
Status	Calculated						
<div> <div>Properties</div> <div>Format Object</div> <div>▼</div> </div>							
<div> <div>1. Connections</div> <table> <tr> <td>Input Stream</td> <td>22</td> </tr> <tr> <td>Output stream</td> <td>12222</td> </tr> <tr> <td>Energy Stream</td> <td>e1</td> </tr> </table> </div>		Input Stream	22	Output stream	12222	Energy Stream	e1
Input Stream	22						
Output stream	12222						
Energy Stream	e1						
<div> <div>2. Parameters of calculation</div> <table> <tr> <td>Pressure drop (Pa)</td> <td>0,0</td> </tr> <tr> <td>Heat Removed (kW)</td> <td>40000,0</td> </tr> <tr> <td>Efficiency (0-100)</td> <td>100</td> </tr> </table> </div>		Pressure drop (Pa)	0,0	Heat Removed (kW)	40000,0	Efficiency (0-100)	100
Pressure drop (Pa)	0,0						
Heat Removed (kW)	40000,0						
Efficiency (0-100)	100						
<div> <div>3. Results</div> <table> <tr> <td>Delta T (K)</td> <td>-7,22698</td> </tr> </table> </div>		Delta T (K)	-7,22698				
Delta T (K)	-7,22698						
<div> <div>Other</div> <table> <tr> <td>Notes</td> <td></td> </tr> </table> </div>		Notes					
Notes							
<div> <div>Heat Removed (kW)</div> <div>Heat removed from the input stream by cooling</div> </div>							

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, where 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.

Selected Object																	
Object	SC-000																
Type	Shortcut Column																
Status	Not Calculated																
<div> <div>Properties</div> <div>Appearance</div> </div>																	
<div> <div>1. Connections</div> <table border="1"> <tr> <td>Feed</td> <td>MAT-001_CLONE</td> </tr> <tr> <td>Distillate</td> <td>2</td> </tr> <tr> <td>Bottoms</td> <td>3</td> </tr> <tr> <td>Condenser Duty</td> <td>21</td> </tr> <tr> <td>Reboiler Duty</td> <td>22</td> </tr> </table> </div>		Feed	MAT-001_CLONE	Distillate	2	Bottoms	3	Condenser Duty	21	Reboiler Duty	22						
Feed	MAT-001_CLONE																
Distillate	2																
Bottoms	3																
Condenser Duty	21																
Reboiler Duty	22																
<div> <div>2. Parameters</div> <table border="1"> <tr> <td>Condenser Type</td> <td>TotalCond</td> </tr> <tr> <td>Reflux Ratio</td> <td>3</td> </tr> <tr> <td>Light Key</td> <td>Carbon Dioxide (CO2)</td> </tr> <tr> <td>Light Key Molar Fraction</td> <td>0.001</td> </tr> <tr> <td>Heavy Key</td> <td>Propane (C3)</td> </tr> <tr> <td>Heavy Key Molar Fraction</td> <td>0.001</td> </tr> <tr> <td>Condenser Pressure (Pa)</td> <td>0.0</td> </tr> <tr> <td>Reboiler Pressure (Pa)</td> <td>0.0</td> </tr> </table> </div>		Condenser Type	TotalCond	Reflux Ratio	3	Light Key	Carbon Dioxide (CO2)	Light Key Molar Fraction	0.001	Heavy Key	Propane (C3)	Heavy Key Molar Fraction	0.001	Condenser Pressure (Pa)	0.0	Reboiler Pressure (Pa)	0.0
Condenser Type	TotalCond																
Reflux Ratio	3																
Light Key	Carbon Dioxide (CO2)																
Light Key Molar Fraction	0.001																
Heavy Key	Propane (C3)																
Heavy Key Molar Fraction	0.001																
Condenser Pressure (Pa)	0.0																
Reboiler Pressure (Pa)	0.0																
<div> <div>Other</div> <table border="1"> <tr> <td>Notes</td> <td></td> </tr> </table> </div>		Notes															
Notes																	
<div> <div>Property Package</div> <table border="1"> <tr> <td>Property Package</td> <td>PP_1</td> </tr> </table> </div>		Property Package	PP_1														
Property Package	PP_1																

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.

Object	DC-000	
Type	Distillation Column	
Status	Calculated	
<div> <div>Properties</div> <div>Format Object</div> </div>		
<div> <div>1. Column Properties</div> <div> <div>Condenser Pressure (Pa)</div> <div>123456</div> </div> <div> <div>Reboiler Pressure (Pa)</div> <div>123456</div> </div> <div> <div>Condenser Type</div> <div>Total_Condenser</div> </div> <div> <div>Condenser Pressure Drop (Pa)</div> <div>0</div> </div> <div> <div>Reflux Ratio</div> <div>5</div> </div> <div> <div>Distillate Flow Rate (mol/s)</div> <div>3000</div> </div> </div>		
<div> <div>2. Stages</div> </div>		
<div> <div>3. Connections</div> </div>		
<div> <div>4. Side Operations</div> </div>		
<div> <div>5. Initial Estimates</div> <div> <div>Use temperature estimates</div> <div>True</div> </div> <div> <div>Use vapor flows estimates</div> <div>True</div> </div> <div> <div>Use liquid flows estimates</div> <div>True</div> </div> <div> <div>Use composition estimates</div> <div>False</div> </div> <div> <div>Initial Estimates</div> <div>Click to edit ...</div> </div> </div>		
<div> <div>6. Tolerances</div> </div>		
<div> <div>7. Solving Method</div> <div> <div>Solving Method</div> <div>Russell_InsideOut</div> </div> <div> <div>Adjust Sb scaling factor</div> <div>True</div> </div> <div> <div>Calculate Kbj by weighted average</div> <div>False</div> </div> <div> <div>Use identity matrix as the first Jacobian inverse</div> <div>False</div> </div> </div>		
<div> <div>8. Results</div> <div> <div>Internal loop iterations</div> <div>4</div> </div> <div> <div>External loop iterations</div> <div>4</div> </div> <div> <div>Condenser Duty (kW)</div> <div>312360,50881</div> </div> <div> <div>Reboiler Duty (kW)</div> <div>5289979.13006</div> </div> </div>		
<div>6. Tolerances</div>		

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 Kb 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.

Object	HE-000													
Type	Heat Exchanger													
Status	Calculated													
<div> <div>Properties</div> <div>Appearance</div> </div>														
<div> <div>1. Connections</div> <table> <tr> <td>Inlet Stream 1</td> <td>1</td> </tr> <tr> <td>Inlet Stream 2</td> <td>2</td> </tr> <tr> <td>Outlet Stream 1</td> <td>3</td> </tr> <tr> <td>Outlet Stream 2</td> <td>4</td> </tr> </table> </div>			Inlet Stream 1	1	Inlet Stream 2	2	Outlet Stream 1	3	Outlet Stream 2	4				
Inlet Stream 1	1													
Inlet Stream 2	2													
Outlet Stream 1	3													
Outlet Stream 2	4													
<div> <div>2. Calculation parameters</div> <table> <tr> <td>Exchanger calculation mode</td> <td>CalcArea</td> </tr> <tr> <td>Hot fluid pressure drop (bar)</td> <td>0</td> </tr> <tr> <td>Cold fluid pressure drop (bar)</td> <td>0</td> </tr> <tr> <td>Cold fluid outlet temperature (°C)</td> <td>70,71823</td> </tr> <tr> <td>Hot fluid outlet temperature (°C)</td> <td>53,59794</td> </tr> <tr> <td>Overall Coefficient (U) (W/[m2.K])</td> <td>5</td> </tr> </table> </div>			Exchanger calculation mode	CalcArea	Hot fluid pressure drop (bar)	0	Cold fluid pressure drop (bar)	0	Cold fluid outlet temperature (°C)	70,71823	Hot fluid outlet temperature (°C)	53,59794	Overall Coefficient (U) (W/[m2.K])	5
Exchanger calculation mode	CalcArea													
Hot fluid pressure drop (bar)	0													
Cold fluid pressure drop (bar)	0													
Cold fluid outlet temperature (°C)	70,71823													
Hot fluid outlet temperature (°C)	53,59794													
Overall Coefficient (U) (W/[m2.K])	5													
<div> <div>3. Results</div> <table> <tr> <td>Area (m2)</td> <td>33,2209</td> </tr> <tr> <td>Log Mean Temperature Difference (LMTD) (°C.)</td> <td>50,4249</td> </tr> </table> </div>			Area (m2)	33,2209	Log Mean Temperature Difference (LMTD) (°C.)	50,4249								
Area (m2)	33,2209													
Log Mean Temperature Difference (LMTD) (°C.)	50,4249													
<div> <div>Other</div> <table> <tr> <td>Notes</td> <td></td> </tr> </table> </div>			Notes											
Notes														
<div> <div>Property Package</div> <table> <tr> <td>Property Package</td> <td>PP_1</td> </tr> </table> </div>			Property Package	PP_1										
Property Package	PP_1													
<div>Property Package</div>														

Figure 19: Heat Exchanger properties.

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

$$Q = UA\Delta T_{ml}, \quad (2.16)$$

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

$$Q = m\Delta H, \quad (2.17)$$

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.

Object	CS-000									
Type	Component Separator									
Status	Calculated									
<div> <div>Properties</div> <div>Appearance</div> <div>▼</div> </div>										
<div>1. Connections</div> <table border="1"> <tr> <td>Inlet Stream</td> <td>MAT-000</td> </tr> <tr> <td>Outlet stream 1</td> <td>MAT-001</td> </tr> <tr> <td>Outlet stream 2</td> <td>MAT-002</td> </tr> <tr> <td>Energy Stream</td> <td>EN-000</td> </tr> </table>			Inlet Stream	MAT-000	Outlet stream 1	MAT-001	Outlet stream 2	MAT-002	Energy Stream	EN-000
Inlet Stream	MAT-000									
Outlet stream 1	MAT-001									
Outlet stream 2	MAT-002									
Energy Stream	EN-000									
<div>2. Calculation parameters</div> <table border="1"> <tr> <td>Specified stream (0 for upper, 1 for lower)</td> <td>0</td> </tr> <tr> <td>Separation specs</td> <td>(Collection) ...</td> </tr> </table>			Specified stream (0 for upper, 1 for lower)	0	Separation specs	(Collection) ...				
Specified stream (0 for upper, 1 for lower)	0									
Separation specs	(Collection) ...									
<div>3. Results</div> <table border="1"> <tr> <td>Energy imbalance (kW)</td> <td>7.11523</td> </tr> </table>			Energy imbalance (kW)	7.11523						
Energy imbalance (kW)	7.11523									
<div>Other</div> <table border="1"> <tr> <td>Notes</td> <td></td> </tr> </table>			Notes							
Notes										
<div>Property Package</div> <table border="1"> <tr> <td>Property Package</td> <td>PP_1</td> </tr> </table>			Property Package	PP_1						
Property Package	PP_1									

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 tapings: select the option which corresponds to the arrangement of the tapings 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 tapings.
- ➔ 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.

Object	OP-000								
Type	Orifice Plate								
Status	Calculated								
<div> <div>Properties</div> <div>Appearance</div> </div>									
<div>1. Connections</div> <table border="1"> <tr> <td>Inlet Stream</td> <td>MAT-001</td> </tr> <tr> <td>Outlet Stream</td> <td>2</td> </tr> </table>		Inlet Stream	MAT-001	Outlet Stream	2				
Inlet Stream	MAT-001								
Outlet Stream	2								
<div>2. Calculation parameters</div> <table border="1"> <tr> <td>Pressure tapplings</td> <td>FlangeTaps</td> </tr> <tr> <td>Orifice diameter (m)</td> <td>0.2</td> </tr> <tr> <td>Beta (d/D)</td> <td>0.75</td> </tr> <tr> <td>Correction factor</td> <td>1.0</td> </tr> </table>		Pressure tapplings	FlangeTaps	Orifice diameter (m)	0.2	Beta (d/D)	0.75	Correction factor	1.0
Pressure tapplings	FlangeTaps								
Orifice diameter (m)	0.2								
Beta (d/D)	0.75								
Correction factor	1.0								
<div>3. Results</div> <table border="1"> <tr> <td>Orifice pressure drop (Pa)</td> <td>60843.84037</td> </tr> <tr> <td>Overall pressure drop (Pa)</td> <td>22765.44959</td> </tr> <tr> <td>Delta T (K)</td> <td>-0.22018</td> </tr> </table>		Orifice pressure drop (Pa)	60843.84037	Overall pressure drop (Pa)	22765.44959	Delta T (K)	-0.22018		
Orifice pressure drop (Pa)	60843.84037								
Overall pressure drop (Pa)	22765.44959								
Delta T (K)	-0.22018								
<div>Other</div> <table border="1"> <tr> <td>Notes</td> <td></td> </tr> </table>		Notes							
Notes									
<div>Property Package</div> <table border="1"> <tr> <td>Property Package</td> <td>PP_1</td> </tr> </table>		Property Package	PP_1						
Property Package	PP_1								

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 (COM-Solver class)

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

2.3 Reactors

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

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

Figure 22: 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 23) along the longitudinal axis of the reactor (assuming the concentration does not vary radially).

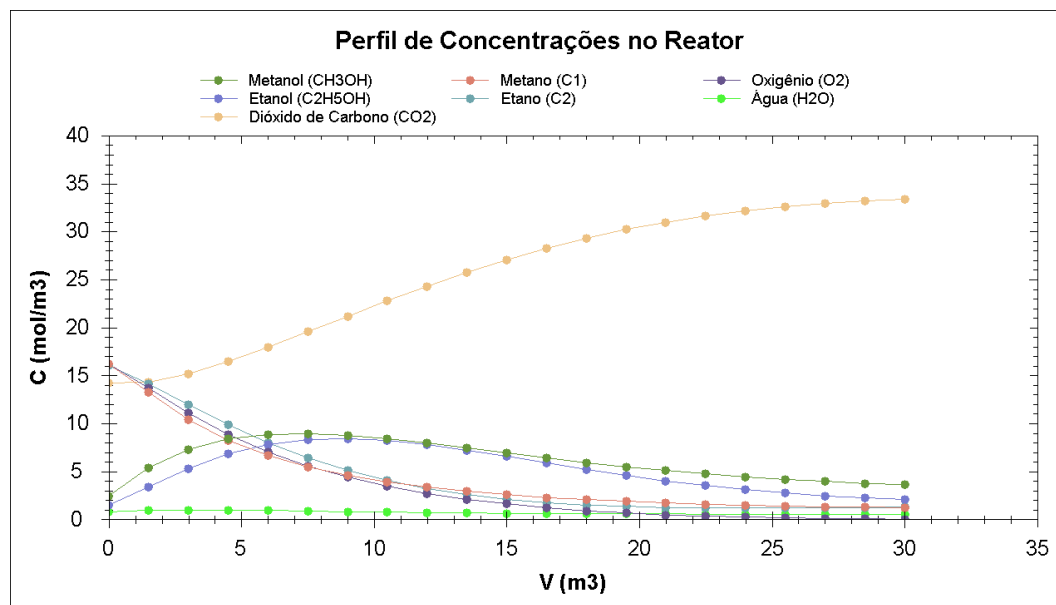


Figure 23: PFR concentration profile.

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 24) is composed by a block in the flowsheet which does convergence verifications in systems where 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.

Object	REC-001								
Type	Recycle								
Status	Calculated								
<div> <div>Properties</div> <div>Format Object</div> </div>									
<div> <div>1. Connections</div> <table> <tr> <td>Input Stream</td> <td>15</td> </tr> <tr> <td>Output stream</td> <td>3</td> </tr> </table> </div>		Input Stream	15	Output stream	3				
Input Stream	15								
Output stream	3								
<div> <div>2. Settings</div> <table> <tr> <td>Method of acceleration</td> <td>Wegstein</td> </tr> <tr> <td>Parameters (Wegstein)</td> <td>(...)</td> </tr> <tr> <td>Type of Flash</td> <td>FlashTP</td> </tr> <tr> <td>Número máximo de iterações</td> <td>10</td> </tr> </table> </div>		Method of acceleration	Wegstein	Parameters (Wegstein)	(...)	Type of Flash	FlashTP	Número máximo de iterações	10
Method of acceleration	Wegstein								
Parameters (Wegstein)	(...)								
Type of Flash	FlashTP								
Número máximo de iterações	10								
<div> <div>3. Parameters of convergence (tolerance)</div> <table> <tr> <td>Temperature (K)</td> <td>0,1</td> </tr> <tr> <td>Pressure (Pa)</td> <td>0,1</td> </tr> <tr> <td>Mass flowrate (kg/s)</td> <td>0,01</td> </tr> </table> </div>		Temperature (K)	0,1	Pressure (Pa)	0,1	Mass flowrate (kg/s)	0,01		
Temperature (K)	0,1								
Pressure (Pa)	0,1								
Mass flowrate (kg/s)	0,01								
<div> <div>4. Results</div> <table> <tr> <td>Required iterations</td> <td>1</td> </tr> <tr> <td>Temperature error (K)</td> <td>-0,05299</td> </tr> <tr> <td>Pressure error (Pa)</td> <td>0</td> </tr> <tr> <td>Mass flowrate error (kg/s)</td> <td>0,00023</td> </tr> </table> </div>		Required iterations	1	Temperature error (K)	-0,05299	Pressure error (Pa)	0	Mass flowrate error (kg/s)	0,00023
Required iterations	1								
Temperature error (K)	-0,05299								
Pressure error (Pa)	0								
Mass flowrate error (kg/s)	0,00023								
<div> <div>Other</div> <div> <div>Method of acceleration</div> <div>Method for accelerating the convergence of recycle.</div> </div> </div>									

Figure 24: 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 25) 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.

Object	AJ000
Type	Adjust
Status	Calculated
<div> <div>Properties</div> <div>Format Object</div> <div>▼</div> </div>	
1. Settings	
Controlled variable	(...)
Controlled variable	Click to select ...
Type of Object	Material Stream
Objeto	2
Property	Pressure
Manipulated variable	(...)
Use as Reference Object?	False
2. Parameters	
Adjustment Value (or Offset)	14325166,95546
Maximum Number of Iterations	10
Tolerance	0,0001
Step Size	0,1
Control Panel	
Other	
Notes	
<div> <div>Controlled variable</div> <div>Select a variable to be controlled by the Adjust.</div> </div>	

Figure 25: 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 26), the user controls the operation convergence. Two convergence methods are available.

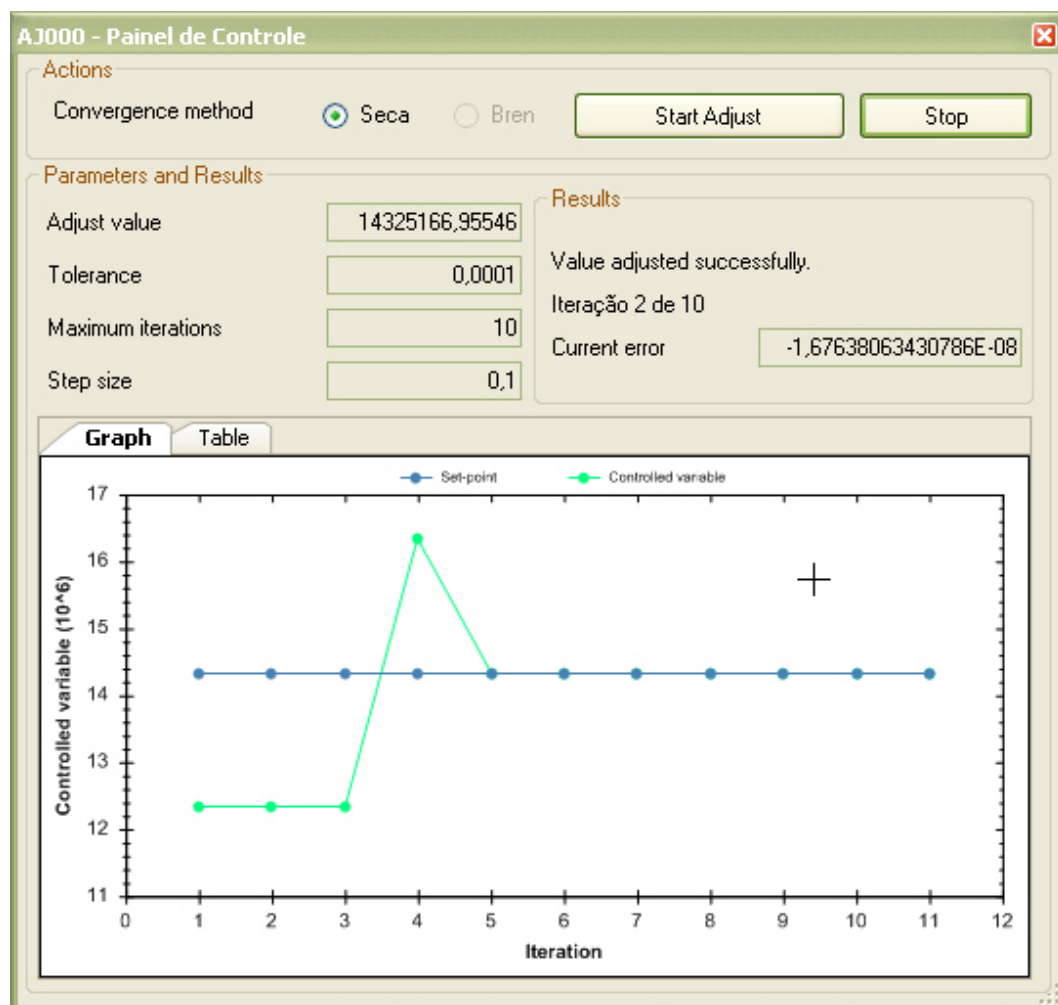


Figure 26: Adjust Control Panel.

2.4.4 Specification

The Specification Logical Operation (Figure 27) 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*.

Object	ES-000	
Type	Specification	
Status	Not Calculated	
<div> <div>Properties</div> <div>Format Object</div> </div>		
<div> <div>1. Settings</div> <div> <div>Source variable</div> <div>(...)</div> <div>Source variable</div> <div>Click to select ...</div> <div>Type of Object</div> <div>Material Stream</div> <div>Objeto</div> <div>1</div> <div>Property</div> <div>Pressure</div> </div> <div>Destination variable</div> <div>(...)</div> <div>Destination variable</div> <div>Click to select ...</div> <div>Type of Object</div> <div>Material Stream</div> <div>Objeto</div> <div>1</div> <div>Property</div> <div>Temperature</div> <div>Active</div> <div>True</div> <div>Calculate target object?</div> <div>False</div> </div>		

Figure 27: 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 28). The user can click on the "Evaluate Expression" to check if the expression is valid.

ES-000 - Painel de Controle		
Details		
Source Object/Variable	1 (Material Stream) / Pressure	
Actual value	14345691,74831 Pa	
Target Object/Variable	1 (Material Stream) / Temperature	
Actual value	340,0 K	
Specification		
Expression	Y =	X/50000
X = Source Variable		
Y = Target Variable	Expressão OK. Resultado: 286,91383	
		Evaluate Expression

Figure 28: Specification Control Panel.

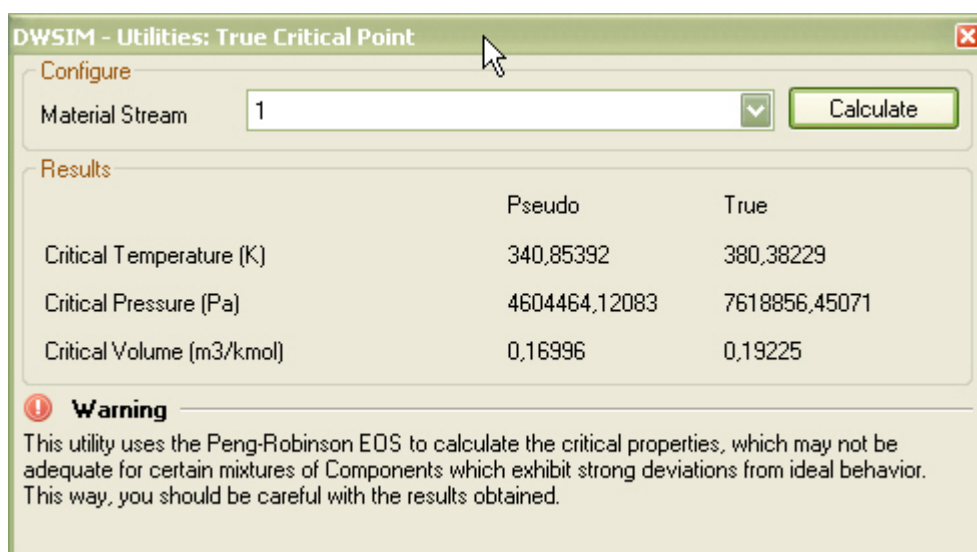
3 Utilities

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 29). The *Peng-Robinson* EOS is used in the calculations.



	Pseudo	True
Critical Temperature (K)	340,85392	380,38229
Critical Pressure (Pa)	4604464,12083	7618856,45071
Critical Volume (m3/kmol)	0,16996	0,19225

Warning
This utility uses the Peng-Robinson EOS to calculate the critical properties, which may not be adequate for certain mixtures of Components which exhibit strong deviations from ideal behavior. This way, you should be careful with the results obtained.

Figure 29: 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.).

DWSIM - Utilities: Hydrate Dissociation Conditions

Configure

Material Stream: 2

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

Calculate

Results

Equilibrium at stream conditions

Hydrate forms: No

Hydrate type: N/A

Equilibrium conditions at stream temperature

Pressure: N/A Pa

Temperature: 322.03889 K

Equilibrium phases: N/A

Details

Equilibrium conditions at stream pressure

Pressure: 1962938.201 Pa

Temperature: 290.8027 K

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

Details

Figure 30: Hydrate calculation interface.

The composition of equilibrium phases and other information can be viewed by clicking in the "Details" button (Figure 31):

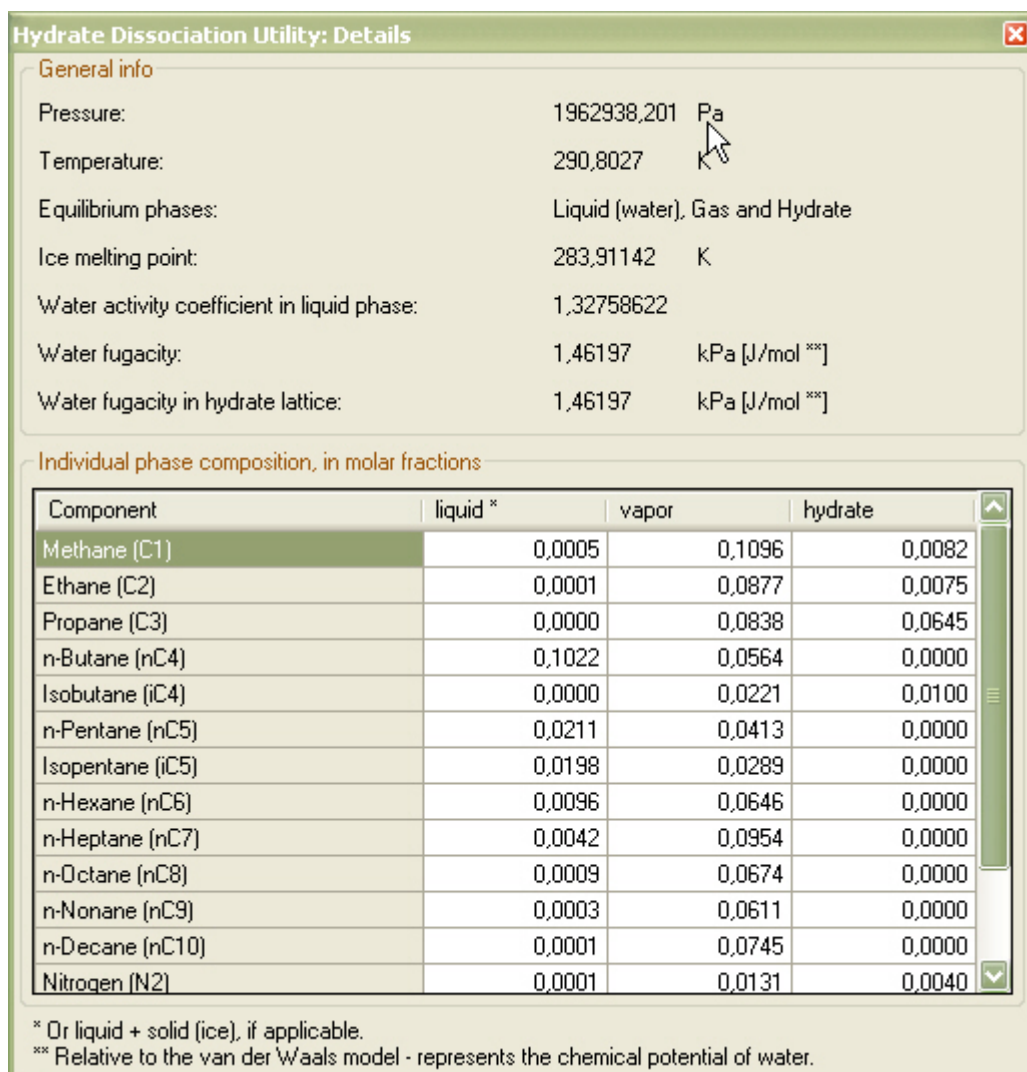


Figure 31: Hydrate equilibrium phase compositions.

3.3 Pure Component Properties

The Pure Component Properties utility is used to view pure component constants and temperature dependent properties like ideal gas C_p , vapor pressure, liquid viscosity and vaporization enthalpy (Figure 32).

DWSIM - Utilities: Pure Component Properties

View
Component: Water (H2O) [Água]

Constants | Ideal Gas Cp | Vapor Pressure | Liquid Viscosity | Enthalpy of Vaporization

Properties

Property	Value	Unit
Molecular Weight	18,015	kg/kmol
Critical Temperature	647,13	K
Critical Pressure	22055000,0	Pa
Critical Compressibility	0,229	-
Acentric Factor	0,34486	-
Ideal Gas Enthalpy of Formation at 25 °C	-13400,0	kJ/kg
Ideal Gas Gibbs Energy of Formation at 25 °C	-7602,03	kJ/kg
Normal Boiling Point,	373,15	K
UNIFAC Ri	0,92	-
UNIFAC Qi	1,4	-

UNIFAC Groups

Group	Quantity
CH3	0
CH2	0
CH	0
OH	0
ACH	0
ACCH2	0
ACCH3	0
ACOH	0
CH3CO	0
CH2CO	0
CH4	0
H2O	1
H2S	0

Figure 32: Pure Component Properties utility.

3.4 Phase Envelope

The Phase Envelope utility (Figure 34) allows the visualization of the existing relations between thermodynamic properties of a mixture of components in a material stream. The following envelopes can be viewed in DWSIM:

- Pressure-Temperature
- Pressure-Enthalpy
- Pressure-Entropy
- Pressure-Volume
- Temperature-Pressure
- Temperature-Enthalpy
- Temperature-Entropy
- Temperature-Volume
- Volume-Pressure
- Volume-Temperature
- Volume-Enthalpy
- Volume-Entropy

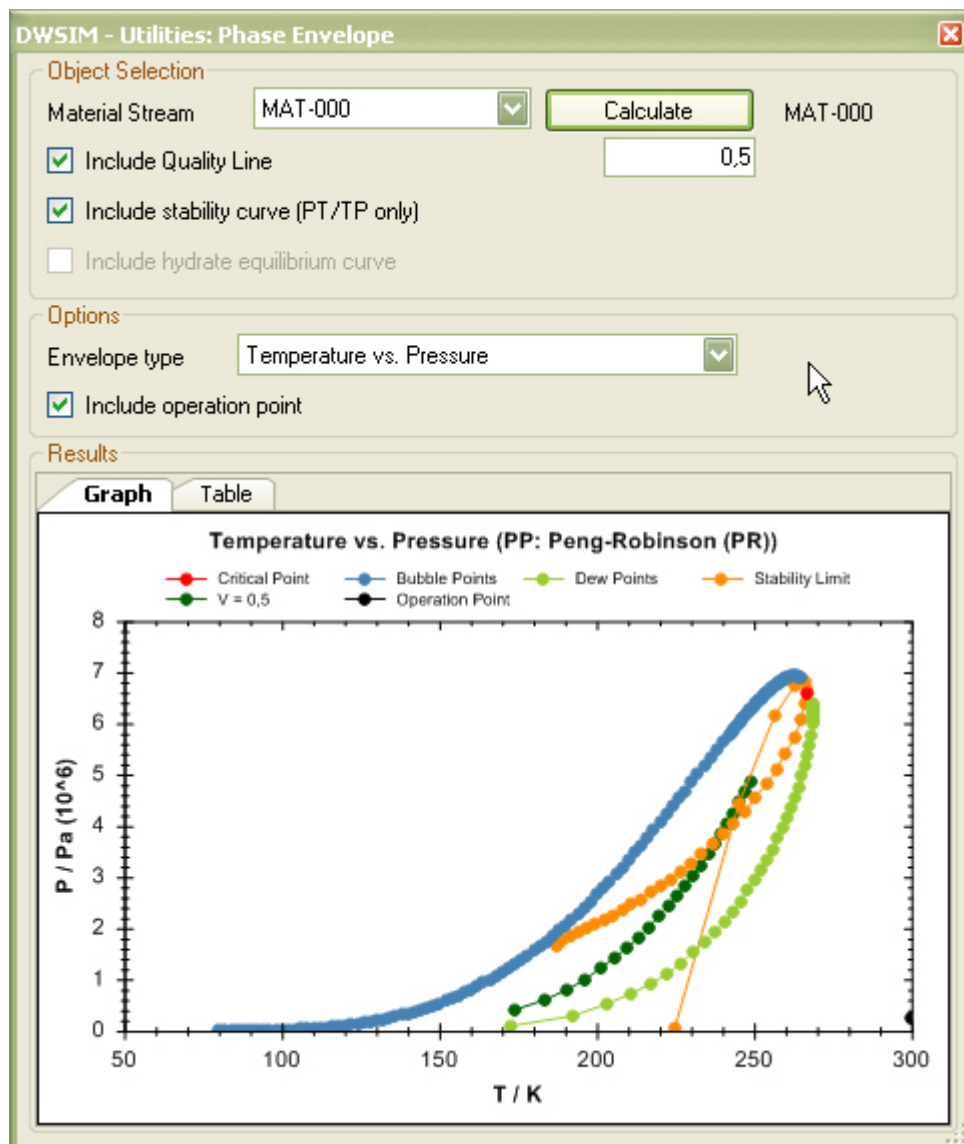


Figure 33: Phase Envelope utility.

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. Some important aspects about this utility must be observed:

- Quality curves can only be calculated by the Peng-Robinson, PR/LK and SRK EOS;
- The stability curve can only be calculated by PR and SRK EOS.

3.5 Binary Envelope

The Binary Envelope utility is nothing more than a specialized envelope builder for viewing specific two-component diagrams (T-x-y, P-x-y, etc.). For the UNIFAC Property Package, a Excess Gibbs Energy option is also available, which can be used to study the stability of the liquid phase in the selected stream.

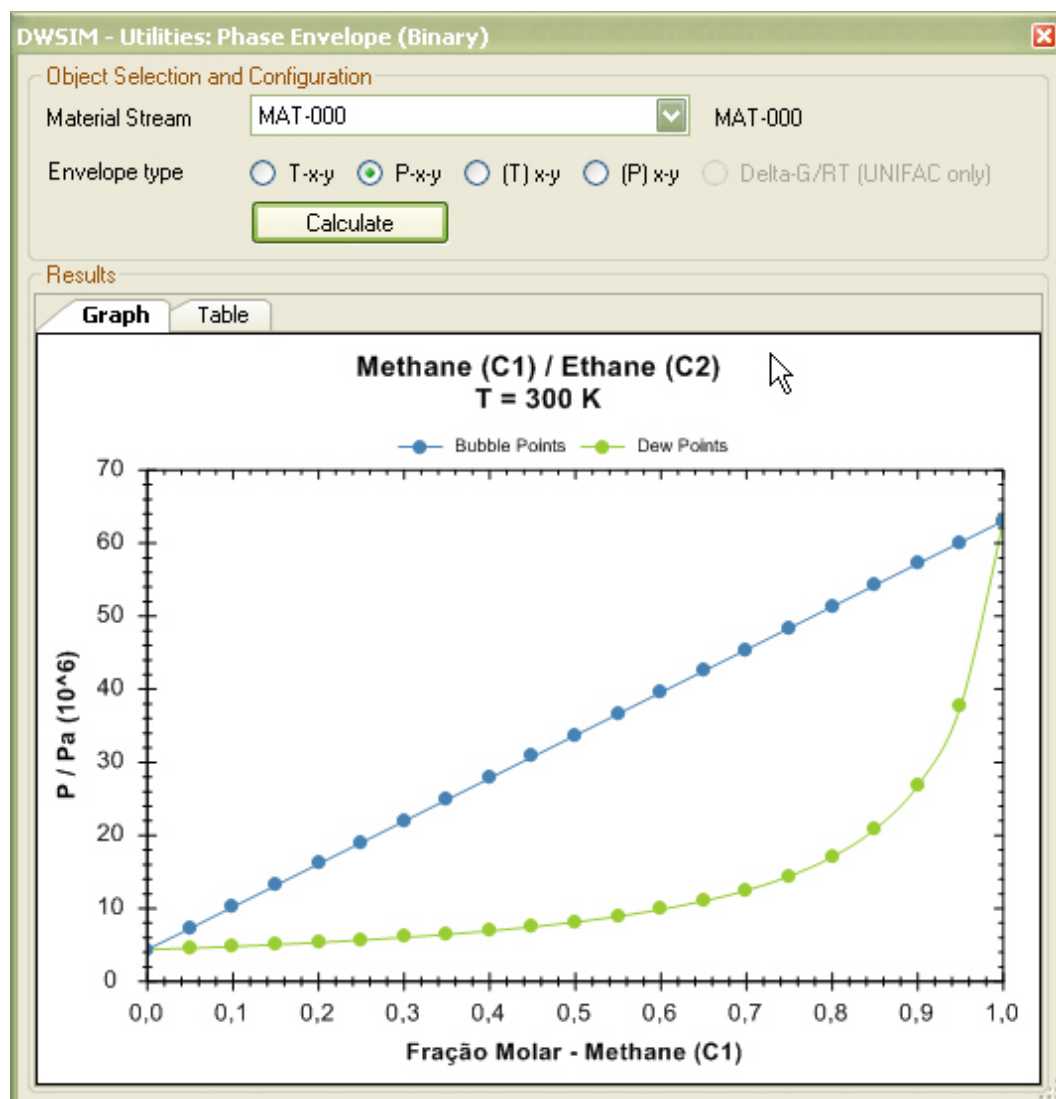
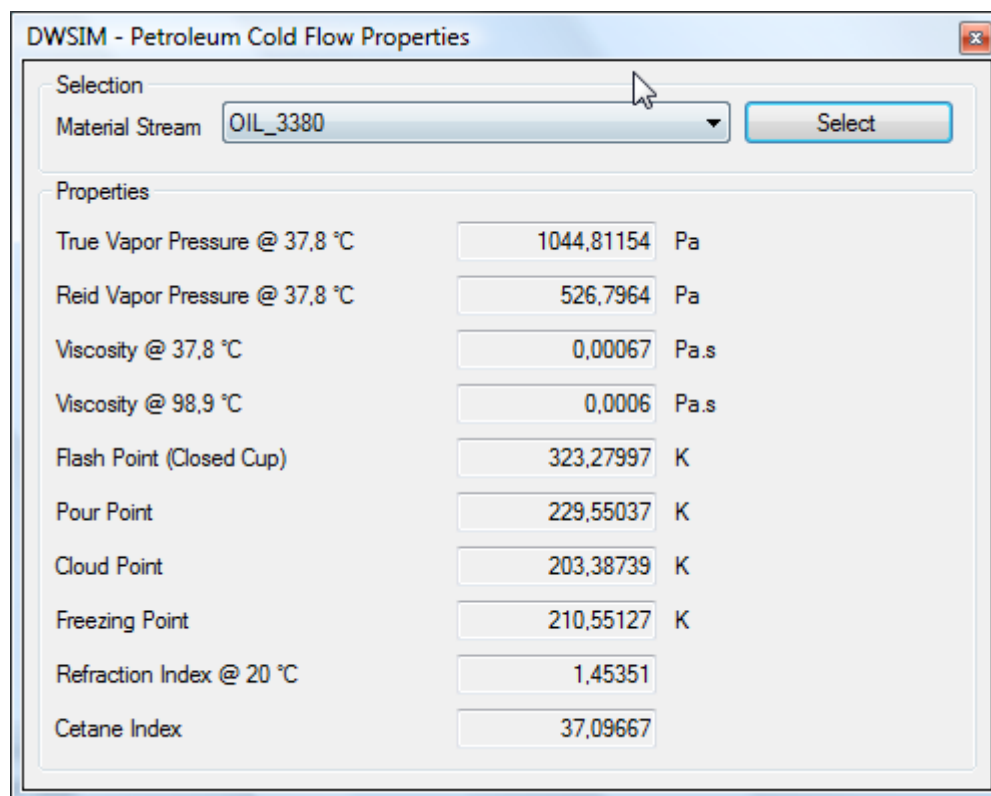


Figure 34: Binary Envelope utility.

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 35).



DWSIM - Petroleum Cold Flow Properties

Selection
Material Stream: OIL_3380 Select

Properties

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

Figure 35: Cold Flow Properties interface.

References

- [1] Kister HZ. *Distillation Design*. McGraw-Hill Professional. 1992.
- [2] Seader JD, Henley EJ. *Separation Process Principles*. Wiley. 2005.
- [3] Tinker T. Shell side characteristics of shell and tube heat exchangers. *Trans ASME*. 1958; 36:80.