



Simulate  
365

# DWSIM Pro

## User's Guide

Version 8.7.1  
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**1. INTRODUCTION**

This user guide details the additional features of DWSIM Pro. For information on features shared between the Open-Source and Pro versions, see the main DWSIM User's Guide.

## 2. REPORTING/DOCUMENTATION TOOLS

### 2.1. Process Flowsheet Diagram

Use this tool (Results menu > Process Flowsheet Diagram) to create a professional-looking Process Flowsheet Diagram (PFD) document that can be exported to a PDF document or to a PNG image.

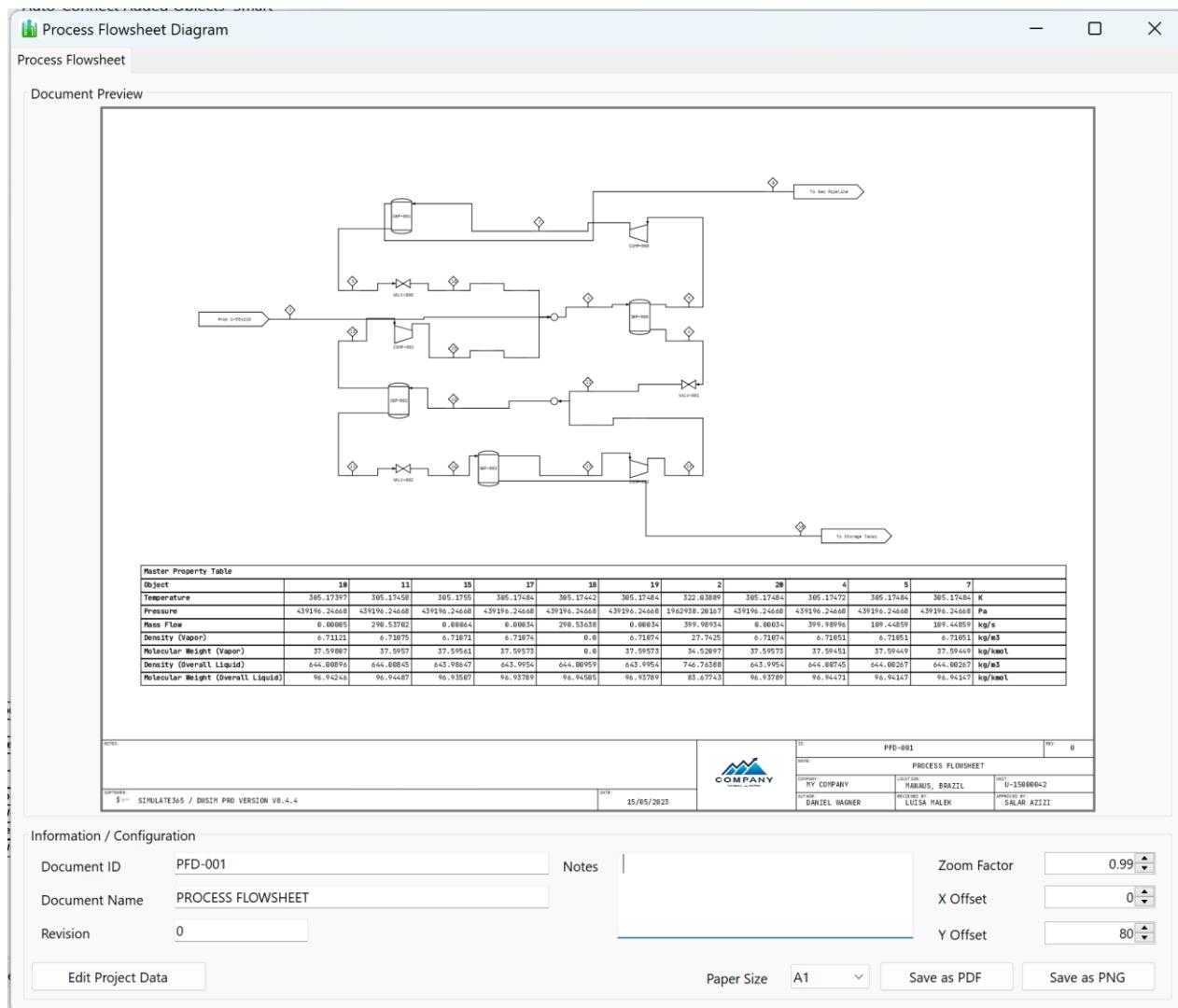


Figure 1 - Process Flowsheet Diagram tool

Use annotations in Material Streams to enter information that will be displayed in the inlet and outlet flags. Edit Project and Company information in the Simulation Settings panel:

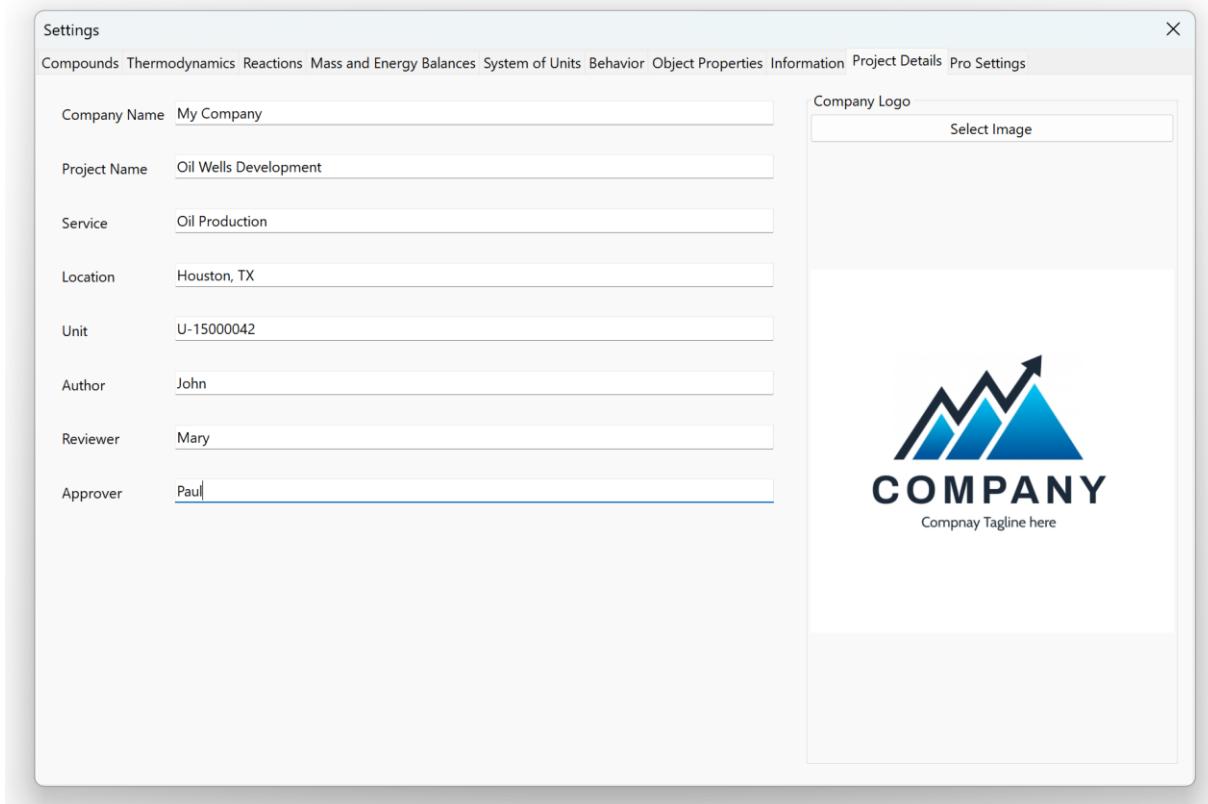


Figure 2 - Project Details panel

## 2.2. Process Datasheets

You can generate Process + Mechanical Datasheets for some selected Unit Operations through the new object editor, “Reports/Sheets” panel. The currently supported Unit Operations are:

- Heat Exchanger
- Air Cooler
- Pump
- Valve

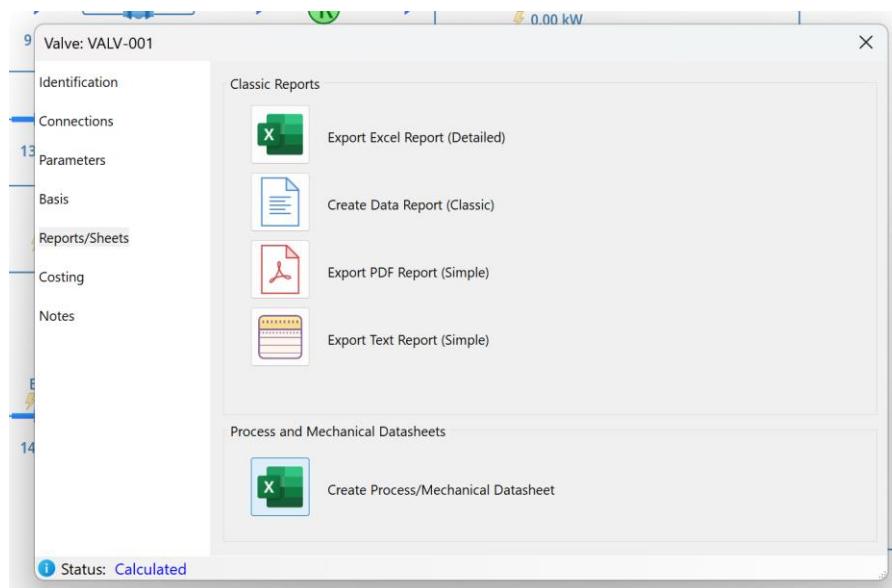


Figure 3 - Create Process/Mechanical Datasheet tool

The Datasheet is filled with process and project information. The Preview window allows you to edit or add more information before exporting the datasheet to a XLSX file or to a PDF file.

Preview Equipment Datasheet		
	A B C D E F G H I J K L M N O P Q R S T U V W X Y Z AA AB AC AD AE AF AG AH AI AJ AK AL AM AN AO AP AQ AR AS AT AU AV AW BI BJ BK BL BM BN BO BP BQ BR BS E	
1	Project Name Oil Wells Development	
2	Document No.	
3	Document Name	
4	P&ID No.	
5	Location/Unit Houston, TX / U-15000042	
6	Tag Number VALV-001	
7	Line Number	
8	Assoc. Equip./Service	
9	<b>SERVICE CONDITIONS</b>	
10	Fluid Name Phase(s) Flow Units 6 2-Ph m <sup>3</sup> /s	
11	Temp., Min. Operating Max. K 275 305 335	
12	Liq. SG @ 60 °F SG @ Op. T Vapor MW 0.66 0.65 37.60	
13	Critical Press., P <sub>c</sub> Op's Viscosity, $\mu$ 3E+06 Pa 0.00045 Pa.s	
14	Flow, Min. Norm. Max. Capacity 0.45	
15	Upstream Pressure @ Flow Pa 4.4E+05	
16	Downstream Pressure @ Flow Pa 4.4E+05	
17	Fluid Density at Inlet T&P, Flow kg/m <sup>3</sup> 643.95	
18	Valve Cv @ Flow (Calculated) 100.00	
19	Maximum Closed $\Delta P$ Fail Position Pa Closed	
20	<b>VALVE SELECTION, FLOW CHARACTERISTICS</b>	
21	Manufacturer Model	
22	Trim Characteristic Flow Direction Linear Under	
23	Bal./Unbal. Body Size Port Size Unbal. in. in.	
24	Trim Size Stroke 25% 50% 90% 100%	
25	Valve Percent Open	
26	Actual Cv @ % Open	
27	End Connections (Size, Rating, Facing) 2" 300# RF	
28	Bonnet Type Number of Ports Extended Two	
29	Lube & Isolating Valve (check) Lube	
30	Packing Type Packing Material Molded V-Ring Graphite Impreg.	
31	<b>MATERIALS</b>	
Fields were already filled with process data. Make the required changes and/or add more information, then click on 'Save to Dashboard'.		
Save as PDF Save as XLSX		

Figure 4 - Preview Datasheet window

## 2.3. Excel Reports

This tool (Results > Excel Reports) can generate reports for all objects on the flowsheet. You can customize the objects and properties to show and select a custom display order.

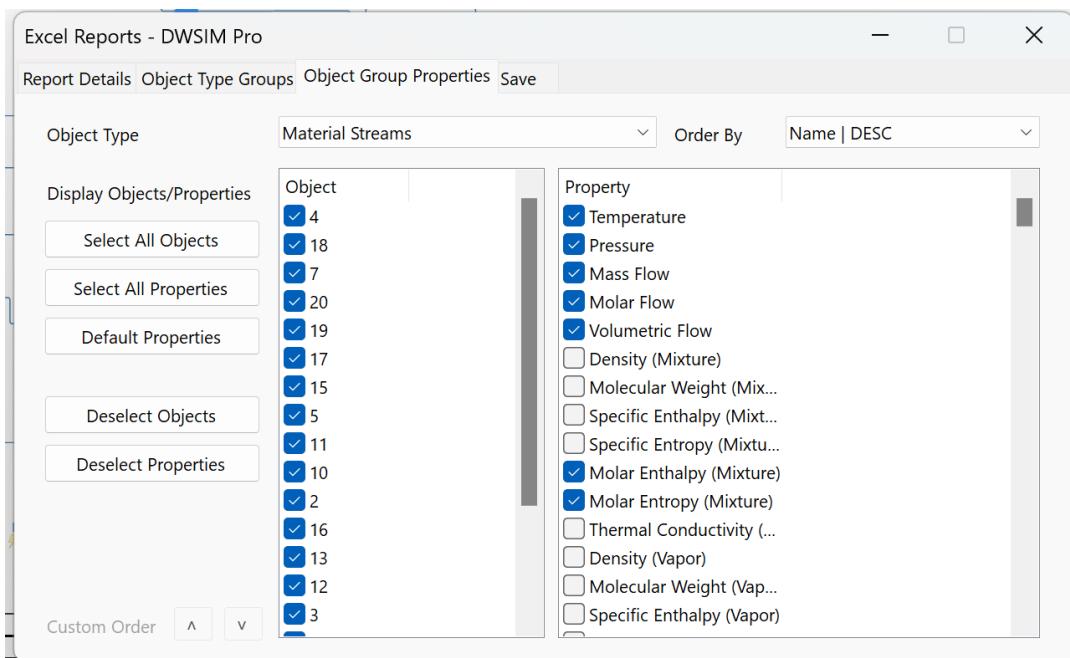


Figure 5 - Excel Reporting tool

The generated report can be saved to a spreadsheet that can be further customized to fulfill your needs. This feature can also be accessed through the Reports/Sheets tab in the new object editors, Export Excel Report (Detailed) item:

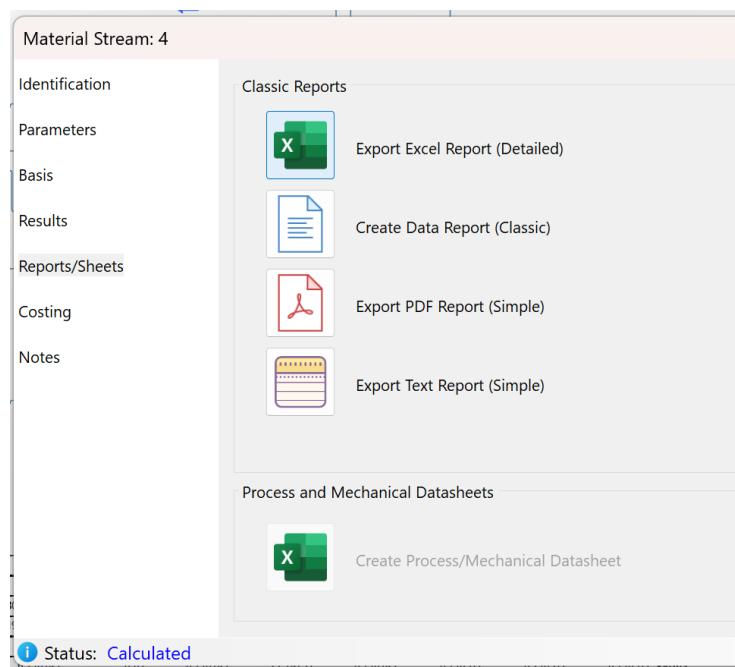


Figure 6 - Excel Reports in new object editors

### 3. FLOWSHEET FEATURES

#### 3.1. Capital Cost Estimator

##### 3.1.1. Introduction

This feature enables estimation of capital and operating costs for a Chemical Processing Plant based on data from the currently active flowsheet.

The costing subsystem includes the following features:

- Capital Cost Estimation
- Yearly Operating Cost Estimation
- Saving/Loading of Cost Reports
- Compare multiple Cost Reports
- Export results to DOC/ODT/XLS/ODS/PDF files
- Automatic mapping for selected equipments, product/raw streams and utilities
- Price correction based on CEPCI and IPC Cost Indexes
- Currency conversion
- User-defined Equipments, Materials and Utilities

##### 3.1.2. Usage Help

A new tab called “Costing” is visible in DWSIM Pro, which holds the Capital Cost Case Manager. The manager allows you to handle multiple cases for the same simulation. Each case is displayed in a different tab. When you create a new simulation, a default case called “MyReport” is already available for editing.

On the “Report Setup” tab, you will enter basic report information like name, description, reference date, cost index selection and currency details.

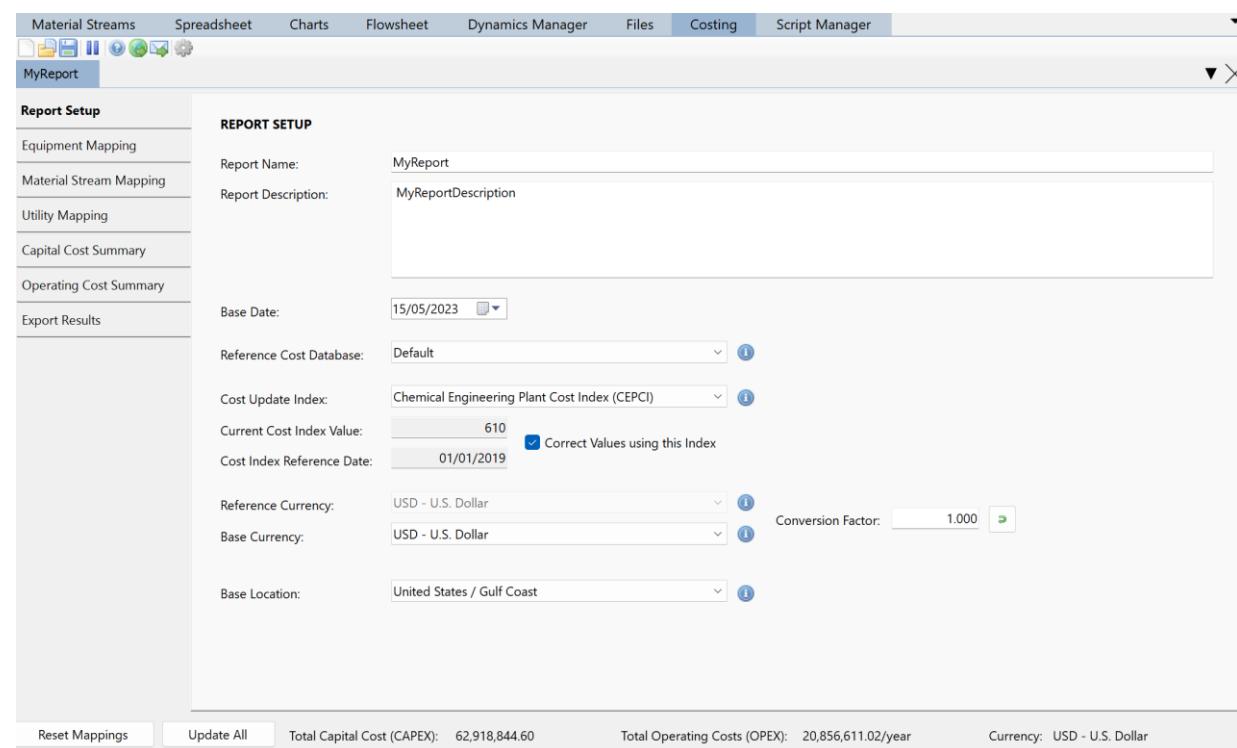


Figure 7 - Capital Cost Estimation Tool

### 3.1.2.1. Equipment Mapping

Some equipments are automatically mapped from Unit Operations, though you can modify the calculated values and change the selected equipments at any time. The correction factors are multiplied by the current prices to form the final total equipment cost.

You can enter equipment information either from the Costing/Equipment Mapping tab or directly through the Costing tab if the ‘New Object Editors’ feature is enabled.

Report Setup		EQUIPMENTS			
Equipment Mapping		Unit Operations from the Flowsheet are automatically mapped to default objects, but can be fully modified. To add a new equipment, start typing on the last row. To remove an exist			
Material Stream Mapping		More equipment prices available online: <a href="http://www.mhhe.com/engcs/chemical/peters/data/ce.html">http://www.mhhe.com/engcs/chemical/peters/data/ce.html</a>			
Equipment Name	Use	Equipment Type	Price, \$		
Gas-Liquid Separator - SEP-000	<input checked="" type="checkbox"/>	Separator / Vertical, cs shell	45,463.38		
Compressor - COMP-001	<input checked="" type="checkbox"/>	Compressor / Centrifugal	4,738,584.99		
Recycle Block - REC-001	<input type="checkbox"/>		0.00		
Stream Mixer - MIST-000	<input checked="" type="checkbox"/>	Mixer / Propeller	17,000.00		
Compressor - COMP-002	<input checked="" type="checkbox"/>	Compressor / Centrifugal	1,784,116.31		
Gas-Liquid Separator - SEP-002	<input checked="" type="checkbox"/>	Separator / Vertical, cs shell	44,896.70		
Valve - VALV-001	<input type="checkbox"/>		0.00		
Stream Mixer - MIST-001	<input checked="" type="checkbox"/>	Mixer / Propeller	17,000.00		
Compressor - COMP-000	<input checked="" type="checkbox"/>	Compressor / Centrifugal	5,881,077.13		
Valve - VALV-000	<input type="checkbox"/>		0.00		
Recycle Block - REC-000	<input type="checkbox"/>		0.00		
Gas-Liquid Separator - SEP-003	<input checked="" type="checkbox"/>	Separator / Vertical, cs shell	37,741.67		
Gas-Liquid Separator - SEP-001	<input checked="" type="checkbox"/>	Separator / Vertical, cs shell	11,600.00		
Valve - VALV-002	<input type="checkbox"/>		0.00		
Recycle Block - REC-002	<input type="checkbox"/>		0.00		
*	<input type="checkbox"/>				

Figure 8 - Equipment Mapping

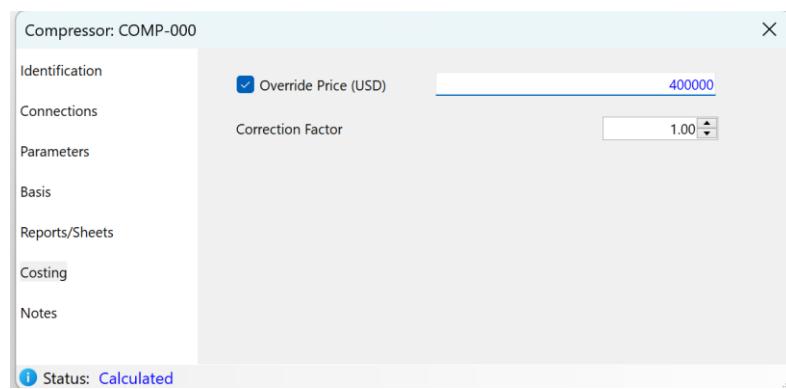


Figure 9 - Overriding an equipment price

### 3.1.2.2. Material Stream Mapping

Material Streams can be mapped to Raw Materials and/or Products, which will be used to calculate Yearly Operating Costs.

You can enter the costing information either from the Costing/Material Stream Mapping tab or directly through the Costing tab if the 'New Object Editors' feature is enabled.

RAW MATERIALS AND PRODUCTS					
To add a new material, start typing on the last row. To remove an existing material, click on the row header and press 'Del'.					
	Stream Name	Use	Type	Material	Price, \$
►	Material Stream - 4	<input type="checkbox"/>	Raw Material	Trichloroethane	13,96
	Material Stream - 18	<input type="checkbox"/>	Raw Material	Trichloroethane	9,02
	Material Stream - 7	<input type="checkbox"/>	Raw Material	Trichloroethane	3,22
	Material Stream - 20	<input type="checkbox"/>	Raw Material	Trichloroethane	45
	Material Stream - 19	<input type="checkbox"/>	Raw Material	Trichloroethane	45
	Material Stream - 17	<input type="checkbox"/>	Raw Material	Trichloroethane	45

Figure 10 - Material Stream mapping

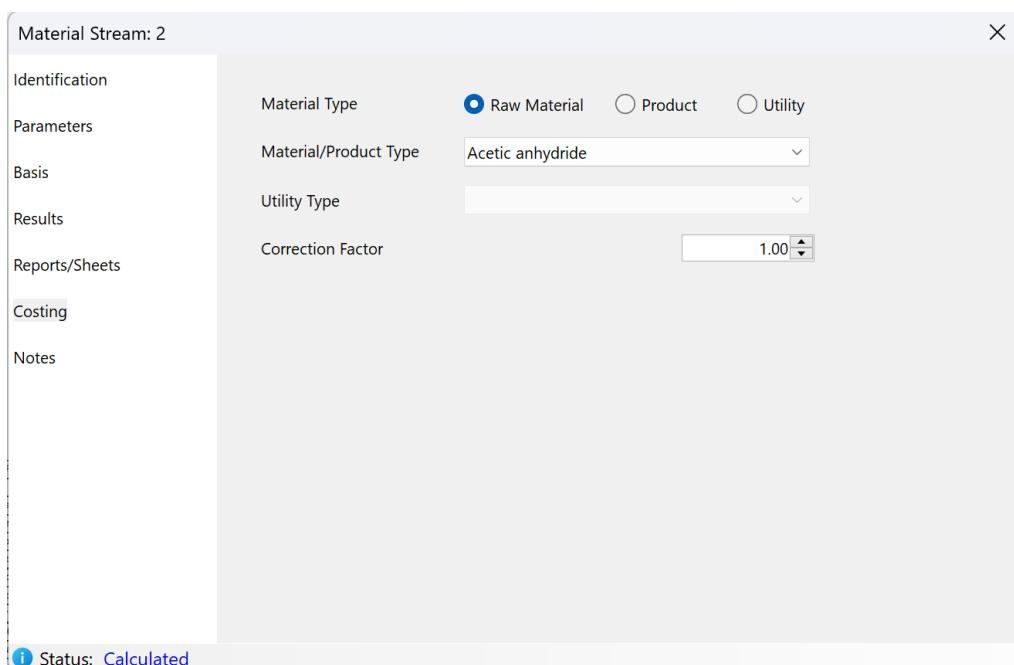
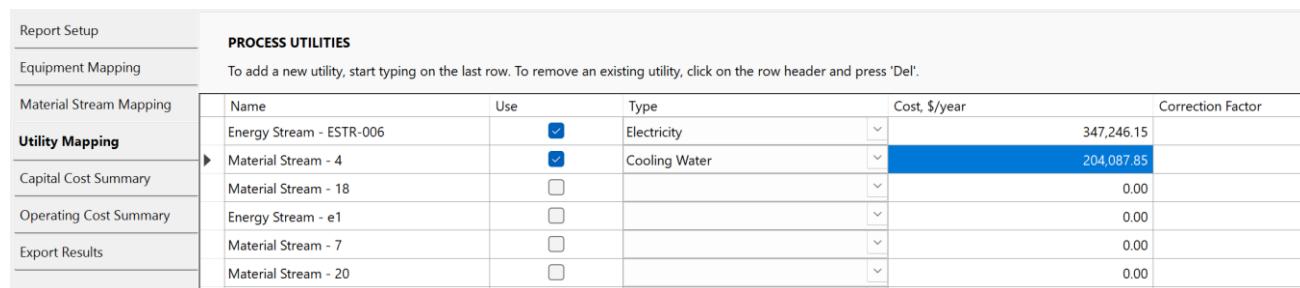


Figure 11 - Entering costing information for Material Streams

### 3.1.2.3. Utility Mapping

You can map Material and Energy Streams to some predefined Process Utilities, and the plugin will automatically calculate the cost based on the mass or energy flow, depending on the stream type.

You can enter the utility information either from the Costing/Utility Mapping tab or directly through the Costing tab if the ‘New Object Editors’ feature is enabled.



PROCESS UTILITIES					
To add a new utility, start typing on the last row. To remove an existing utility, click on the row header and press 'Del'.					
	Name	Use	Type	Cost, \$/year	Correction Factor
Material Stream Mapping	Energy Stream - ESTR-006	<input checked="" type="checkbox"/>	Electricity	347,246.15	
<b>Utility Mapping</b>	Material Stream - 4	<input checked="" type="checkbox"/>	Cooling Water	204,087.85	
Capital Cost Summary	Material Stream - 18	<input type="checkbox"/>		0.00	
Operating Cost Summary	Energy Stream - e1	<input type="checkbox"/>		0.00	
Export Results	Material Stream - 7	<input type="checkbox"/>		0.00	
	Material Stream - 20	<input type="checkbox"/>		0.00	

Figure 12 - Utility Mapping

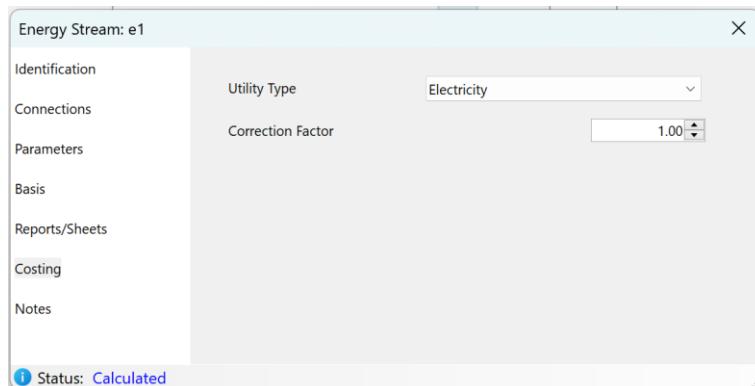


Figure 13 - Entering Costing information for Utility Streams

### 3.1.2.4. Capital Cost Summary

Here you'll see a summary of the items that make up the Total Capital Cost. You can change the calculation basis (Percentage or Absolute value) for most items, except for those who are calculated based on the previously mapped items.

Report Setup	<b>CAPITAL COST ESTIMATION</b>		
Equipment Mapping	<b>Direct Costs</b>		
Material Stream Mapping	Equipment (Total Purchased Cost) <span style="color: blue;">i</span>		
Utility Mapping	Update <span style="float: right;">43,392,306.62</span>		
<b>Capital Cost Summary</b>	Equipment Erection <span style="color: blue;">i</span>		
Operating Cost Summary	Update <span style="float: right;">12,577,480.18</span>		
Export Results	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">45.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">70.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">20.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">10.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">15.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">50.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">15.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">5.00</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">15.00</span>		
	<b>Indirect Costs</b>		
	Design and Engineering <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">30.00</span>		
	Contractor's Fee <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">5.00</span>		
	Contingency <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">10.00</span>		
Reset Mappings	Update All	Total Capital Cost (CAPEX):	62,918,844.60
		Total Operating Costs (OPEX):	20,856,611.02/year
		Currency:	USD - U.S. Dollar

Figure 14 - Capital Cost Summary

### 3.1.2.5. Yearly Operating Cost Summary

Here you'll see a summary of the items that make up the Total Yearly Operating Cost. You can change the calculation basis (Percentage or Absolute value) for most items, except for those who are calculated based on the previously mapped items.

Report Setup	<b>ANNUAL OPERATING COST ESTIMATION</b>		
Equipment Mapping	<b>Fixed Costs</b>		
Material Stream Mapping	Maintenance <span style="color: blue;">i</span>		
Utility Mapping	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">10.00</span>		
<b>Capital Cost Summary</b>	Operation <span style="color: blue;">i</span>		
Operating Cost Summary	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">15.00</span>		
Export Results	Laboratory <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">3.00</span>		
	Supervision <span style="color: blue;">i</span>		
	<input type="radio"/> Percentage <input checked="" type="radio"/> Absolute <span style="float: right;">50,000.00</span>		
	Plant Overheads <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">50.00</span>		
	Capital Charges <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">10.00</span>		
	Rates / Taxes <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">2.00</span>		
	Insurance <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">1.00</span>		
	Licensing Fees / Royalty Payments <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">1.00</span>		
	<b>Variable Costs</b>		
	Raw Materials <span style="color: blue;">i</span>		
	Update <span style="float: right;">0.00</span>		
	Other Materials <span style="color: blue;">i</span>		
	<input checked="" type="radio"/> Percentage <input type="radio"/> Absolute <span style="float: right;">10.00</span>		
	Utilities <span style="color: blue;">i</span>		
	Update <span style="float: right;">0.00</span>		
	Shipping and Packaging <span style="color: blue;">i</span>		
Reset Mappings	Update All	Total Capital Cost (CAPEX):	62,918,844.60
		Total Operating Costs (OPEX):	20,856,611.02/year
		Currency:	USD - U.S. Dollar

Figure 15 - Operating Cost Summary

### 3.1.2.6. Export Results

You can export the calculated results to a document file (DOC, ODT, PDF) or a spreadsheet file (XLS, ODS).

### 3.1.3. Cost Estimation Basis

Most of the calculation methods on this tool are based on the Factorial Method described on the Chemical Engineering Design book by R. K. Sinott, which you should refer to for more information. (Towler, et al.)

#### 3.1.3.1. Introduction

Cost estimation is a specialised subject and a profession in its own right. The design engineer, however, needs to be able to make quick, rough, cost estimates to decide between alternative designs and for project evaluation. Chemical plants are built to make a profit, and an estimate of the investment required, and the cost of production are needed before the profitability of a project can be assessed.

#### 3.1.3.2. Accuracy and Purpose of Capital Cost Estimates

The accuracy of an estimate depends on the amount of design detail available: the accuracy of the cost data available; and the time spent on preparing the estimate. In the early stages of a project only an approximate estimate will be required, and justified, by the amount of information by then developed.

Capital cost estimates can be broadly classified into three types according to their accuracy and purpose:

- Preliminary (approximate) estimates, accuracy typically 30 per cent, which are used in initial feasibility studies and to make coarse choices between design alternatives. They are based on limited cost data and design detail.
- Authorization (Budgeting) estimates, accuracy typically 10-15 per cent. These are used for the authorization of funds to proceed with the design to the point where an accurate and more detailed estimate can be made. Authorization may also include funds to cover cancellation charges on any long delivery equipment ordered at this stage of the design to avoid delay in the project. In a contracting organization this type of estimate could be used with a large contingency factor to obtain a price for tendering. Normally, however, an accuracy of about 5 per cent would be needed and a more detailed estimate would be made, if time permitted. With experience, and where a company has cost data available from similar projects, estimates of acceptable accuracy can be made at the flow-sheet stage of the project. A rough P&I diagram and the approximate sizes of the major items of equipment would also be needed.
- Detailed (Quotation) estimates, accuracy 5-10 per cent, which are used for project cost control and estimates for fixed price contracts. These are based on the completed (or near complete) process design, firm quotations for equipment, and a detailed breakdown and estimation of the construction cost.

The cost of preparing an estimate increases from about 0.1 per cent of the total project cost for 30 per cent accuracy, to about 2 per cent for a detailed estimate with an accuracy of 5 per cent.

### **3.1.3.3. Cost Escalation (Inflation)**

The cost of materials and labor has been subject to inflation since Elizabethan times. All cost-estimating methods use historical data, and are themselves forecasts of future costs. Some method has to be used to update old cost data for use in estimating at the design stage, and to forecast the future construction cost of the plant.

The method usually used to update historical cost data makes use of published cost indices. These relate present costs to past costs, and are based on data for labor, material and energy costs published in government statistical digests.

Chemical plant cost indexes are dimensionless numbers employed to updating capital cost required to erect a chemical plant from a past date to a later time, following changes in the value of money due to inflation and deflation. Since, at any given time, the number of chemical plants is insufficient to use in a preliminary or predesign estimate, cost indexes are handy for a series of management purposes, like long-range planning, budgeting and escalating or de-escalating contract costs. (Estimating Plant Construction Costs, 1997)

A cost index is the ratio of the actual price in a time period compared to that in a selected base period (a defined point in time or the average price in a certain year), multiplied by 100. Raw materials, products and energy prices, labor and construction costs change at different rates, and plant construction cost indexes are actually a composite, able to compare generic chemical plants capital costs.

### **3.1.3.4. Calculation methods**

Although the available indexes are compiled in several ways, they are defined to encompass a specific set of conditions and items. Prices for these items can be obtained either through company's purchasing department data or through published indexes, like those published by the Bureau of Labor Statistics (BLS) (Humphreys, 2005). Both the CE and the IC indexes, from Chemical Engineering and Intratec, respectively, employs BLS' data.

The weighting of such factors, which is defined by the realized degree of importance of each component in the specific index (or sub-index), aims to represent the costs variations typically found for chemical plants.

### **3.1.3.5. Using a cost index**

To update an item cost (equipment, projects) from period A to period B, is necessary to multiply period A's cost by the ratio of period B's index over period A's index, according to the following equation:

$$\text{Cost at } B = \text{Cost at } A \frac{\text{index at } B}{\text{index at } A}$$

As a rule-of-thumb, cost indexes permit fairly accurate estimates for cost escalation if the difference between period A and period B is less than 10 years. Differences between the actual equipment and labor prices and those predicted by the index tend to grow over the years, surpassing the typical error verified in budget-level estimates (Peters, et al., 2004) (Updating the CE Plant Cost Index, 2002).

### 3.1.3.6. Cost Indexes in Engineering

The selection of the proper index to use depends on the industry in which it is applied. For example, while CE, M&S or IC Index are typically employed for chemical process industries, the ENR (Engineering News-Record) construction index is used for general industrial construction and takes in account the prices for fixed amounts of structural steel, cement, lumber and labor.

The majority of cost indexes demonstrate a time lag, due to data collection and its compilation for publishing. As stated before, some indexes use information published by other organizations and a delay in data may be verified (like those provided by the BLS). Exceptions to this are the ENR construction and the IC indexes, which present relatively current values.

The main indexes available for process industries include:

- Chemical Engineering Index, CEPCL: composed of 4 major components – equipment, construction labor, buildings, and engineering and supervision – the index is employed primarily as a process plant construction index, was established using a base period of 1957-1959 as 100. The CE Index is updated monthly and it lags in time by about 3 months. The CE Index was revised in 1982, to account for changes in labor productivity and, again, in 2002. (Couper, 2003) Published in each issue of Chemical Engineering (Albright, 2008) (Access Intelligence, 2023).
- Marshall and Swift Cost Index, M&S (originally known as Marshall and Stevens Index): a composite of two major components - process-industry equipment average and all-industry equipment average - was established in 1926 with a value of 100. Some industries considered in the process-industry equipment average are chemicals, petroleum products, rubber and paper. The all-industry average encompasses 47 different types of industrial, commercial and housing equipment. Published monthly in each issue of Chemical Engineering until April 2012.
- Intratec Chemical Plant Construction Index, IPC: a process plant construction index developed by Intratec, a chemical consulting company. Although cost indexes do not usually forecast future escalation, the IC Index stands out for presenting a smaller delay between release date and index date, besides a 12 months forecast. On the other hand, the index is only available from January 2000 (with a value of 100). A sample is available at Intratec's website (Intratec, 2023).
- Nelson-Farrar Indexes, NF (originally known as the Nelson Refinery Construction Indexes): established in 1946 with a value of 100, the index is more suitable for petroleum or petrochemical business. Published once a month in the Oil and Gas Journal.

#### 3.1.3.6.1. Location Factor

In order to be able to use the available standard indexes to locations where index data is not available, we have to incorporate a new term called the Location Factor (LF) to the standard index value. It is a dimensionless value for a particular location relative to either of the above-mentioned basis:

$$\text{Cost in } A = \text{Cost in USGC} \cdot LF(A)$$

where  $A$  is the location for which cost is being evaluated and  $LF(A)$  is the location factor for the location  $A$  relative to USGC.

Location factors are greatly influenced by currency exchange rates due to their significant effect on Index value and hence vary drastically with time. Over the past couple of decades the location factors for various locations are trending close to the value 1. However location factor for a particular region within a country can be easily determined by adding 10% to the index of the reference location for every 1000 miles. The reference location is usually a major industrial location closest to the location where the index is being determined. Location factors for various locations have been published and updated in various journals as in Aspen Richardson's "International Construction Cost Factor Location Manual (2003)".

### 3.1.3.7. The Factorial Method for Capital Cost Estimation

Capital cost estimates for chemical process plants are often based on an estimate of the purchase cost of the major equipment items required for the process, the other costs being estimated as factors of the equipment cost. The accuracy of this type of estimate will depend on what stage the design has reached at the time the estimate is made, and on the reliability of the data available on equipment costs. In the later stages of the project design, when detailed equipment specifications are available and firm quotations have been obtained, an accurate estimation of the capital cost of the project can be made.

### 3.1.3.8. Lang factors

The factorial method of cost estimation is often attributed to Lang (1948). The fixed capital cost of the project is given as a function of the total purchase equipment cost by the equation:

$$Cf_D = f_L \cdot C_e$$

where  $Cf_D$  is fixed capital cost,  $C_e$  is the total delivered cost of all the major equipment items: storage tanks, reaction vessels, columns, heat exchangers, etc. and  $f_L$  is the Lang factor, which depends on the type of process.

The values given above should be used as a guide; the factor is best derived from an organization's own cost files. The above equation can be used to make a quick estimate of capital cost in the early stages of project design, when the preliminary flowsheets have been drawn up and the main items of equipment roughly sized.

### 3.1.3.9. Detailed factorial estimates

#### 3.1.3.9.1. Direct costs

To make a more accurate estimate, the cost factors that are compounded into the “Lang factor” are considered individually. The direct-cost items that are incurred in the construction of a plant, in addition to the cost of equipment are:

- Equipment erection, including foundations and minor structural work.
- Piping, including insulation and painting.
- Electrical, power and lighting.
- Instruments, local and control room.
- Process buildings and structures.
- Ancillary buildings, offices, laboratory buildings, workshops.
- Storages, raw materials and finished product.
- Utilities (Services), provision of plant for steam, water, air, firefighting services (if not costed separately).
- Site, and site preparation.

The contribution of each of these items to the total capital cost is calculated by multiplying the total purchased equipment by an appropriate factor. As with the basic “Lang factor”, these factors are best derived from historical cost data for similar processes. Typical values for the factors are given in several references, Happle and Jordan (1975) and Garrett (1989). Guthrie (1974), splits the costs into the material and labour portions and gives separate factors for each. In a booklet published by the Institution of Chemical Engineers, IChemE (1988), the factors are shown as a function of plant size and complexity.

The accuracy and reliability of an estimate can be improved by dividing the process into sub-units and using factors that depend on the function of the sub-units; see Guthrie (1969). In Guthrie’s detailed method of cost estimation the installation, piping and instrumentation costs for each piece of equipment are costed separately. Detailed costing is only justified if the cost data available are reliable and the design has been taken to the point where all the cost items can be identified and included.

In addition to the direct cost of the purchase and installation of equipment, the capital cost of a project will include the indirect costs listed below. These can be estimated as a function of the direct costs.

#### 3.1.3.9.2. Indirect costs

Design and engineering costs, which cover the cost of design and the cost of “engineering” the plant: purchasing, procurement and construction supervision. Typically 20 per cent to 30 per cent of the direct capital costs. Contractor’s fees, if a contractor is employed his fees (profit) would be added to the total capital cost and would range from 5 per cent to 10 per cent of the direct costs. Contingency allowance, this is an allowance built into the capital cost estimate to cover for unforeseen circumstances (labor disputes, design errors, adverse weather). Typically 5 per cent to 10 per cent of the direct costs.

### 3.1.3.10. Operating Costs

An estimate of the operating costs, the cost of producing the product, is needed to judge the viability of a project, and to make choices between possible alternative processing schemes. These costs can be estimated from the flow-sheet, which gives the raw material and service requirements, and the capital cost estimate.

The cost of producing a chemical product will include the items listed below. They are divided into two groups.

- Fixed operating costs: costs that do not vary with production rate. These are the bills that have to be paid whatever the quantity produced.
- Variable operating costs: costs that are dependent on the amount of product produced.

#### **3.1.3.10.1. Fixed costs**

- Maintenance (labor and materials).
- Operating labor.
- Laboratory costs.
- Supervision.
- Plant overheads.
- Capital charges.
- Rates (and any other local taxes).
- Insurance.
- License fees and royalty payments.

#### **3.1.3.10.2. Variable costs**

- Raw materials.
- Miscellaneous operating materials.
- Utilities (Services).
- Shipping and packaging.

The division into fixed and variable costs is somewhat arbitrary. Certain items can be classified without question, but the classification of other items will depend on the accounting practice of the particular organization.

The items may also be classified differently in cost sheets and cost standards prepared to monitor the performance of the operating plant. For this purpose the fixed-cost items should be those over which the plant supervision has no control, and the variable items those for which they can be held accountable.

The costs listed above are the direct costs of producing the product at the plant site. In addition to these costs the site will have to carry its share of the Company's general operating expenses. These will include:

- General overheads.

- Research and development costs.
- Sales expenses.
- Reserves.
- How these costs are apportioned will depend on the Company's accounting methods. They would add about 20 to 30 per cent to direct production costs at the site.

### 3.2. Greenhouse Gas (GHG) Emissions Estimation

#### 3.2.1. Introduction

This feature enables estimation of greenhouse gas emissions from equipments and streams in the process being modeled so you can analyze and optimize it based on the total emissions of the plant.

#### 3.2.2. GHG Emissions workflow

- **Emissions compositions:**

In Flowsheet Analysis > GHG Compositions Editor, you can enter various GHG compositions that can be later associated with objects in the flowsheet:

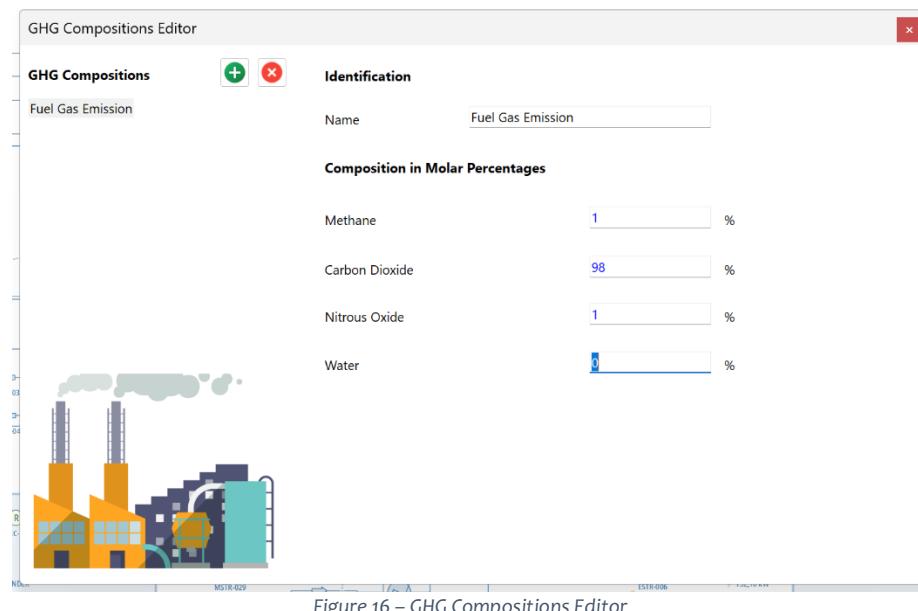


Figure 16 – GHG Compositions Editor

- **Setup GHG Emissions for Flowsheet Objects:**

Right-click on an object and select GHG Emissions Editor in the context menu. It will open a window where you can edit the emission details for the selected object, including the associated composition, emission factor and other parameters.

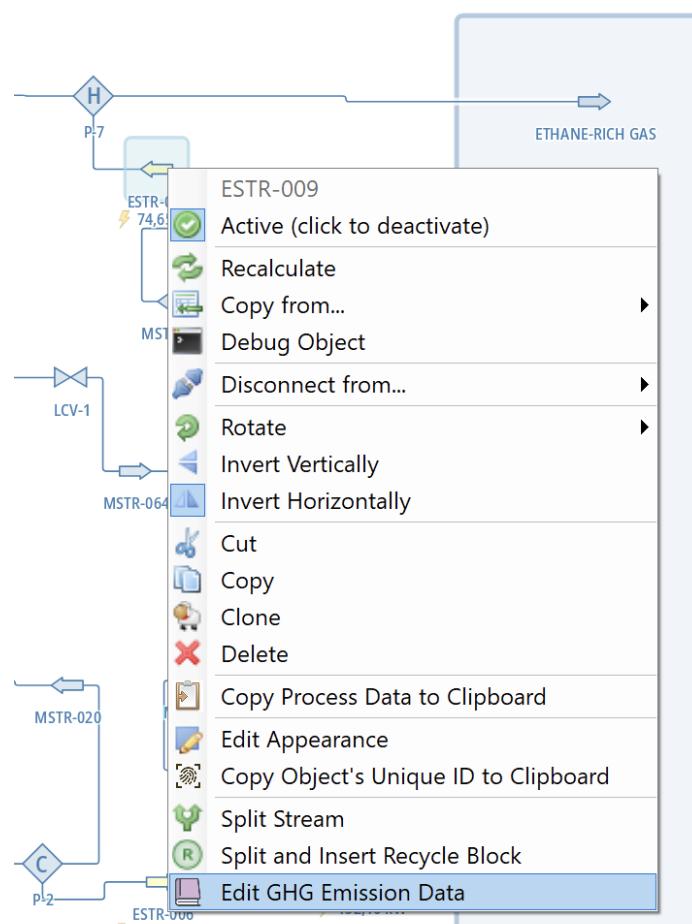


Figure 17 – Edit GHG Emission Data menu item

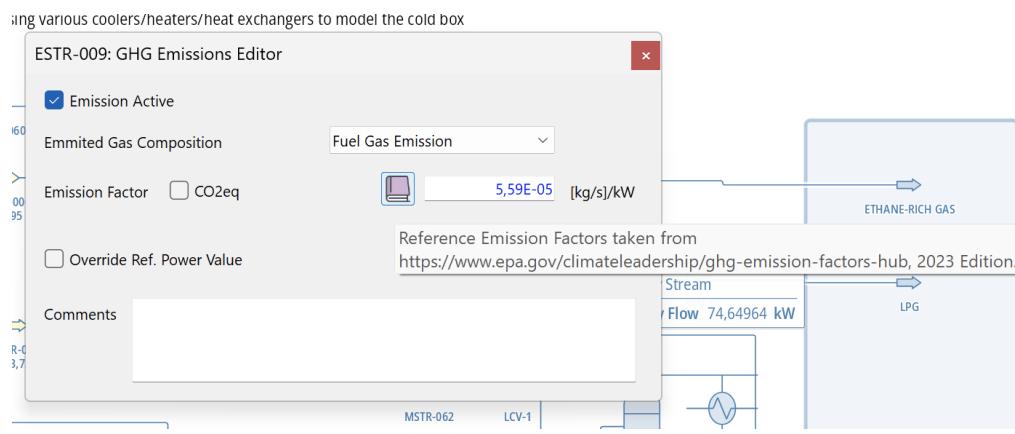


Figure 18 – Edit GHG Emission Data window

### - Viewing Total GHG Emissions from the Flowsheet:

In the GHG Emissions tab, you can visualize the emissions for all emission-enabled objects and the overall emissions from the flowsheet.

Material Streams	Charts	Dynamics Manager	Files	Spreadsheet	Flowsheet	Script Manager	GHG Emissions	
Greenhouse Gas Emissions Summary								
Update								
Object	Type	Reference Power/Heat	Emission Factor	Mass GHG Emissions	Mass GHG Emissions (CO2eq)	Molar GHG Emissions	Molar GHG Emissions (CO2eq)	Comments
ESTR-009	Energy Stream	74,64964	0,00006	15,02233	57,38529	198,32206	757,59028	

Figure 19 – GHG Emission panel

Overall emissions from the flowsheet can be later used in Optimization and Sensitivity studies:

Material Streams   Charts   Dynamics Manager   Files   Spreadsheet   Flowsheet   Script Manager

Case Manager

New SACase0

Copy

Save

Delete

Name and Description (Selected Case)

Name SACase0

Description

Independent Variables   Dependent Variables   Results   Chart

Variables    Expression

Add/Remove Variables   Expression Parameters

	Object	Property	Unit
▶	Flowsheet Result	Total GHG Mass Emissions	kg/s

Name	Obj

Figure 20 – Selecting Total GHG Emissions property

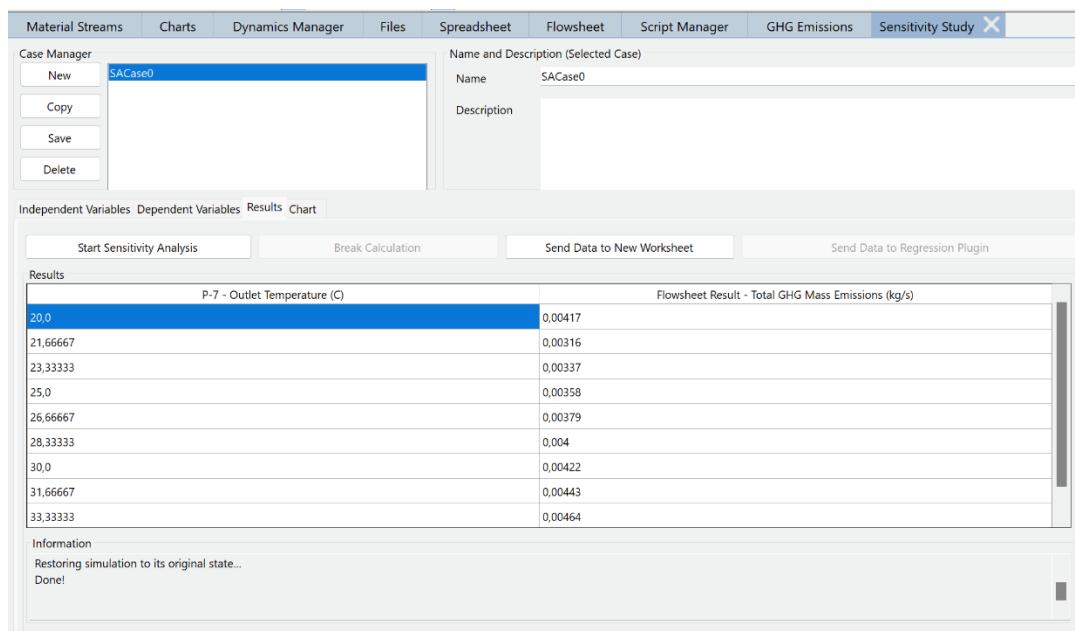


Figure 21 – Analyzing Total GHG Emissions

### 3.3. New Object Editors

DWSIM Pro contains a new set of object editors, activated by default on new and existing simulations. These editors can be accessed with a double mouse-click over the object and replace the previous sidebar editors from the open-source version of DWSIM.

The new editors add new panels so you can include the new features and tools from DWSIM Pro in your workflow, which are: Costing and Reports/Sheets.

Status: Calculated

Figure 22 - New Object Editor for Material Streams

To disable or enable the new editors, go to the Simulation Settings Panel > Pro Features tab:

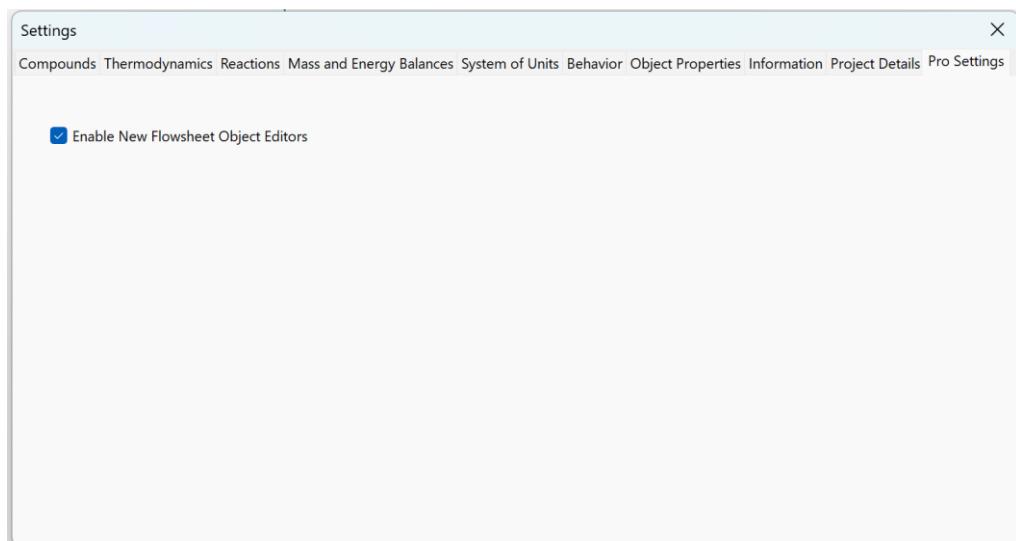


Figure 23 - Enable/Disable New Object Editors

### 3.4. Bidirectional Solver

#### 3.4.1. Introduction

The Bidirectional Solver allows you to define/calculate unit operation blocks with indirect specifications, that is, information travelling backwards. Material flow information is propagated forwards and backwards across the flowsheet according to your inputs.

The Bidirectional Solver includes an all-new object editor style which is compatible with the industry standards.

In the screenshot below, the Heater block is calculated using flow information defined in stream 2 and temperature defined in stream 6. The pressure drop in VALVE-1 is calculated using the pressure informed by the user for stream 4.

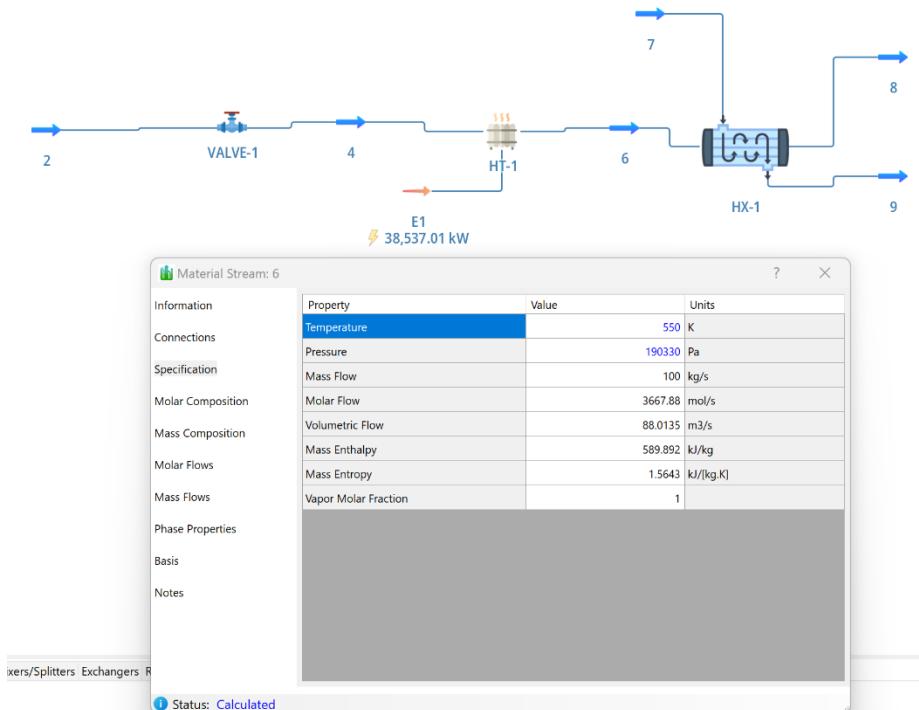


Figure 24 - Bidirectional Solver in action

### 3.4.2. General Usage Guidelines

After enabling the Bidirectional Solver, double-click on an object to open its property editor.

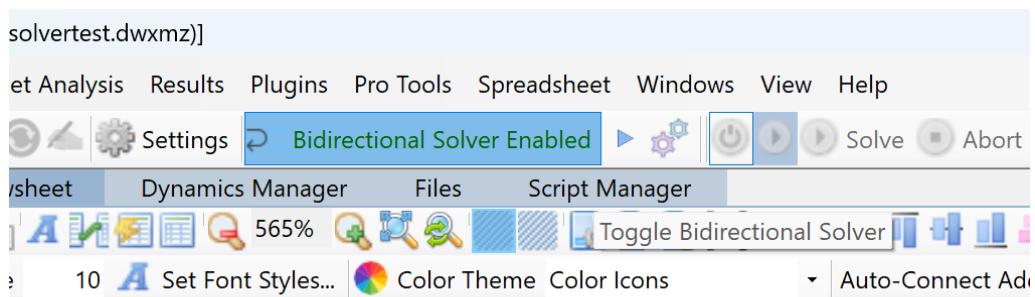


Figure 25 - Bidirectional Solver toolbar

The bidirectional Solver runs every time you change a property from an object. The objects are calculated according to the available information "travelling" back and forth across the flowsheet. You can also force a solver run by pressing the corresponding button in the toolbar.

When defining material streams, give preference to inputting molar fractions, temperature, pressure and overall mass flow. Leave one of the molar fractions blank and the solver will calculate it automatically, otherwise the stream will not be calculated due to overspecification.

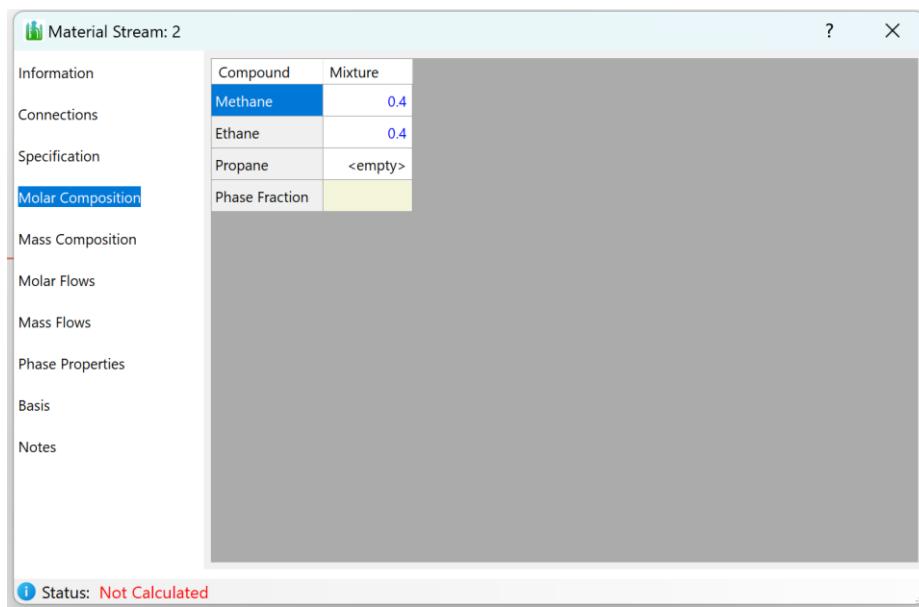


Figure 26 - Entering molar fractions for a Material Stream when the Bidirectional Solver is enabled

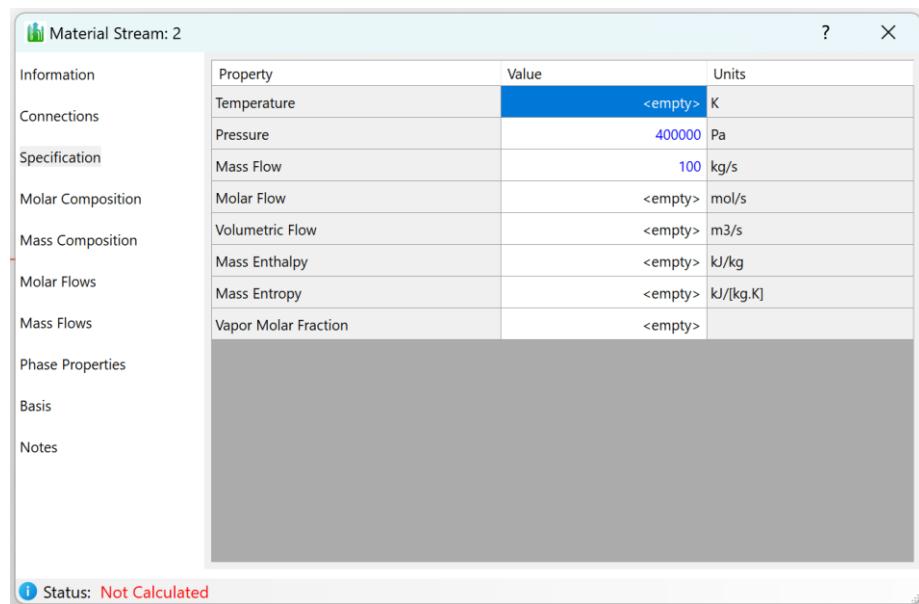


Figure 27 - Entering Stream properties when the Bidirectional Solver is enabled

If the stream has enough information, it will be automatically calculated, and you'll be able to see its properties.

Material Stream: 2		
	Property	Value
Information	Temperature	400 K
Connections	Pressure	400000 Pa
Specification	Mass Flow	100 kg/s
Molar Composition	Molar Flow	3667.88 mol/s
Mass Composition	Volumetric Flow	30.1889 m3/s
Molar Flows	Mass Enthalpy	204.522 kJ/kg
Mass Flows	Mass Entropy	0.525346 kJ/(kg.K)
Phase Properties	Vapor Molar Fraction	1
Basis		
Notes		

>Status: Calculated

Figure 28 - Calculated Material Stream

Supported Unit Operations can be solved by entering indirect specifications, that is, defining properties on outlet streams. For instance, you can calculate a Heater by defining the temperature of its outlet stream.

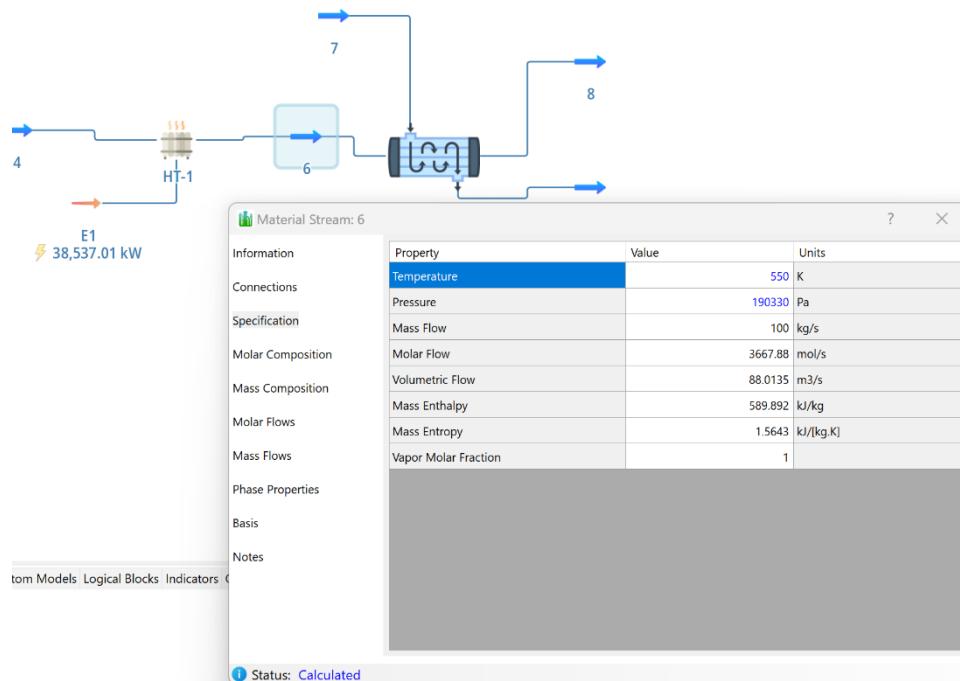


Figure 29 - Bidirectional Solver editor for supported objects

Unsupported Unit Operations will always be calculated using information collected from their inlet streams and own parameters. The editor window will let you know if the selected object is supported or not.

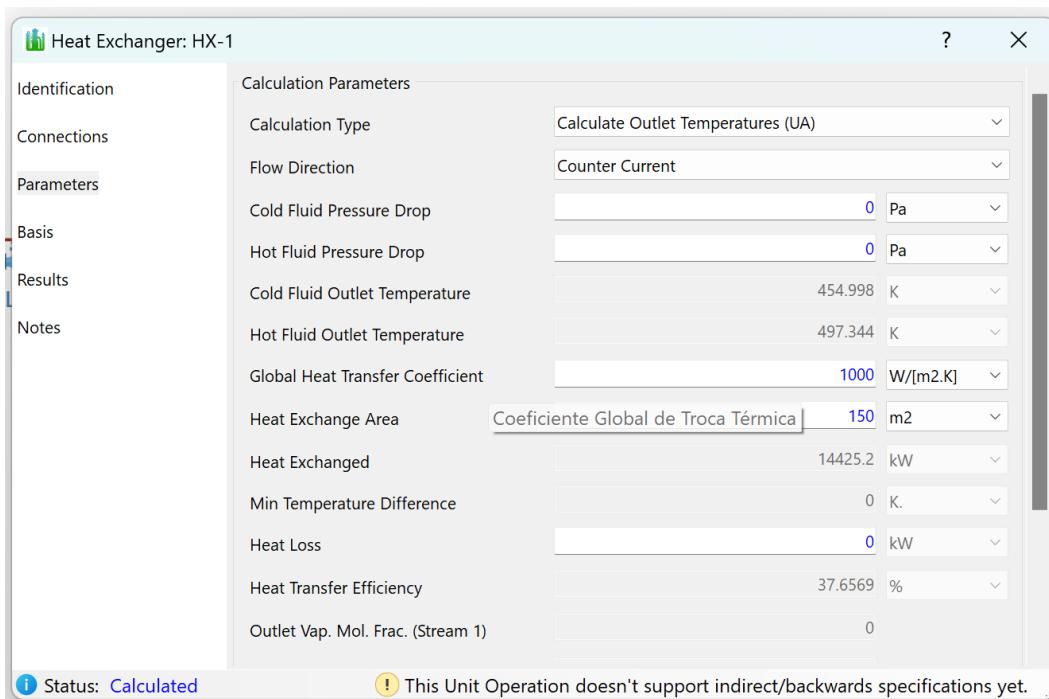


Figure 30 - Bidirectional Solver editor for unsupported objects

### 3.4.3. Supported Objects

- Material Stream
- Energy Stream
- Valve
- Pump
- Compressor
- Expander
- Heater
- Cooler
- Gas-Liquid Separator
- Mixer
- Splitter

### 3.4.4. Limitations

- For Material Streams, only Molar/Mass Fractions + Temperature + Pressure + Mass/Molar Flow definitions are supported.
- Not all calculation modes are supported by the Bidirectional Solver for the currently supported Unit Operations. If you want to use these modes, disable the Bidirectional Solver and proceed with the specifications using the regular editors + flowsheet solver.
- Logical blocks were not tested (Recycle, Controller/Adjust, Specification).

- The Bidirectional Solver behavior when working with flowsheets containing unsupported Unit Operations is unpredictable. If you find any problems, please disable the Bidirectional Solver and proceed with the specifications using the regular editors + flowsheet solver.

### 3.4.5. Solver Configuration

In the Solver Configuration window, you can clear all specified variables at once, define the indirect specification solver parameters and request/suggest a new feature to be added in the next releases.

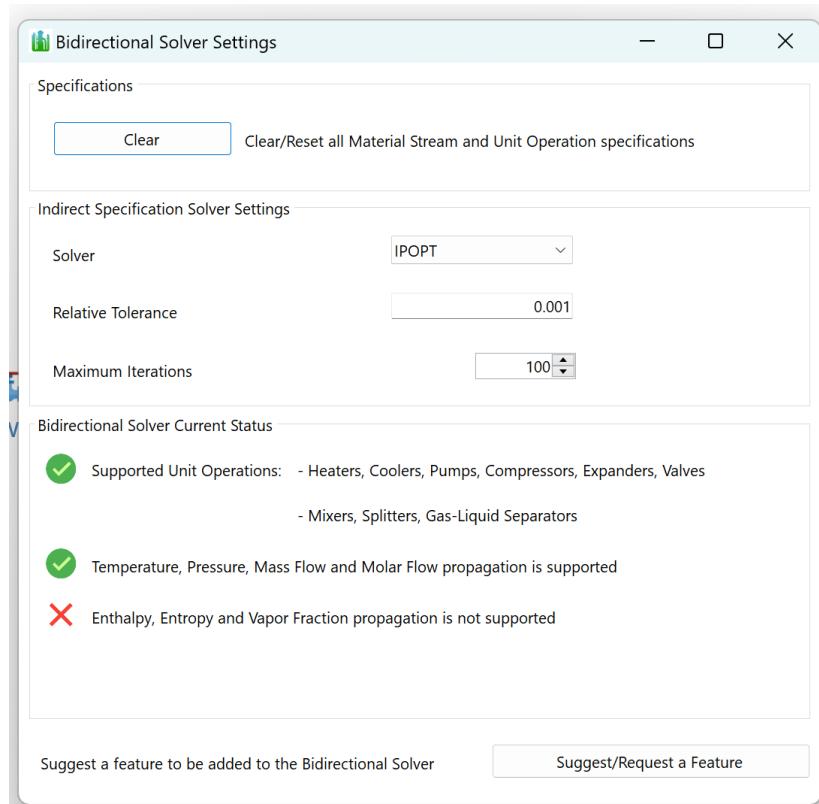


Figure 31 - Bidirectional Solver configuration window

### 3.5. Single Object Calculation Mode

This feature allows you to perform calculations in a unit operation as if it was the only block added to the flowsheet, that is, you can edit its inlet material streams to perform sensitivity analyses even if they are connected to another unit operation. Except for the unit operation itself and its connected streams, all the other objects will be disabled and will not be calculated/updated. To enable this feature, select a unit operation and click on 'Single Object Calculation Mode' toolbar item:

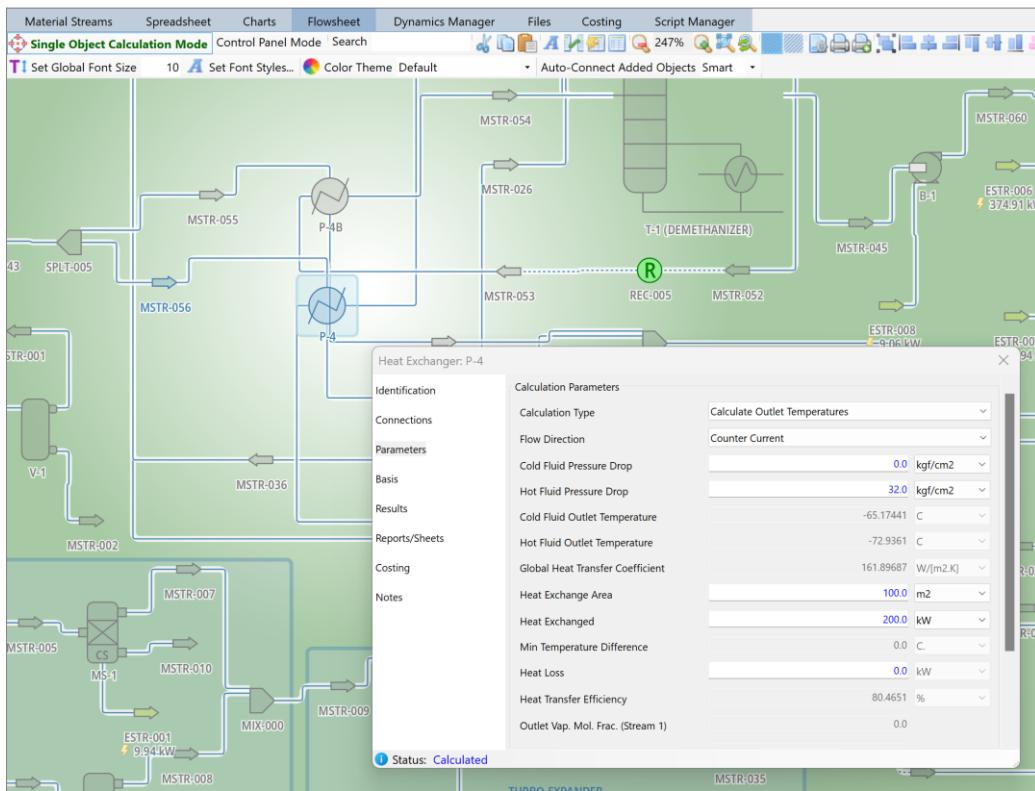


Figure 32 - Single Object Calculation Mode

### 3.6. Heatmaps

Add a Heatmap Layer to the flowsheet to have a visual representation of how Temperature, Pressure, Flow and Compound Concentration changes across the process model.

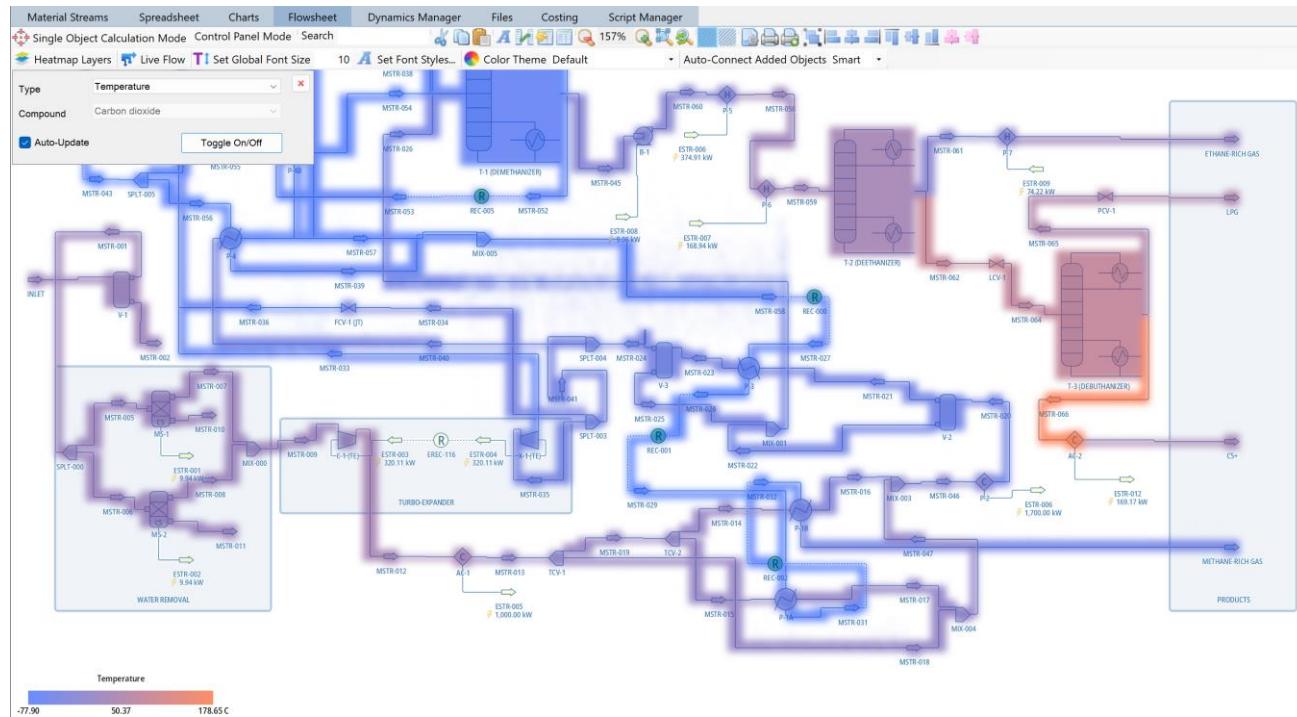


Figure 33 - Flowsheet Heatmaps

### 3.7. Live Flows

The Live Flows feature adds animated arrows to the Material Stream connection lines to enhance the visualization of the material and energy flowing across the flowsheet. The bigger the arrows, the higher the flow rate.

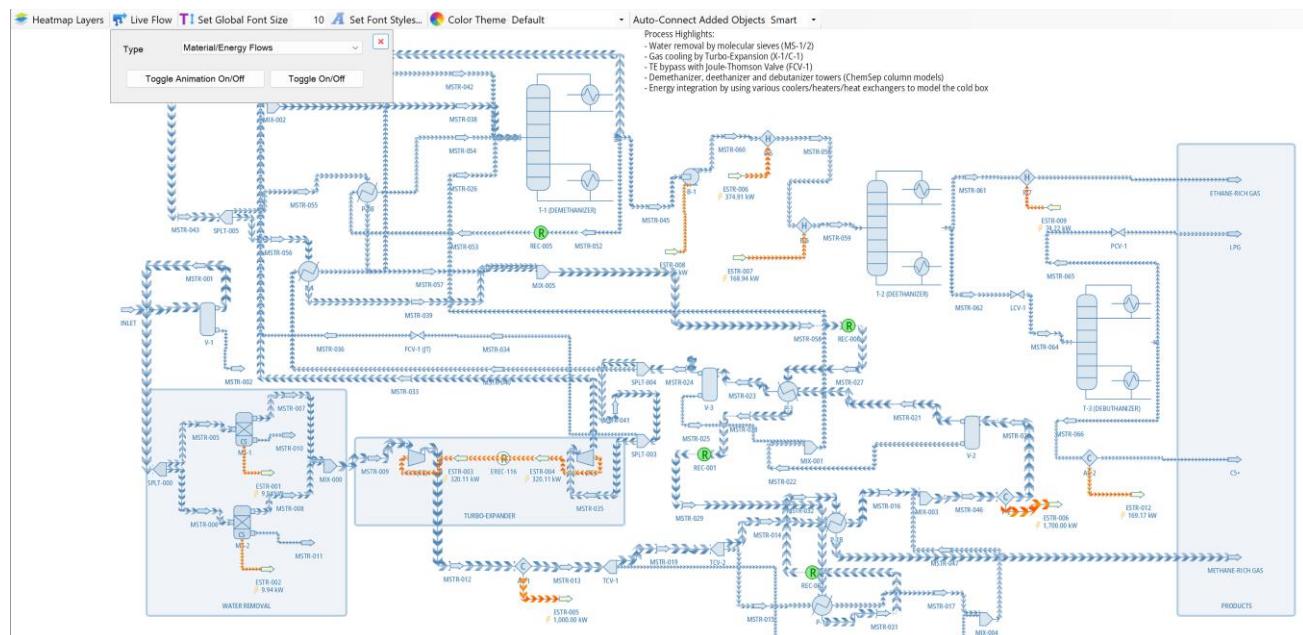


Figure 34 - Live Flows

### 3.8. Material Stream Data Importing Tool

You can use this tool to import Material Stream data from an Excel Spreadsheet to the flowsheet, including temperature, pressure, mass/molar/volumetric flow and molar/mass composition.

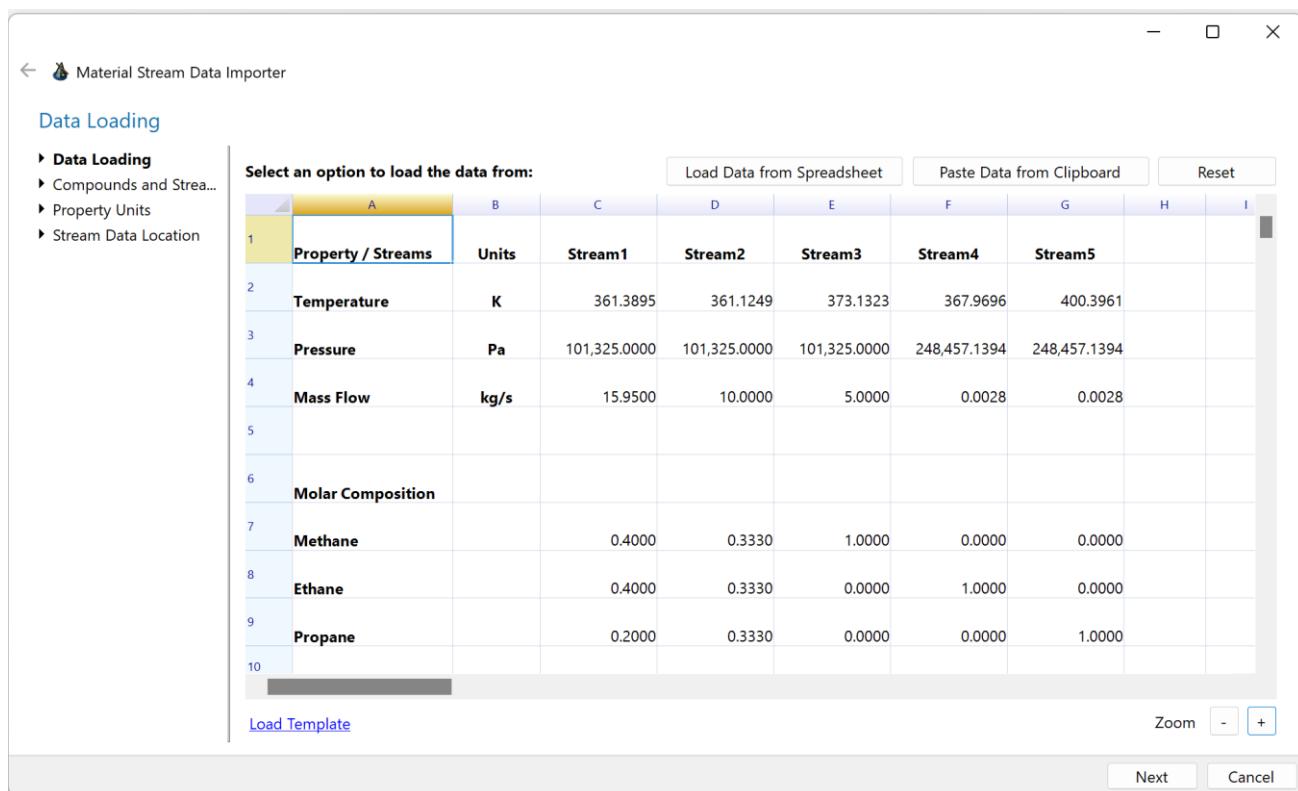


Figure 35 – Material Stream Data Importer Tool

### 3.9. Other Features

#### 3.9.1. Find Tear Streams

This feature can be accessed through the flowsheet context menu. Clicking on it will make DWSIM Pro look for the minimum amount of recycle blocks that needs to be added to the flowsheet so it can be calculated.

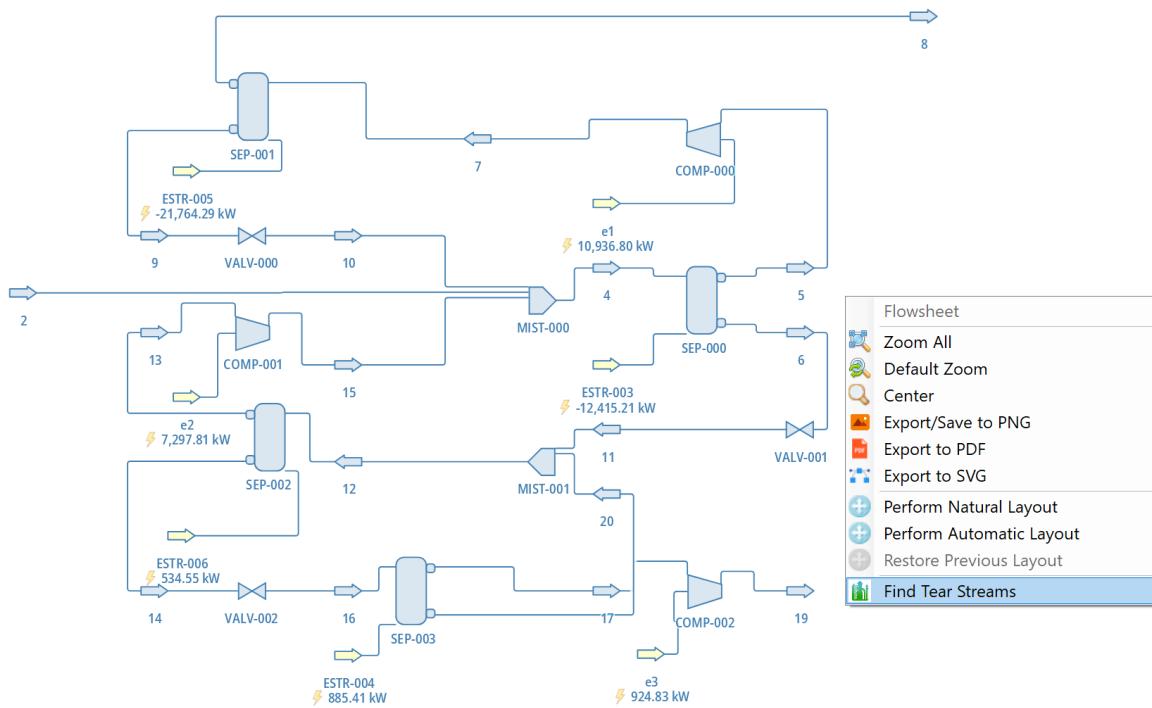


Figure 36 - Accessing the 'Find Tear Streams' tool

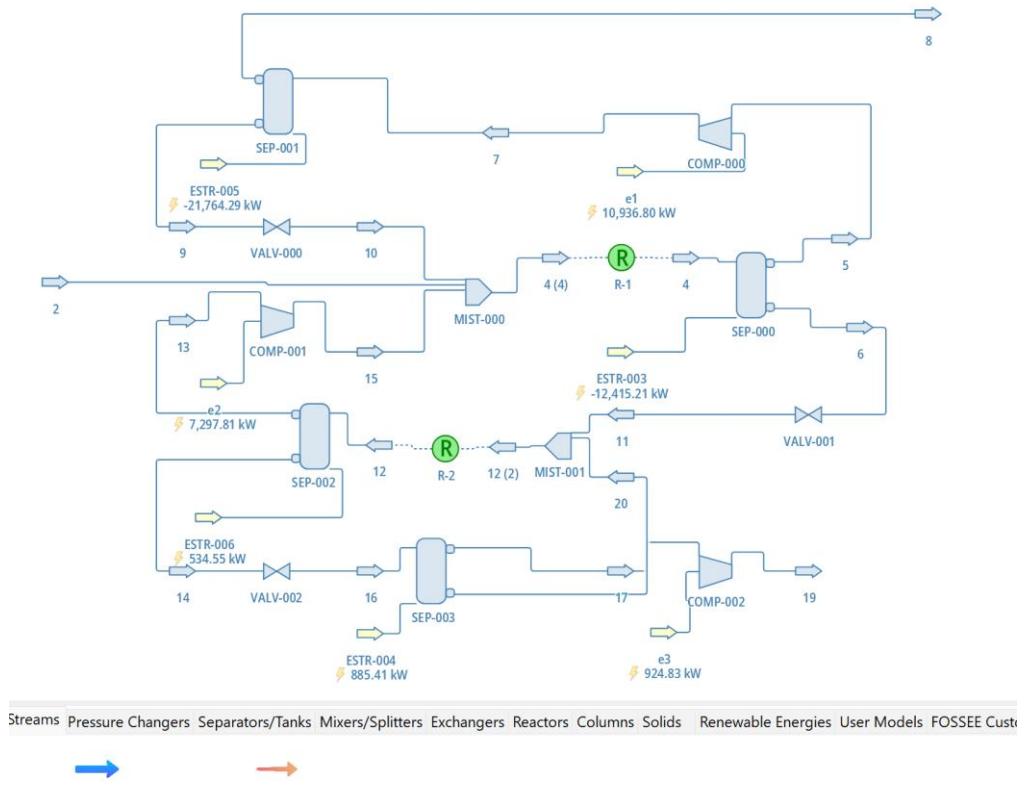


Figure 37 - Flowsheet with recycle blocks automatically added by the 'Find Tear Streams' tool

### 3.9.2. Export to PNG Image

Use this feature to export the current Flowsheet viewing area to a PNG image.

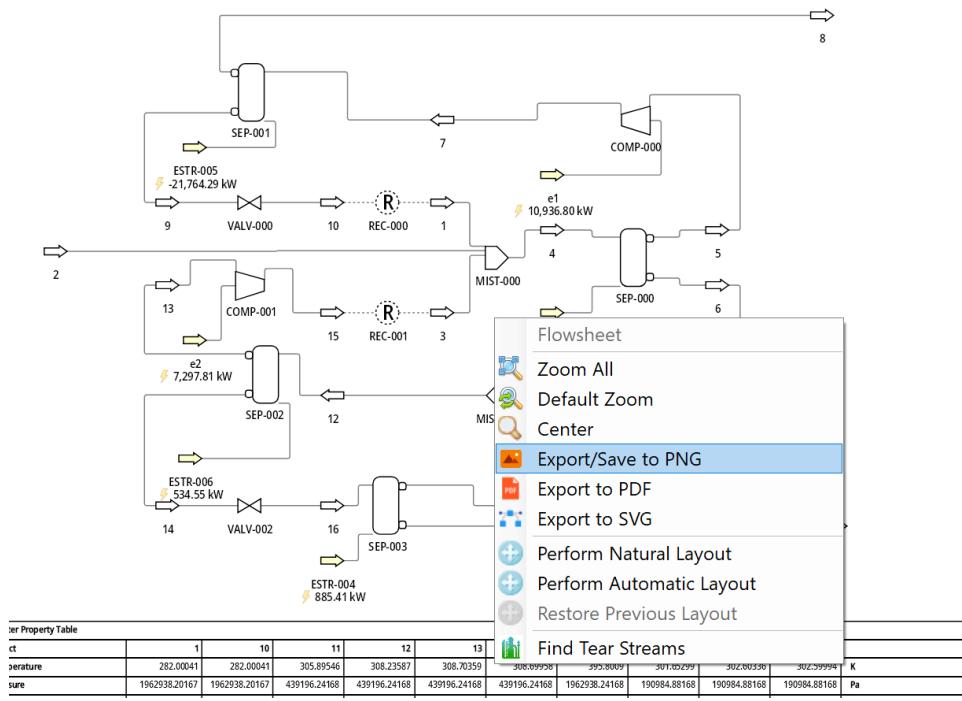


Figure 38 - Export Flowsheet to PNG Image

## 4. UNIT OPERATIONS

### 4.1. Three-Phase Reactive Distillation Column

The Three-phase Reactive Distillation Column is an enhanced column model supporting two liquid phases and reactive mixtures. You can define which stages are reactive and which ones support two liquid phases. The model supports kinetic and heterogeneous catalytic reactions, defined through the Reactions Manager.

### 4.2. PPBDesigner Column: Advanced L-L extraction simulation

PPBDesigner is a highly specific unit-operation to simulate L-L Extraction Columns (LLEC) of different types (mechanical / packed columns). The model is based on the **population balance framework**, which is a novel modeling approach that describes the evolution of a particle or a droplet size distribution of a dispersed phase (single particles or particles in swarm) in a continuous phase.

The population balance model accounts for different phenomena that occur in LLEC like, the buoyancy-driven motion of drops, axial dispersion, mass transfer, breakage, and coalescence of droplets. Therefore, many correlations and input parameters are required by the model to simulate your column module and provide reliable results.

#### 4.2.1. PPBDesigner Editor

In the current version of PPBDesigner, Agitated columns such as Rotating Disk Contactor (RDC) and Kühni column are supported.

Depending on the column type of your choice, you need to define different input parameters to model and simulate a Liquid-Liquid extraction column using PPBDesigner.

By default, PPBDesigner Editor is displayed in a standard mode where important but not necessary parameters are hidden for a simple simulation environment. The advanced mode shows all input parameters of the column module. (Advanced mode is recommended when sufficient data is available).

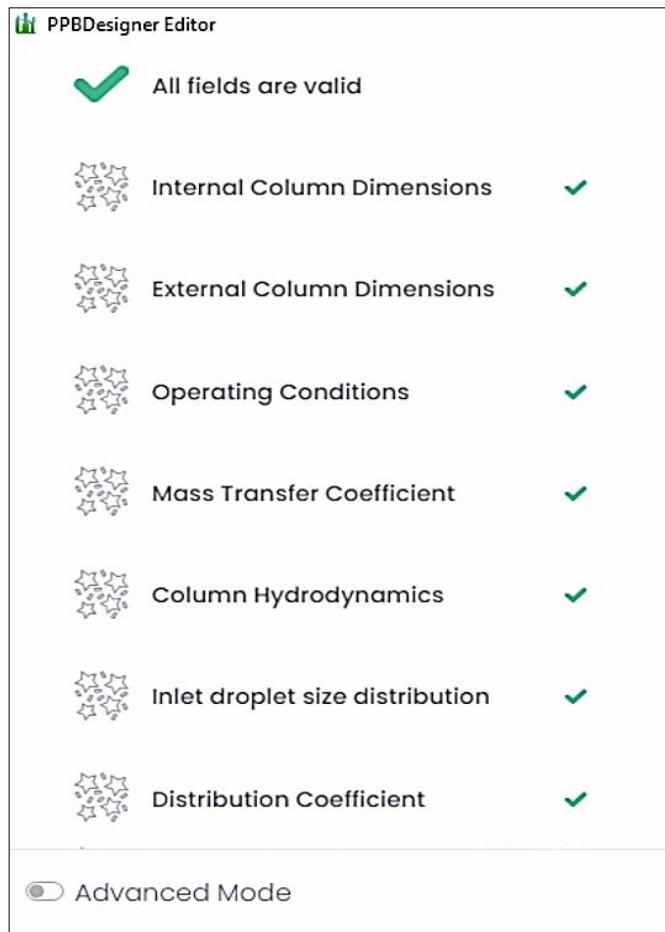


Figure 39: PPBDesigner Editor

#### 4.2.2. Internal and external Geometry

The internal geometry of the column makes the Population Balance Equation (PBE) specific for each column type. Therefore, you specify the Internal Column Dimensions of your column module as shown in figure 33.



Figure 40: Internal column dimensions (Kühni column internals).

You define the column diameter, upper and lower settling zones diameters, which are respectively the zones above and below the column active height. If your column does not have a settling zone, you define the diameter of the settling zones as the column diameter.

**External Column Dimensions**

Column Diameter (m)	1.6
Upper Settling Zone Diameter (m)	1.6
Lower Settling Zone Diameter (m)	1.6

Figure 41: External Column Dimensions.

Two options are available to define the **External Column Dimensions**. You can choose between the actual number of compartments or numerical Cells method (Figure 35). The number of numerical cells in Option two is a numerical parameter used internally by the solver to discretize the external coordinate (column height Z). High number numerical of cells leads to an accurate simulation but results in a high computational time. You can adjust this parameter for an optimal simulation setting.

**Spatial Discretization**

<input type="radio"/> Actual Number of Compartments	Number of Compartments 88
	Heavy Phase Inlet Compartment 70
	Light Phase Inlet Compartment 17
<input checked="" type="radio"/> Numerical Cells	Column Height (m) 4.4
	Heavy Phase Inlet Height (m) 3.8
	Light Phase Inlet Height (m) 0.85
	Number of Numerical Cells 50

Figure 42: External Column Dimensions.

#### 4.2.3. Operating conditions

In the operating conditions Rubric, you define the rotor speed, and you choose which phase is the dispersed phase. The choice of the dispersed phase may be based on the phase volume ratio for example.

**Operating Conditions**

Dispersed Phase *	<input type="radio"/> Heavy Phase <input checked="" type="radio"/> Light Phase
Rotor Speed (l/min)	200

Figure 43: Operating conditions section.

All other operating conditions are defined in DWSIM-Pro flowsheet environment, in the inlet streams sidebar (Mass flow, temperature, pressure ... ).

#### 4.2.4. Mass Transfer

Mass transfer coefficients for the continuous and dispersed phase are selected in the Mass Transfer Coefficient rubric. The choice of a correlation to estimate the mass transfer coefficient depends on the behaviour of the single droplet, whether it acts as a rigid, circulating, or oscillating droplet. Important correlations for both continuous and dispersed phase are respectively classified in Table 1 and Table 2.

You have the option to include or exclude Mass transfer phenomena depending on your simulation purposes. If mass transfer is included, you define the mass transfer direction of the solute whether is from the continuous to the dispersed phase or in the opposite direction.

Figure 44: Mass Transfer Coefficient rubric.

Continuous Phase correlations	Specifications
Garner and Tayeban	Rigid drops, $80 < Re < 800$
Kronig and Brink	Circulating drops
Treybal	Circulating drops- Swarm effect included
Heetjes et al.	Transition from spherical to circulating drops
Kumar & Hartland	Wide range from stagnant to oscillating drops
Clift et al.	Oscillating drops

Table 1: Correlations for mass transfer coefficient calculation for the continuous phase.

Dispersed Phase correlations	Specifications
Handlos and Baron	Oscillating drops by Considering the creation of turbulent eddies. Drop diameter range: 2.5-5 mm
Kronig and Brink	Considers circulation inside drops due to the buoyancy-driven motion
Laddha	Circulating drops- empirical model derived from the penetration theory
Pilhofer and Mewes	Empirical model- Oscillating drops
Kumar & Hartland	Wide range from stagnant to oscillating drops. swarm effect and energy dissipation included
Slater	Correlation includes a contamination factor
Simplified Grober	Stagnant drops. Assumptions: 1- No resistance in the continuous phase. 2- Long contact time
Seibert and Fair	Oscillating drops.

Table 2: Correlations for mass transfer coefficient calculation for the dispersed phase.

#### 4.2.5. Hydrodynamics

Column Hydrodynamics rubric contains correlations for breakage, coalescence, and correlations for axial dispersion coefficients, **Erro! Fonte de referência não encontrada.**. To explore the effect of these mechanisms on your column performance, you have the option whether including or excluding droplet interaction (breakage and coalescence) and axial dispersion.

Column Hydrodynamics			
Droplets Interaction	Include Breakage & Coalescence		
Breakage Frequency	Schmidt, Simon & Bart (2003)		
Coalescence Frequency	Coulaloglou & Tavlarides (1977)		
Coulaloglou & Tavlarides (1977) ①	C1 0.015	C2 1830	
Axial Dispersion	Include for both phases Hydro and Mass		
Heavy Phase Axial Dispersion Correlation	Kumar and Hartland (1994)		
Light Phase Axial Dispersion Correlation	Modes		

Figure 45: Breakage, coalescence, and axial dispersion correlations.

The coalescence rate in the correlation of Coulaloglou & Tavlarides has two adjustable constants to fit the model parameters to the corresponding experimental hydrodynamics data. The correlation of Coulaloglou & Tavlarides is the most used in literature and expressed as:

$$\omega(d, d', \emptyset_y) = \left[ C_1 \frac{\varepsilon^{\frac{1}{3}}}{1 + \emptyset_y} (d + d')^2 \left( d^{\frac{2}{3}} + d'^{\frac{2}{3}} \right)^{\frac{1}{2}} \right] \times \left[ \exp \left( -\frac{C_2 \eta_x \rho_x \varepsilon}{\sigma^2 (1 + \emptyset_y)^3} \right) \left( \frac{dd'}{d + d'} \right)^4 \right]$$

Many experimental works are conducted to estimate the constants  $C_1$  and  $C_2$ , which are dependent from the chemical system used and the type of the extraction column. Table 3 summarizes the founded constants values in literature.

Reference	Constant value		Conditions for determining the adjustable constants
	$C_1(-)$	$C_2(m^{-2})$	
Simon (2004)	$1.80 \cdot 10^{-2}$	$1.88 \cdot 10^{11}$	RDC, DN-150; Toluene (d)-Water
	$1.41 \cdot 10^{-2}$	$1.18 \cdot 10^{10}$	RDC, DN-150; butyl acetate(d)-water
Attarakih et al (2006) <a href="#">Ilecmod</a>	$6.94 \cdot 10^{-2}$	$1.3 \cdot 10^{11}$	RDC, DN-150; butyl acetate(d)-water
Schmidt et al. (2006)	$9.859 \cdot 10^{-2}$	$1.646 \cdot 10^{11}$	RDC, DN-150; toluene (d)-water

<b>Bart et al. (2004)</b>	$3.6 \cdot 10^{-2}$	$1.00 \cdot 10^{12}$	RDC; DN-80,100,150; toluene (d)-acetone-water
<b>Jaradat et al. (2012)</b>	$3.60 \cdot 10^{-2}$	$1.152 \cdot 10^{11}$	RDC; DN-150; butyl acetate(d)-water
<b>Gomes et al. (2006)</b>	2.312	$1.62 \cdot 10^{12}$	Kühni column; DN-150; toluene(d)-water
<b>Steinmetz (2007)</b>	0.79	$5.40 \cdot 10^{11}$	Kühni column; DN-32; toluene(d)-water
	0.98	$1.00 \cdot 10^{10}$	Kühni column; DN-32; butyl acetate(d)-water
<b>Drumm and Bart (2007)</b>	$0.50 \cdot 10^{-2}$	$1.00 \cdot 10^{11}$	RDC; DN-150; toluene(d)-water
<b>Attarakih et al (2012)</b>	$0.5 \cdot 10^{-2}$	$1.33 \cdot 10^{11}$	Kühni; DN-80; toluene(d)-acetone-water
<b>Attarakih et al. (2013) ppblab:</b>	$3.00 \cdot 10^{-2}$	$1.83 \cdot 10^{13}$	RDC; DN-80; toluene(d)-acetone-water

Table 3: Adjustable constants for the correlation of Coulaloglou&amp;Tavlarides.

Hydrodynamics rubric also includes droplet velocity models, Figure 8. You select a correlation to calculate the terminal velocity and you define the slowing factor model or its value to calculate the relative velocity. For the continuous phase, you choose a velocity model as well. You have the option between the oscillatory model or the steady state model (Oscillatory model is used only with dynamic simulation).



Figure 46: Models for droplet and continuous phase velocity.

Single droplet velocity (Terminal velocity) characterises the motion of single droplets in the column without internal effect. It depends mainly on the drop diameter and the properties of the chemical system (calculation of the inverse of Morton Number  $Mo = \frac{g \Delta \rho \eta_c^4}{\rho_c^2 \sigma^3}$ ). Therefore, different models are available for the user which are described in Table 4.

Droplet terminal velocity model	Specification
Rigid sphere (Wesselingh&Bollen (1999))	<ul style="list-style-type: none"> <li>- Rigid drops.</li> <li>- <math>Mo^{-1} &gt; 10^{11}</math></li> </ul>
Vignes Law (1965)	<ul style="list-style-type: none"> <li>- Circulating drops</li> <li>- High interfacial tension</li> <li>- <math>10^7 &lt; Mo^{-1} &lt; 10^{11}</math></li> </ul>
Klee and Treybal (1956)	<ul style="list-style-type: none"> <li>- Circulating and Oscillating drops.</li> <li>- Medium interfacial tension.</li> <li>- <math>10^5 &lt; Mo^{-1} &lt; 10^7</math></li> </ul>
Grace Law (1976)	<ul style="list-style-type: none"> <li>- Oscillating drops.</li> <li>- Low interfacial tension.</li> <li>- <math>Mo^{-1} &lt; 10^5</math></li> </ul>
Drag coefficient-based	Correlation based on drag coefficient

Table 4: Available terminal velocity models in PPBDesigner.

In the **inlet droplet size distribution** rubric, three options available for the inlet feed distribution (Normal, Lognormal and Weibull distribution). With the advanced mode, you define the following parameters: the normalization factor, the population mean diameter, and the population standard deviation. You specify the minimum and the maximum diameter of your droplet class.

Figure 47: Parameters for the inlet feed distribution.

The number of pivots is a numerical parameter used by the solver to discretize the internal coordinate (drop diameter). Using high number of pivots results in more accurate results but higher computational time.

#### 4.2.6. Distribution coefficient (Partition ratio)

In the distribution coefficient rubric, you have three options to define the distribution coefficient of your chemical system. The first option is to use the UNIQUAC property package to estimate the interaction parameters to be used for distribution coefficient estimation. As a second option, a correlated equation of the distribution coefficient as function of the solute concentration is used. The user provides the distribution coefficient value, as a third option, if available.

**Distribution Coefficient**

UNIQUAC Populate

UNIQUAC Parameters

R-Heavy Phase	0	R-Light Phase	0	R-Solute	0
Q-Heavy Phase	0	Q-Light Phase	0	Q-Solute	0

Interaction Parameters

A12	0	A21	0	A23	0	A32	0
-----	---	-----	---	-----	---	-----	---

Function of Solute Concentration ⓘ

a	-2.1567	b	0.0027	c	0	<span style="background-color: #0070C0; color: white; padding: 2px 10px; border-radius: 5px;">Estimate</span>
---	---------	---	--------	---	---	---

User Defined (Constant Value)

K-Value Cy/Cx (kg/kg)	0.7
-----------------------	-----

Figure 48: Distribution coefficient- Estimation options.

#### 4.2.7. Solver settings

The solver settings rubric (**Erro! Fonte de referência não encontrada.** 42) provides a set of adjustable numerical parameters and different solvers. You can adjust the final simulation time, the solver time step, and the initiate from previous result option (reduced the computational time). In most cases, solver settings are kept by default.

**Solver Settings**

Select PPE Solver	EFPMT
Grid Type	Uniform Grid
Initiate from previous result	No
Number of Quadrature Points	2
Number of Gauss Quadrature	5
Final Simulation Time (s)	7000
Solver Time Step (s)	5

Figure 49: Solver settings rubric.

#### 4.2.8. View and export of results

Different tabs are available to view your simulation results. By clicking on results in the PPBDesigner column sidebar (figure 43), you can see important results, in addition to the holdup and solute concentration profiles.

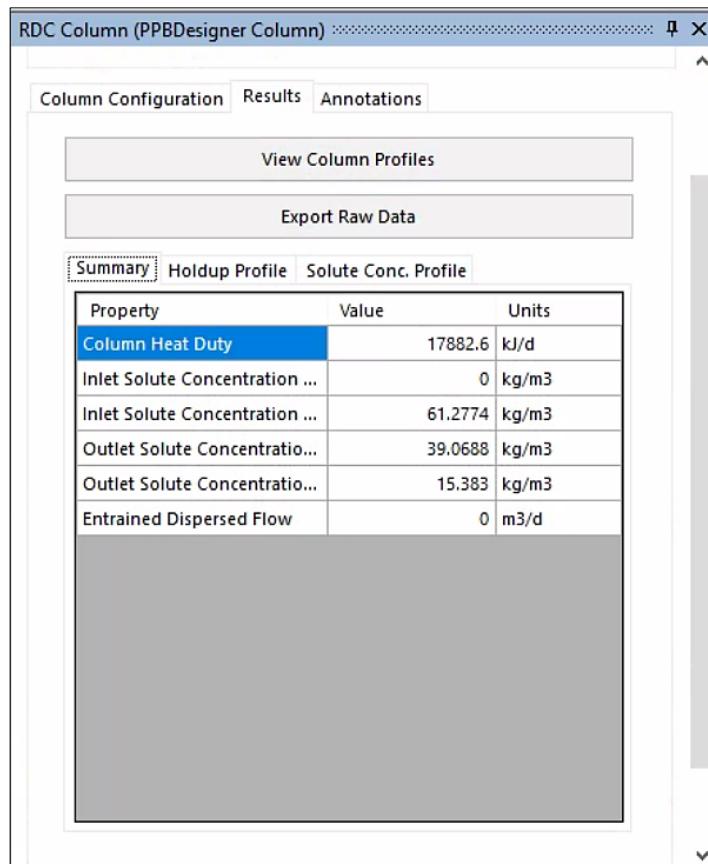


Figure 50: Results Tab in the PPDesigner column sidebar.

By clicking on **view column profiles** button, more results related to hydrodynamics and mass transfer in the column (droplet' diameter, droplet volume distribution, equilibrium concentration...) are displayed as function of the column height. Charts and tables for these results are generated.

You can export all properties of the studies chemical system and results of the simulation as a text file by simply clicking on **Export Raw Data**.

## 4.3. Pipe Network

### 4.3.1. Introduction

Pipe networks are structures built to transport fluids between several supply and demand points. Transmission and distribution of natural gas are examples of services provided by pipeline networks.

In fluid dynamics, pipe network analysis is the analysis of the fluid flow through a hydraulics network, containing several or many interconnected branches. The aim is to determine the flow rates and pressure drops in the individual sections of the network. This is a common problem in hydraulic design.

### 4.3.2. Model Features

The Pipe Network Unit Operation allows modelling and simulation of pipe networks connected through nodes with multiple sources and sinks. Rigorous compositional fluid property calculations are done by DWSIM Property Packages. It has the following features:

- Supports Pipe Segments with Rigorous Heat Transfer calculations, Valves, Pumps, Compressors and Gas-Liquid Separators.
- Rigorous fluid properties and phase distribution calculated with DWSIM Property Packages
- Fully featured Graphical Network Designer.
- Supports Pressure and Mass/Molar/Volumetric Flow specification on endpoints (Sources and Sinks).

#### 4.3.3. Usage Help

Create a new simulation or open an existing one. Add a Pipe Network block and connect material streams to it. Open the Network Designer:

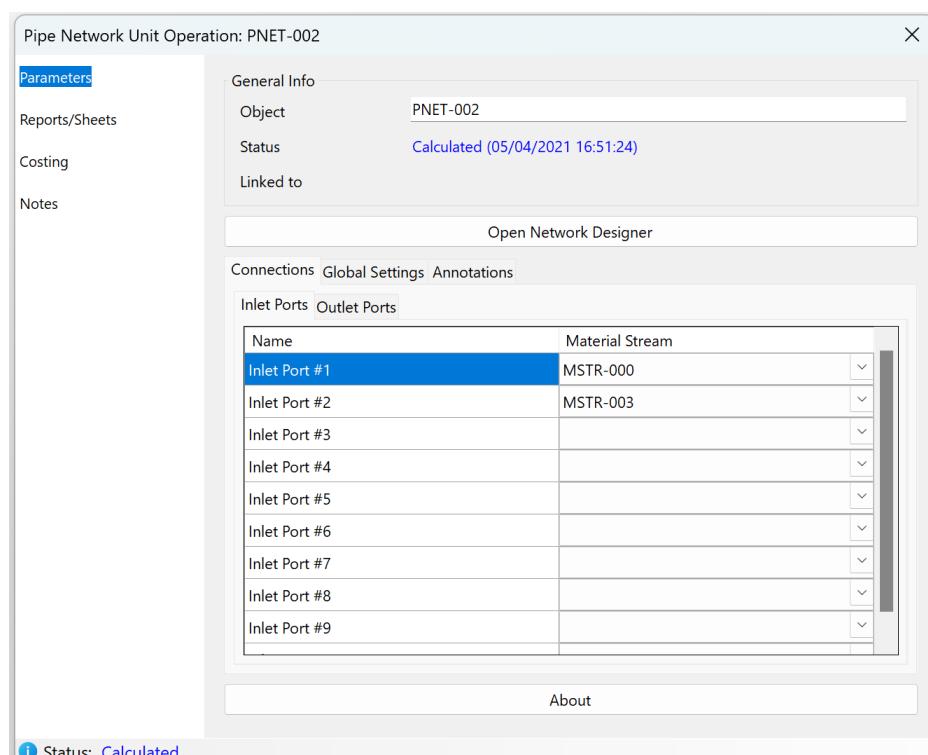


Figure 51 - Pipe Network editor

Drag and drop network objects to the Designer area and connect them to each other. Sources and Sinks are used to link the inputs and outputs to the connected material streams. Bridges are used to connect source and sink nodes to the rest of the network.

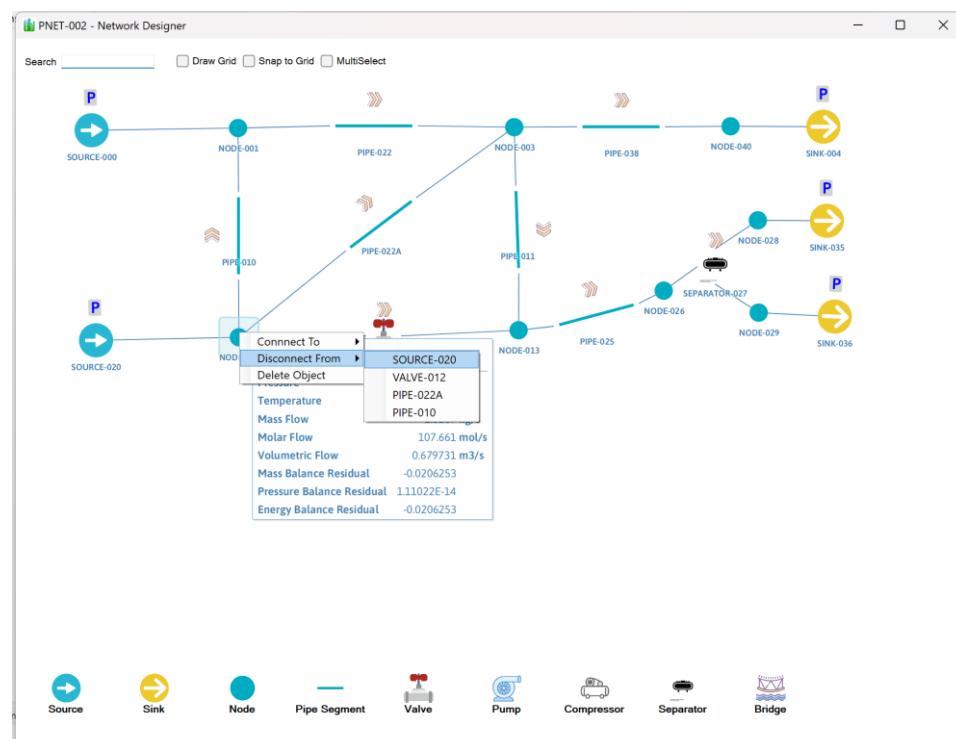


Figure 52 - Network Designer

Double-click on an object to define its parameters:

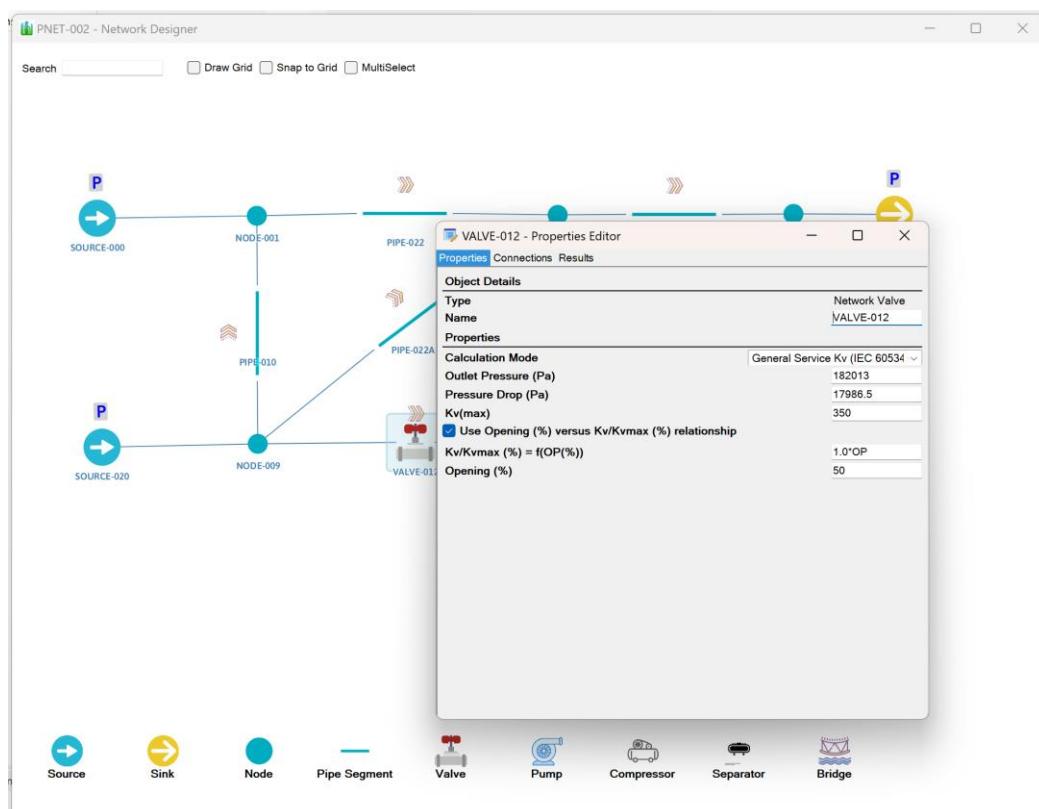


Figure 53 - Network Object editor

When all parameters are set, close the Network Designer, and request a flowsheet calculation. It can take a few minutes. If any error appears, go back to the designer, and make the required corrections before trying again.

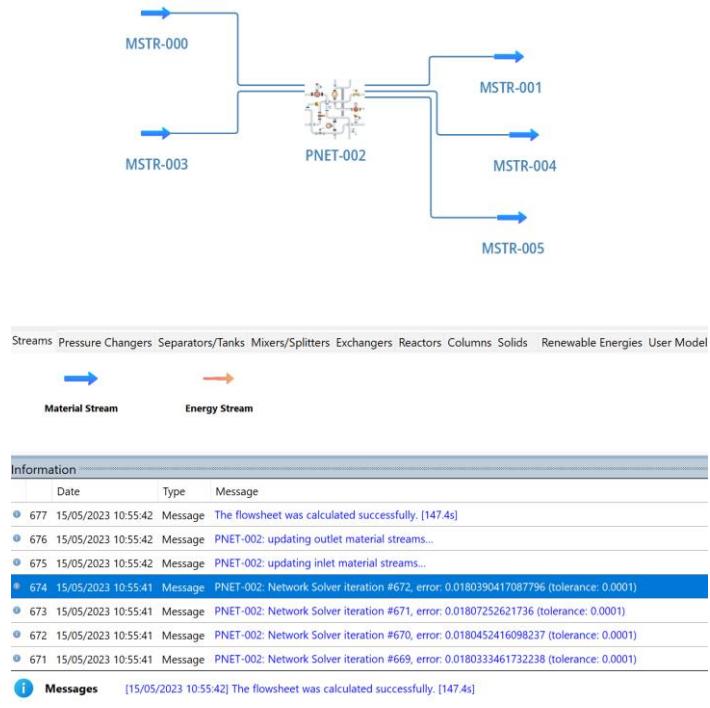


Figure 54 - Solving a Pipe Network block

After the network is solved, you can go back to the designer and view the results by block/object. Inspect the outlet Material Streams to see the network outputs.

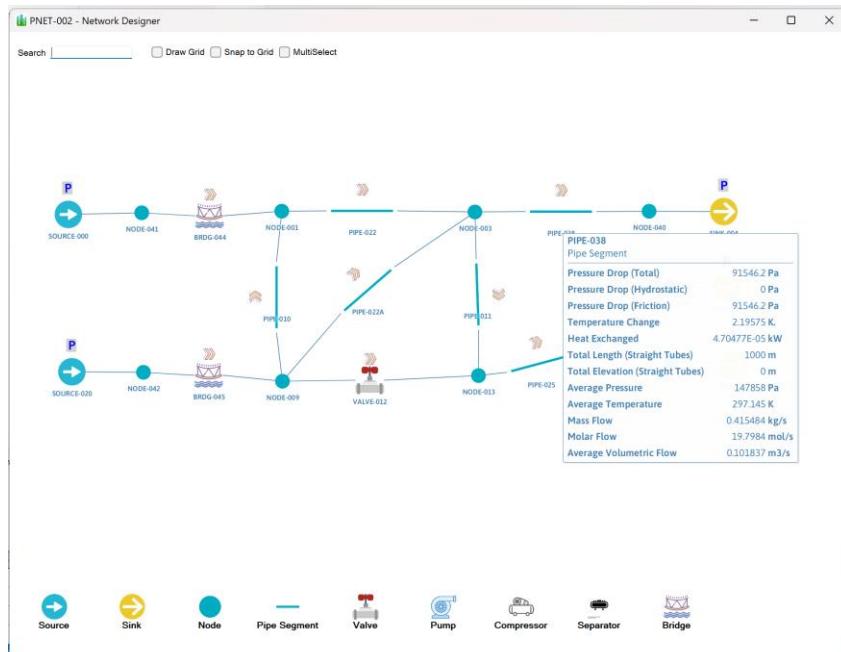


Figure 55 - Viewing results from a calculated Pipe Network object

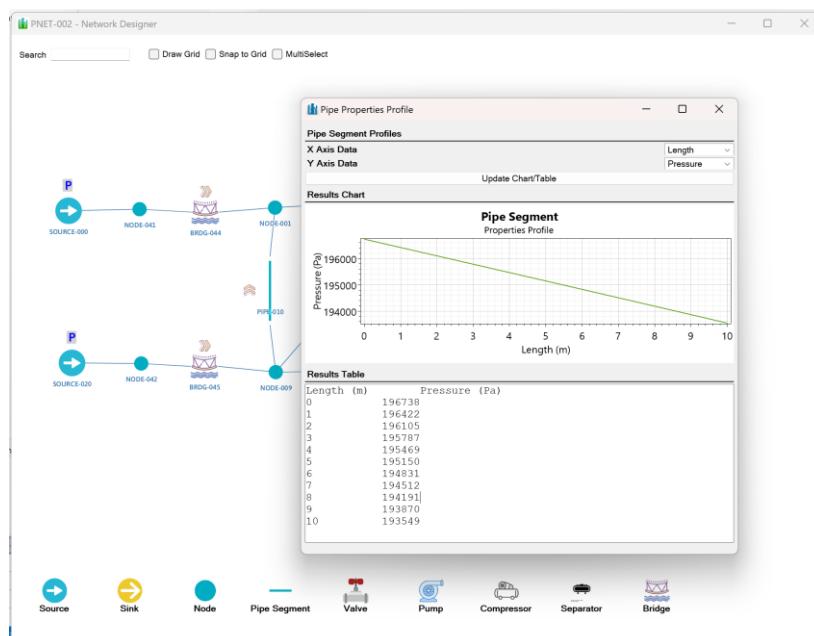


Figure 56 - Viewing results from a calculated Pipe Network object (2)

#### 4.4. (Semi)Batch Reactor

The (Semi)Batch reactor (referred to as SBR) is a dynamic Unit-Operation in DWSIM Pro for batch simulation. The reactor works as batch by defining the reactor content, or as semi-batch which enables feeding the reactor continuously by one (or multiple) reactant.

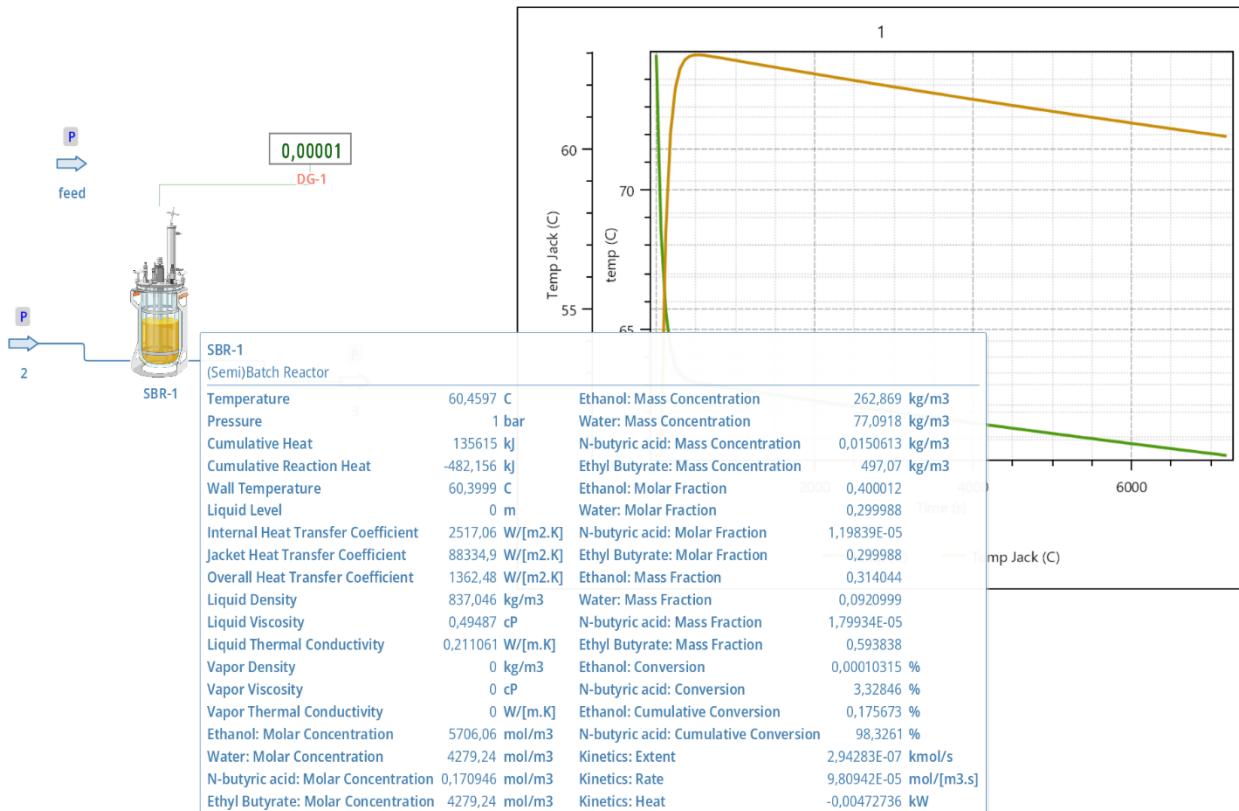


Figure 57 -(Semi)Batch Reactor model.

For more information on how to set-up a dynamic simulation, refer to Dynamic modelling and simulation (section 14: Dynamic simulation structure and configuration) of DWSIM Open-Source User Guide.

#### 4.4.1. Operation Modes

The SBR supports three operation modes:

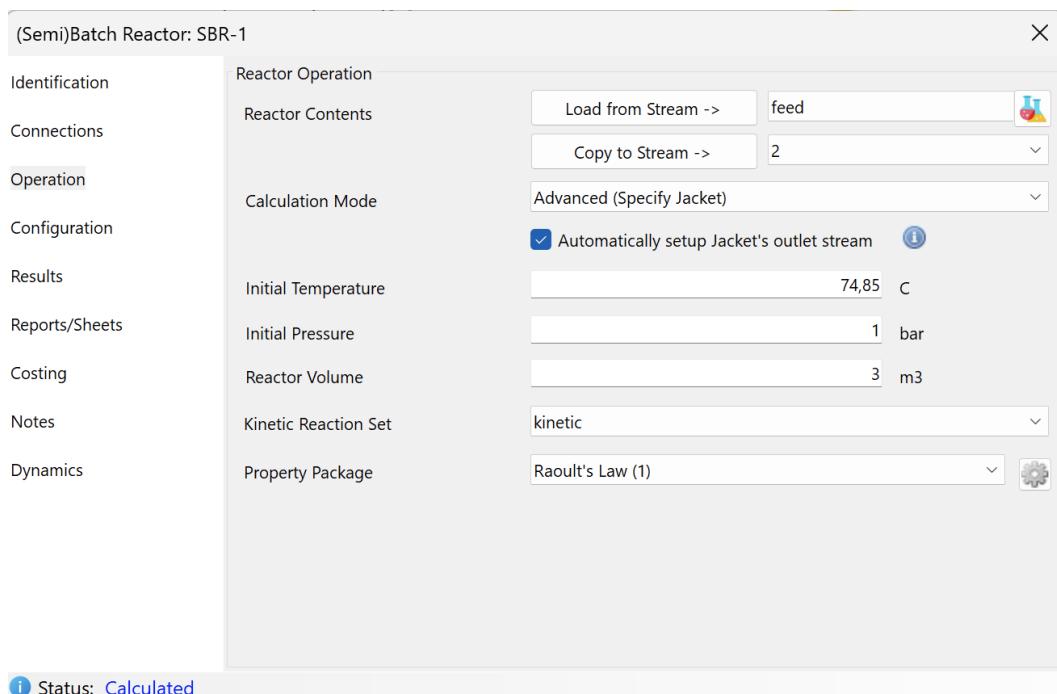


Figure 58 –(Semi)Batch Reactor operation settings.

**Isothermal operation:** The SRB content is perfectly Mixed. During the first few moments of operation the concentrations of the reactants decrease, the concentrations of the products increase, and the temperature remains constant.

**Adiabatic operation:** The SBR is considered well insulated. The temperature of the reactor content may increase or decrease depending on the nature of the reaction if it is an exothermic or endothermic reaction.

**Advanced operation (Use of Jacket):** The SBR is considered non-isothermal and the control of the temperature' content requires the use of Batch reactor with jacket to cool-down or heat-up the content based on the kinetic behavior of a typical reaction. This operation mode requires an advanced design of the reactor, jacket, and the agitation to estimate the overall heat transfer coefficient.

When the advanced operation mode is selected, the Reactor Configuration Tab in the SBR main window is enabled. For the isothermal and adiabatic operation modes, the Tab is disabled by default. Note: The reactor is designed with a dished bottom.

**Reactor Geometry:** The Geometry Tab allows for defining design parameters of the SBR (add screenshot). The parameters are used to calculate Heat transfer area. The following equations are used depending on the filling level:

For  $V_{min} < V < V_{max}$ :

$$A = \frac{V - V_{min}}{V_{max} - V_{min}} * (A_{max} - A_{min}) + A_{min}$$

For  $V < V_{min}$ :

$$A = \frac{V}{V_{min}} * A_{min}$$

**Agitator:** Agitation is considered for Internal heat transfer calculation inside the SBR. Three types of agitators are available: Turbine with six flat blades, Impeller with three tilted blades, and Anchor agitator. The power of the agitator is included in the energy balance equation of the reactor. Note: The agitation is not considered for the mass transfer calculations in the reactor.

**Jacket:** The reactor jacket comes with three different types: Simple Unbaffled, Dimple baffled and Half-pipe coil. Also, different wall materials are provided. The internal cooling/heating is not supported, but only external Heat exchange.

Parameter	Description	Value	Units
Volume	Internal Jacket Volume	2	m³
Height	Jacket Height	3	m
Annulus	Jacket Annulus	100	mm
Inlet Diameter	Jacket Inlet Diameter	100	mm
Inner Pipe Diameter	for Half-Pipe Coil Type	10	mm
Heat Loss	Jacket Heat Loss	0	kW

Figure 59 -(Semi)Batch Reactor Jacket configuration.

#### 4.4.2. Thermodynamic Calculations

The SBR supports Vapor-Liquid phase equilibrium and the presence of solids in the reactor allowing different applications and reaction types (Chemical and Bio-Chemical reactions). The liquid phase is by default defined for the reactor. In the reaction settings, the reactive phases can be changed.

By default, the first property package in the Thermo-package list is selected. It is possible to switch to another property package if it is in the list of the thermos-package directly from the Operation Tab of the reactor.

#### 4.4.3. Initial charge

To specify the initial charge of the reactor, use a material stream to define: Temperature, pressure, and the initial composition. In the operation Tab of the SBR, Load the material stream to the Reactor and define the initial quantity (Mole, mass, or volume basis).

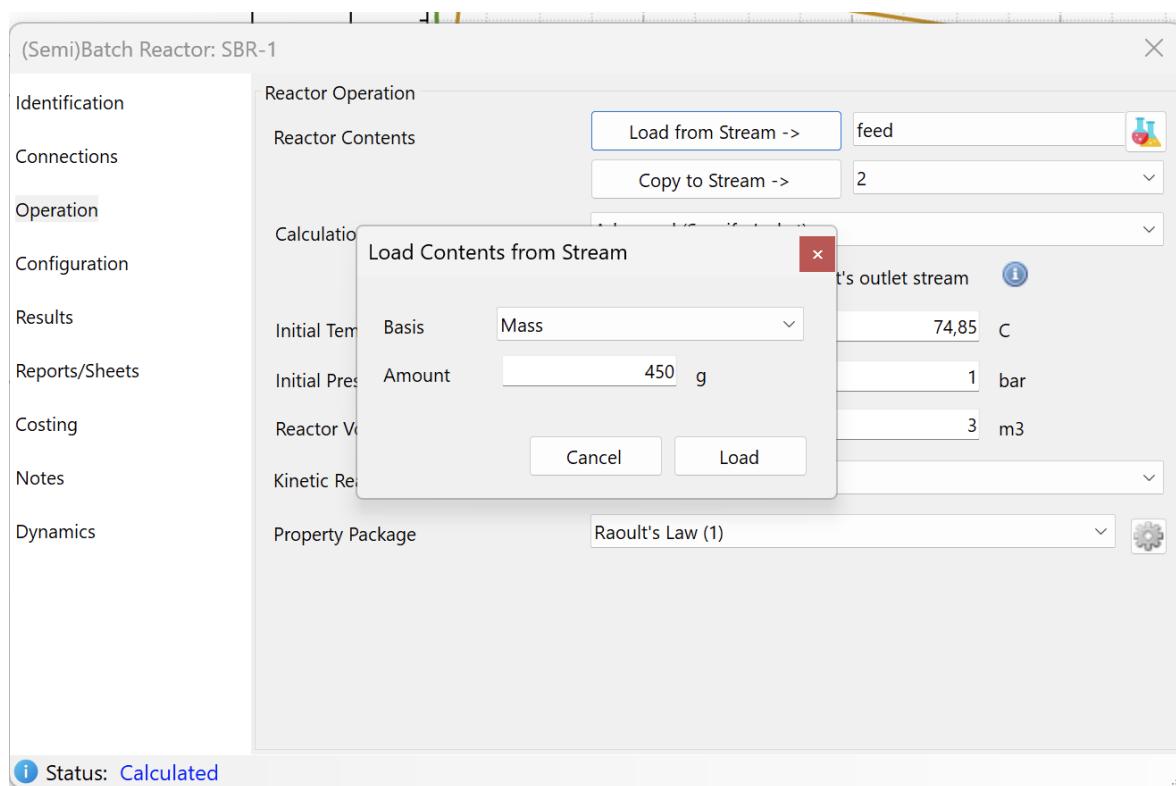


Figure 60 –(Semi)Batch Reactor initial charge input window.

It is possible to redefine different initials for the reactor temperature and pressure from the Material steam being loaded. In addition, the reactive volume of the reactor is to be defined. Those specifications are valid for the three operation modes.

To get the final content of the reactor in a stream, use the copy to stream function by choosing the appropriate stream you created for this purpose. Units are to be defined in the system of units Tab in the Settings window for: Time, Volume, and the loading quantity (Mole or Mass basis).

#### 4.4.4. Kinetic Reaction Set

The kinetic Reaction set is automatically selected based on the definition of the reaction system in the reaction Tab in the Settings window. The SBR supports parallel reactions or in series mode. The user can define kinetic rate-base reaction or heterogeneous rate-base reaction.

For more information on how to set-up the reaction rates, refer to Chemical Reactions (2.8 section) of DWSIM Open-Source User Guide.

#### 4.5. Falling Film Evaporator

A falling film evaporator is an industrial device to concentrate solutions, especially with heat sensitive components. The evaporator is a special type of heat exchanger. It supports four different calculation modes:

- **Outlet Temperature (1):** specify the outlet temperature for the concentration fluid and the heat load will be calculated. Requires an energy stream connected to the evaporator.
- **Outlet Vapor Fraction (2):** specify the amount of vapor that will be evaporated, ranging from 0.0 (0% evaporation) to 1.0 (100% evaporation), so the heat load will be calculated. Requires an energy stream connected to the evaporator.
- **Energy Stream (3):** The evaporator will read the amount of heat available from the energy stream and use it to calculate the amount of evaporation. Requires an energy stream connected to the evaporator.
- **Direct Steam (4):** Directly connect material streams to the evaporator for the steam utility and use it to evaporate the liquid. Requires a material stream connected to the “Steam Inlet” port and another one connected to the “Condensate Outlet” port.

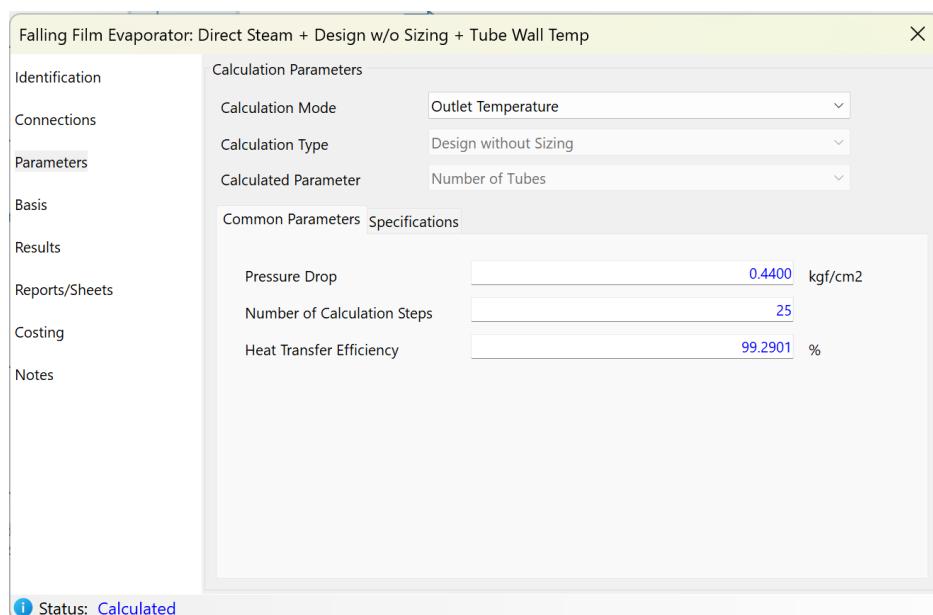


Figure 61 - Falling Film Evaporator Unit Operation – Common Input parameters

The pressure drop for the liquid stream can be specified for all calculation modes. By defining the number of calculation steps you will get an evaporation profile that can be used for further sizing calculations or more detailed analysis.

EV-01 (C6) - Evaporation Profile						
Temperature (C)	Pressure (kgf/cm2)	Heat Added (kW)	Heat of Vaporization (kJ/kg)	Vapor Molar Fraction	Vapor Mass Fraction	Vapor Molar Weight (kg/kmol)
102.4849	2.5127	1,107.9660	2,046.7688	0.0000	0.0000	0.0000
118.4653	2.4687	1,107.9660	1,977.3038	0.0000	0.0000	0.0000
126.1479	2.4247	1,107.9660	2,132.6341	0.0176	0.0161	18.0153
125.5621	2.3807	1,107.9660	2,132.1180	0.0534	0.0490	18.0153
124.9681	2.3367	1,107.9660	2,131.4675	0.0892	0.0818	18.0153
124.3657	2.2927	1,107.9660	2,130.6662	0.1249	0.1146	18.0153
123.7548	2.2487	1,107.9660	2,129.6951	0.1607	0.1474	18.0153
123.1350	2.2047	1,107.9660	2,128.5323	0.1963	0.1801	18.0153
122.5063	2.1607	1,107.9660	2,127.1520	0.2320	0.2128	18.0153
121.8684	2.1167	1,107.9660	2,125.5241	0.2676	0.2454	18.0153

Figure 62 - Falling Film Evaporator Unit Operation – Evaporation Profile

#### 4.5.1. Details of Calculation Modes 1, 2 and 3

The basic equation for heat transfer is:

$$Q = W \times (H_{out} - H_{in}) \times \eta,$$

where  $Q$  is the heat transferred,  $W$  is the feed mass flow,  $H_{out}$  is the outlet enthalpy,  $H_{in}$  is the inlet enthalpy and  $\eta$  is the heat transfer efficiency.

The calculation steps subdivide the heat exchanger into segments. For calculation modes 1, 2 and 3,  $H_{out}$  is calculated for every segment. In modes 1 and 2, the heat exchanger outlet conditions are defined by either the temperature or vapor fraction, and  $Q$  can be calculated. For mode 3,  $Q$  is provided, and  $H_{out}$  can be calculated for every segment.

There is an option to define the Tube Wall Temperature, which allows the calculation of some additional parameters using predefined default values for the Reynolds Number (1000), Tube Internal Diameter (50 mm), Tube Material (Stainless Steel) and Tube Thickness (2.5 mm):

- Overall Heat Transfer Coefficient, ignoring the contribution from external side (steam side)
- Internal Heat Transfer Coefficient
- Average Film Thickness
- Average Film Velocity
- Temperature Difference

The above properties are stored and can be seen in the Evaporation Profile.

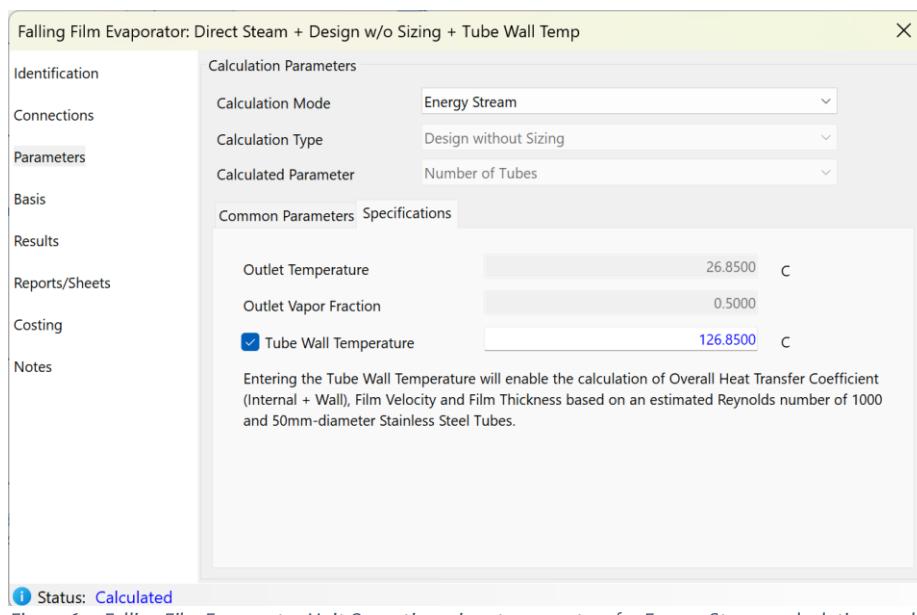


Figure 63 - Falling Film Evaporator Unit Operation – input parameters for Energy Stream calculation mode

#### 4.5.2. Direct Steam calculation mode details

The Direct Steam calculation modes provides further options to include or calculate the dimensions of the heat exchanger in the Falling Film Evaporator. There are three calculation types available:

- **Evaluation (A):** Evaluate a heat exchanger of given design information (Number of Tubes, Tube Internal Diameter, Tube Thickness, Tube Length and Tube Material).

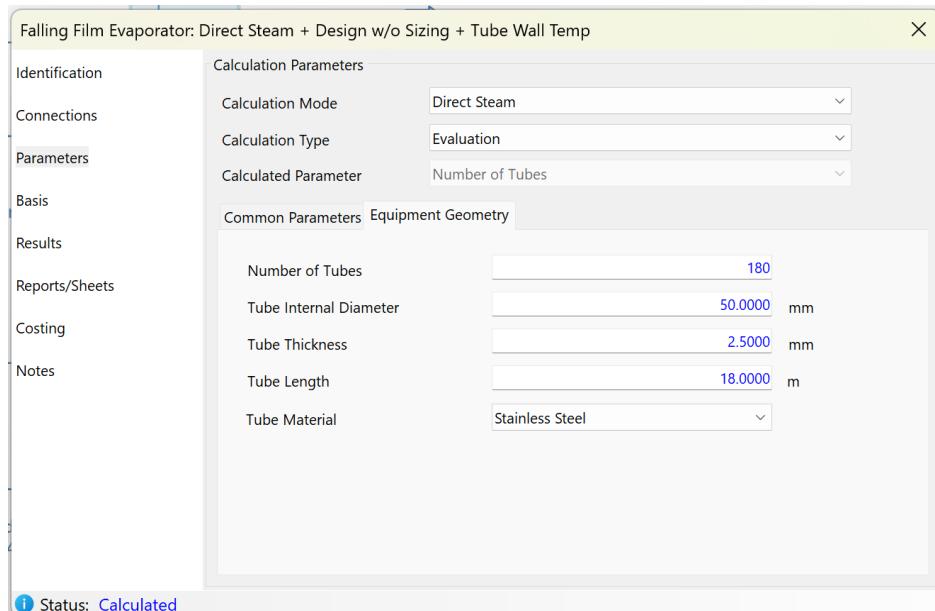


Figure 64 - Falling Film Evaporator Unit Operation – input parameters for Direct Steam + Evaluation calculation mode

- **Design (B):** Calculate the Tube Length, Tube Internal Diameter or Number of Tubes based on the outlet characteristics of the steam.

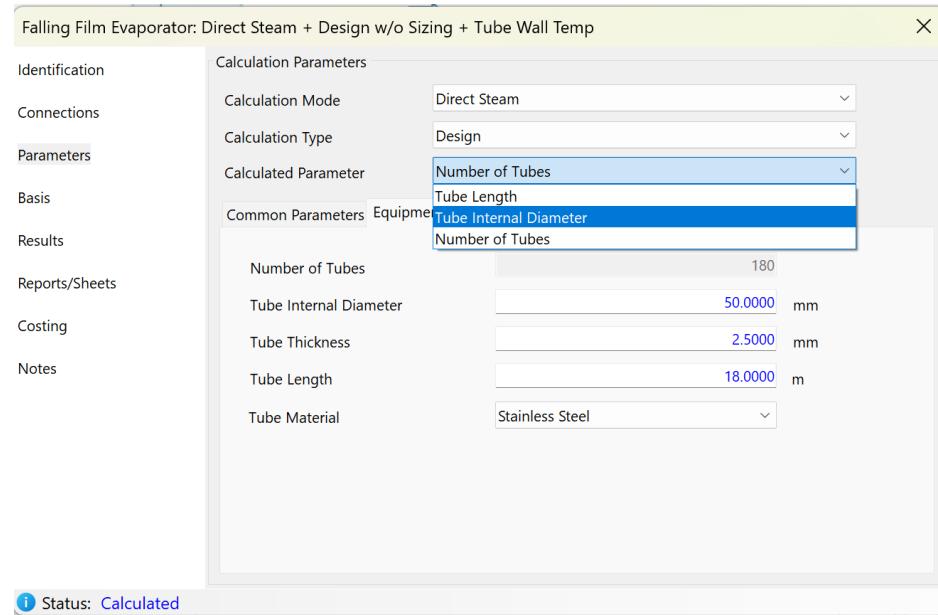


Figure 65 - Falling Film Evaporator Unit Operation – input parameters for Direct Steam + Design calculation mode

- **Design without sizing (C):** Calculate the heat load based on the outlet characteristics of the steam. This calculation type does not require design information and does not update values for  $U$  and  $A$ , but does require the definition of the efficiency.

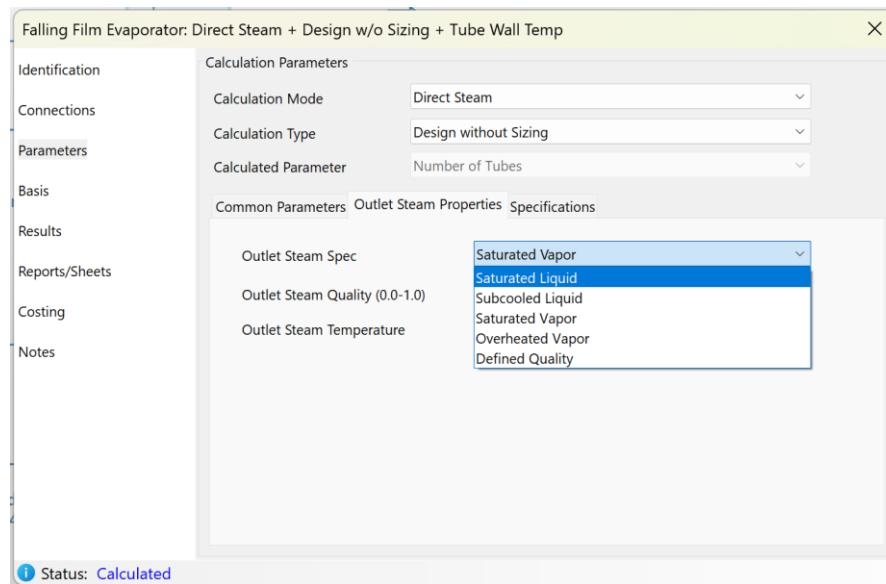


Figure 66 - Falling Film Evaporator Unit Operation – input parameters for Direct Steam + Design without Sizing calculation mode

The calculation step subdivides the tube length into segments for options A and B. For each segment, the heat balance and corresponding heat exchanger parameters are calculated. The governing equation is

$$Q = U \times A \times \Delta T,$$

where  $Q$  is the heat load,  $U$  is the overall heat transfer coefficient,  $A$  is the heat exchange area and  $\Delta T$  is the temperature difference.  $A$  is calculated from the tube geometrical data and  $\Delta T$  from the

temperatures of the steam and fluid at the current segment.  $U$  is calculated from external convection (steam), internal convection (fluid) and tube wall conduction using the following equations:

$$\frac{1}{U} = \frac{1}{h_o} + \frac{D_e}{k_w} \ln \frac{D_e}{D_i} + \frac{D_e}{D_i h_i},$$

where:

$$h_i = 62.09 Re_L^{-0.01239} Re_V^{0.3427}$$

$$h_o = 53200 Re_C^{-0.1418} Pr_C^{-3.1975}$$

Option C calculates properties for each segment similarly to Calculation Modes 1-3, except that we first calculate the heat exchanged from the specified outlet steam conditions + defined efficiency. After calculating  $Q$ , the rest of the calculations proceed as if we had an energy stream connected to the FFE, including the option to consider the tube wall temperature to calculate the additional parameters.

The following Outlet Steam Specifications are available for Option B and C:

- Saturated Liquid
- Subcooled Liquid
- Saturated Vapor
- Overheated Vapor
- Defined Quality (ranging from 0.0 to 1.0)

The subcooled liquid temperature can't be lower than the feed temperature and the overheated vapor temperature can't be higher than the steam inlet temperature.

Falling Film Evaporator: Direct Steam + Evaluation		
Identification Connections Parameters Basis Results Reports/Sheets Costing Notes	Results	
	View Evaporation Profile	
	Parameter	Value
	Heat Exchange	13,078.3006 kW
	Maximum Heat Exchange	13,171.8051 kW
	Thermal Efficiency	99.2901 %
	Heat Transfer Area	534.3849 m <sup>2</sup>
	Overall Heat Transfer Coefficient	1,259.7571 W/[m <sup>2</sup> .K]
	Average Temperature Difference	19.4272 C.
Costing		
Notes		

i Status: Calculated

Figure 67 - Falling Film Evaporator Unit Operation – Typical Results

#### 4.6. Material/Energy Stream Switch

The Stream Switch (Material and Energy) Logical Blocks route (redirect) an inlet stream to one of two outlet streams according to the result of a logical expression entered by the user.

#### 4.7. Material Stream Mapper

This block can be used to transfer information from a Material Stream to another while overriding some properties in between.

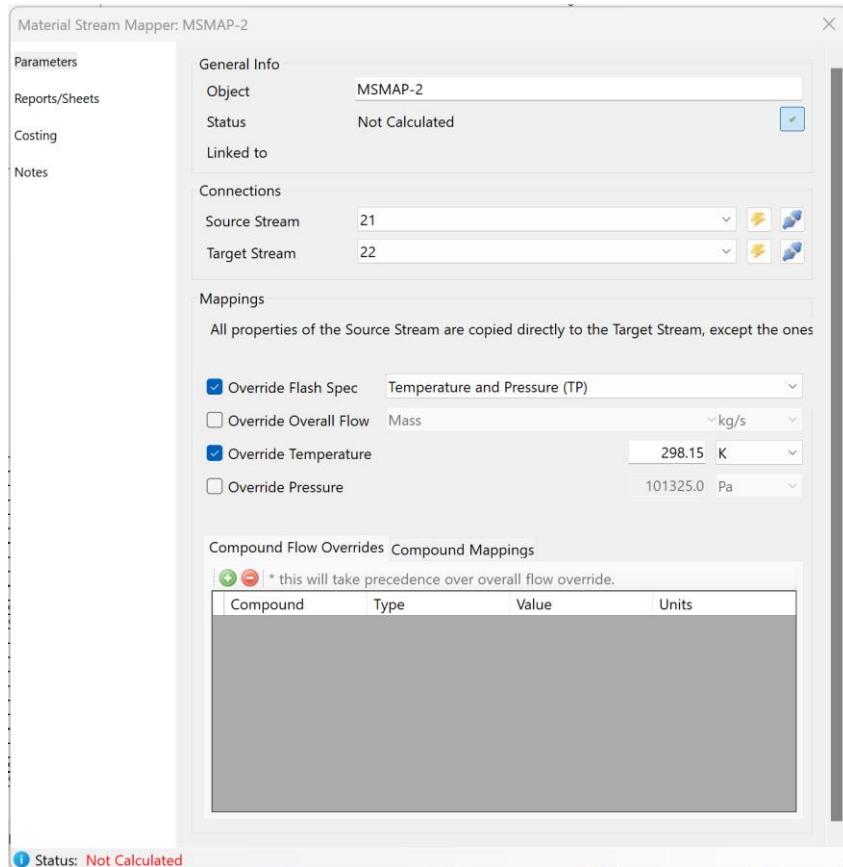


Figure 68 - Material Stream Mapper editor

#### 4.8. Energy Stream Splitter

This block splits an energy stream into two or more streams according to a split factor defined by the user.

#### 4.9. Thermo Property Editor

This logical block exposes property package model parameters for usage with sensitivity analysis and flowsheet-wide optimization tools. You can use it to tune binary interaction parameters from the thermo models using a property of a flowsheet object or a combination of object properties as the objective function. You can also use it to study the influence of the binary interaction parameters on stream properties or unit operation performance metrics.

Make sure to connect this block to the first inlet material stream on the flowsheet.



## 5. EXTERNAL MATH SOLVERS

DWSIM Pro includes two additional sets of math solvers (ODE, Non-Linear Optimization and Non-Linear Systems of Equations) that can be used by some Unit Operation blocks, which are:

- Extreme Optimization Solvers (Exo Solvers)
- SciPy Python Solvers

You can use external solvers with selected Unit Operations, including:

- Plug-Flow Reactor: Exo and SciPy ODE solvers
- Rigorous Distillation Column: Exo and SciPy Non-Linear System of Equations Solvers
- Equilibrium Reactor: Exo and SciPy Non-Linear System of Equations Solvers
- Gibbs Reactor: Exo and SciPy Local and Global Non-Linear Minimization Solvers

Once in the editors for these unit operations, you'll see a dropdown menu called "External Solver", from which you can select the solver to be used:

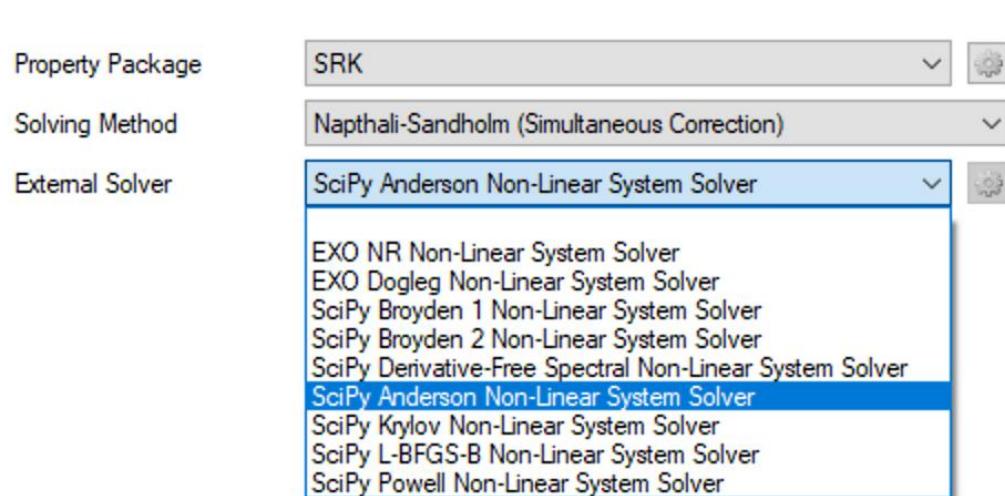


Figure 69 - External Solver selection

Besides being more reliable and having better convergence characteristics, the external solvers can be up to 3,5 times faster than the default open-source solvers, depending on the simulation characteristics and associated unit operation.

## 6. PROPERTY PACKAGES

### 6.1. Amines

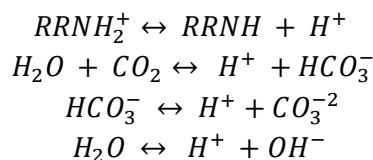
The Amines Property Package is used to model CO<sub>2</sub> and H<sub>2</sub>S capture processes with amines. The following amine compounds are supported:

- Monoethanolamine (MEA)
- Diethanolamine (DEA)
- Methyl Diethanolamine (MDEA)
- Piperazine (PZ)

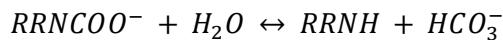
The DWSIM Pro implementation is based on a semi-empirical Kent-Eisenberg model (KEM) modified for estimating high-load equilibria at high-pressure (Humbul Suleman, 2021).

#### 6.1.1. Model Description

Various chemical reactions occur in the alkanolamine solutions to absorb carbon dioxide:



For Primary and secondary alkanolamines, another reaction (carbamate reaction) is added to the chemical system of reactions.



Equilibrium and Henry's constants are estimated based on an equation of the following form:

$$K_i = \exp\left(\frac{A_i}{T} + B_i \ln(T) + C_i T + D\right)$$

#### 6.1.2. Model Applicability Range and Limitations

The model is validated against the corresponding experimental data in the following ranges:

	MDEA	MEA	DEA
<b>Temperature (°C)</b>	<b>30 - 125</b>	<b>30 -120</b>	<b>30-120</b>
<b>Amine concentration (weight%)</b>	<b>5 - 50</b>	<b>5 - 80</b>	<b>10 - 45</b>
<b>Maximum tested CO<sub>2</sub> loading (mol CO<sub>2</sub>/mol amine)</b>	<b>1.56</b>	<b>0.85</b>	<b>1.1</b>

## 6.2. REFPROP

REFPROP is a computer program, distributed through the Standard Reference Data program of NIST, that provides thermophysical properties of pure fluids and mixtures over a wide range of fluid conditions including liquid, gas, and supercritical phases.

The REFPROP Property Package allows DWSIM Pro to request and receive thermophysical properties calculated by REFPROP.

## 6.3. Enhanced Property Packages

An enhanced/modified version of the Peng-Robinson Property Package is available for oil and gas industry simulations. It allows you to use a single property package to predict hydrocarbon gas/liquid properties, water/hydrocarbon mutual solubilities and pure water properties with improved accuracy (Whitson, 2013)).

DWSIM Pro also includes faster versions of the most popular property packages:

- Peng-Robinson (1978)
- Soave-Redlich-Kwong
- NRTL
- UNIQUAC
- UNIFAC
- Modified UNIFAC (Dortmund)
- Modified UNIFAC (NIST)

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