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55. Sim Dynamic Simulations

55.1. Introduction

HSC Sim has tools for dynamic calculations for both minerals processing and species type of units. There are also tools to collect data, set up different calculation scenarios, set deviation for different parameters and to create events based on discrete conditions.

55.2. Dynamic simulation as an initial value problem

Dynamic process simulation often involves the solution of differential equations. These equations, which describe how certain variables change over time, are solved as an initial value problem. An initial value problem is an ordinary differential equation, Eq. (1), together with a specified value, (t_0, y_0), called the initial condition, of the

$$y'(t) = \frac{dy}{dt} = f\big(t, y(t)\big) \tag{1}$$

unknown function $y(t)$ at a given point in the domain of the solution.

A solution to an initial value problem is a function y that is a solution to the differential equation and satisfies

$$y(t_0) = y_0. \tag{2}$$

Thus, simulating the dynamic behavior of a system frequently amounts to solving an initial value problem. The solution of an initial value problem is an equation that is an evolution equation specifying how the system will evolve with time, given the initial conditions.

55.3. Numerical methods

Some initial problems can be solved algebraically. However, for many of the differential equations we need to solve in the real world, there is no algebraic solution. On the other hand, even if we can solve some differential equations algebraically, the solutions may be quite complicated and thus are not very useful. In such cases, a numerical approach gives us a good approximate solution. As a result, we need to resort to using numerical methods for solving such differential equations. There are different numerical methods to solve an initial value problem. HSC Sim uses Euler's Method.
Euler's Method assumes our solution is written in the form of a Taylor's series:

$$y(t+h) \approx y(t) + hy'(t) + \frac{h^2 y'(t)}{2!} + \frac{h^3 y'''(t)}{3!} + \frac{h^4 y^{\mathrm{iv}}(t)}{4!} + \cdots \tag{3}$$

This gives us a reasonably good approximation if we take plenty of terms, and if the value of *h* is reasonably small. *h* is an increment of an independent variable and can also be denoted as Δt , i.e., as a time step.
For Euler's Method, we take the first two terms of the series.

$$y(t+h) \approx y(t) + h\frac{dy}{dt} \tag{4}$$

Euler's Method provides accuracy sufficient for most industrial applications. Another of its advantages is that it is fast and works well in computerized modeling.

55.4. Dynamic unit operation: mass and energy balance

The basis for the dynamic simulation in HSC Sim is the total mass, component, and energy balance equations:

$$\frac{dm}{dt} = m_{in} - m_{\text{out}} \tag{5}$$

$$\frac{dn_A}{dt} = F_{\text{A,in}} - F_{\text{A,out}} + G_A \tag{6}$$

$$\frac{dH}{dt} = V_R \frac{dP}{dt} + \sum_{i=1}^{N} F_i^0 \overline{H}_i^0 - \sum_{i=1}^{N} F_i \overline{H}_i + \dot{Q} \tag{7}$$

where m –mass; *H* -- the enthalpy which is a function of temperature, pressure, and composition; H_i – the partial molar enthalpy of species; V_R – volume; *P* – pressure; F_i – molar flow; and $\dot{Q}$ – heat flux.
These equations are automatically formed and solved by HSC Sim after the user has specified the operations in the dynamic unit.

55.5. Dynamic Calculation Settings

The goal of the HSC Sim dynamic simulation is to model the evolution of a system over time, as opposed to the static simulations that are used to simulate the system until convergence. Every dynamic calculation round (or timestep) simulates what happens in a single timestep (1 second, 3 seconds, 2 minutes, etc). Dynamic simulation can be applied to all kinds of units (reaction unit, a distribution unit, mineral processing DLL), however, some dynamic settings are supported only in a dynamic unit (dynamic units are described in 55.6. section).

Dynamic simulation of a flowsheet can be configured through the **"Dynamic Settings"** button in the upper toolbar (Fig. 1).

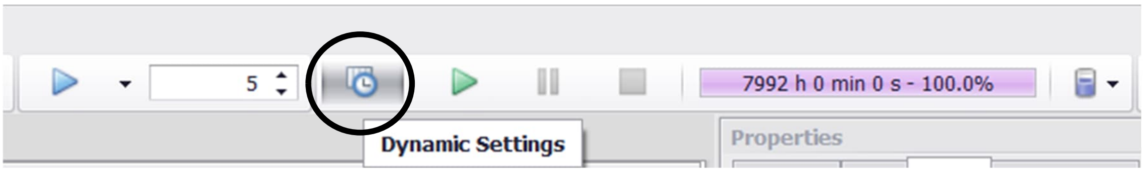

Figure 1: Dynamic Settings

Dynamic Settings allow for scenario configuration simulating the evolution of the flowsheet model over time. As opposed to the scenario editor in static simulation, dynamic settings allow for accurate control over time steps, simulation speed, delays, etc. The scenario is configured using various sheets.

Table 1: Sheets in Dynamic settings

Sheet Name	Description
Get sheet	Is used to collect data from flowsheets references.
Set sheet	Is used to assign specific values for flowsheets variables.
Event sheet	Is used to configure events and conditions under which a particular event happens.
Monte Carlo sheet	Is used to introduce stochasticity into a system that allows for the fluctuation of specified variables.
Tank level sheet	Allows to set the level of tanks in a unit *NOTE: This sheet should be used for the units that support tank simulation inside unit settings. Currently, Materials and Dynamic Units support tanks level control.*
Streams	Is used to introduce delays into streams, so that material enters the assigned destination after a specified time.

Dynamic settings consist of Run Options, Simulation Settings, Tank Levels, Data Settings, Monte Carlo, Chart Settings and Report Tools (Fig. 2).

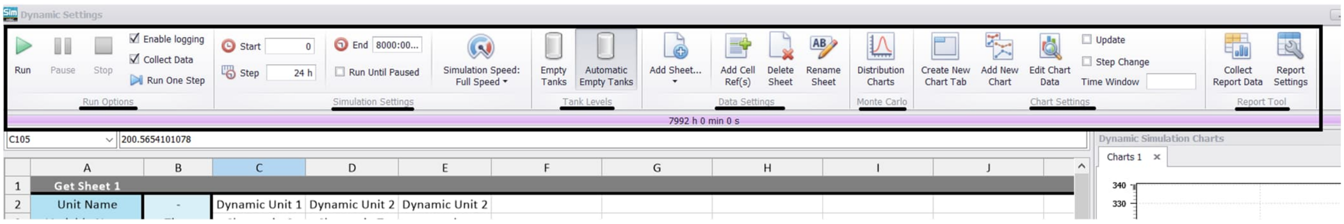

Figure 2: Dynamic Settings toolbar

Run Options

In the Run Options section (Fig. 3), dynamic scenarios for flowsheet simulation can be run with the **Run** button, paused with the **Pause** button, and stopped with the **Stop** button. Also, selecting the checkbox **Enable logging** allows log data to be viewed in the Log Viewer, and the checkbox **Collect data** enables the viewing of calculation data in the sheet at each timestep. Disabling the Collect Data and Enable logging options can prevent memory overload in case of long calculations. The **Run one step** option (or Alt + -> shortcut) allows for test running of a single timestep only.

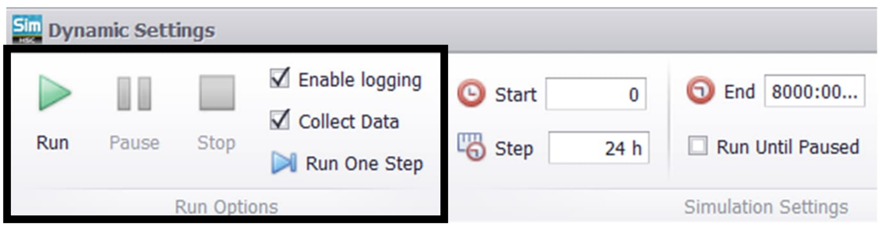

Figure 3: Run Options in Dynamic Settings

Simulation Settings

The timesteps can be specified in Simulation Settings (Fig. 4). The **Step** field corresponds to the timestep size in hours (h), minutes (min), or seconds (s). In the **Start** field, the beginning of the scenario simulation is specified in the same format as the step size. It is possible to either run the model until the Pause button is pressed by selecting **Run until paused** checkpoint or by specifying the end time in the **End** field in hours (h), minutes (min), or seconds (s). The speed of the simulation can be specified in the **Simulation Speed** selection list.

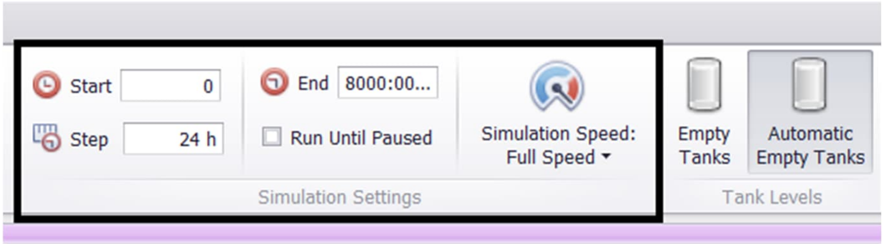

Figure 4: Simulation Settings toolbar section in Dynamic Settings. Here, full speed simulates the model at the full speed of the computer simulation. The simulation speed can also be changed to Real Time.

Tank Levels

NOTE: *These settings can be used for all units, but they affect the simulation only for the units that support tank simulation inside unit settings.*

The Tank Levels settings section allows for manipulations with tanks in units that support tanks logic. The **Empty Tanks** option is used to empty all the tanks in all the units of the flowsheet, and the **Automatic Empty Tanks** option will empty tanks before the calculation starts (flowsheet simulation will run with emptied tanks). The logic of tanks is explained in detail in the Dynamic Unit section.

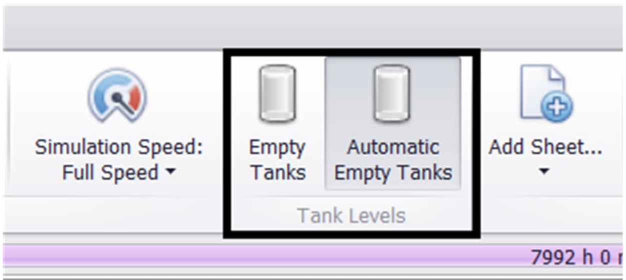

Figure 5: Tank levels toolbar section in Dynamic Settings. Automatic Empty Tanks is activated.

Data Settings

The Data Settings option is used to add sheets to the dynamic simulation scenarios. All the possible sheets that can be added are listed in Table 1. The **Add Sheet** option allows selection of a new sheet to add, **Rename Sheet** and **Delete Sheet** are used respectively to rename or delete the sheet that is currently active. The Option **Add Cell Ref (s)** is used to add a reference to a particular cell. This option is equivalent to the **Paste Cell Reference** that is done with a right click.

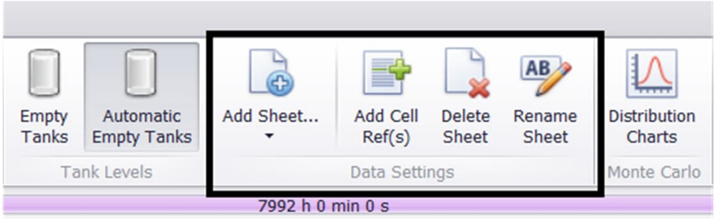

Figure 6: Data Settings toolbar section in Dynamic Settings

To add a sheet to the Dynamic Settings, **Add Sheet** should be pressed, and the desired sheet selected (Fig. 7).

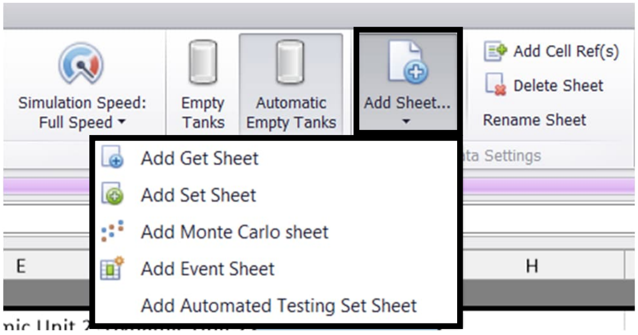

Figure 7: Add Sheet selection list

Chart Settings

The Chart Settings option (Fig. 8) allows visualization of dynamic simulation results. **Create New Chart Tab** allows the user to add separate chart tabs to the Dynamic Simulation Charts window (Fig. 9).

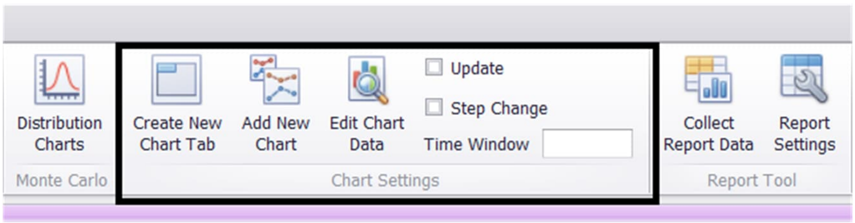

Figure 8: Chart Settings toolbar section in Dynamic Settings.

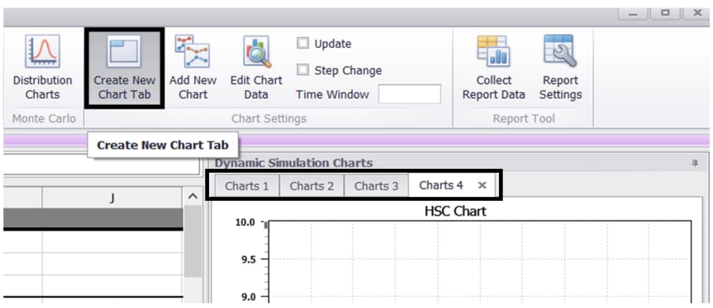

Figure 9: Adding a new chart tab in the Chart Settings section of the Dynamic Settings toolbar. In the Dynamic Simulation Charts window, 'Charts 1', 'Charts 2', 'Charts 3', and 'Charts 4' are separate chart tabs.

The **Add New Chart** option allows the insertion of a new chart within one chart tab panel (Fig. 10).

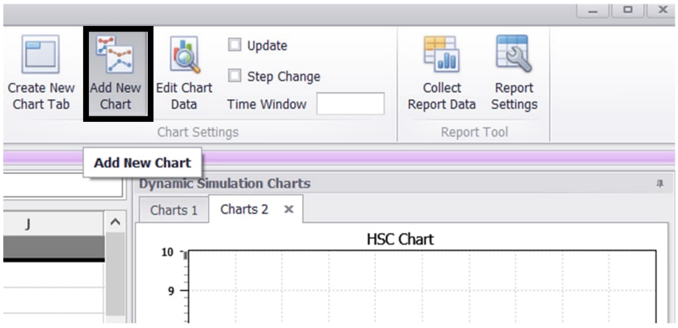

Figure 10: Add a new chart to a chart tab panel. New HSC charts can be added to the 'Charts 1' and 'Charts 2' tab panels.

The **Update** checkbox enables continuous updating of all the charts during a simulation run. The **Step Change** checkbox allows data representation in the form of a step function, in which Y-axis values are updated after each step, but not continuously. Fig. 11 and Fig. 12 show an example graph with an enabled and disabled **Step Change** checkbox.

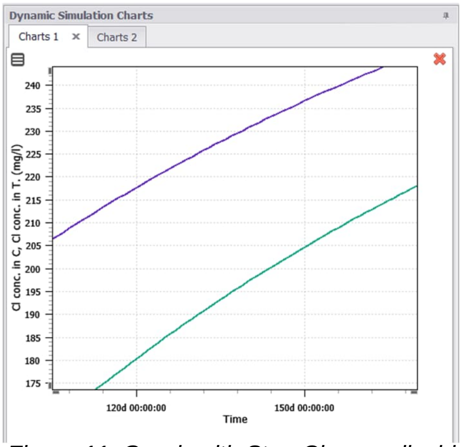

Figure 11: Graph with Step Change disabled.

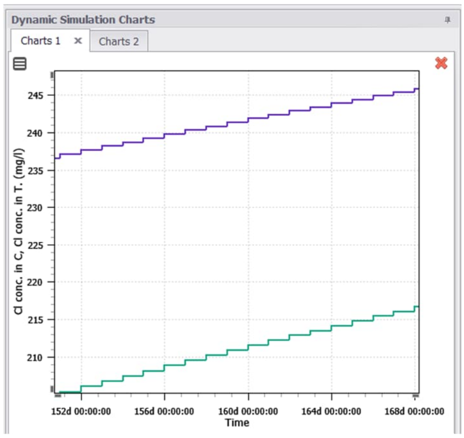

Figure 12: Graph with Step Change enabled.

A chart can be edited with the **Edit Chart Data** option. For each Chart tab, the chart properties can be specified in the Edit Chart Data menu for each graph (Fig. 13). By default, the column for the X-axis is for time, so only Y-axis data should be assigned in this menu. Also, charts can be edited with the Chart Menu button in the top left corner of the chart and deleted with the Close Chart button in the top right corner (Fig. 14).

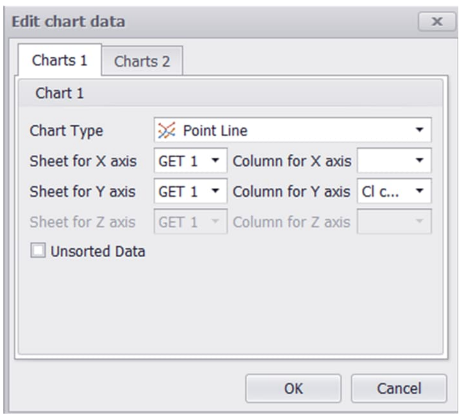

Figure 13: Edit Chart Data menu.

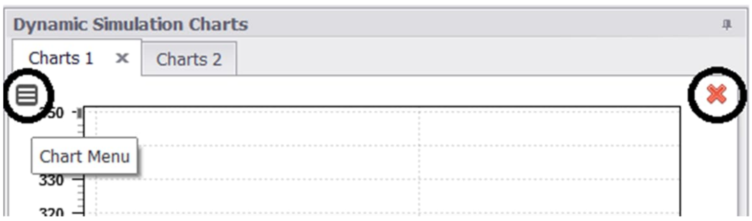

Figure 14: Chart menu in Dynamic Simulation Charts panel. Chart Menu button and Close Chart button are circled.

In the chart menu, the selected chart can be downloaded, copied, printed, or reformatted (Fig. 15). Also, there is an option called **Crosshair** that upon activation inserts a vertical line and the coordinates of the intersection points (Fig. 16).

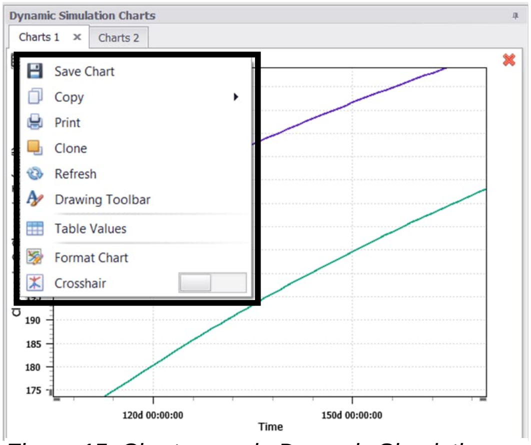

Figure 15: Chart menu in Dynamic Simulation Charts

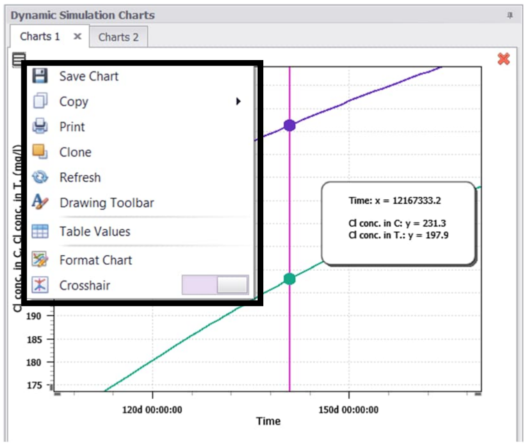

Figure 16: Crosshair tumbler in Chart menu

The chart style can be edited using the **Format Chart** option (Fig. 17).

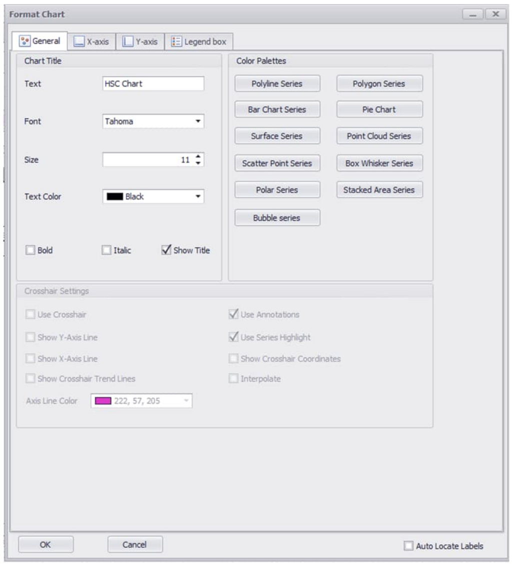

Figure 17: Format Chart option in Chart menu in a dynamic unit.

Report Tool

The Report Tool function (Fig. 18) allows the creation of a report about the results of a simulation by pressing the **Collect Report Data** (Fig. 19) option. In the Report Settings menu, the tanks and streams which are needed for the report can be specified.

Please note that collecting the report data may decrease the calculation speed.

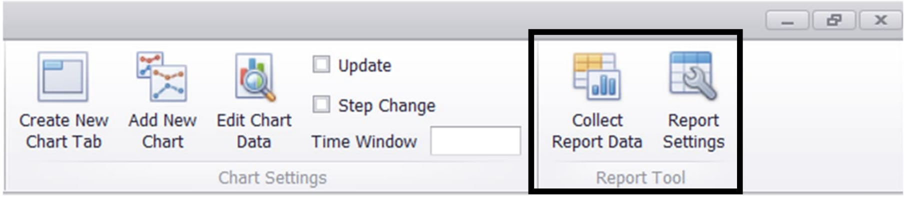

Figure 18: Report Tool section in Dynamic Settings.

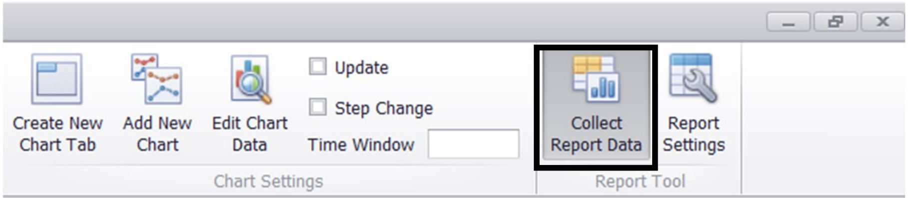

Figure 19: Collect Report Data option in Report Tool

55.6. Dynamic Calculation Unit

Dynamic Unit Overview

As opposed to static units (e.g., reaction unit, distribution unit, or minerals processing DLL), dynamic units support the accumulation of mass and energy within a unit. This is implemented by Tank logic, meaning that tanks serve as mass and energy storage inside a dynamic unit, and it is possible to perform specified operations with the accumulated material in the tanks.

Creation of a Dynamic Unit

A dynamic unit is created with the **Draw Dynamic Unit** option in the left-side toolbar (Fig. 20). As for other units, streams are added with the **Draw Streams** option in the same toolbar. The **Unit Editor** can be opened by double-clicking the unit (Fig. 21).

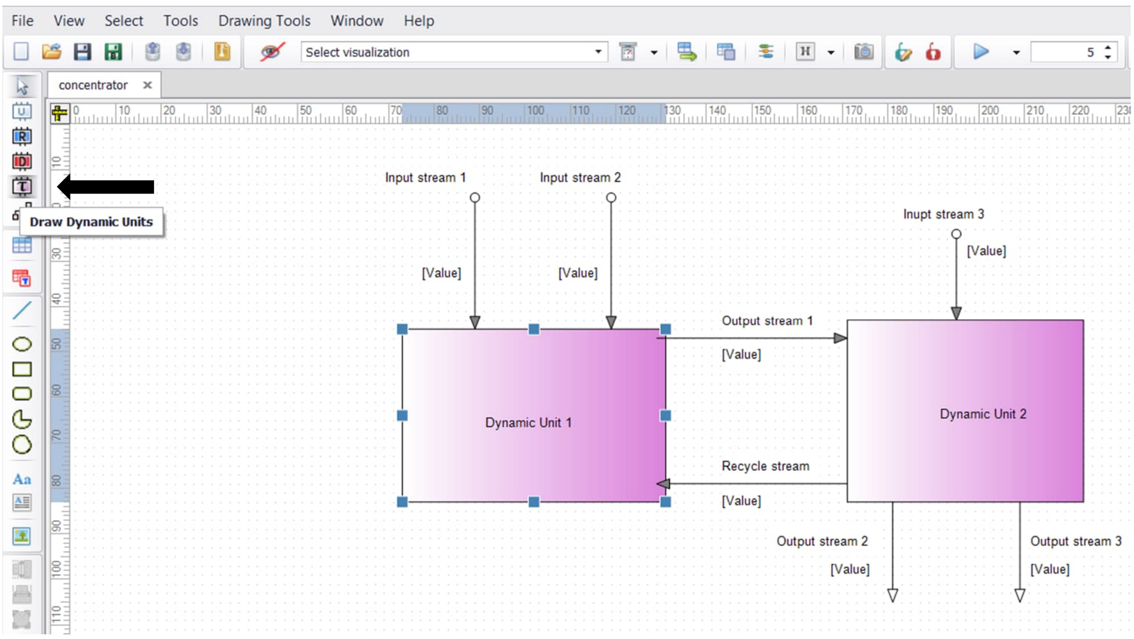

Figure 20: Creation of a dynamic unit

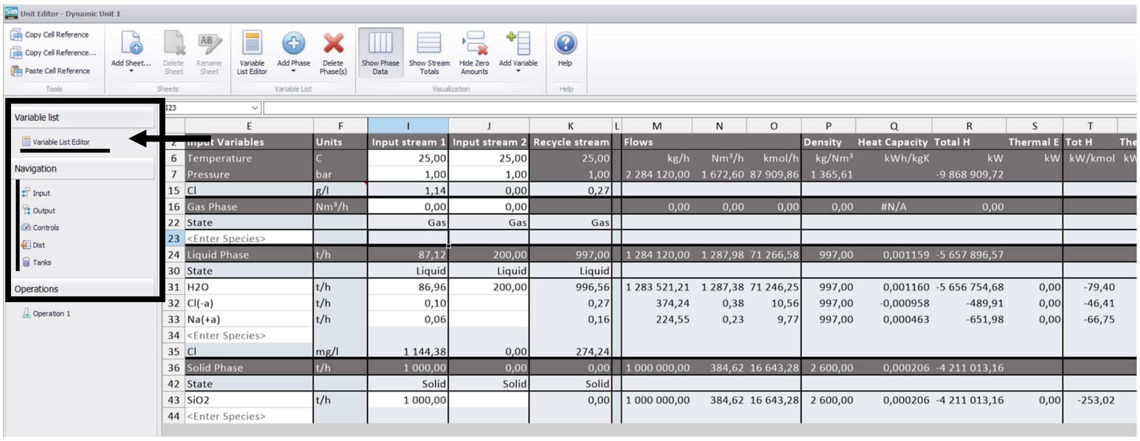

Figure 21: The main components of Unit Editor are the Variable list and various sheets, including Input, Output, Controls, Distributions, and Tanks sheets.

Unit Editor

Unit Editor allows the configuring of input and output streams, specifying tank and output stream distributions as well as tank configuration.

Variable List Editor in Dynamic Units

Species can be added with the help of Variable List Editor (Fig. 22) or inserted manually into the Input sheet. However, Variable List Editor provides very broad functionality and multiple additional variable options, so the usage of Variable List Editor is recommended. After the variables are added to the Input sheet either manually or through Variable List Editor, the species are transferred to the Output and Tanks sheets automatically as well as to other connected units.

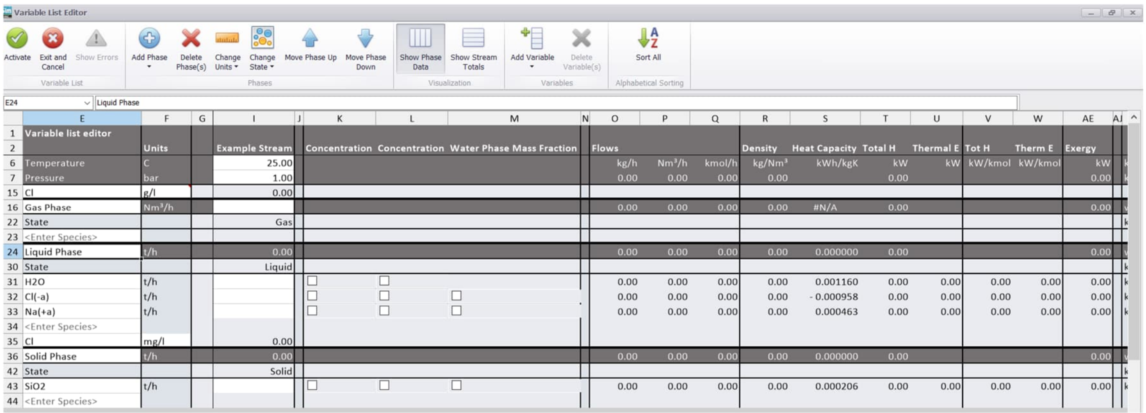

Figure 22: Variable List editor in Unit editor

Distribution of variables into phases in dynamic units

In a dynamic unit, all species are distributed into phases in all Input, Output, and Tanks sheets. So, while inserting species in the *<Enter Species>* field, there is no need to add solid (s), liquid (l), or gas (g) state to the species as it is for the reaction units. In a dynamic unit, species need to be allocated to the correct phase. However, for ion species the charge should be specified in brackets and aqueous species should be specified with (a).

In Variable List Editor, phases can be edited using the **Phases** upper toolbar section (Fig. 23). In order to activate the **Phases** toolbar, a cell in the phase needs to be selected with a left mouse click. Phases can be added with the **Add Phase** option, deleted with the **Delete Phase(s)** option, and the order of phases can be changed with the **Move Phase Up** and **Move Phase Down** options. Also, the measurement units of a phase can be changed with the **Change Units** option. In a dynamic unit, the phase amounts can be measured in percentages (as for distribution units) or in absolute mass (the same as for reaction units).

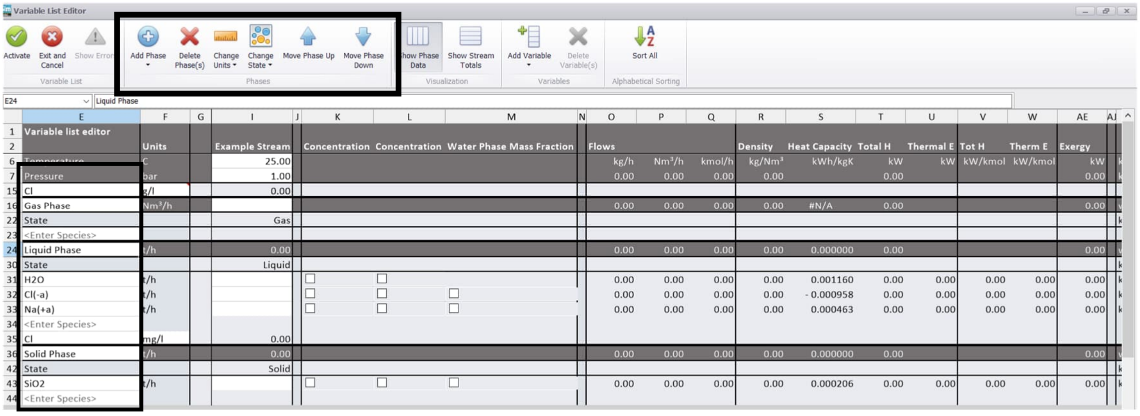

Figure 23: Edit phases in Variable List Editor within Unit Editor

Variables in Dynamic Unit

Apart from species, many other variables can be added using **Variable List Editor**, e.g., element or species concentration, heat or electricity flow, etc. Importantly, it is critical which row is selected when adding a new variable, because the new variable is added to the phase that is currently selected (e.g., a new variable is added to the Gas Phase in Fig. 24). In order to add a new variable to all phases, any variable common to all phases should be selected when adding a new one, e.g., Pressure in Fig. 24. A variable can be deleted with the **Delete Variable(s)** option when the corresponding cell is selected (Fig. 25). A complete list of available variables is presented in Table 2 and Table 3.

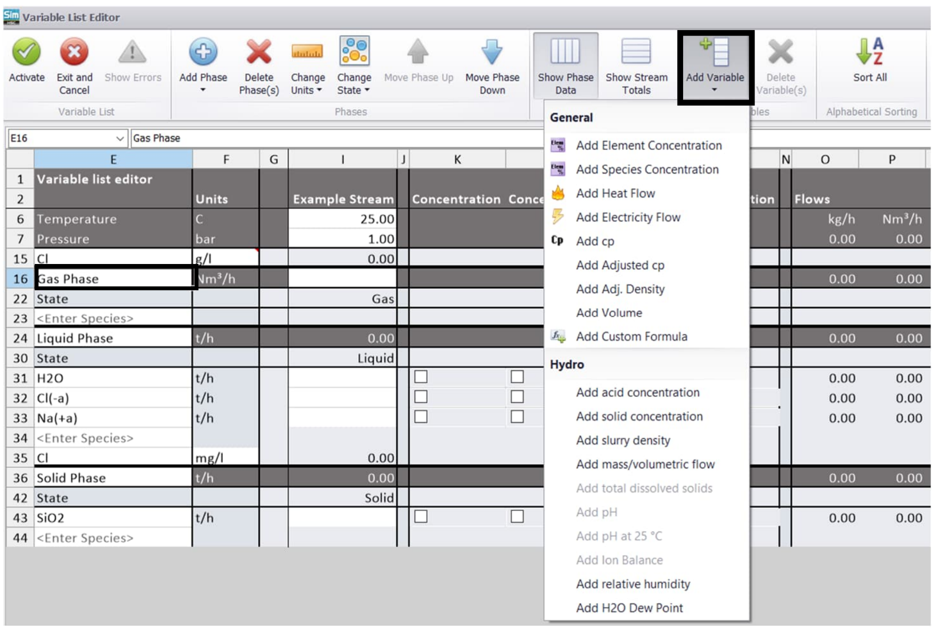

Figure 24: Adding a new variable. Here, the gas phase is selected, so the new variable will be added to the gas phase.

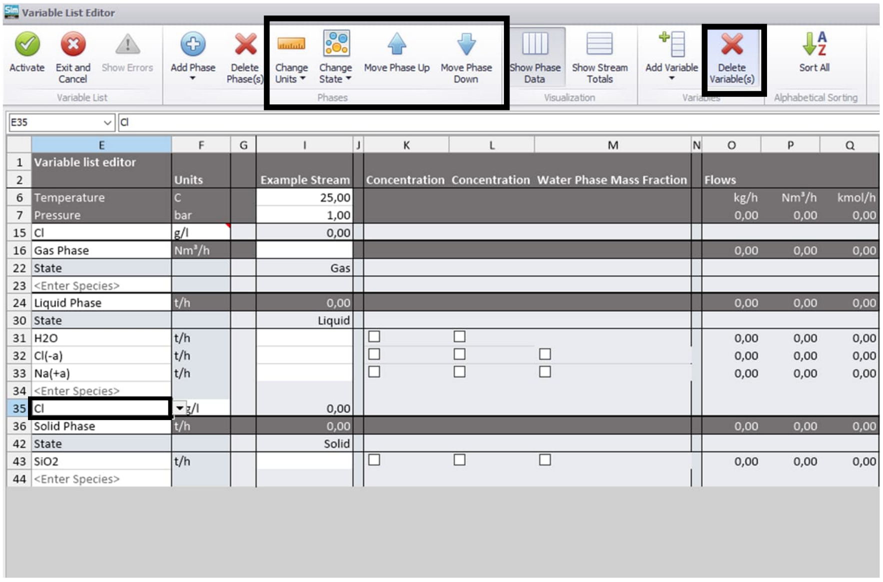

Figure 25: Delete Variable and edit phases options in Variable List Editor.

Also, a phase's state, units, and order can be edited with the Phases section of the upper toolbar (Fig. 25). In order to edit phases, any state variable can be selected.

Table 2: Complete list of general variables in Variable List Editor within Dynamic Unit Editor.

General Variables	Description
Element Concentration	Can be added to any phase, an element is selected after adding a new variable (Fig. 26). The concentration for a particular element can also be added by selecting the checkboxes shown in Fig. 28. *NOTE: Concentration is calculated for a selected phase. If the selected cell is within common variables, the total concentration is calculated.*
Species Concentration	Can be added to any phase; species are selected after adding a new variable (Fig. 27). *NOTE: Concentration is calculated for a selected phase. If the selected cell is within common variables, the total concentration is calculated.*
Heat Flow	Heat flow variable can be used to input or extract heat from the unit. Usually this is used to calculate heat losses, cooling or heating effect of the indirect heat exchanger modeled as a separate unit. *NOTE: Heat loss value can be added only to streams that do not contain mass flow.*
Electricity Flow	The electricity flow variable can be used to input or extract enthalpy from the unit.

	Electricity flow differs from Heat flow only in the way exergy is calculated.
Cp	Average Cp shows the heat capacity of the water phase at average NTP temperature (20 °C) and stream temperature. This is used to show the Cp value that can be compared to the adjusted average Cp variable.
Adjusted Cp	Adjusted average Cp is used to change the Cp value from the calculated value. Adjusted average Cp is a constant Cp value throughout the temperature range. The average Cp variable is calculated in the same way as the adjusted average Cp variable and therefore they are comparable with each other. When there is a value in this cell, it is used in the calculations. If there is no value, the calculated Cp is used instead. This value needs to be entered manually for all streams.
Adjusted Density	Adjusted density is an overwriting variable for the calculated density. The value of the adjusted density needs to be added manually to the streams. If this cell is not filled, the original calculation is used.
Volume	Ideal gas volume uses gas phase flow information, temperature, and pressure to calculate the volume flow of the gas phase with the ideal gas law formula.
Custom	This type of variable adds an empty cell to the variable list, where any formula can be typed. This cell needs to be filled individually in every unit.

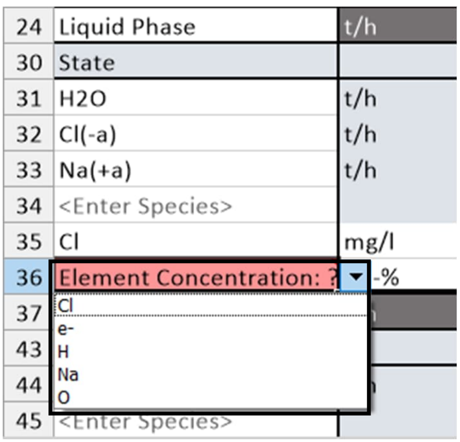

Figure 26: Selection of element in Element Concentration variable

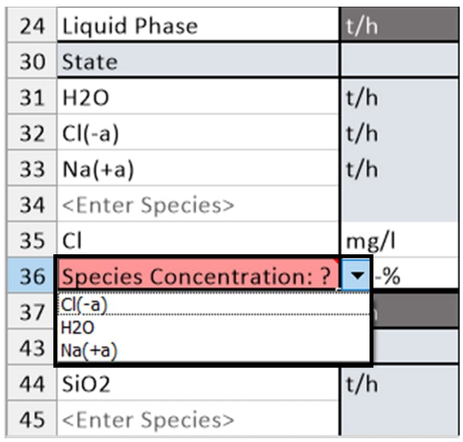

Figure 27: Selection of species in Species Concentration variable

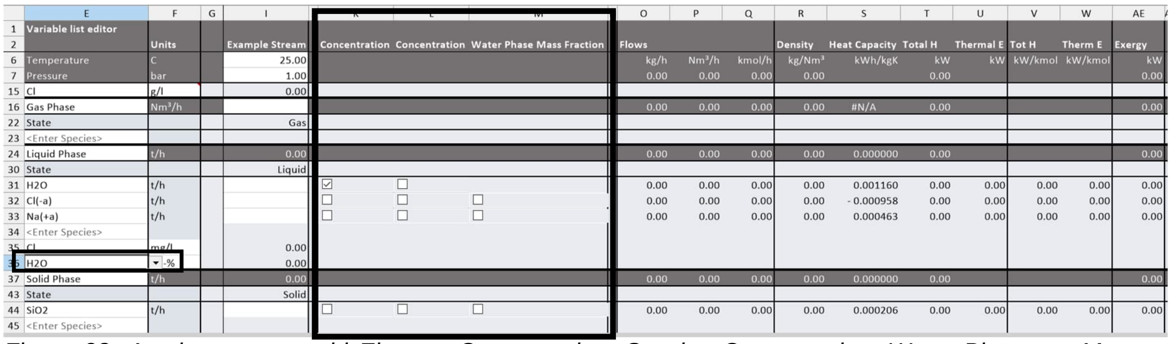

Figure 28: Another way to add Element Concentration, Species Concentration, Water Phase, or Mass fraction variables. Here, by activating the Concentration checkbox for the H2O, the new H2O concentration variable is added to the Liquid phase list of variables.

Table 3: Complete list of Hydro Variables in Variable List Editor within Dynamic Unit Editor.

Hydro Variables	Description
Acid concentration	Calculates the acid concentration in a phase. The compounds (H2SO4, HCl, or HNO3) that are used to calculate the acid concentration can be chosen afterwards.
Solid concentration	Calculates the solid concentration in a phase.
Slurry density	Slurry density is calculated using all water, solid, organic, and particles phases in the model.
Mass/Volumetric flow	Flow of material in mass or volumetric measurement units.
Total dissolved solids	Total dissolved solids use the H2O compound and assume everything else in the water phase to be dissolved solids.
pH	pH calculation uses the compounds H(+a) and OH(-a) and stream temperature to calculate the pH at the stream temperature. *NOTE: The pH value is not temperature compensated, it is the pH at the stream temperature. This uses $K_w(T)$.* *NOTE: Laboratory equipment often gives the pH reading as converted to 25 °C temperature and this variable gives pH at the stream temperature.* *For acidic solutions, the effect of temperature is significant only in very dilute solutions, but for basic solutions the effect is significant in all concentrations.*
pH at 25℃	pH calculation uses the compounds H(+a) and OH(-a) and stream temperature to calculate the pH. This uses K_w(25 °C). *NOTE: Laboratory equipment often gives the pH reading as converted to 25 °C*

	temperature and this variable makes the same conversion. For acidic solutions, the effect of temperature is significant only in very dilute solutions, but for basic solutions the effect is significant in all concentrations
Ion balance	Ion balance uses all ions in the water phase and shows the possible offset of anions and cations. A null value for this variable means that there is an equimolar number of anions and cations in the solution.
Relative humidity	Relative humidity uses only the H2O(g) compound, the stream temperature, and pressure in the calculation and assumes everything else in the gas phase to be air.
H2O dew point	H2O dew point uses the H2O(g) compound and stream temperature in the calculation. Shows the dew point of water at the stream temperature.
Mass Fraction	Mass fraction is used to calculate aqueous solution density. The phase is always the water phase. It is recommended to first select the compound from the variable list, the box on the right, and then the compound from the database, the box in the middle. Available compounds in these boxes are filtered according to the other selection. For example, Na(+a) ions in the variable list to be Na2SO4, all Na(+a) ions are assumed to be Na2SO4. In cases when you also have another sodium compound like NaOH and you want to specify that also, it is recommended to use, for example, NaOH(a) compound to enable the specification of both sodium-containing compounds in the same variable list.

After all the variables have been specified, they can be activated with the **Activate** button or discarded with the **Exit and Cancel** option.

Input sheet in Dynamic Unit

After the variables have been added, the input sheet can be configured by inserting initial values for the variables (Fig. 29). Apart from adding variables, the visualization section in the upper toolbox provides the opportunity to visualize the data. **Show Phase Data** allows the visualization of additional information about phases, including Flows, Density, Heat Capacity, etc., and the **Show Streams Totals** option inserts total amounts into the common variables section (Fig. 30). Also, the **Hide Zero Amounts** option hides the variables and their values if they equal zero, which can be convenient when dealing with many species.

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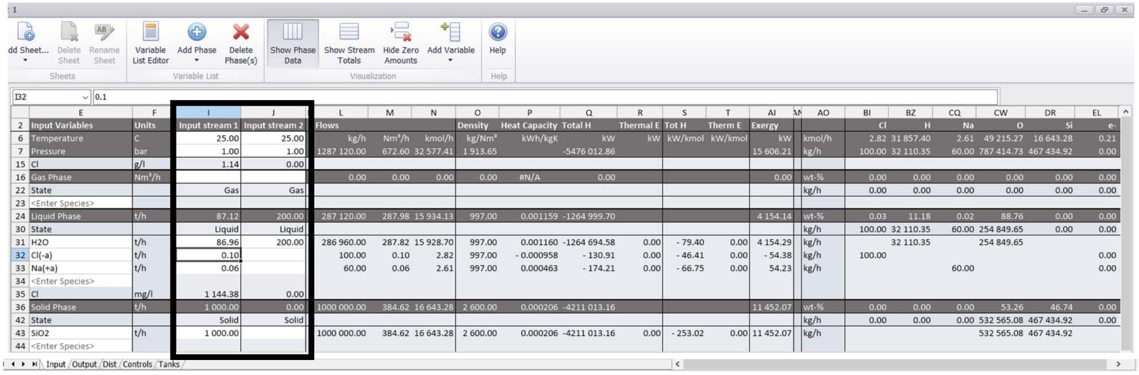

Figure 29: Input sheet in a Dynamic Unit. Examples of initial values for input streams are highlighted.

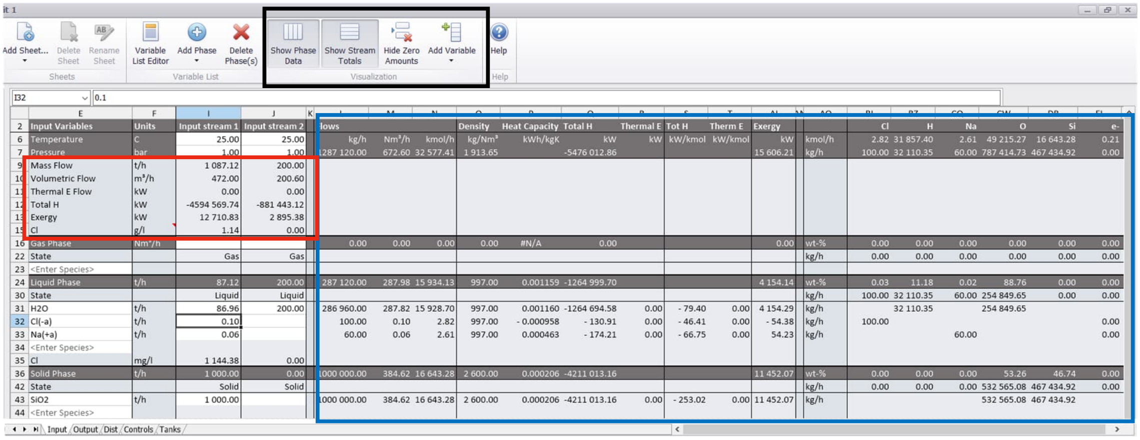

Figure 30: Visualization options for input and output sheets. Streams totals are highlighted in red, while phase data is in blue

Output sheet in Dynamic Units

All added variables are automatically transferred into the Output sheet of the dynamic unit and connected units.

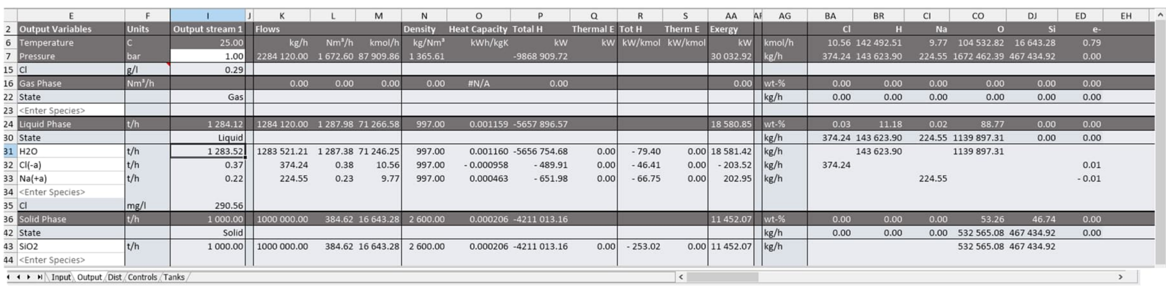

Figure 31: Output sheet in a Dynamic Unit

Dist sheet in Dynamic Units

In the distribution sheet (or Dist sheet), all the inputs can be distributed into output streams and tanks. The distribution sheet makes it possible to perform operations with different inputs within the tank.

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	Tank 1	Output stream 1
Input stream 1	0	100
Input stream 2	0	100

Input / Output / Dist / Controls / Tanks

Figure 32: Dist sheet in a Dynamic Unit. Here, 100% of the inputs are assigned to the output stream, meaning that all material goes to the output, not to Tank 1.

Tanks sheet in Dynamic Unit

Tanks serve as the material and energy storage inside a dynamic unit.
As in the input and output sheets, in the Tanks sheet the species are distributed into phases.

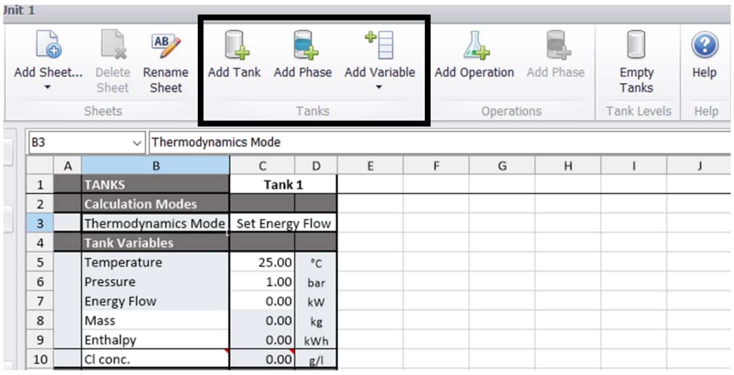


Figure 33: Tanks section in Tanks sheet within Dynamic unit

A tank can be added by pressing the **Add Tank** option in the Tanks section of the upper toolbar (Fig. 33). A new phase can be added by the **Add Phase** option that serves as a tanks-specific phase and is not transferred to either input or output. For every phase there is a **State Type** field (Fixed or Float), which means whether phase transitions are possible (float) or not (fixed). In the case of a float phase, the melting or boiling temperatures need to be specified as well (Fig. 35). Variables can be added with the **Add Variable** option to either Tank Variables (which are common for all phases) or phase-specific variables. All the variables related to tanks are listed in Table 4.

At all times, the dynamic unit automatically tracks the energy balance inside the units. This means that either the energy or the temperature inside the tanks changes automatically. The user can define which variable (energy or temperature) changes during the calculation by using the **Thermodynamic Mode** option. By default, the thermodynamic mode is set as **Set Energy Flow**. If the thermodynamic mode chosen is **Set Temperature**, the temperature remains constant during the calculation, and the energy is adjusted.

Within each tank, different operations can be performed with all materials of any phase that are sent to the tank. Operations can be added by pressing **Add Operation** in the Operation section in the upper toolbox (Fig. 36); a new Operation sheet will be added, and the operation will be added as a variable to the tank's phases (Fig. 35). As can be seen from Fig. 34, the operation variable serves as the operation rate in percentages of the phase materials that are to be involved in the operation. For example, as shown in Fig. 34, operation 1 is performed with 60% of the liquid phase of the tank 1.

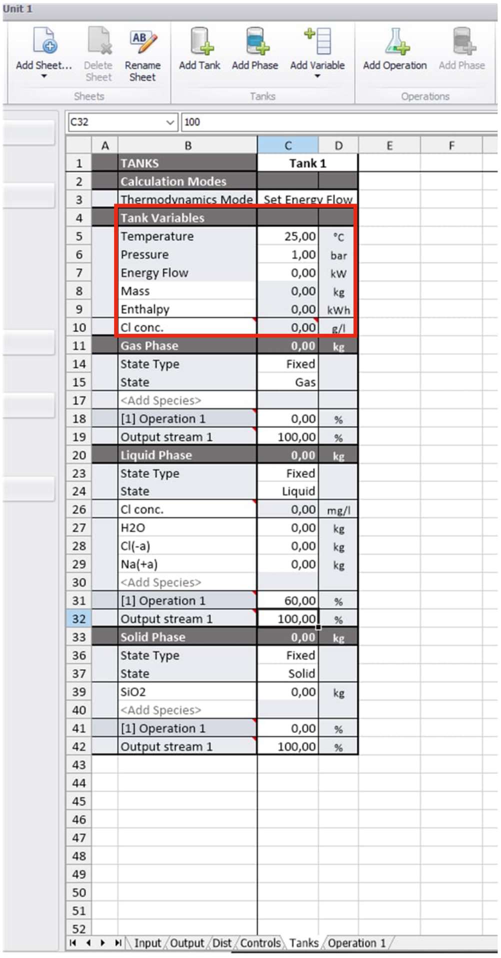


Figure 34: Tanks sheet with Operation in a dynamic unit. Here, tank variables that are common for all phases are highlighted.

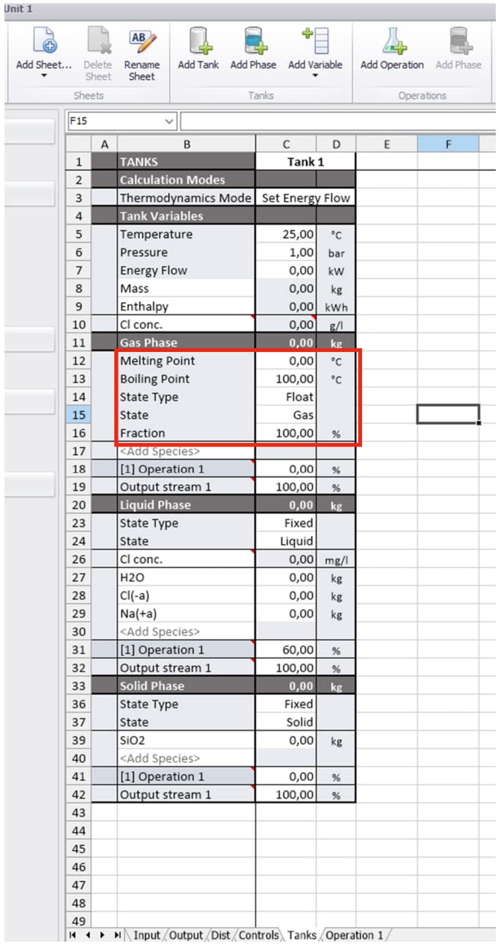


Figure 35: Tanks sheet in a dynamic unit. Here, the gas phase has the state type Float.

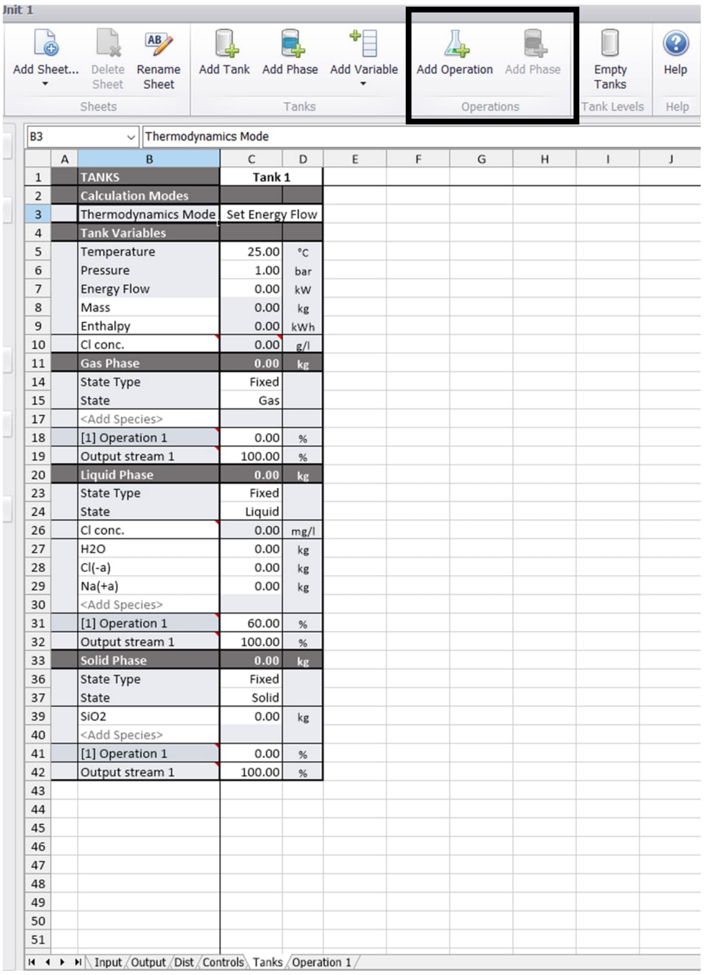


Figure 36: Adding Operation in Tanks sheet within a Dynamic Unit. Here, the Operation 1 sheet is created by pressing Add Operation, and after adding the operation, it becomes visible in the Tanks sheet as well.

Table 4: Tank variables in Tanks sheet of a Dynamic Unit

Tank level and Overflow variables	Description
Allow Empty Tanks	OFF or ON modes. Allows the emptying of only particular tanks before each calculation run by turning OFF this variable for the tanks that are supposed to stay filled.
Tank Level	Sets the particular level of a tank. Can be useful when a particular action needs to be performed at a certain tank level.
Tank Size	Sets a tank to be of a particular size. By default, a tank's size is infinite. If the tank is full, the excess exits via overflow.
Overflow Priority	Phase-specific variable that is used to specify which phases overflow first. Phases with a low priority number overflow before phases with a high priority number.
Overflow Amount	Goes hand in hand with Tank Size. If a tank is full, the overflow amount will be shown.
Overflow destination	Is used to specify the destination of the overflow amount.

Water Vapor Balance	Is used as a mechanism to simulate the vaporization of water, keeping the relative water humidity of the gas at 100%. *NOTE: It is possible to use Water Vapor Balance in combination with Calculate Gas Pressure and Shared Gas Tank variables.*
Calculate Gas Pressure	Is used to consider pressure changes after water evaporation. Also, it pressurizes the gas when there is no vapor balance configured. *NOTE: The Calculate Gas Pressure variable only works when the tank size is specified.*
Shared Gas Tank	Is used to assign one of the tanks as a shared gas tank for all other tanks, i.e., the other tanks are connected so that the gas is mixed for all tanks.

Operations sheet in Dynamic Units

Operations sheets establish the operations that are performed in the tanks. The input for the operations is set in the Tanks sheet, while the operation itself and the output distribution are described in separate Operation sheets. The operation could be of various types, including reactions, element distribution, ideal mixer, ideal heat mixer, chemical equilibrium, and species converter.

- **Reactions** operation is executed similarly to the hydro (reaction) units in which the chemical reactions are defined.
- **Ele dist** (Element distribution) operation is based on the distribution of elements in the same way as it is for pyro units.
- **Species Converter** provides conversion analysis between elements and species.
- **Ideal mixer** allows for mass and heat mix/transfer between tanks.
- **Ideal heat mixer** allows for heat transfer only; the mass remains within the initial tank.
- **Chem EQ** (chemical equilibrium) operation simulates the equilibrium of the system.

In the following sections, these operation types are covered in more detail.

Initialization of operations in the tanks

The **Add Operation** option in the Operations toolbar section (Fig. 37) allows the addition of a new operation. A new phase can be added with the **Add Phase** option. This newly added phase will be transferred to the tank's phases in the Tanks sheet if the material of this phase is produced during the simulation (but also if the return mode (see Table 5) is NOT advanced). Otherwise, this new phase serves as an operation-specific phase.

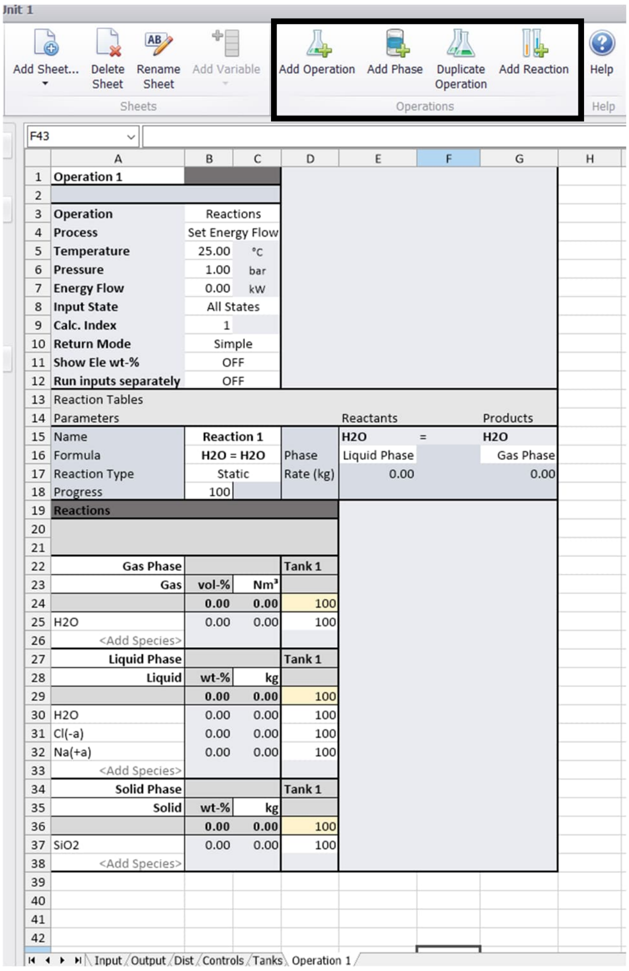


Figure 37: Reactions operation sheet in a dynamic unit. Here, Reaction 1 is added by default, and more reactions can be added with the Add Reaction option.

The **Duplicate Operation** option creates an identical copy of the current operation as a new Operation sheet. The **Add Reaction** option works only with the Reactions type of operations, and it adds a new reaction to the **Reaction Tables** in the reaction operation sheet. A complete list of operations for parameters for all operation types is presented in Table 5.

For all operations, the operation output distribution can be specified in the section highlighted in Fig. 38. Most importantly, all the operation products should be assigned to go back to tanks so that 100% of all input material is distributed back into some tank.

For example, as can be seen from Fig. 38, after Operation 1 has been performed, all the reaction products will be equally distributed to Tank 1 and Tank 2. If the sum of percentages returned to the tanks is not equal to 100%, the values will be normalized so that all the material is returned to the tanks.

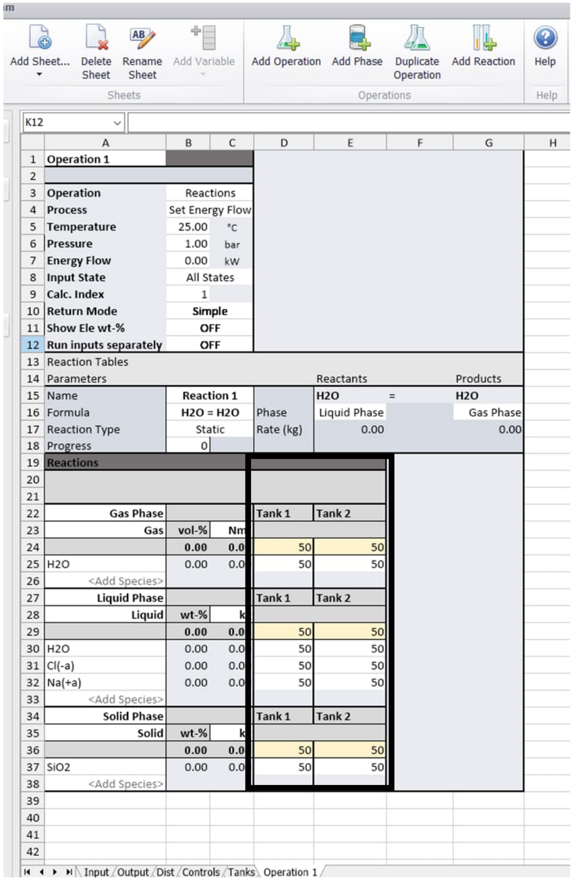


Figure 38: Operation sheet in a dynamic unit. Here, in the highlighted area, the reaction products' destination is defined as 50% of the reaction output species going to Tank 1 and the remaining 50% of the reaction output going to Tank 2.

Table 5: Parameters of operations in tanks in Dynamic unit

Operations parameters	Description
Operation	Is used to set the type of operation.
Process	Energy Flow or Set Temperature. Energy Flow mode allows for temperature adjustment, while Set Temperature mode calculates the required energy flow for a specified constant temperature.
Temperature	Is used to set temperature in *°C* or *°K*
Pressure	Is used to set pressure in *bar*
Energy Flow	Is used to set the energy in *kW*
Input State	This parameter establishes which phases are involved in the operation, e.g., solids only, liquids only, etc.
Calc. Index	The order of operation execution. For example, assuming that there are several operations inside the tank, if the calculation index for all operations is 1, the operations will be performed simultaneously. Otherwise, if operations are numerated sequentially, they

	will be executed one by one starting from the smallest number.
Return Mode	Simple or Advanced. Advanced mode allows species to be moved between phases when returning them to the tanks. In Simple mode, species that are in a specific phase are always returned to the corresponding phase in the tank.
Show Ele wt-%	ON or OFF modes. If ON, shows elemental distribution in the operation's output.
Run inputs separetely	ON or OFF modes. Variable specific for Chem EQ that allows calculation of activity coefficient estimates of elements in chemical equilibrium based on the specified target concentration.
AC Back calculation	ON or OFF modes. Variable specific for Chem EQ that allows to calculate activity coefficients estimates of elements in chemical equilibrium based on the specified target concentration.
Constraints	ON or OFF modes. Variable specific for Chem EQ (chemical equilibrium) type of operations. If ON, Error handling allows calculation of the system with or without constraints.
Exact O (H) measurement	ON or OFF modes. Variable-specific for species converter type of operations. If ON, it allows specification of the amount of Oxygen (Hydrogen) as the exact or minimum amounts entered. For more details, please visit the *Species Converter Module* page.

Reactions type of operation

A reactions type of operation works similarly to the reactions (hydro) unit. A new reaction can be added to the **Reaction Tables** in the Operation sheet (Fig. 39). For each reaction in the reaction table, the reaction details are specified, including Formula, Progress, and Reaction Type.

The reaction's formula should be specified in a way that reactants and products are separated by '=', and for liquid, solid, and gaseous phases the phase types is selected in a special field. **Progress** (in %) is the percentage of the operation's input involved in the reaction. The **Reaction type** can be *Static, Dynamic, or Equilibrium.*

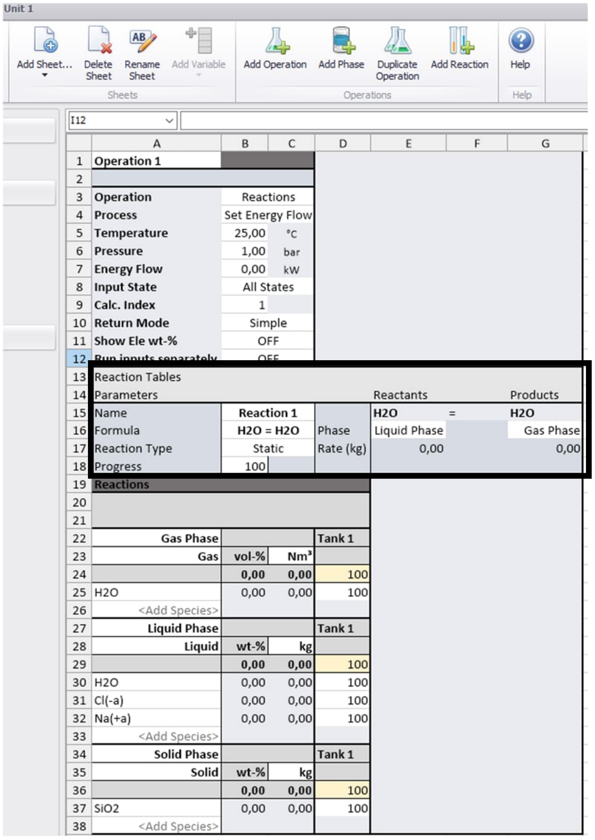


Figure 39: Reaction type of operation in a dynamic unit.

Overall, the difference between static and dynamic reactions is that static reactions happen in one direction, meaning that reactants are converted into the products of the reaction. On the other hand, dynamic reactions can happen in both directions depending on the initial volume of the reactants and products. Thus, in dynamic equilibrium both reaction rates become the same (or almost the same), while the static reaction equilibrium refers to a state of the system in which there are no reactants left to be turned into reaction products.

Static reactions use **Progress** % to calculate how much of the first reactant is consumed in the reaction. However, if there is not enough of the other reactants, the reaction will stop when one of the reactants is totally consumed. Reactions happens from top to bottom row-wise.

The dynamic reaction calculations are simulated with the following *Arrhenius Equation* (Fogler, 2010) for the reaction rate constant for the specified temperature:

$$K(T) = k_a * e^{\left(\frac{1000*E_a}{R}*\left({}^{1}/_{T_0}-{}^{1}/_{T}\right)\right)}$$

where K(T) – is the specific reaction rate, k_a – is the frequency factor, E_a – is the activation energy (in kJ), T_0 – is the rate constant temperature in °C.

In dynamic units, all the parameters for the dynamic reaction are specified in the reaction tables (Fig. 40). Also, the **Reference Volume**, which is the volume used for the reactant concentration calculations, should be specified. The reactant concentration is calculated with the following formula (Fogler, 2010):

$$C[Reactant] = \frac{AC*Mol}{RefVol},$$

where C – is the concentration, AC – is the activity coefficient of the reactant, Mol is the target species amount in Moles, and RefVol is the Reference Volume value.

A reference volume can be chosen as the tank volume of Liquid, Gas volume or Custom volume value. The Custom volume should be then defined in the **Custom Vol** field.

The dynamic reactions are simulated by applying numerical computational methods (Runge-Kutta, Euler or Heun's methods) that can be specified with the **ODE method** option, and the number of ODE steps can be defined with the **ODE Steps** option. These options become visible when the dynamic reaction type selected is **Dynamic reaction** or (dynamic) **Equilibrium**. As a result, during the calculation, every timestep is split into sub-steps (dt) based on the specified ODE step value, and then the chosen ODE method is applied to each sub-step (Fig. 40, Fig. 41).

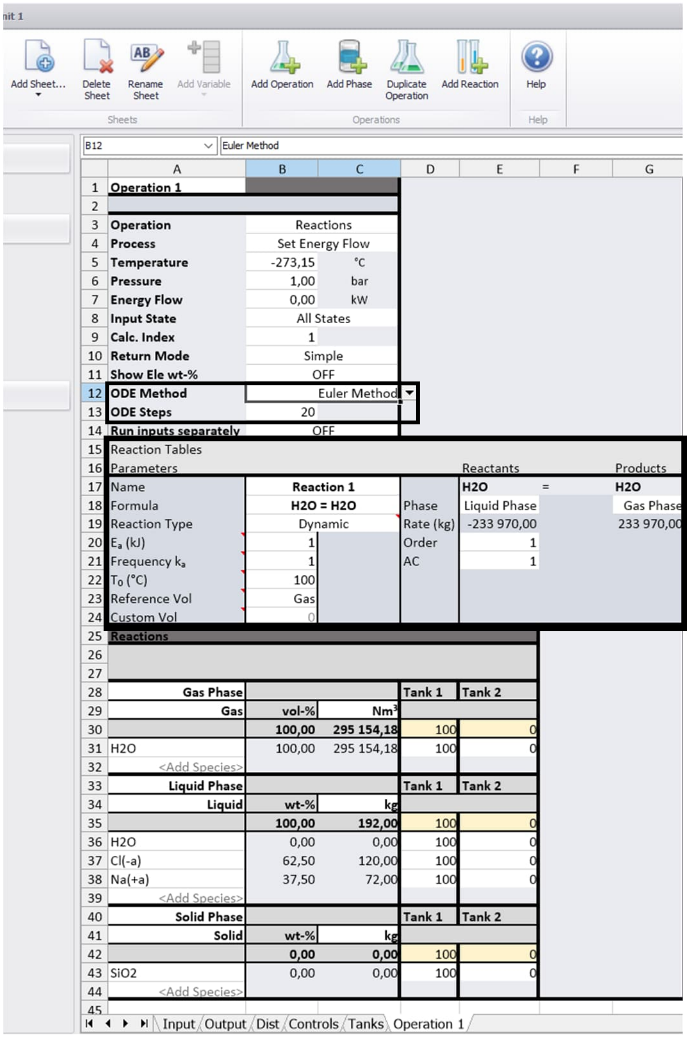


Figure 40: Dynamic type of reaction operation in a dynamic unit. Here, the dynamic reaction type is selected, and the method of solving the differential equation of dynamic reaction is highlighted.

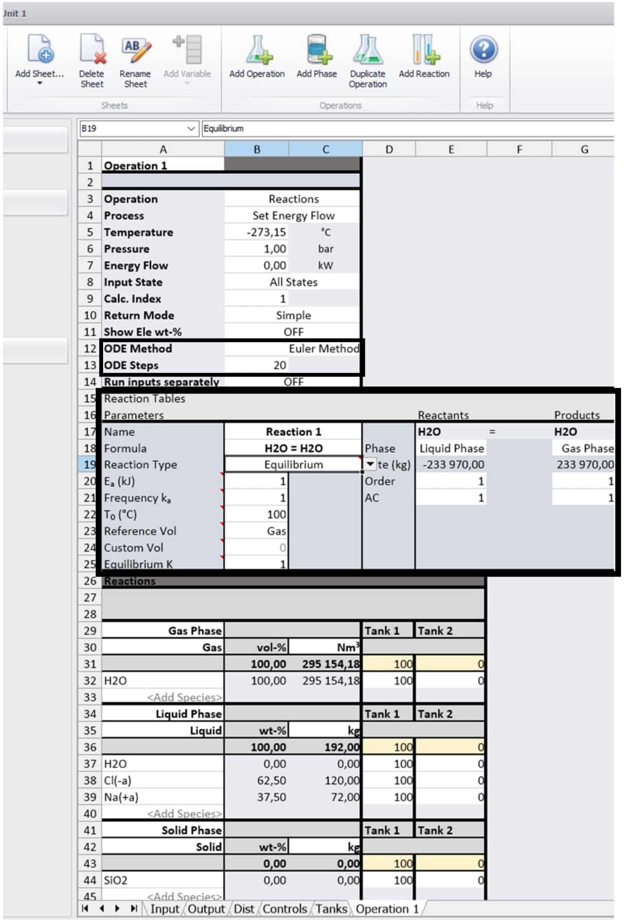


Figure 41: Equilibrium type of eaction operation in a dynamic unit. Here, the reaction type selected is Dynamic equilibrium, and the method of solving the differential equation of dynamic reaction is highlighted.

After the reactant concentration is calculated, the product concentration is calculated in accordance with the Power Law model using the following equation:

$$C[Product] = C[Reactant_1]^{Order1} * C[Reactant_2]^{Order2} * \dots * C[Reactant_N]^{OrderN},$$

where C - is the concentration, and the Order of the reactant is specified in the Order field for each reactant in the reaction.

The final formula for the **Dynamic** reaction type for the reaction rate for a reactant is the following (Fogler, 2010):

$$Rate_{Reactant_i} = K(T) * C[Product] * RefVol * \frac{a_i}{|a_1|}$$

where $RefVol$ is the reference volume for the current state of the system, and a_i - is the i^{th} reactant's coefficient in the reaction.

Meanwhile, for the **Equilibrium** reaction type, the product concentration is calculated separately for the reactants with a positive concentration $C_+[Product]$ and negative concentration value $C_-[Product]$.

Then, the reaction rate can be written as follows (Fogler, 2010):

$$Rate_{Reactant_i} = K(T) * \frac{(C_+[Product] - C_-[Product])}{K_{eq}} * RefVol * \frac{a_i}{|a_1|}$$

where K_{eq} is the equilibrium constant that is specified only for the reaction of Equilibrium type.

NOTE: Reference Volume should not be zero. In order to prevent that, make sure that the amount in the input sheet for the reference volume species is not specified with zero value.

Chem EQ type of operation

Equilibrium calculations are based on Gibbs free energy minimization problem. Activity coefficients for Gibbs free energy can be either specified for mixed phases (Fig. 42) or estimated with **AC Back Calculation** option under possible **Constraints** (Fig. 43).

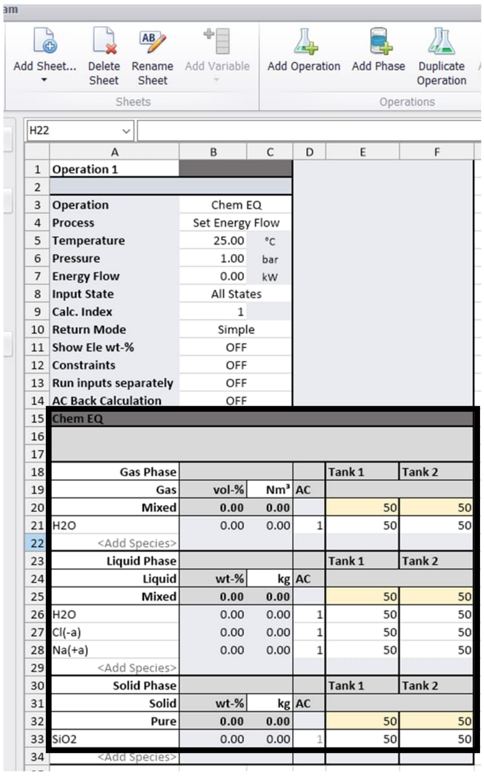


Figure 42: Chemical equilibrium type of operation in a dynamic unit. Here, the activity coefficients are specified for mixed phases. The AC back calculation is OFF.

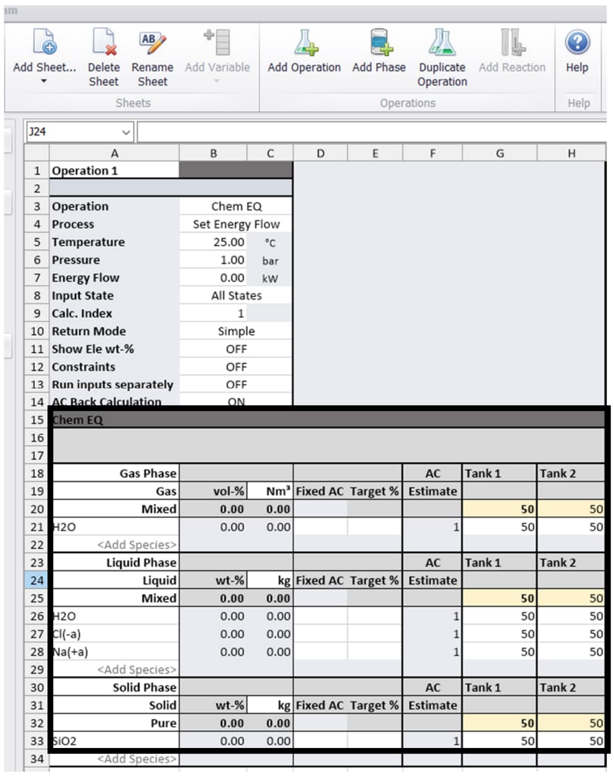


Figure 43: Chemical equilibrium operation in a dynamic unit. Here, the AC back calculation is ON, meaning the activity coefficients are estimated based on target concentration percentages.

Ele Dist type of operation

An **Ele Dist (Element distribution)** type of operation is very similar to distribution (pyro) units, in which the state (Fixed, Float, and Rest) should be assigned for each element as well as the distribution of elements between phases and species (Fig. 44). The only difference here with pyro units is that the output should be assigned to the corresponding tanks after the element distribution has been defined.

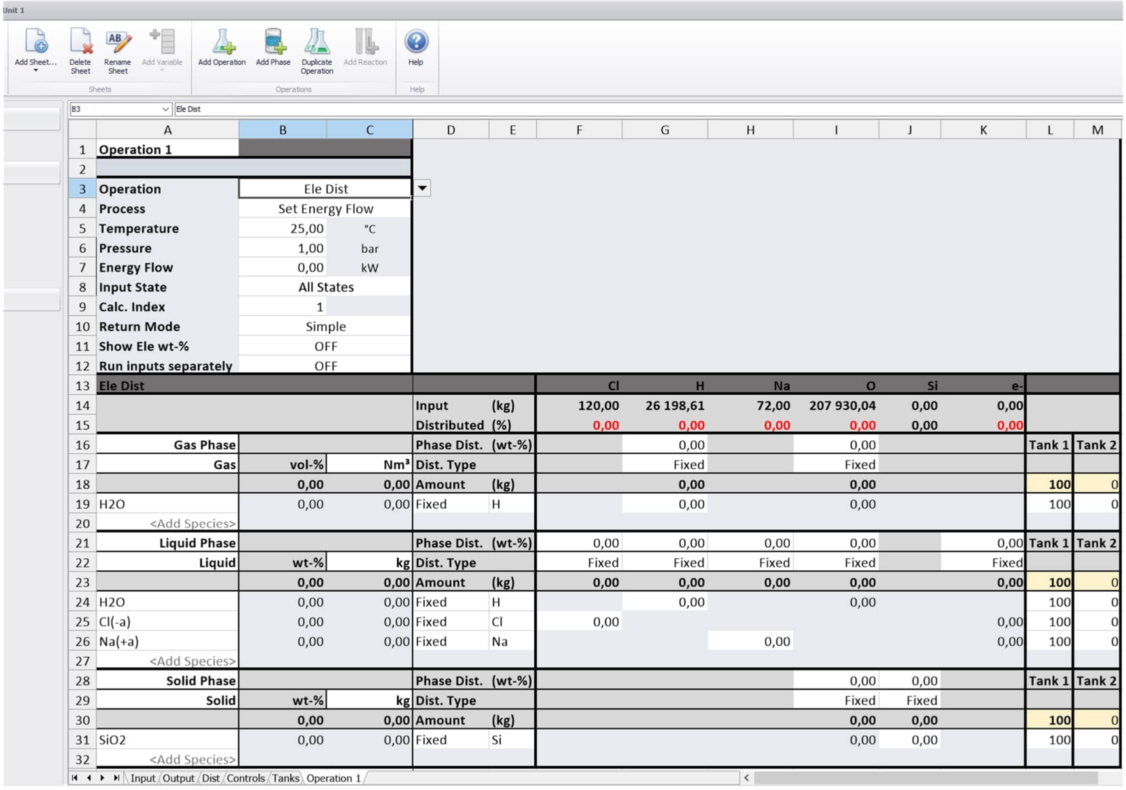


Figure 44: Element Distribution operation type in a dynamic unit.

Ideal Mixer and Ideal Heat Mixer types of operation

Ideal Mixer allows the mixing of heat and mass between tanks, while in Ideal Heat Mixer only heat is exchanged between materials. More specifically, in Ideal Heat Mixer, all the mass is assigned to the operation's input with their respective temperatures and heat values. The heat is mixed so that the material's temperature equalizes, and then the materials are assigned back to the tanks that they initially came from.

As can be seen from Fig. 45 and Fig. 46, for the **Ideal Mixer** it is possible to specify the tank to which the mixed material is transferred after the mixing operation is finished, while for the **Ideal Heat Mixer**, the output material goes to the initial tanks by default.

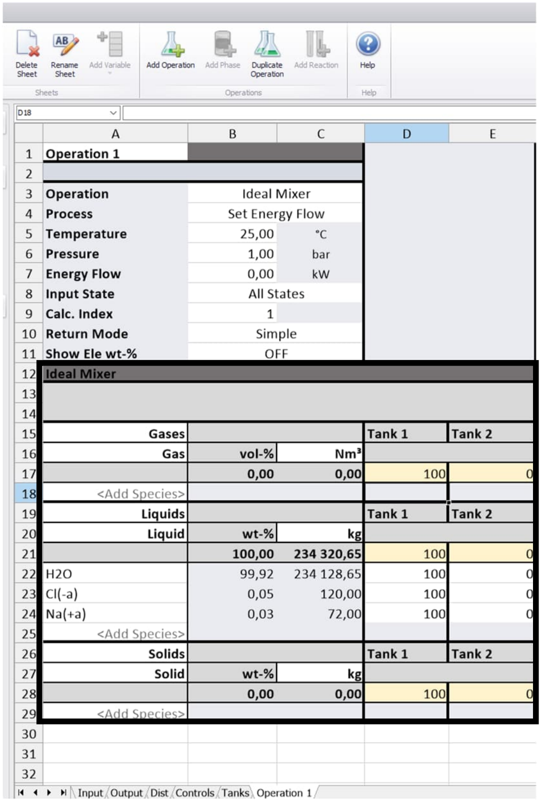


Figure 45: Ideal Mixer operation in a dynamic unit.

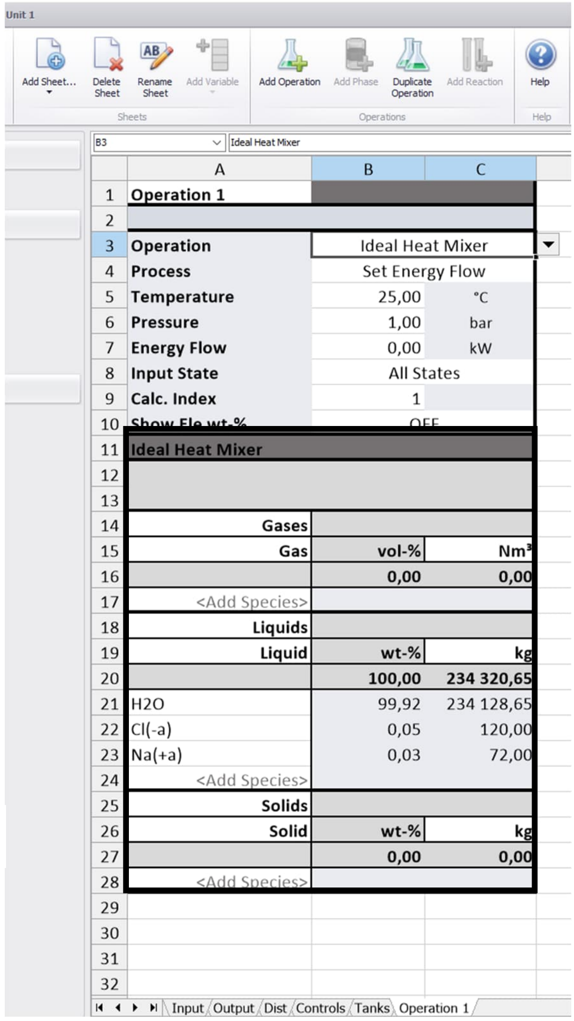


Figure 46: Ideal Heat Mixer operation in a dynamic unit.

Species Converter type of operation

As described on the *Species Converter Module* page, Species Converter allows transitioning between elemental analysis to species analysis and vice versa. Fig. 47 shows the species converter operation in the tank within a Dynamic Unit, in which the data for input and output analysis can be specified in the highlighted sections. For the output analysis, it is possible to specify the target of the output result that can be achieved by defining a **target wt-%** combined with a higher **Weight** for a particular species.

Also, as in the Species Converter module, in the operation's parameters section, there are **Exact O and H measurement** options, which allow the user to specify the amounts of oxygen and hydrogen as exact amounts entered in the input analysis or as minimum amounts.

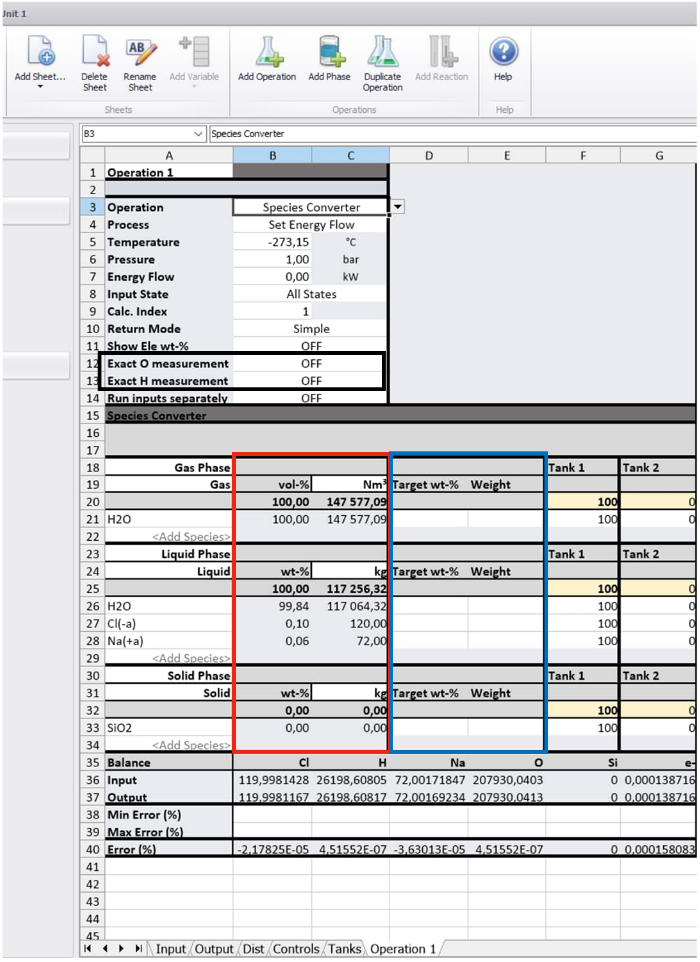


Figure 47: Species Converter type of operation in a dynamic unit. Here, the sections for input (total wt-% or vol-%) and output (weighting coefficients) analysis are highlighted in red and blue, respectively. Also, the exact O and H measurement options are highlighted.

Event sheet in Dynamic Units

An event in a dynamic unit consists of several blocks (Fig. 48). The first block is a monitored variable that corresponds to a variable that needs to be adjusted in order to satisfy the conditions or target variables. The value of the monitored variable is inserted into the **Monitored reference**, and **Relation** establishes the logical operation for comparison between the **Monitored reference** and **Value (Min)** (and optionally **Max** for BETWEEN and NOT IN BETWEEN relations).

Then, there are target variables blocks, in which the variable and target values are specified. Please note that there are two blocks for target variables depending on whether the **Target reference** should be equal (true) or not equal (false) to the target **Value**. An event's firing is specified with the **Event fire** binary option. An event can be fired either **Always** (every calculation step) or **On status change** (every calculation step in which the event status changes).

An event can be switched on and off with the **Mode** option, and if the event needs more comparison, then the **Condition link to the next Event** logic operation can be specified as AND, OR, or NONE, meaning that there is no relation with the next events. The status of comparison for all the events linked with a condition link to the next event is shown in

Condition link status. Please note that this status is not updated all the time, but only after the whole sheet has been calculated.

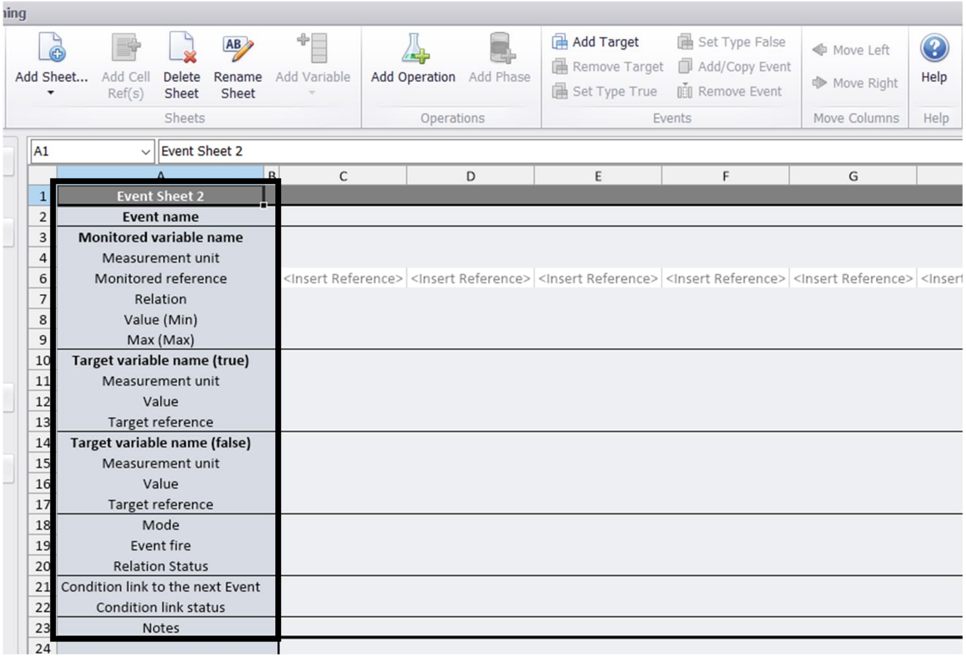


Figure 48: Event sheet in Dynamic unit.

Set sheet in Dynamic Units

Set sheets serve as predefined schedules for changes within a dynamic unit. There are several **Run Modes** for a set sheet, which set the occurrence of changes (Fig. 49). For example, the run mode **Once** means that changes happen only once, while **Repeat** mode allows for recurring changes.

Also, there is a **Stopwatch** mode that creates a separate counter for each set column to the top row (Fig. 50). The stopwatch counter can be used to perform particular events when a specific number of seconds has passed since the start of the simulation. The counter can also be reset to zero by creating an event with the counter as a cell reference (cell C1 for the example in Fig. 50). A more detailed example on how the stopwatch set sheet can be used is described later in the leaching example section.

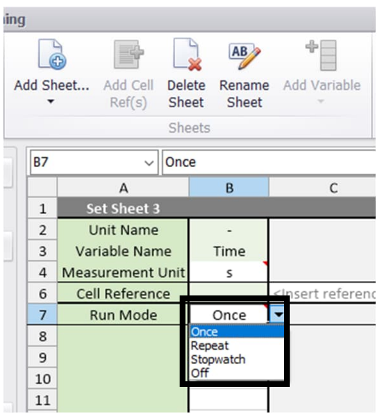


Figure 49: Set sheet in a dynamic unit.

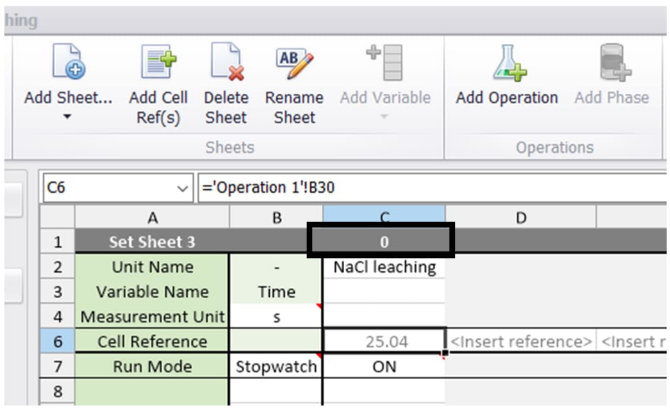


Figure 50: Stopwatch Run mode in Set sheet in a dynamic unit. Here, the stopwatch second counter is highlighted.

Batch sheet in Dynamic Units

The Batch sheet allows the definition of a specific amount of material of a particular phase that is to be added to the input. For example, let us define a model (Fig. 51) that consists of a dynamic unit and an input stream. The gas flow of Input stream 1 is 100 Nm^3/h (Fig. 52). In addition to the input amount of gas, the amount of 55 Nm^3 gas also needs to be added within 10 seconds of starting the calculation. In this case, it can be configured by using the Batch sheet (Fig. 53). As a result, the flow of Input stream 1 has to be adapted so that the specified amount enters the system along with the regular gas flow. Thus, after 1 hour the gas amount is 155 Nm^3 (Fig. 54).

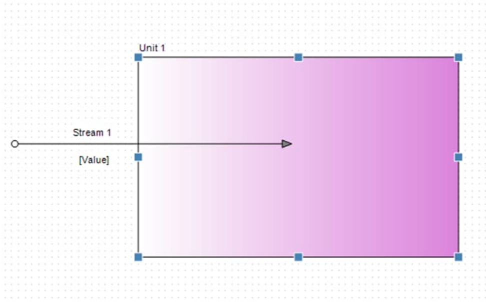
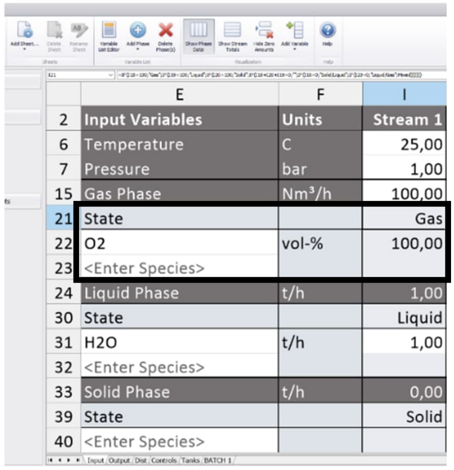
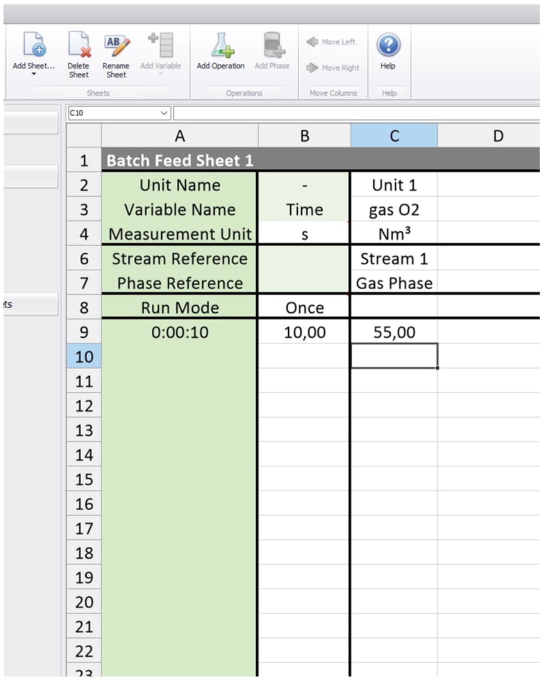


Figure 51: Example model for Batch sheet demonstration.



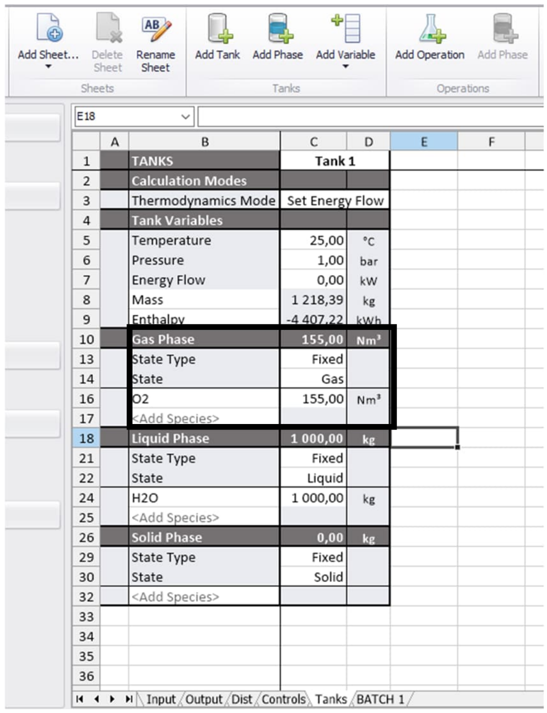
	E	F	I
2	Input Variables	Units	Stream 1
6	Temperature	C	25,00
7	Pressure	bar	1,00
15	Gas Phase	Nm³/h	100,00
21	State		Gas
22	O2	vol-%	100,00
23	<Enter Species>		
24	Liquid Phase	t/h	1,00
30	State		Liquid
31	H2O	t/h	1,00
32	<Enter Species>		
33	Solid Phase	t/h	0,00
39	State		Solid
40	<Enter Species>		

Figure 52: Input sheet for the Batch sheet demonstration model. Here, the initial input for gas is defined as 100 Nm^3/h.



	A	B	C	D
1	Batch Feed Sheet 1			
2	Unit Name	-	Unit 1	
3	Variable Name	Time	gas O2	
4	Measurement Unit	s	Nm³	
6	Stream Reference		Stream 1	
7	Phase Reference		Gas Phase	
8	Run Mode	Once		
9	0:00:10	10,00	55,00	

Figure 53: Batch sheet in a dynamic unit. Here, an amount of 55 Nm^3 is added to Input stream 1 ten seconds after the beginning of the simulation.



	B	C	D
1	TANKS	Tank 1	
2	Calculation Modes		
3	Thermodynamics Mode	Set Energy Flow	
4	Tank Variables		
5	Temperature	25,00	°C
6	Pressure	1,00	bar
7	Energy Flow	0,00	kW
8	Mass	1 218,39	kg
9	Enthalpy	-4 407,22	kWh
10	Gas Phase	155,00	Nm³
13	State Type	Fixed	
14	State	Gas	
16	O2	155,00	Nm³
17	<Add Species>		
18	Liquid Phase	1 000,00	kg
21	State Type	Fixed	
22	State	Liquid	
24	H2O	1 000,00	kg
25	<Add Species>		
26	Solid Phase	0,00	kg
29	State Type	Fixed	
30	State	Solid	
32	<Add Species>		

Figure 54: Tanks sheet after 1 hour of simulation. Here, the amount of gas phase is the sum of the initial gas input (100 Nm^3) and the additional 55 Nm^3 specified in the Batch sheet.

Schematic representation of tank and operations calculation

An operation can be considered as an isolated system inside the tank, meaning that there is no energy and mass exchange between the operation and the tank until the material has been transferred back to the tank. Overall, the process within a tank can be described as follows. First, the inputs are distributed into the tanks, in which the operations are defined either subsequently or simultaneously with the help of a calculation index (written in square brackets before the operation). Then, the species are assigned to the operations, and the operations are performed as isolated systems. After the operations have been done, the mass and energy are transferred into the specified tanks. After all the operations within the tanks have finished, the material is sent to the specified outputs from the tanks (Fig. 55).

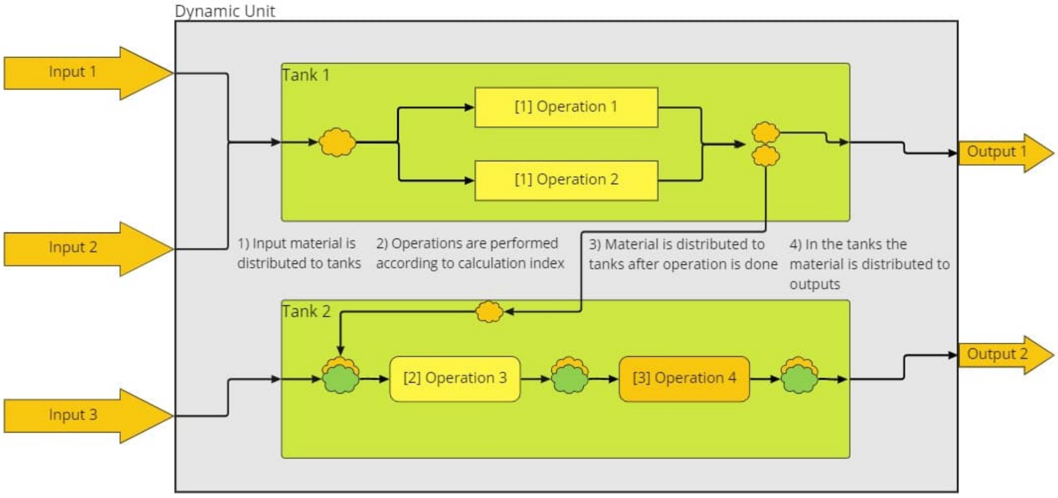


Figure 55: Schematic representation of a dynamic unit example.

Leaching example

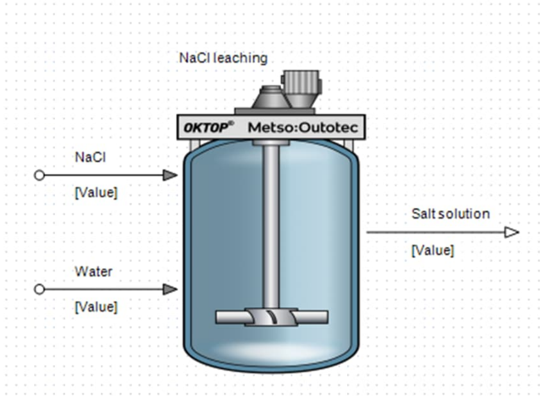
Here, a leaching example is considered in order to demonstrate the reaction operation in a dynamic unit. This example is a simple case of NaCl leaching in batches to produce a salt solution.

Model definition:

1. NaCl is leached in a 100 m^3 reactor.
2. The batch is started when the reactor is 50% full and ended when the reactor is 90% full. First solid salt is added and then water. The batch is mixed for 5 minutes before discharge.
3. The desired final NaCl concentration is a 25 wt-% solution.
4. The reactor is emptied to 50% and the making of the batch is started again.
5. Feed flows are 150 t/h for solid salt and 200 m^3/h for water.
6. The output flow is 120 m^3/h.

Overall, in this leaching example, the sodium chloride is leaching and producing a salt solution, so the reaction type of operation is needed with the reaction: $NaCl \rightarrow NaCl(a)$. Also, according to the model definition (3), the final NaCl concentration is to be tracked, so the **Total Dissolved Solids** variable is also needed. The other conditions, such as mixing and tank emptying, must be configured with the event sheet.

First, the dynamic unit model is drawn (Fig. 56). In Dynamic Unit Editor, the input variables should be considered first. In this example, the variable list includes species (H2O, NaCl(a), and NaCl) and the **Total Dissolved Solids** variable for the liquid phase (Fig. 57).



Inputs	Outputs
NaCl	Salt solution
Water	

Figure 56: Example model of leaching.

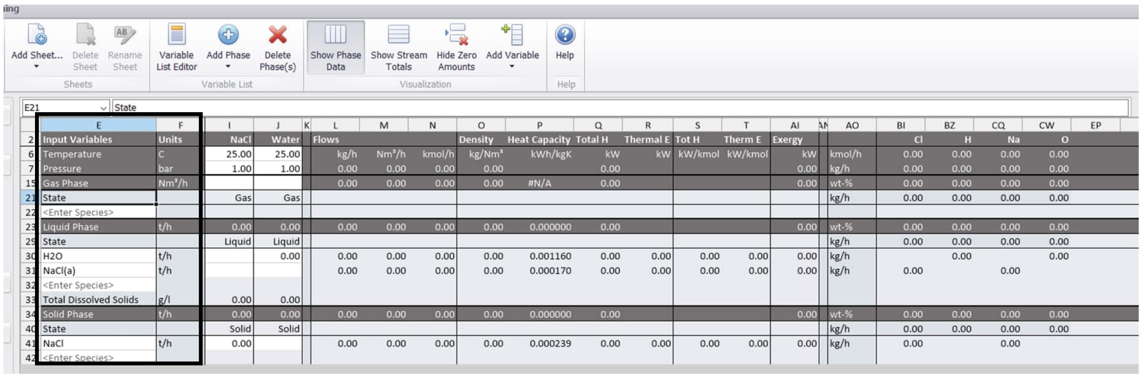


Figure 57: Input sheet for leaching example.

Having all the variables automatically transferred to the Output and Tank sheets, the Dist sheet can be configured right after the Input sheet. In this example, all the input material is to be distributed to a tank (Fig. 58).

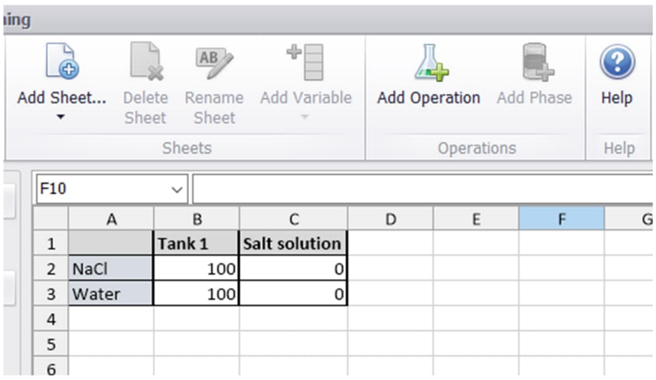


Figure 58: Dist sheet for leaching example.

Then, the tank logic can be configured. According to the model definition (1), the reactor's tank should be of a definite size, so the **Tank Size** variable is needed. It can be added with the **Add Variable** option in the Tanks sheet. The **Overflow destination** is specified as Tank 1, meaning that overflow material is accumulated in the tank. Also, in this example, the tank's level needs to be controlled, and some actions (model definition (2) and (4)) should be done at specific levels of the tank. Therefore, the **Tank level** variable has to be added. As a result, all the required tank variables are configured (Fig. 59). After that, the reaction operation has to be configured.

A reactions type of operation is similar to a reaction unit. A new reaction is added to the **Reaction Tables** in the operation sheet. In the reaction table, the formula of the reaction is typed as shown in Fig. 60 (reactants and products are separated by '='). Please note that phases are specified as a separate reaction parameter, so there is no need to add (s), (g), or (l) to the reaction species. In the **Progress** field of the reaction, the reaction rate (in %) is specified. This defines the percentage of the species sent to the operation that are to be involved in the reaction. Finally, all of the reaction output is assigned to Tank 1.

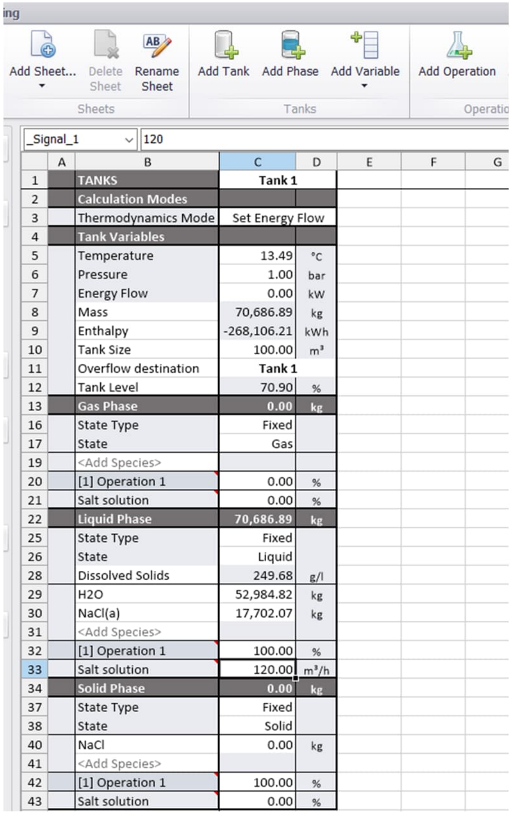


Figure 59: Tank sheet for leaching example.

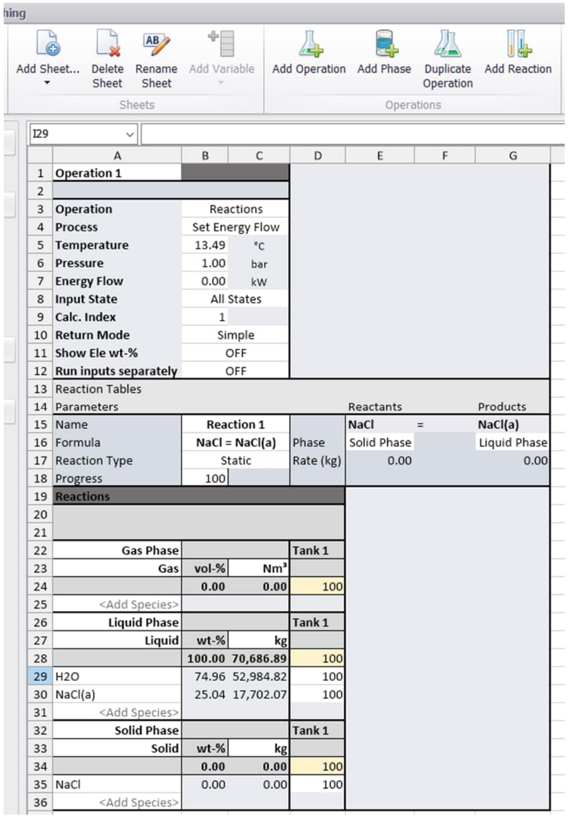
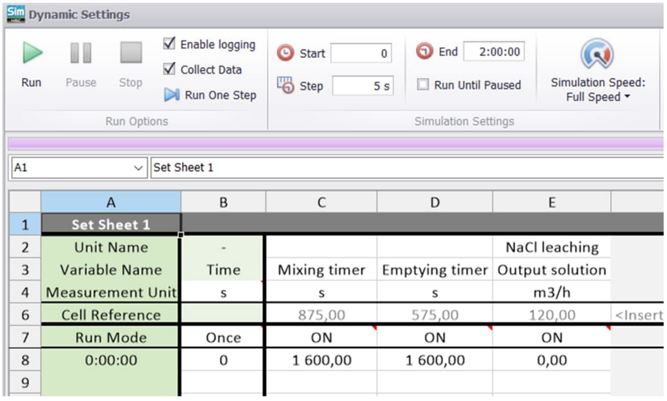


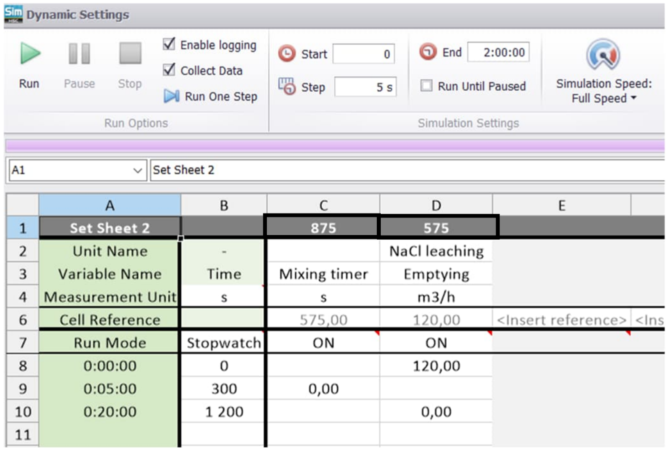
Figure 60: Operation (Reaction) sheet for leaching example

Finally, the events can be defined for the leaching example. In this example, the initial mixing time and emptying time as well as the initial output flow need to be specified in the Set 1 sheet (Fig. 61). As can be seen from the figure, the initial values for the second counters are set to 1600 s, and the simulation runs in descending order. Please note that initialization happens only once, so the Run Mode is set to Once. Then, in the Set 2 sheet, mixing at 5 min before discharge is set as well as tank emptying (Fig. 62).



	A	B	C	D	E
1	Set Sheet 1				
2	Unit Name	-			NaCl leaching
3	Variable Name	Time	Mixing timer	Emptying timer	Output solution
4	Measurement Unit	s	s	s	m3/h
6	Cell Reference		875,00	575,00	120,00
7	Run Mode	Once	ON	ON	ON
8	0:00:00	0	1 600,00	1 600,00	0,00
9					

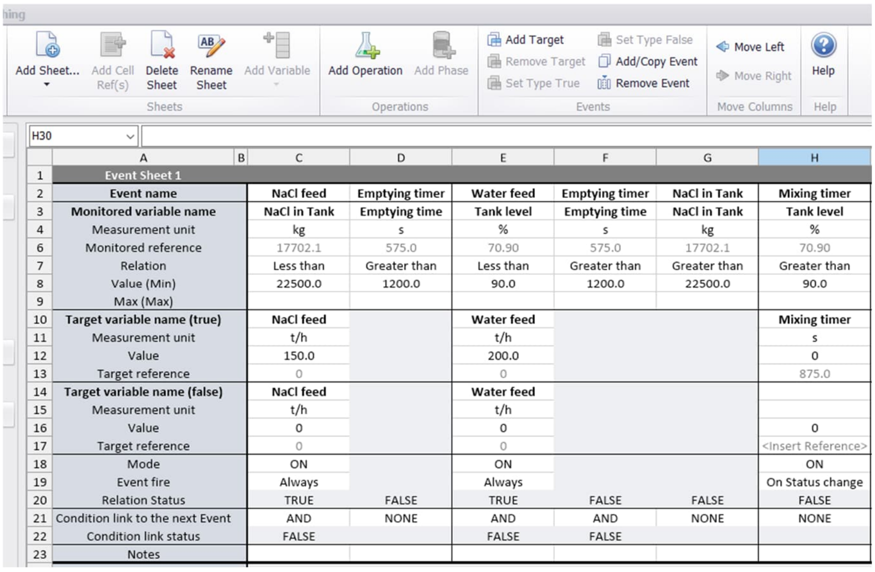
Figure 61: Set 1 sheet for leaching example. Here, the cell references for the mixing timer and emptying timer are referenced to the second counters in the Set 2 sheet.



	A	B	C	D	E
1	Set Sheet 2		875	575	
2	Unit Name	-		NaCl leaching	
3	Variable Name	Time	Mixing timer	Emptying	
4	Measurement Unit	s	s	m3/h	
6	Cell Reference		575,00	120,00	<Insert reference>
7	Run Mode	Stopwatch	ON	ON	
8	0:00:00	0		120,00	
9	0:05:00	300	0,00		
10	0:20:00	1 200		0,00	
11					

Figure 62: Set 2 sheet for leaching example. Here, the second counters for the mixing and emptying timers are highlighted.

As a result, the example model is almost configured, and the final event sheet can be specified (Fig. 63). In this example, events include NaCl and water feed flows (model definition (5)), tank emptying (model definition (2) and (4)) and mixing (model definition (2)).



	A	C	D	E	F	G	H
1	Event Sheet 1						
2	Event name	NaCl feed	Emptying timer	Water feed	Emptying timer	NaCl in Tank	Mixing timer
3	Monitored variable name	NaCl in Tank	Emptying time	Tank level	Emptying time	NaCl in Tank	Tank level
4	Measurement unit	kg	s	%	s	kg	%
6	Monitored reference	17702.1	575.0	70.90	575.0	17702.1	70.90
7	Relation	Less than	Greater than	Less than	Greater than	Greater than	Greater than
8	Value (Min)	22500.0	1200.0	90.0	1200.0	22500.0	90.0
9	Max (Max)						
10	Target variable name (true)	NaCl feed		Water feed			Mixing timer
11	Measurement unit	t/h		t/h			s
12	Value	150.0		200.0			0
13	Target reference	0		0			875.0
14	Target variable name (false)	NaCl feed		Water feed			
15	Measurement unit	t/h		t/h			
16	Value	0		0			0
17	Target reference	0		0			<Insert Reference>
18	Mode	ON		ON			ON
19	Event fire	Always		Always			On Status change
20	Relation Status	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE
21	Condition link to the next Event	AND	NONE	AND	AND	NONE	NONE
22	Condition link status	FALSE		FALSE	FALSE		
23	Notes						

Figure 63: Event sheet for leaching example.

References

Chapra, S. C., & Canale, R. P. (2006). Numerical methods for engineers. Boston: McGraw-Hill Higher Education.
Skogestad, S. (2009). Chemical and Energy Process Engineering. Boca Raton, FL, USA: CRC Press, https://doi.org/10.1201/9781420087567
Fogler, H. S. (2010). Essentials of Chemical Reaction Engineering. Pearson Education.