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55. Sim Dynamic Simulations

55.1. Introduction

The goal of the HSC Sim dynamic simulation is to model the evolution of a flowsheet state over time. Thus, at each discrete moment in time, the system state is calculated based on previous system states. This can be opposed to static steady-state simulations, where the aim is to solve values for process variables so that mass and energy balances are maintained.

HSC Sim offers tools for dynamic calculations for both particle and species units. Additionally, it provides functionality to collect data, configure various dynamic simulation scenarios, assign time-dependent values to different parameters, and create events based on discrete conditions.

55.1.1. Dynamic simulation as an initial value problem

Dynamic process simulation 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 unknown function y(t) at the given point in the domain of the solution.

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

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.

55.1.2. Numerical methods

Some initial problems can be solved algebraically. However, for many of the differential equations we encounter in the real world, there is no straightforward algebraic solution. Even when there are algebraic solutions available, these solutions often become too complex and are not practically useful. Therefore, we rely on numerical **Runge-Kutta (RK)** methods to provide approximate solutions for differential equations in HSC Sim.

Most numerical methods assume that our solution can be expressed in the form of a Taylor series:

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

This advancing approach yields a reasonably good approximation when we include an adequate number of terms and maintain a small value for h, which represents a time increment of an independent variable per discrete simulation step. This value, also denoted as Δt, corresponds to the **Time Step** in the dynamic simulation settings within HSC Sim software.

The simplest RK method, **Euler's Method**, uses the first two terms of the series:

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

This method provides sufficient accuracy for most industrial applications. Another advantage is that it is fast and works well in computerized modeling. Therefore, we utilize this method to simulate mass and energy accumulators called **'Tanks'** in a dynamic unit.

55.1.3. Mass and energy balance

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

$$\frac{dm}{dt} = m_{in} - m_{\text{out}} \quad (5)$$

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

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

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.

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55.2. Dynamic Scenario Editor (Dynamic Dialog)

Dynamic simulation of a flowsheet can be configured through the Dynamic Scenario Editor button in the upper toolbar (**Fig. 1**) or via "Calculate" menu. This tool allows for dynamic scenario configuration to set delays for streams, assign time-dependent values for referenced cells, define conditional or stochastics events, record values from referenced cells, and plot the system behavior over time.

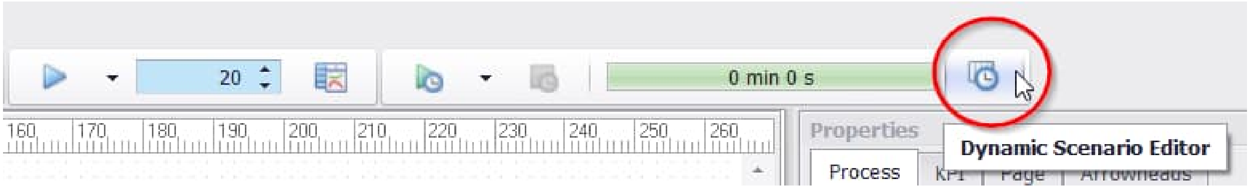

Figure 1: Dynamic Scenario Editor

Scenarios are configured in various spreadsheets, which can be added using the "Add Sheet" button on the top toolbar (**Fig. 2**). "Rename Sheet" and "Delete Sheet" functions are used respectively to rename or delete the sheet that is currently active.

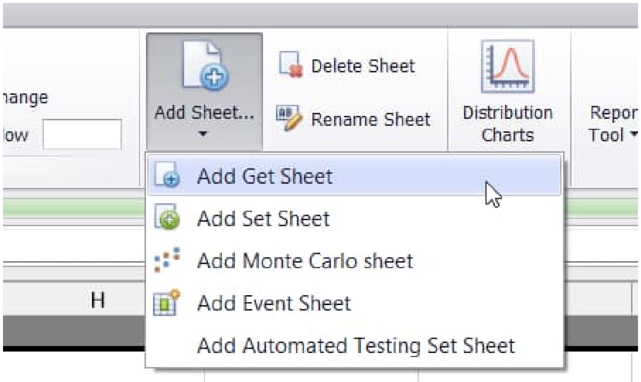

Figure 2: Add Sheet

1. **Set Sheet**

   Assign time-dependent values to the referenced cells.

2. **Get Sheet**

   Collect time-dependent values from the referenced cells.

   NOTE: This sheet can be deactivated either from the top toolbar or from the "Results" menu in the main window by checking the "Collect Data" checkbox.

3. **Monte Carlo Sheet**

   Assign time-dependent random values to the referenced cells, based on the selected probability distribution.

4. **Event Sheet**

   Define events to assign values for referenced cells based on conditional logic.

5. **Tank Level Sheet**

   Fill selected tanks on units that support mass and energy accumulators defined in the **tank sheets** withing Unit Editor.

6. **Stream Sheet**

   Define delays for streams, so that material enters the assigned destination after a specified time. This can also be accomplished in a flowsheet by right-clicking a stream and selecting **Stream Properties**.

   NOTE: The delay larger than the simulation time step allows HSC to parallelize calculations, potentially improving dynamic simulation speed.

55.3. Running Dynamic Simulation

Dynamic Simulation settings can be configured in Dynamic Scenario Editor (**Fig. 3**), or directly in “Calculate” menu on Sim main window.

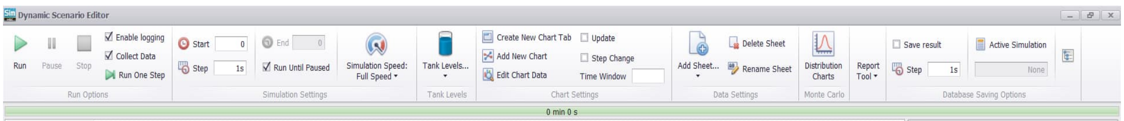

Figure 3: Dynamic Scenario Editor top toolbar.

The most important controls and settings for a dynamic simulation are listed here.

1. **Start / Pause Dynamic Simulation**

   Simulates system behavior over time.

   NOTE: Run a single simulation step by using the key binding **Alt + Arrow Right**.

2. **Stop Dynamic Simulation**

   Resets the simulation clock.

3. **Enable LCA Updates**

   If this option is enabled, the Life Cycle Assessment (LCA) tool is updated on each simulation step.

4. **Simulation Speed**

   Dynamic simulation speed is defined as a multiplier of real speed. For example, 2x speed means that the simulation clock will tick twice as fast as the real clock.

5. **Start Time**

   Specifies the start time of the dynamic simulation in the format *<hours>:<minutes>:<seconds>*.

6. **Time Step**

   Determines the time increase (dt) per discrete simulation step (measured in seconds, minutes, or hours)

7. **Run Until Paused**

   If this option is selected, the simulation will run until the pause or stop button is pressed.

8. **Step Count**

   The number of discrete calculation steps.

9. **End Time**

   Specifies the time when the simulation is set to end, also in the format *<hours>:<minutes>:<seconds>*.

The **Clear Internal Streams** functionality removes particles and delayed content from all flowsheet streams. Correspondingly, the **Empty Tanks** function 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 after the stop button is pressed. The logic of tanks is explained in detail in the Dynamic Unit section.

55.4. Plotting the Simulation Results

The Chart Settings option in **Dynamic Scenario Editor** (**Fig. 4**) 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. 5**).

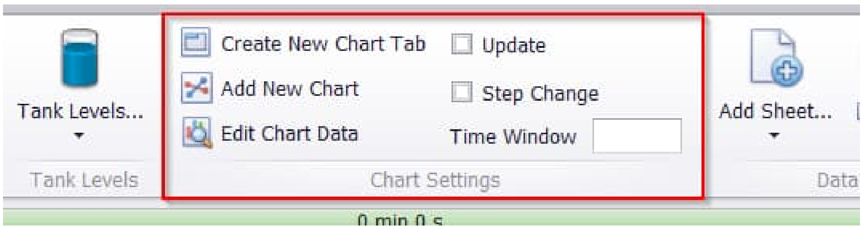

Figure 4: Chart Settings toolbar section in Dynamic Scenario Editor.

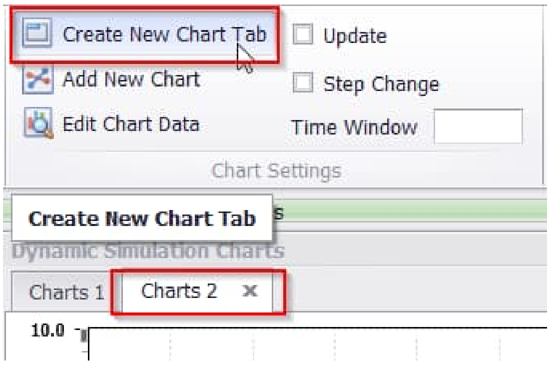

Figure 5: Adding a new chart tab in the Chart Settings section of the Dynamic Settings toolbar. In the Dynamic Simulation Charts window, 'Charts 1', 'Charts 2', 'Charts 3', and 'Charts 4' are separate chart tabs.

The **Add New Chart** option allows the insertion of a new chart within one chart tab panel (**Fig. 6**).

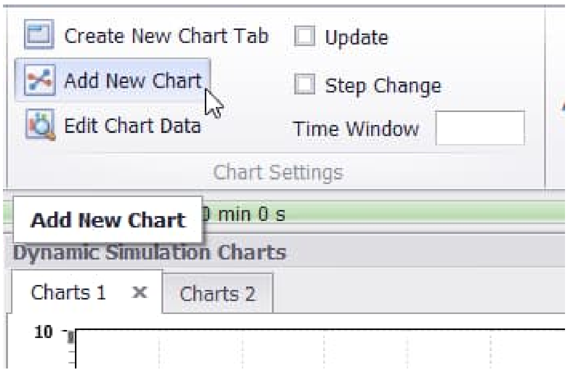

Figure 6: Add a new chart to a chart tab panel. New HSC charts can be added to the 'Charts 1' and 'Charts 2' tab panels.

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.

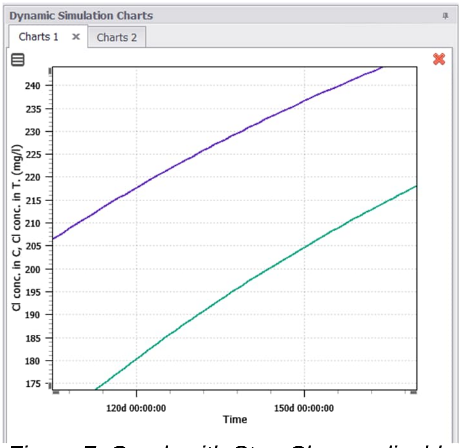

Figure 7: Graph with Step Change disabled.

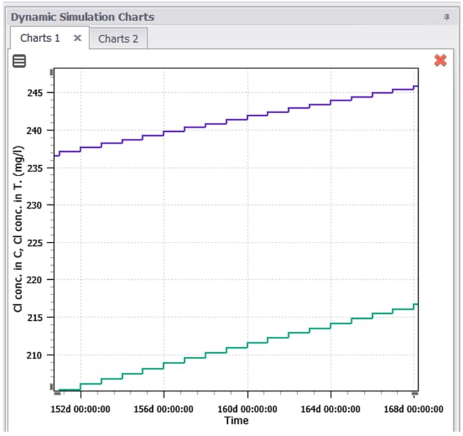

Figure 8: Graph with Step Change enabled.

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. 9**). 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. 10**).

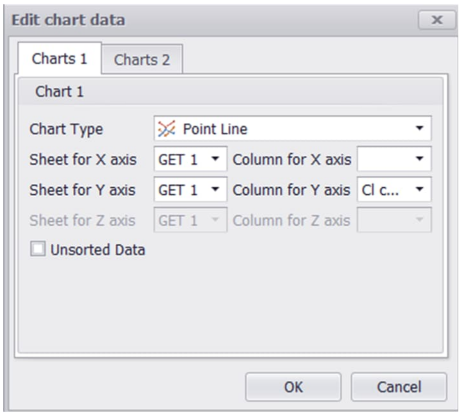

Figure 9: Edit Chart Data menu.

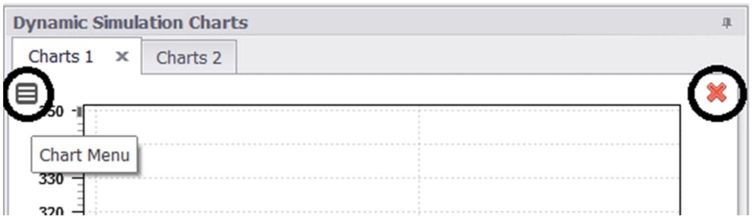

Figure 10: Chart menu in Dynamic Simulation Charts panel. Chart Menu button and Close Chart button are circled.

In the chart menu, the selected chart can be downloaded, copied, printed, or reformatted (**Fig. 11**). Also, there is an option called **Crosshair** that upon activation inserts a vertical line and the coordinates of the intersection points (**Fig. 12**).

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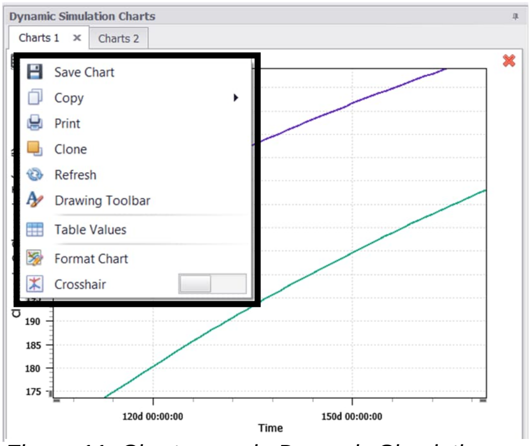

Figure 11: Chart menu in Dynamic Simulation Charts

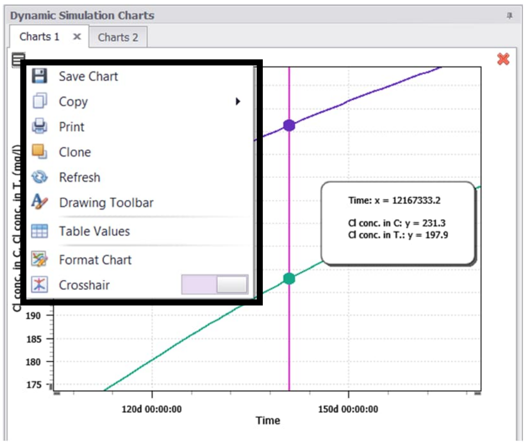

Figure 12: Crosshair tumbler in Chart menu

The chart style can be edited using the **Format Chart** option (**Fig. 13**).

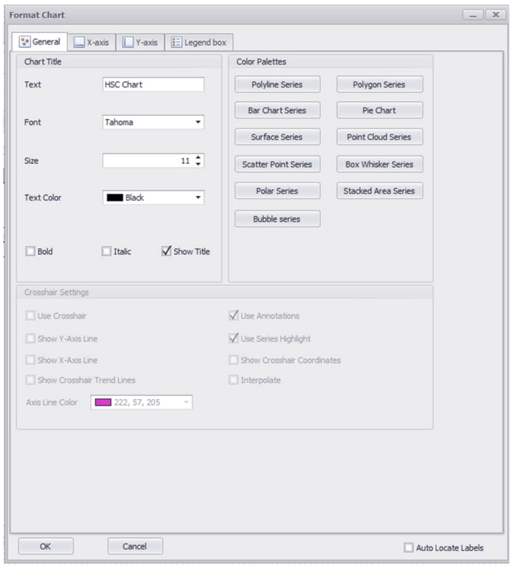

Figure 13: Format Chart option in Chart menu in a dynamic unit.

55.5. Reporting Simulation Results

The Report Tool function in **Dynamic Scenario Editor** (**Fig. 15**) allows the creation of a report about the results of a simulation by pressing the **Collect Report Data** (**Fig. 16**) option. In the Report Settings menu, the tanks and streams which are needed for the report can be specified.

Note: Collecting the report data may decrease the calculation speed.

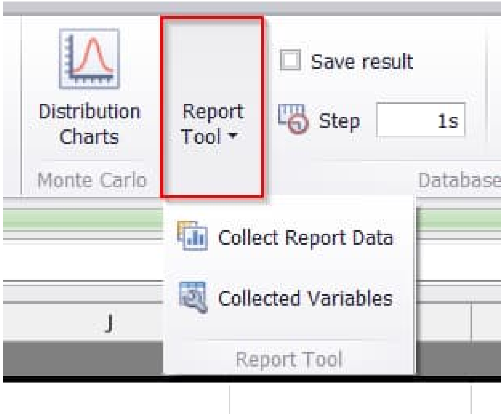

Figure 15: Report Tool section in Dynamic Settings.

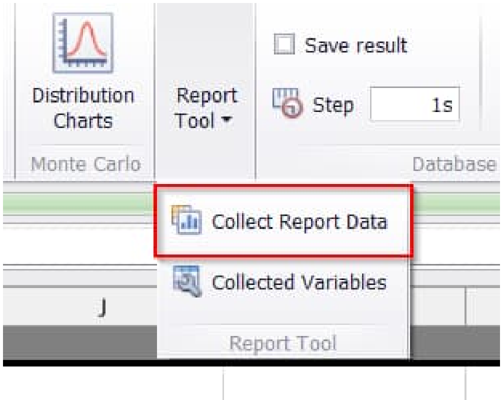

Figure 16: Collect Report Data option in Report Tool

55.6. Dynamic Calculation Unit

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.

A dynamic unit is created with the **Draw Dynamic Unit** option in the left-side toolbar (**Fig. 17**). 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. 18**).

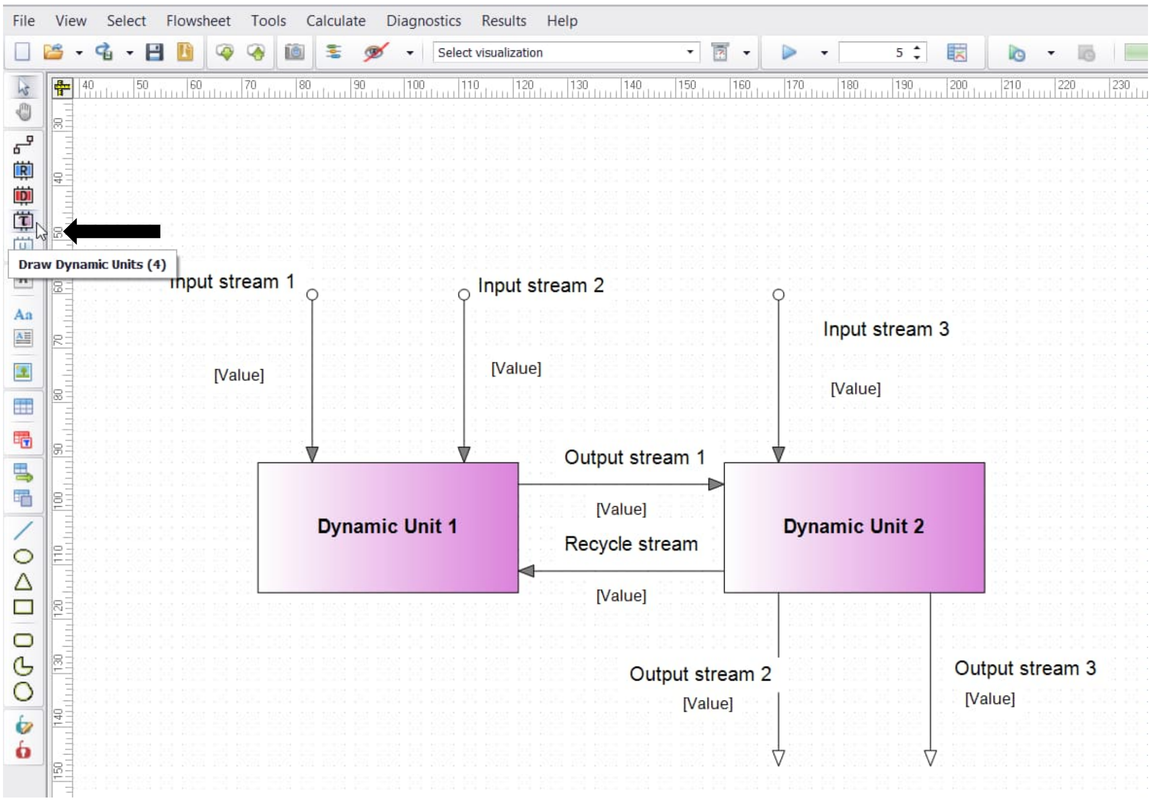

Figure 17: Creation of a dynamic unit

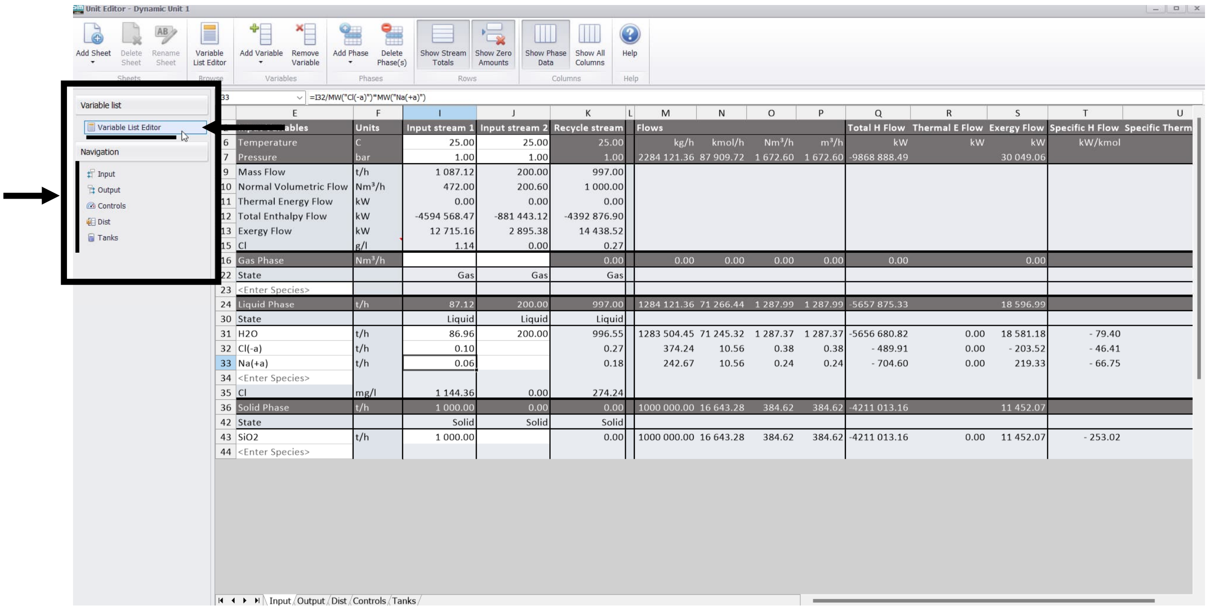

Figure 18: The main components of Unit Editor are the Variable list and various sheets, including Input, Output, Controls, Distributions, and Tanks sheets.

55.7. Global Variable List in Dynamic Unit

Species can be added with the help of **Variable List Editor** (**Fig. 19**) or inserted directly into the **Input, Output,** or **Tanks** sheets. 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.

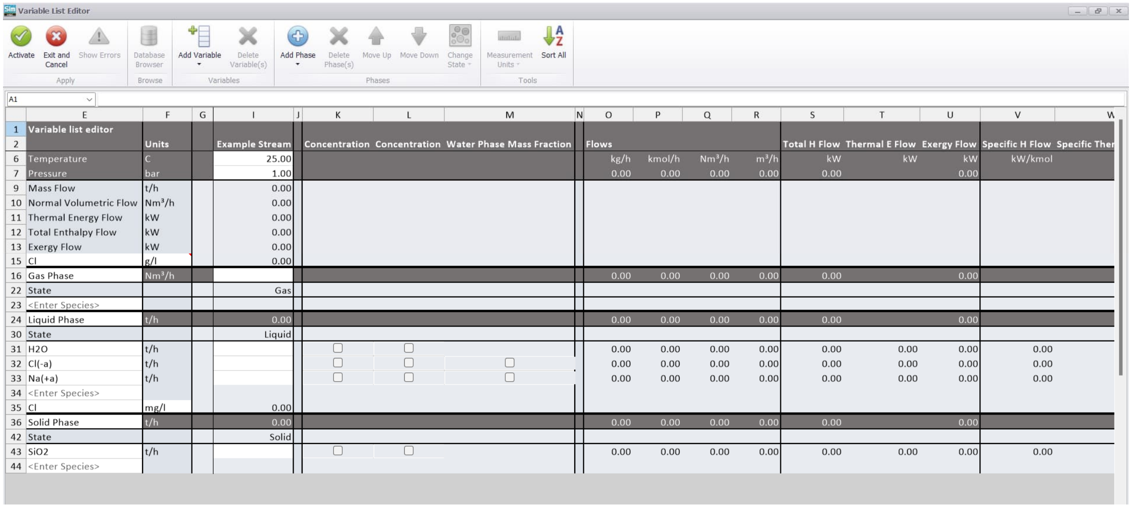

Figure 19: Variable List editor in Unit editor

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. 20**). 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.

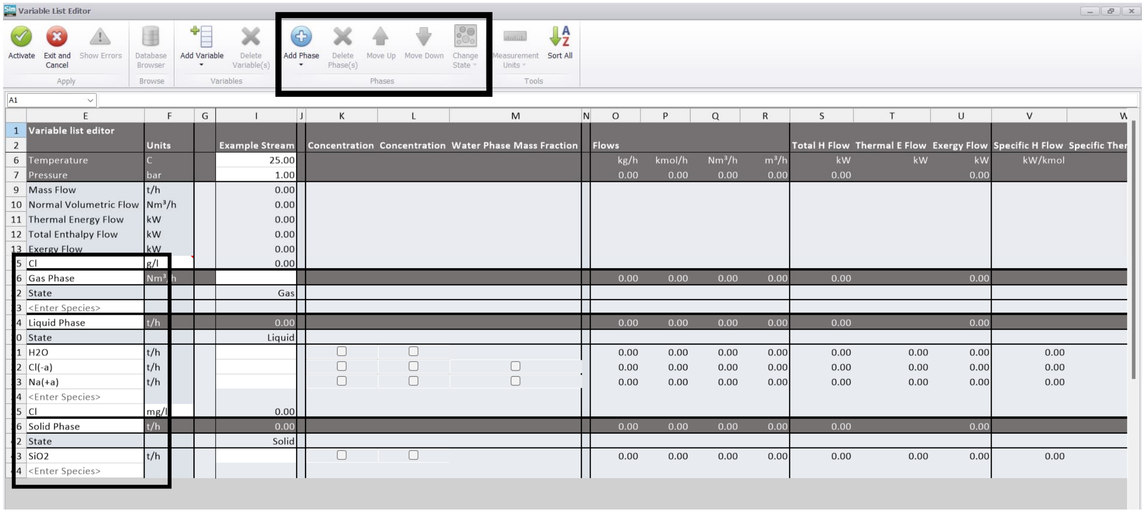

Figure 20: Edit phases in Variable List Editor within Unit Editor

Apart from species, other variables can be defined by using the '**Add Variable**' button on the **Dynamic Unit Editor**, or by opening a **Variable List Editor**. 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.** Correspondingly, to add a new variable common to all phases, any common variable on top rows should be selected when adding a new one (**Fig. 21**).

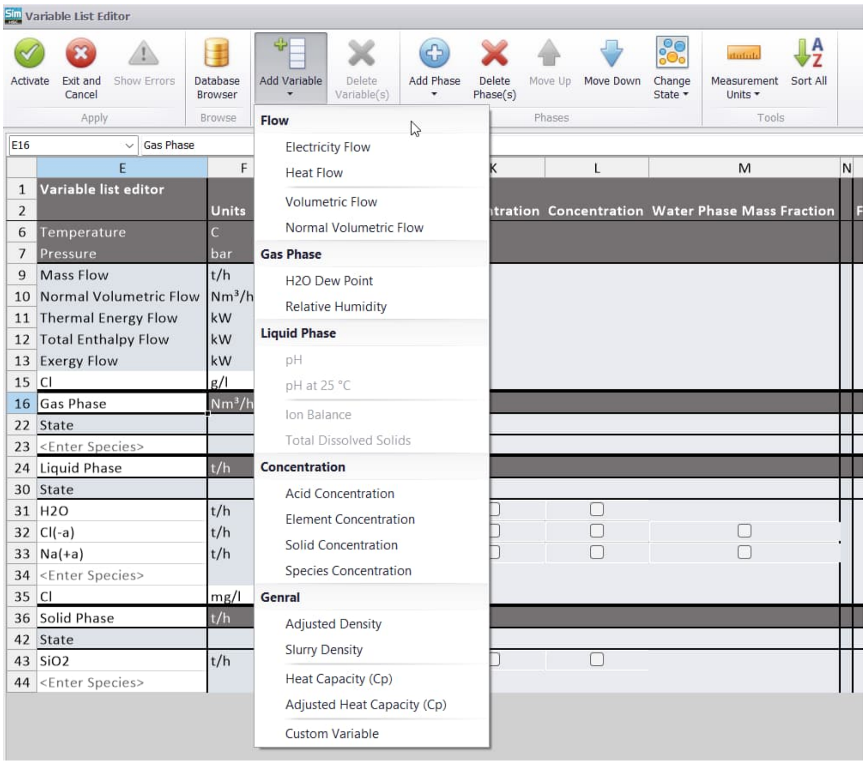

Figure 21: Adding a new variable. Here, the gas phase is selected, so the new variable will be added to the gas phase.

To delete a variable, select the corresponding cell and use the **Delete Variable(s)** option. Additionally, you can modify the measurement units of a phase by using the **Change Units** option in the **Variable List Editor**. In a dynamic unit, amounts can be expressed either as percentages (similar to distribution units) or in absolute mass (similar to reaction units). (**Fig. 22**)

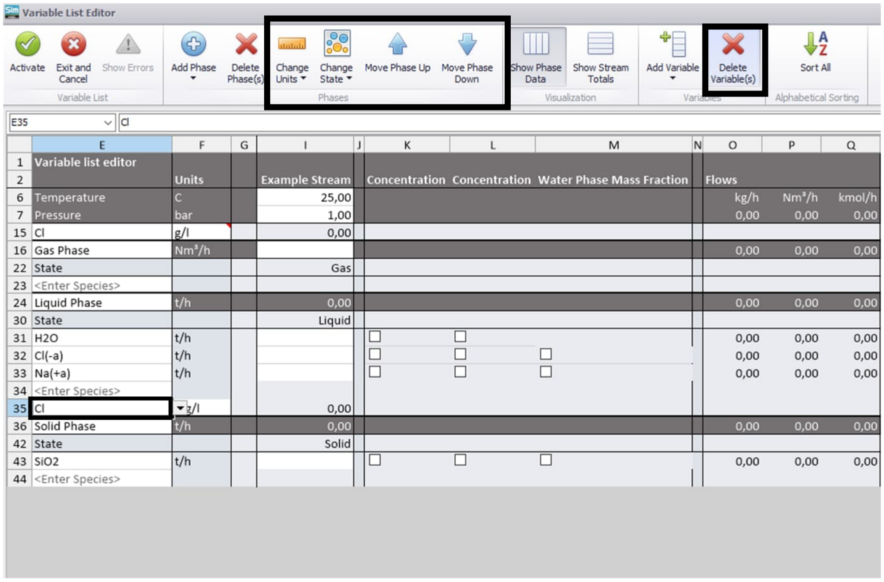

Figure 22: Delete Variable and edit phases options in Variable List Editor.

A complete list of available global variables is presented below:

Flow Variables

1. Electricity Flow

Non-convective energy transfer that can be used to input or extract enthalpy from the unit. Electricity flow differs from Heat Flow only in the way exergy is calculated.

NOTE: This variable can have values only for streams that do not contain mass flow.

2. Heat Flow

Non-convective energy transfer that can be used to input or extract heat from the unit. Usually, this is used to calculate heat losses, cooling, or the heating effect of the indirect heat exchanger modeled as a separate unit.

NOTE: This variable can have values only for streams that do not contain mass flow.

3. Volumetric Flow

Total Volumetric flow at current temperature and pressure in selected phase.

4. Normal Volumetric Flow

Total Volumetric flow at 0 °C (273.15K) and 1 bar pressure in selected phase.

Gas Phase Variables

5. H2O Dev Point

The temperature at which the selected gas phase becomes saturated with current amount of water vapor. Cannot be calculated if the gas phase does not contain H_2O(g).

6. Relative Humidity

The water vapor content in the selected gas phase, expressed as a percentage of the maximum vapor amount needed to achieve saturation at the current temperature. Uses H_2O(g) compound, the stream temperature, and pressure in the calculation and assumes everything else in the gas phase to be air.

Liquid Phase Variables

7. pH

pH at actual stream temperature. Calculation uses the concentrations of H(+a) and OH(-a) species, one of which must exist in the liquid phase.

NOTE: The pH value is not temperature compensated; it represents the pH at the stream temperature (Kw(T)).

NOTE: Laboratory equipment often provides the pH reading converted to 25°C temperature, whereas this variable gives the 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 across all concentrations.

8. pH at 25 °C

pH at 25 °C temperature. Calculation uses the concentrations of H(+a) and OH(-a) species, one of which must exist in the liquid phase.

NOTE: Laboratory equipment often provides the pH reading 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 across all concentrations.

9. Ion Balance

Shows the possible offset of anions and cations in the water phase, expressed in moles. A null value for this variable means that there is an equimolar number of anions and cations in the solution.

10. Total Dissolved Solids

Total dissolved solids use the H2O compound and assume everything else in the water phase to be dissolved solids. This is computed as an amount of non-water species divided by the total amount of species in the liquid phase, expressed in a user-defined measurement unit.

Concentration Variables

11. Acid Concentration

Estimated amount of acid divided by the total amount of substance in the selected phase. The amount of acid is estimated by the quantities of acid molecules and H+ ions, which are assumed to originate from the acid. Species (H_2SO_4, HCl, or HNO_3) are selected in a separate dialog after the variable is added.

12. Element Concentration

The total amount of an selected element in a selected phase, divided by the total amount of substance in that phase. An element is selected in a separate dialog after the variable is added.

NOTE: The concentration for a particular element can also be added in Variable List Editor by selecting the checkboxes shown in **Fig. 23**.

13. Solid Concentration

The total amount of substances in solid phases, divided by the total amount of substances in liquid phases.

14. Species Concentration

The amount of a chemical species in a selected phase, divided by the total amount of species in that phase. Species are selected in a separate dialog after the variable is added.

NOTE: The concentration for a particular species can also be added in Variable List Editor by selecting the checkboxes shown in **Fig. 24**.

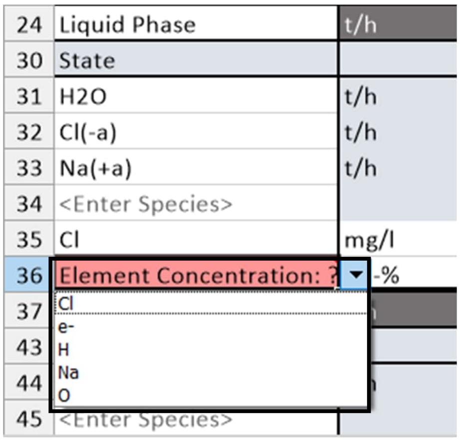

Figure 23: Selection of element in Element Concentration variable

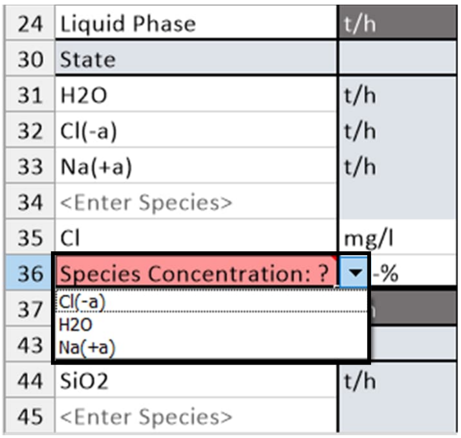

Figure 24: Selection of species in Species Concentration variable

General Variables

15. Adjusted Density

User-specified custom value for the density of a selected phase at current temperature and pressure.

16. Slurry Density

The total mass of all liquid and solid phases, divided by the total volume of all liquids and solids at current temperature and pressure.

17. Heat Capacity (Cp)

Total heat capacity of a selected phase, computed at the current stream temperature.

18. Adjusted Heat Capacity (Cp)

User-specified value for Adjusted Cp of a selected phase is applied for the enthalpy calculations in the range starting from the reference point (at 25°C) to the current temperature of the stream. In this range, the pressure is assumed to stay at the current stream pressure.

H (at current T and P) = reference H (at 25° C and current P) + H added by adjusted Cp (25→T)

19. Custom Variable

User-specified custom variable that must be defined in the **Variable List Editor**. Custom variable is just an empty cell in the variable list, where any formula can be typed. This cell needs to be filled individually in every unit.

The density of an aqueous solution can be interpolated based on experimental solution data stored in the database. To achieve this, select the checkbox for **Water phase mass fractions** in the **Variable List editor**, and then choose the appropriate experimental dataset from the drop-down menu (**Fig 25**).

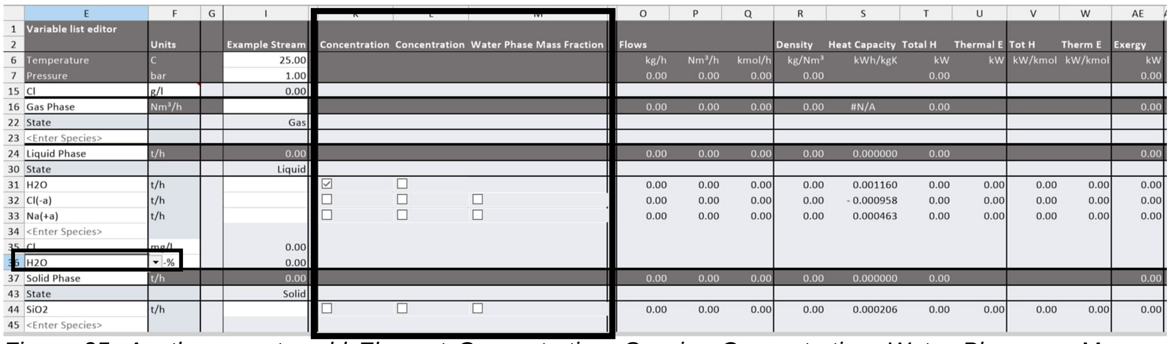

Figure 25: Another way to add Element Concentration, Species Concentration, Water Phase, or Mass fraction variables. Here, by activating the Concentration checkbox for the H2O, the new H2O concentration variable is added to the Liquid phase list of variables.

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.

55.8. 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. 26**). 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. 27**). 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.

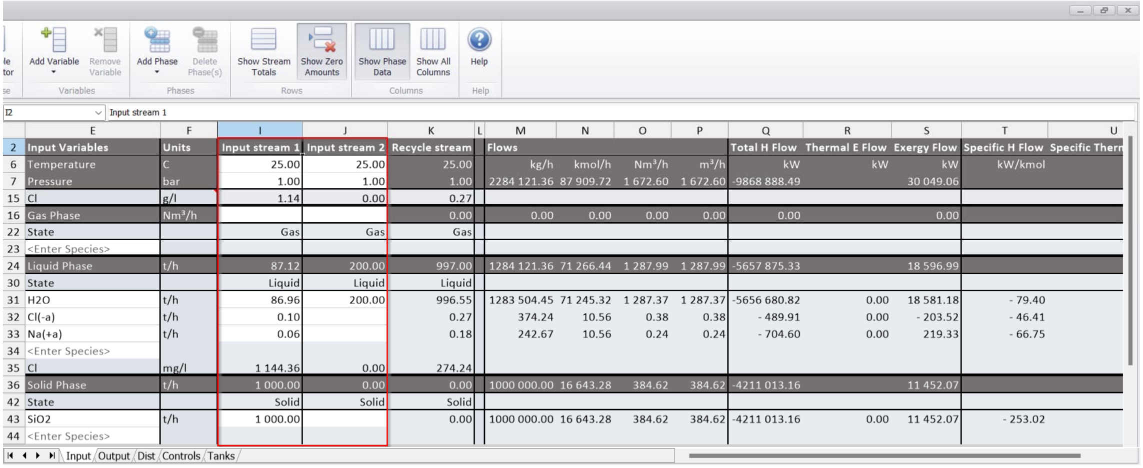

Figure 26: Input sheet in a Dynamic Unit. Examples of initial values for input streams are highlighted.

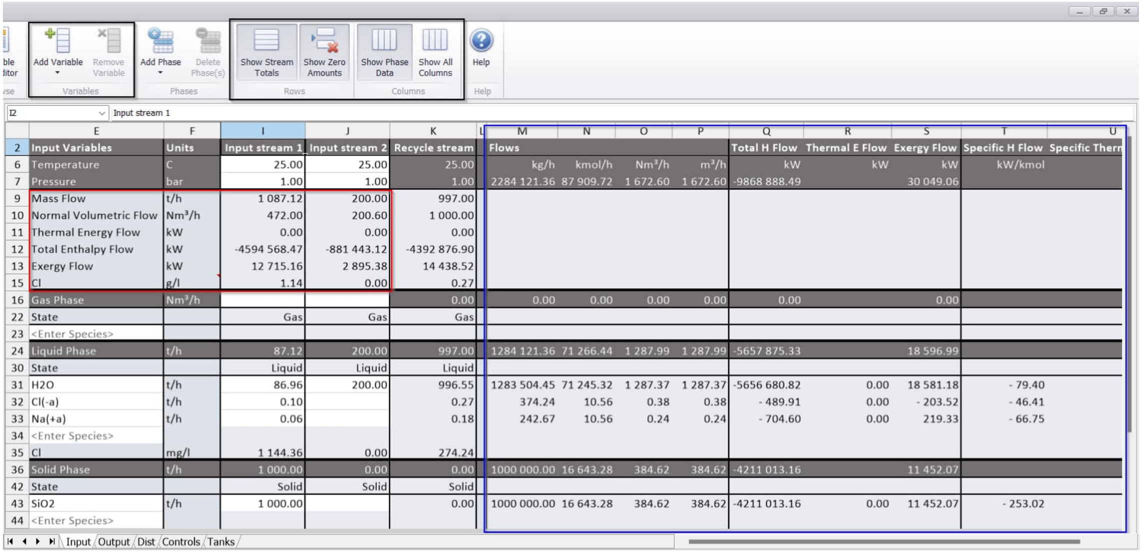

Figure 27: Visualization options for input and output sheets. Streams totals are highlighted in red, while phase data is in blue

55.9. Output Sheet in Dynamic Unit

All added variables are automatically transferred into the Output sheet of the dynamic unit (**Fig. 28**), which is similar to the input sheet.

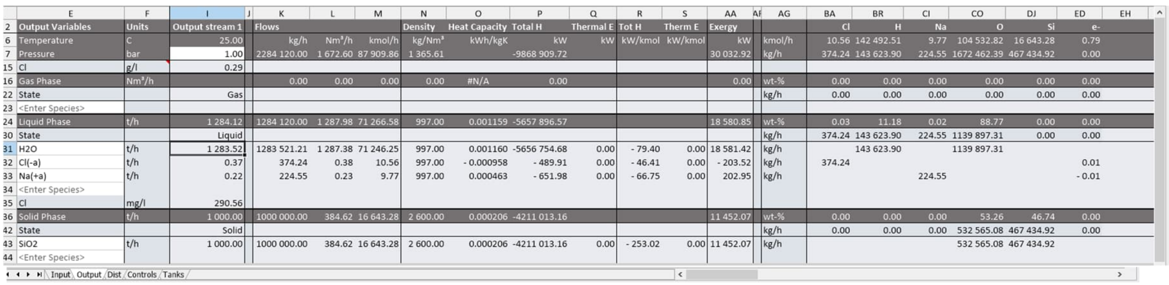

Figure 28: Output sheet in a Dynamic Unit

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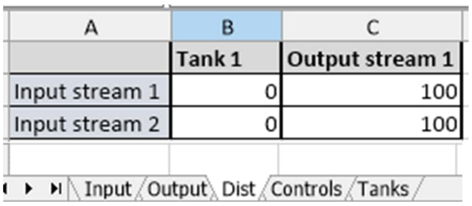
55.10. Dist Sheet in Dynamic Unit

In the distribution sheet (or Dist sheet), all the inputs can be distributed into output streams and tanks (**Fig. 29**). The distribution sheet makes it possible to perform operations with different inputs within the tank.



A	B	C
	Tank 1	Output stream 1
Input stream 1	0	100
Input stream 2	0	100

Figure 29: 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.

55.11. 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.

A tank can be added by pressing the **Add Tank** option in the Tanks section of the upper toolbar (**Fig. 30**). 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. Variables can be added with the **Add Variable** option to either Tank Variables (which are common for all phases) or phase-specific variables.

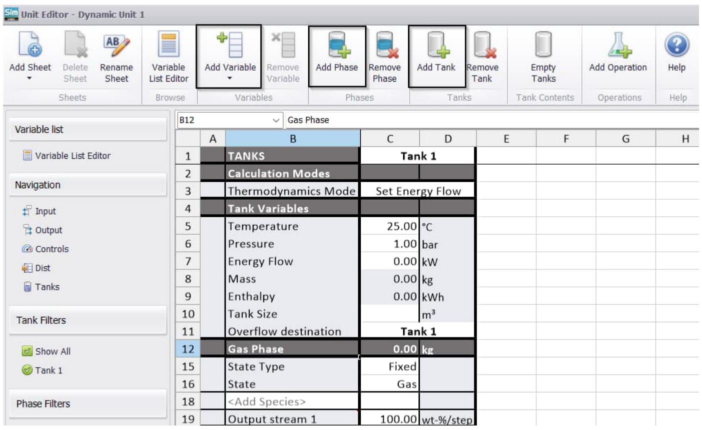


Figure 30: Tanks section in Tanks sheet within Dynamic unit

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. 33**); a new Operation sheet will be added, and the operation will be added as a variable to the tank's phases. As can be seen from **Fig. 31**, 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. 32**, operation 1 is performed with 60% of the liquid phase of the tank 1.

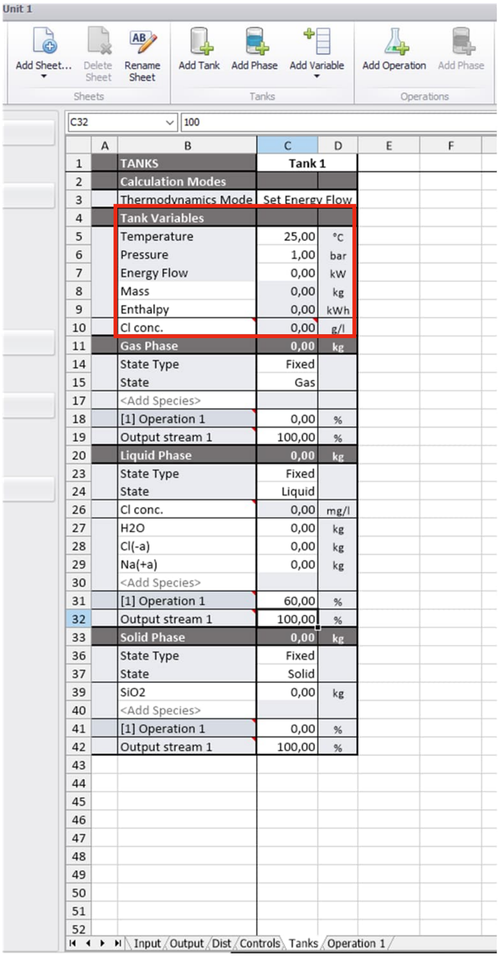


Figure 31: Tanks sheet with Operation in a dynamic unit. Here, tank variables that are common for all phases are highlighted.

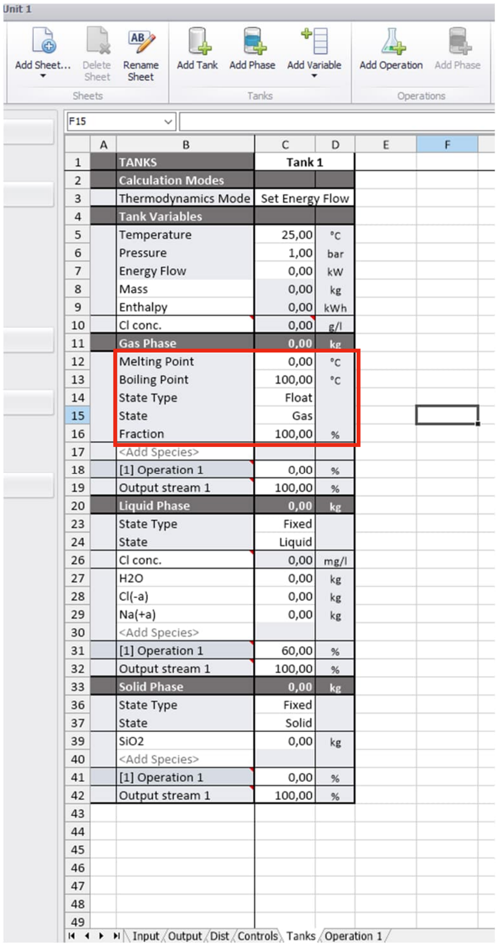


Figure 32: Tanks sheet in a dynamic unit. Here, the gas phase has the state type Float.

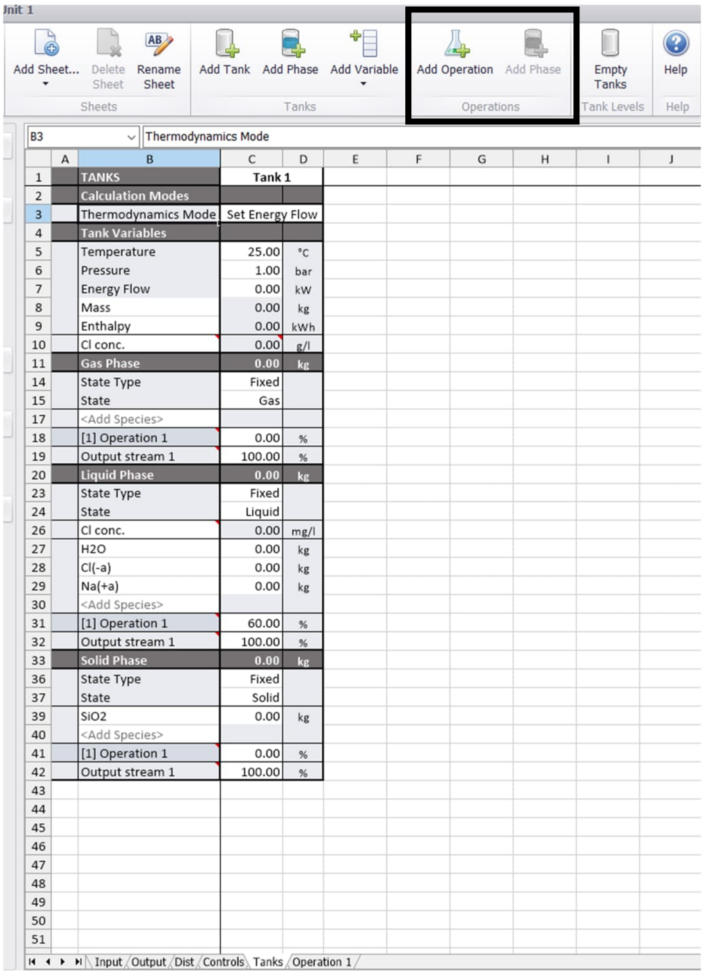


Figure 33: Adding Operation in Tanks sheet within a Dynamic Unit. Here, the Operation 1 sheet is created by pressing Add Operation, and after adding the operation, it becomes visible in the Tanks sheet as well.

55.12. Local Tank Variables

Input and output sheet variables are always shared among all interconnected units. However, local tank variables are only visible on the "Tanks" sheet, which means that the tank variables are always unit-specific. Additionally, global variables are also listed in the tanks sheet user interface, and both local and global variables are visible in the "Add-Variable" menu on the "Tanks" sheet. Available tank variables are listed below:

Tank Properties

1. **Tank Size**

   Sets a tank to a specific size. By default, a tank's **size is infinite**. If the tank becomes full, the excess content exits **via overflow.**

2. **Calculate Ideal gas Pressure.**

   Computes an ideal gas pressure when there is no vapor balance configured. Is used to consider pressure changes after water evaporation.

   NOTE: The “Calculate Gas Pressure” variable only works when **the tank size** is specified.

3. **Allow Empty Tanks**

   Select which tanks are allowed to empty when the “**Empty Tanks**” button is pressed or the “**Empty Tanks Before Calculation Starts**” feature is activated.

4. **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.

5. **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.

Amount in a Tank

6. **Enthalpy**

   Total enthalpy in selected phase.

7. **Mass**

   Total Mass in selected phase.

8. **Volume**

   Total volume in selected phase at current temperature and pressure.

9. **Total Accumulated Mass**

   Represents the total mass that has been fed into the tank over its operational history.

10. Tank Level

Represents the current tank level as a percentage value. This information can be particularly useful when specific actions need to be taken at certain tank levels.

Tank Flow

11. Mass Transfer

Mass transfer from a selected tank to a chosen destination, which can be another tank, a stream, or an operation. The specific settings for are configured in a separate dialog after the variable is added.

12. Mass Multiplier

Multiplies the mass by a user-specified factor on each simulation step.

13. Overflow Amount

If the tank becomes full, the excess content exits via overflow, the amount of which is expressed by this variable.

14. Overflow Calculation Order

Specify when the overflow is calculated and the mass is transferred into the overflow stream:

- **New Mass:** Incoming mass is moved into overflow if it does not fit into the tank.
- **New Mass and Energy:** Incoming mass and energy are moved into overflow if the incoming mass does not fit into the tank.
- **Old Mass and Energy:** Existing mass and energy stored into tank are moved into overflow if the incoming mass does not fit into the tank.
- **Overflow at the End of Round:** Excess mass and energy are moved into overflow at the end of the round. (Default option)

15. Overflow Phase 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.

55.13. Operations Sheet in Dynamic Unit

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.

The **Add Operation** option in the Operations toolbar section (**Fig. 34**) 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 1**) is NOT advanced). Otherwise, this new phase serves as an operation-specific phase.

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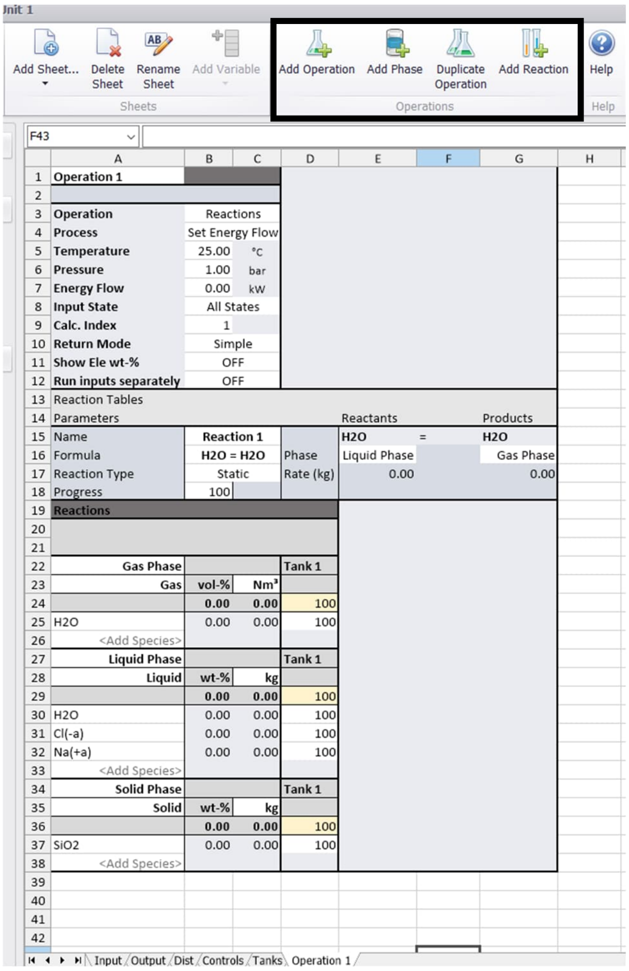

Figure 34: Reactions operation sheet in a dynamic unit. Here, Reaction 1 is added by default, and more reactions can be added with the Add Reaction option.

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 1.

For all operations, the operation output distribution can be specified in the section highlighted in **Fig. 35**. 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. 35**, 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.

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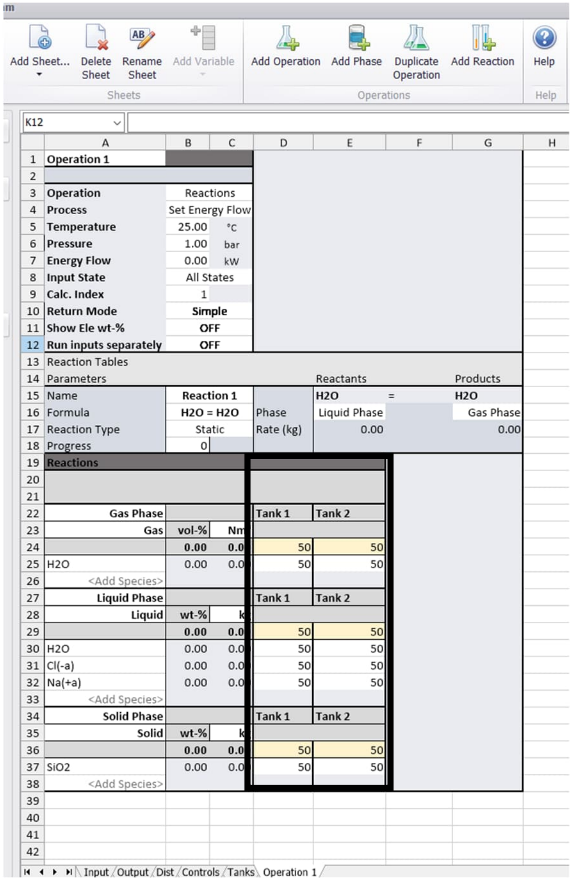

Figure 35: Operation sheet in a dynamic unit. Here, in the highlighted area, the reaction products' destination is defined as 50% of the reaction output species going to Tank 1 and the remaining 50% of the reaction output going to Tank 2.

Table 1: Parameters of operations in tanks in Dynamic unit

Operations parameters	Description
Operation	Is used to set the type of operation.
Process	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	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-%	If ON, shows elemental distribution in the operation’s output.
Run inputs separetely	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	Variable specific for Chem EQ that allows to calculate activity coefficients estimates of elements in chemical equilibrium based on the specified target concentration.
Constraints	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	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.

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55.14. 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. 36**). 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.*

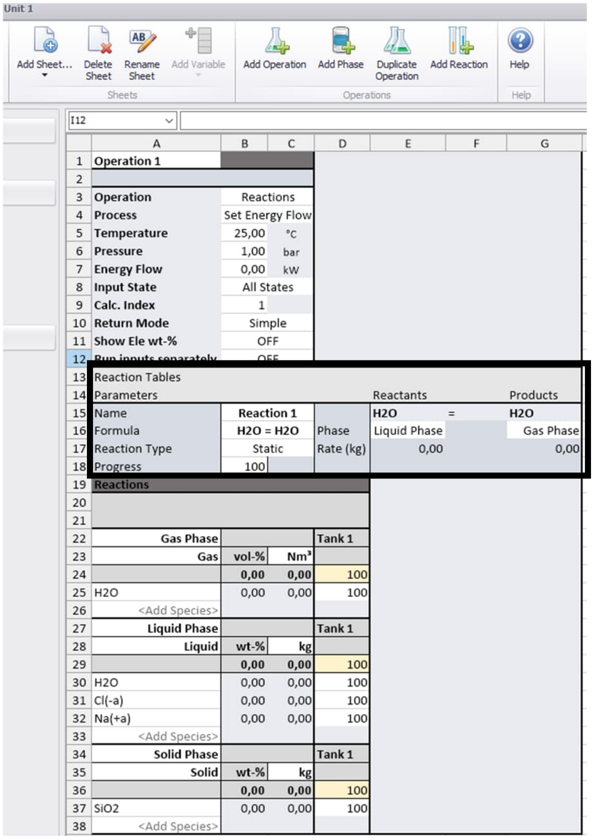

Figure 36: Reaction type of operation in a dynamic unit.

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:

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

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. 37**). 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. 37, Fig. 38**).

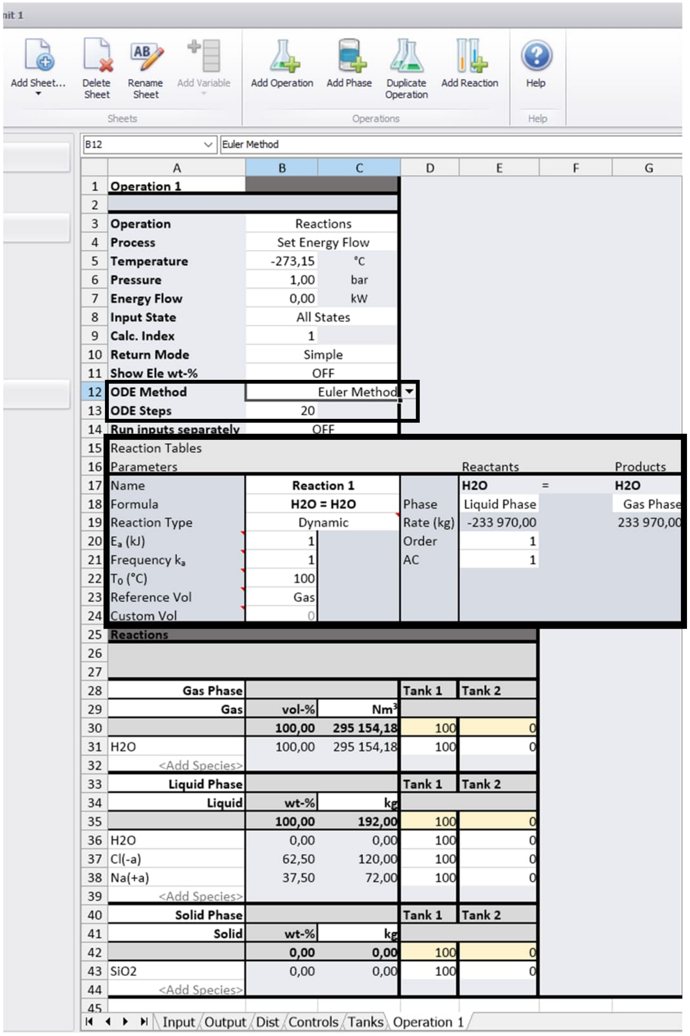

Figure 37: Dynamic type of reaction operation in a dynamic unit. Here, the dynamic reaction type is selected, and the method of solving the differential equation of dynamic reaction is highlighted.

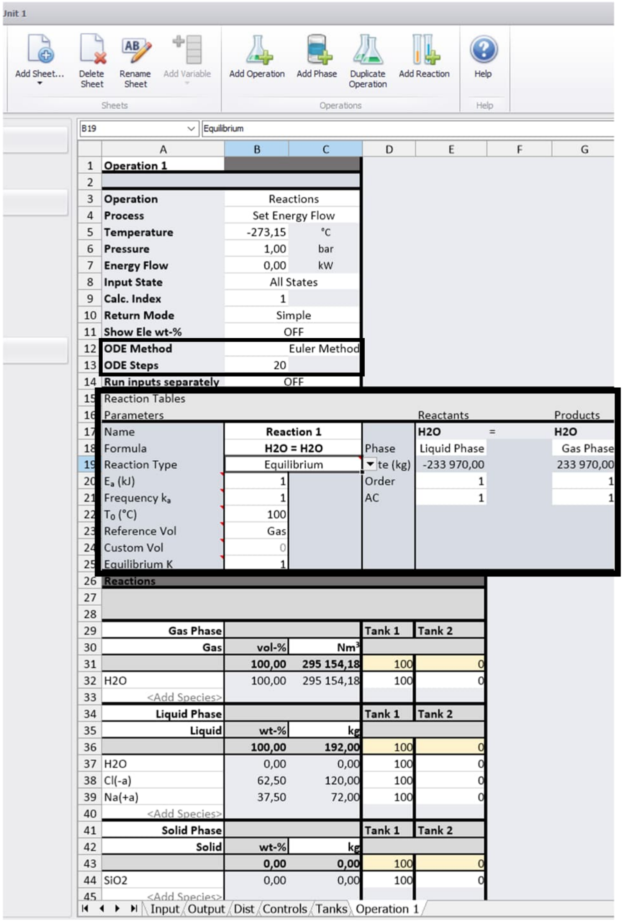

Figure 38: Equilibrium type of eaction operation in a dynamic unit. Here, the reaction type selected is Dynamic equilibrium, and the method of solving the differential equation of dynamic reaction is highlighted.

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):

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

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.

55.15. 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. 39**) or estimated with **AC Back Calculation** option under possible **Constraints** (**Fig. 40**).

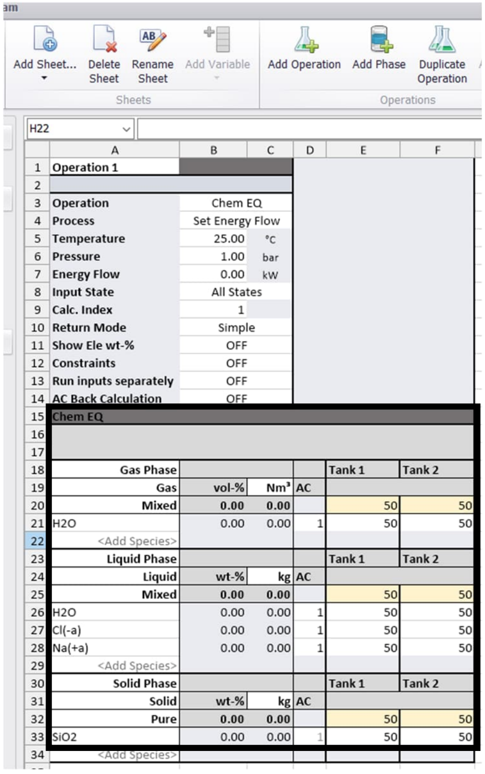

Figure 39: Chemical equilibrium type of operation in a dynamic unit. Here, the activity coefficients are specified for mixed phases. The AC back calculation is OFF.

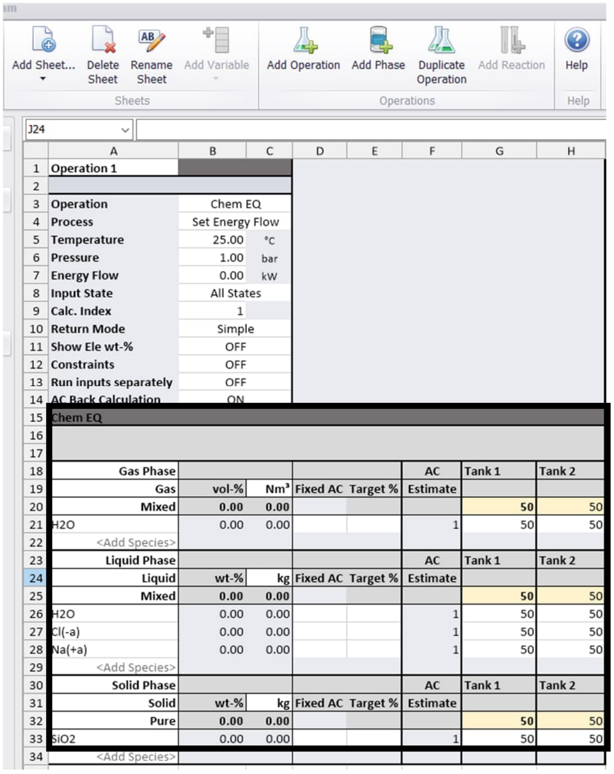

Figure 40: Chemical equilibrium operation in a dynamic unit. Here, the AC back calculation is ON, meaning the activity coefficients are estimated based on target concentration percentages.

55.16. 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. 41**). 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.

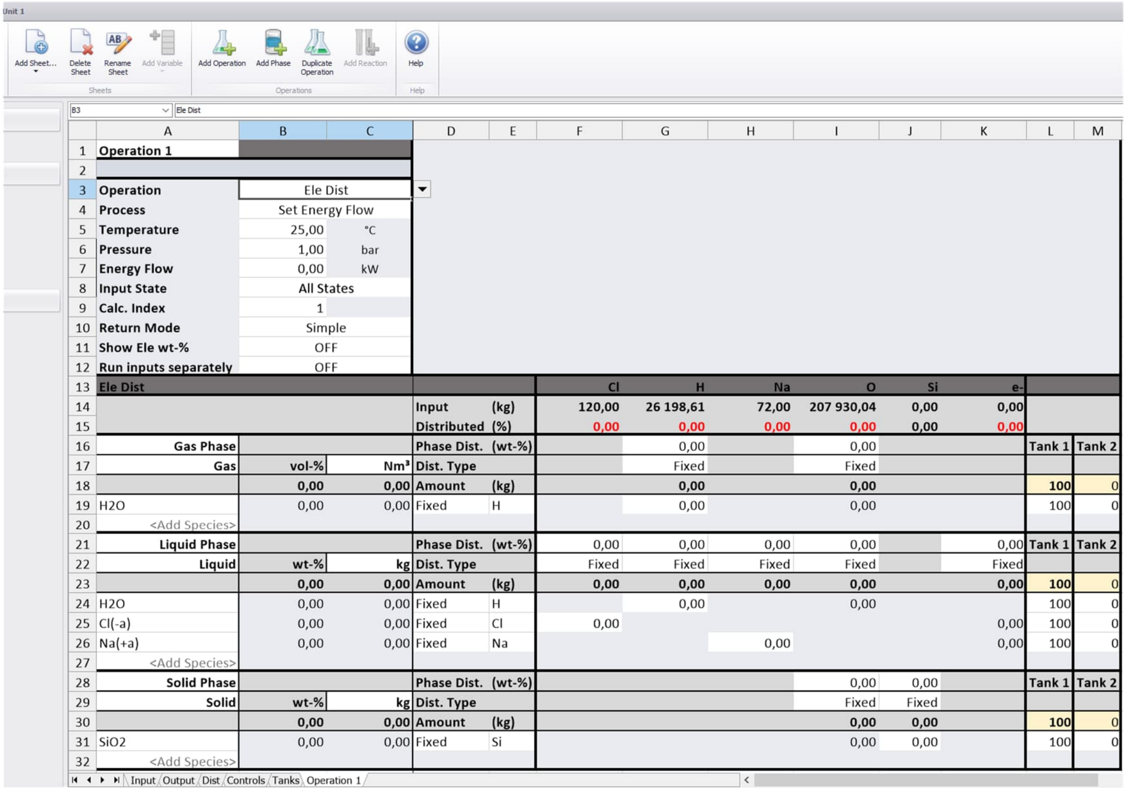

Figure 41: Element Distribution operation type in a dynamic unit.

55.17. Ideal Mixer and Ideal Heat Mixer Type 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. 42** and **Fig. 43**, 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.

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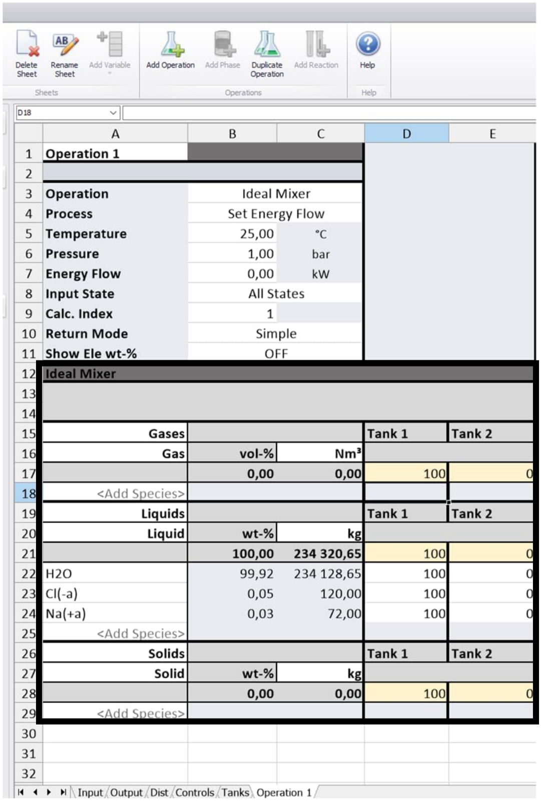

Figure 42: Ideal Mixer operation in a dynamic unit.

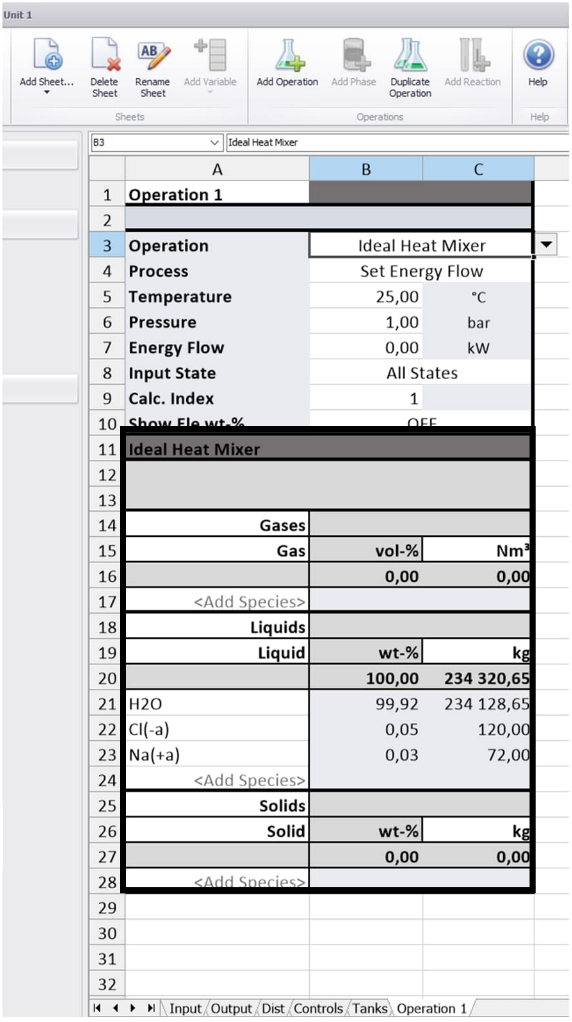

Figure 43: Ideal Heat Mixer operation in a dynamic unit.

55.18. 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. 44** 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.

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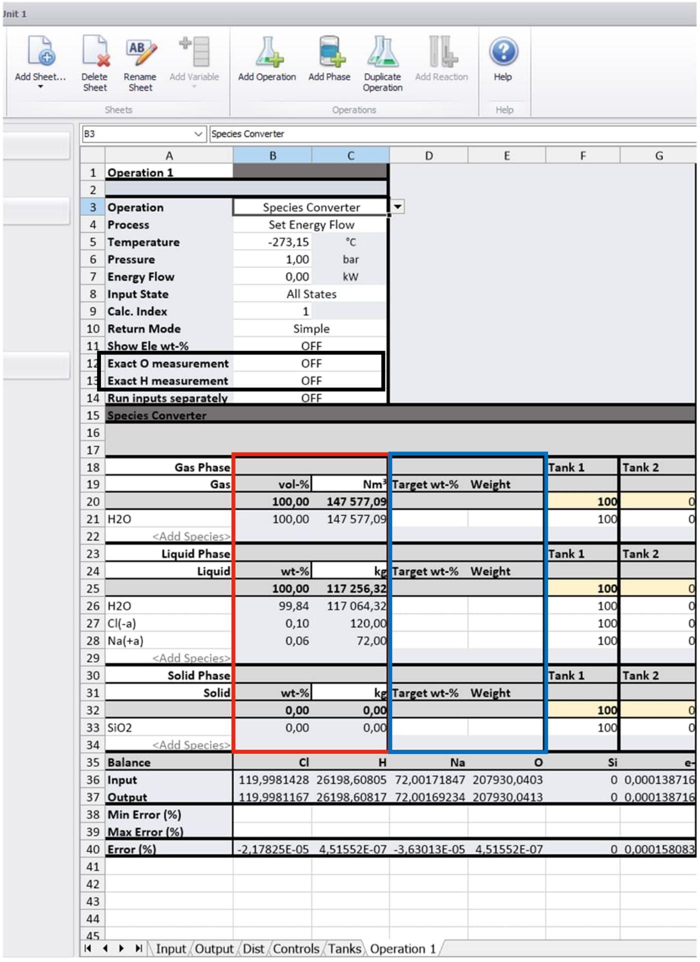

Figure 44: Species Converter type of operation in a dynamic unit. Here, the sections for input (total wt-% or vol-%) and output (weighting coefficients) analysis are highlighted in red and blue, respectively. Also, the exact O and H measurement options are highlighted.

55.19. Schematic representation of tank and operation 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. 45**).

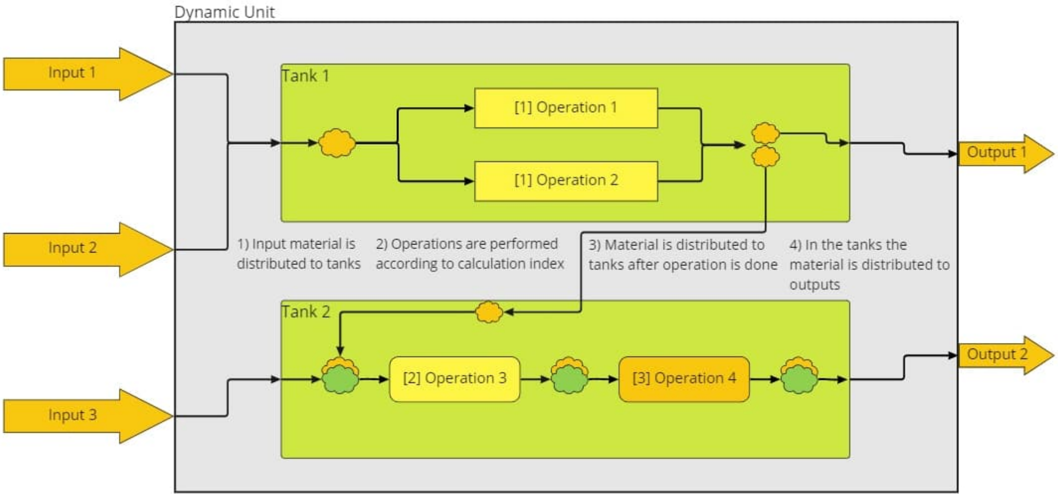

Figure 45: Schematic representation of a dynamic unit example.

55.20. Event Sheet in Dynamic Unit

An event in a dynamic unit consists of several blocks (**Fig. 46**). 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.

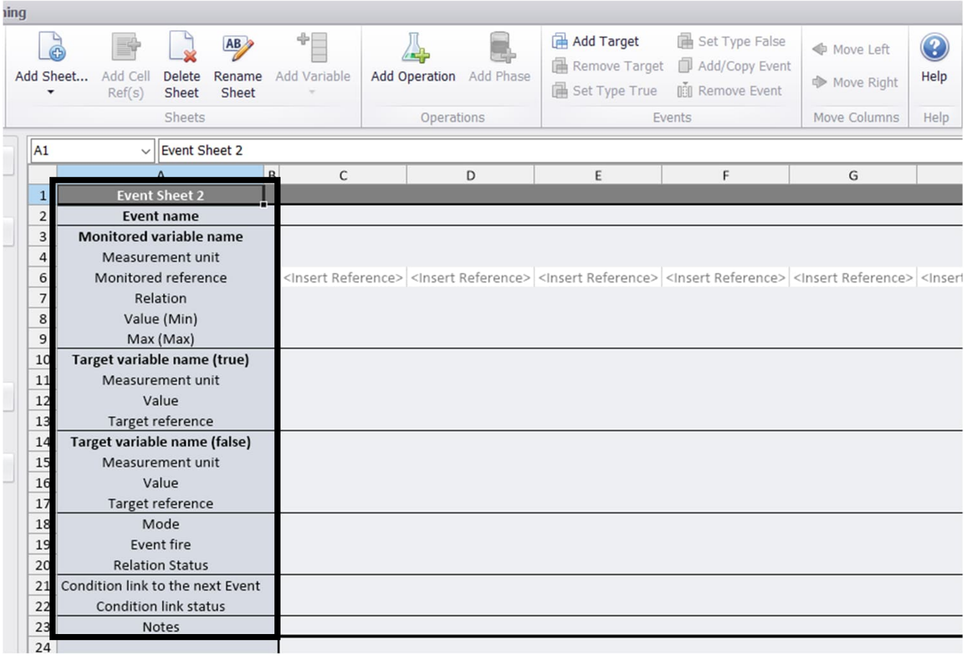

Figure 46: Event sheet in Dynamic unit.

55.21. Set Sheet in Dynamic Unit

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. 47**). 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. 48**). 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. 48**). A more detailed example on how the stopwatch set sheet can be used is described later in the leaching example section.

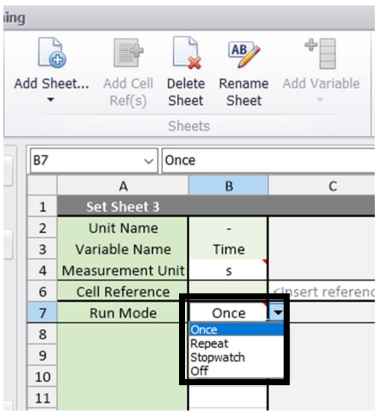

Figure 47: Set sheet in a dynamic unit.

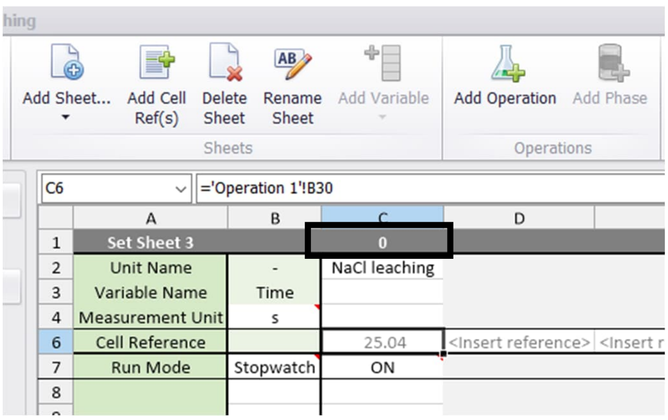

Figure 48: Stopwatch Run mode in Set sheet in a dynamic unit. Here, the stopwatch second counter is highlighted.

55.22. Batch sheet in Dynamic Unit

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. 49**) that consists of a dynamic unit and an input stream. The gas flow of Input stream 1 is 100 Nm^3/h (**Fig. 50**). 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. 51**). 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. 52**).

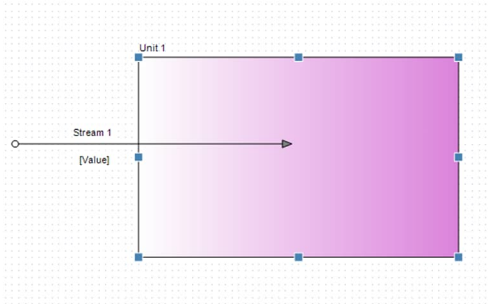

Figure 49: Example model for Batch sheet demonstration.

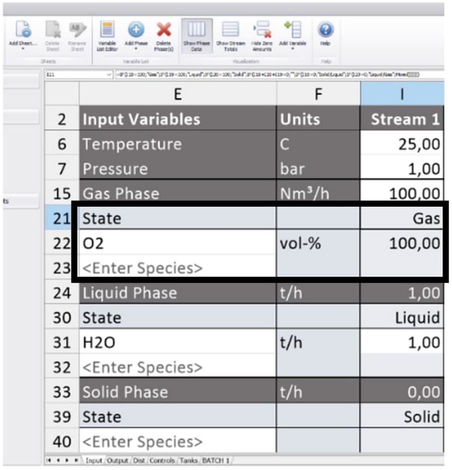

Figure 50: Input sheet for the Batch sheet demonstration model. Here, the initial input for gas is defined as 100 Nm^3/h.

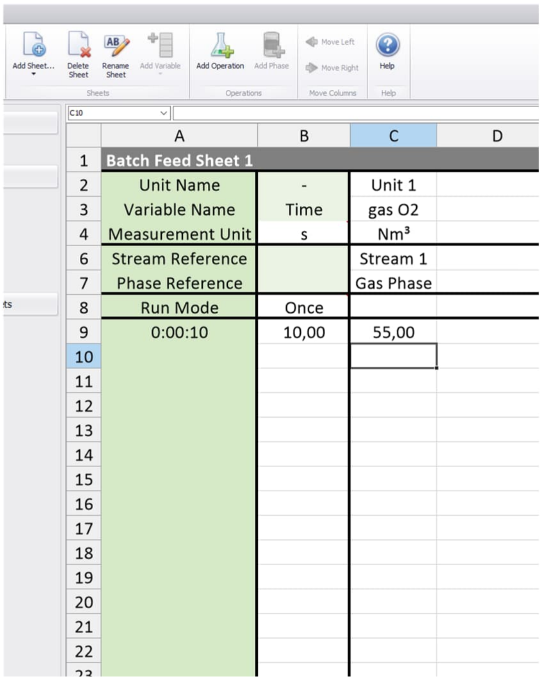

Figure 51: Batch sheet in a dynamic unit. Here, an amount of 55 Nm^3 is added to Input stream 1 ten seconds after the beginning of the simulation.

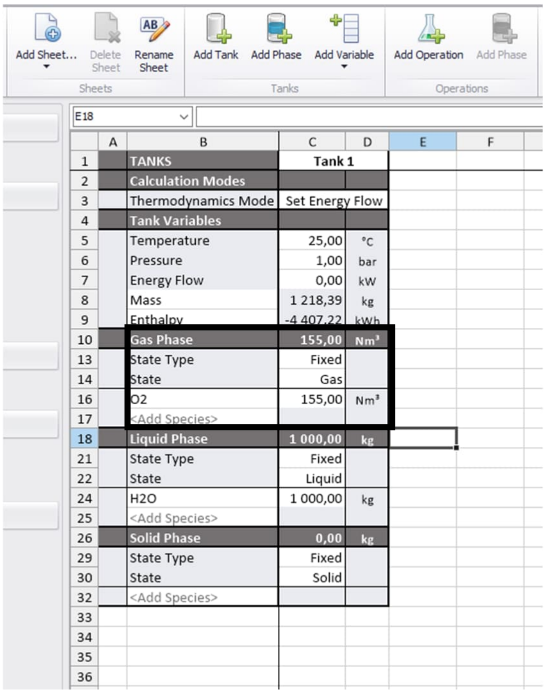

Figure 52: Tanks sheet after 1 hour of simulation. Here, the amount of gas phase is the sum of the initial gas input (100 Nm^3) and the additional 55 Nm^3 specified in the Batch sheet.

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55.23. Leaching Example

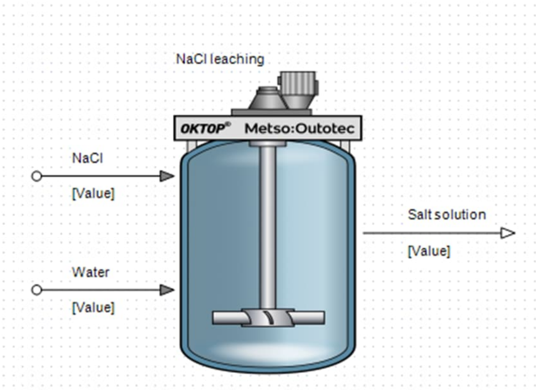
Here, a leaching example is considered in order to demonstrate the reaction operation in a dynamic unit. This example is a simple case of NaCl leaching in batches to produce a salt solution.

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
3. 90% full. First solid salt is added and then water. The batch is mixed for 5 minutes before discharge.
4. The desired final NaCl concentration is a 25 wt-% solution.
5. The reactor is emptied to 50% and the making of the batch is started again.
6. Feed flows are 150 t/h for solid salt and 200 m^3/h for water.
7. 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. 53**). 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. 54**).



Inputs	Outputs
NaCl	Salt solution
Water	

Figure 53: Example model of leaching.

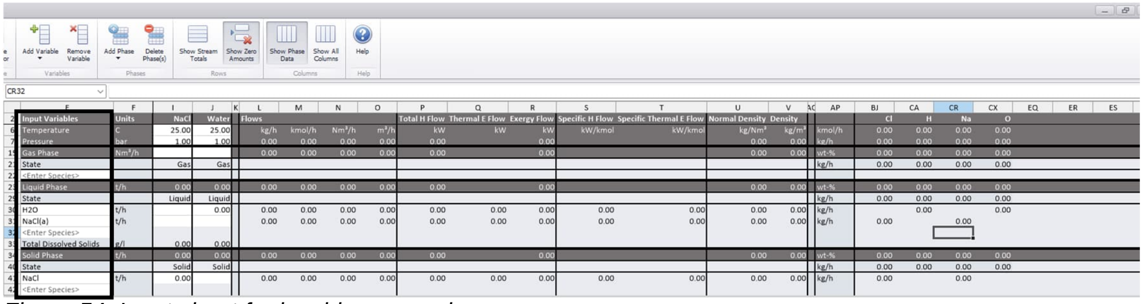


Figure 54: Input sheet for leaching example.

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. 55**).

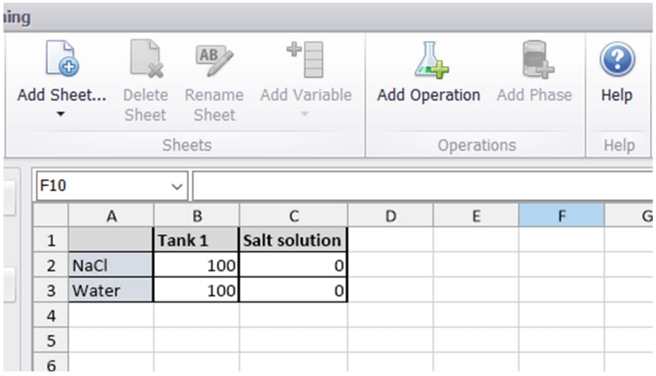


Figure 55: Dist sheet for leaching example.

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. 56**). 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. 57** (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.

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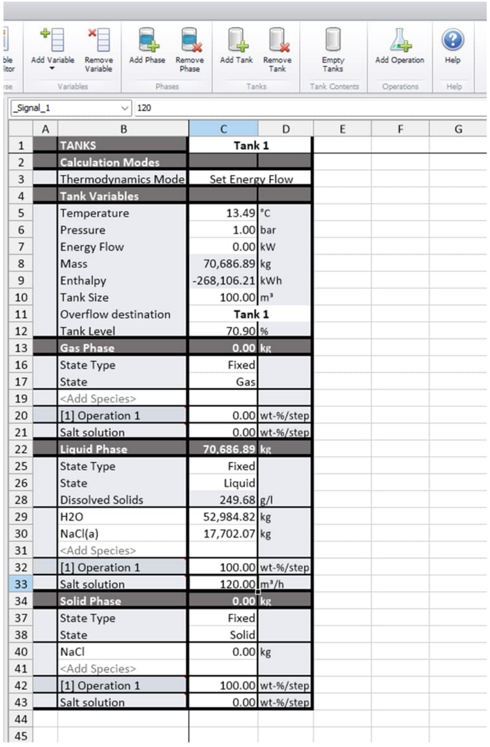


Figure 56: Tank sheet for leaching example.

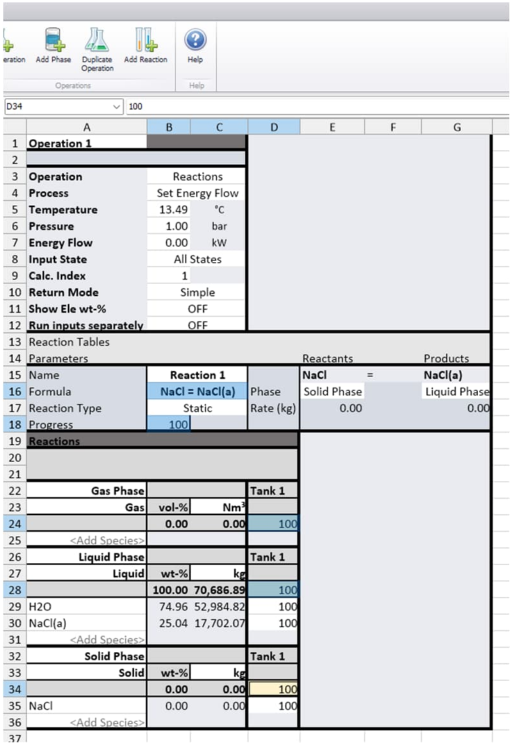


Figure 57: Operation (Reaction) sheet for leaching example

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. 58**). 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. 59**).

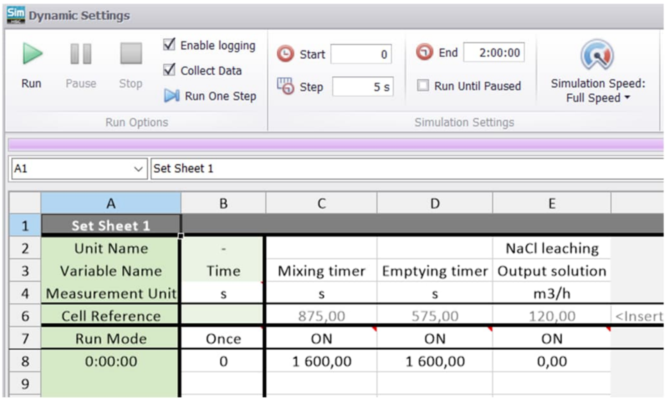
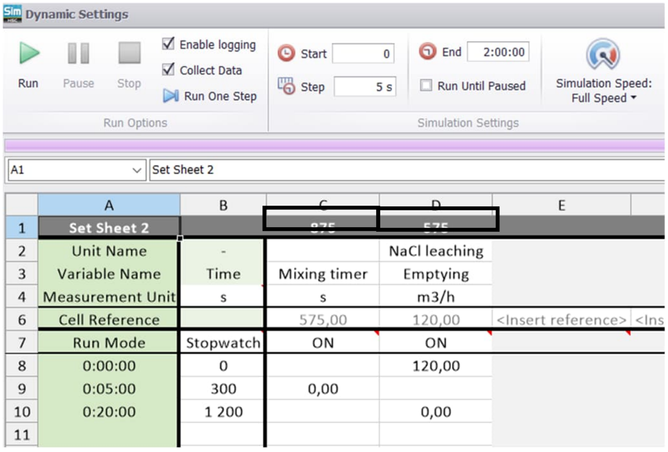


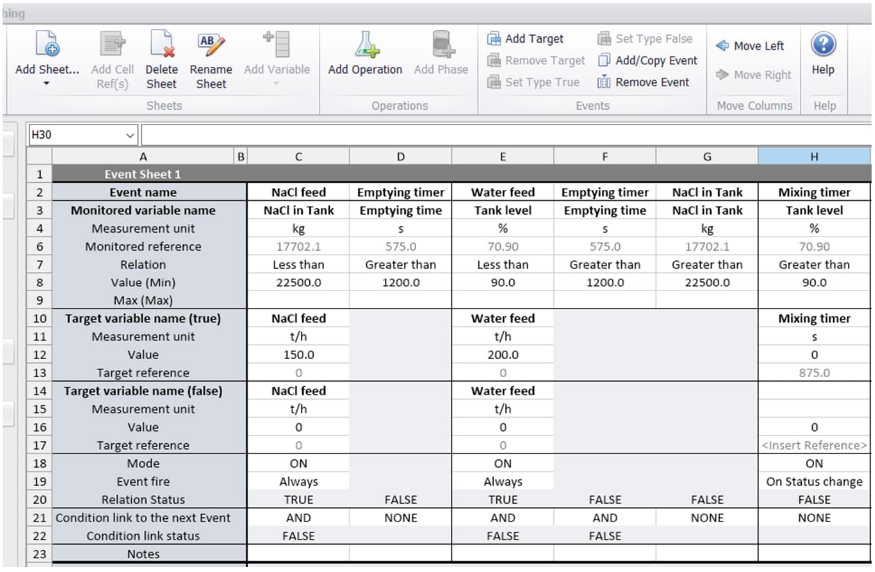
Figure 58: Set 1 sheet for leaching example. Here, the cell references for the mixing timer and emptying timer are referenced to the second counters in the Set 2 sheet.



	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 59: 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. 60**). 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 60: Event sheet for leaching example.

55.24. 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.