OLI Flowsheet

Modeling Basics Course

V11

think simulation

getting the
chemistry right

OLI Flowsheet Modeling Basics Course

© 1997-2021 OLI Systems, Inc.

The enclosed materials are provided to the lessees, selected individuals and agents of OLI Systems, Inc. The material may not be duplicated or otherwise provided to any entity without the expressed permission of OLI Systems, Inc.

Contact Information

Visit the Contact OLI Systems page at https://www.olisystems.com/techsupport to submit general inquiries, contact Technical Support, or search for an address and phone number.

If you need to contact Support, you can submit an online request via OLI Portal: https://portal.olisystems.com/

Other useful links and resources are:

- OLI Systems Portal – How to create and account: http://downloads.aqsim.com/Client%20Portal%20Instruction%20Manual.pdf
- Product Downloads: http://downloads.olisystems.com/
- OLI Systems YouTube Channel: https://www.youtube.com/OLISystems
- OLI Systems Wiki page: http://wiki.olisystems.com/wiki/Main_Page

Disclaimer

This manual was produced using the OLI ESP FS 11.0 build 1 (11.0.1). As time progresses, new data and refinements to existing data sets can result in values that you obtain being slightly different than what is presented in this manual. This is a natural progress and cannot be avoided. When large systematic changes to the software occur, this manual will be updated.

Chapter 1 Removing Hardness from Water

The Application

The simplest ESP calculation is the adiabatic mixing of two streams. We will use this calculation to see ESP's general workings. Figure 1-1 is a process diagram containing two inlet streams, a mixer, a separator and two outlet streams. The Hard Water stream contains substantial amounts of dissolved calcium and magnesium. Adding sodium carbonate will precipitate $CaCO_3$ and $Mg(OH)_2$ by providing a source of carbonate and by raising the pH. The goal is to reduce the total dissolved calcium and magnesium concentrations in the hard water to less than 10 mg/l on a combined basis.

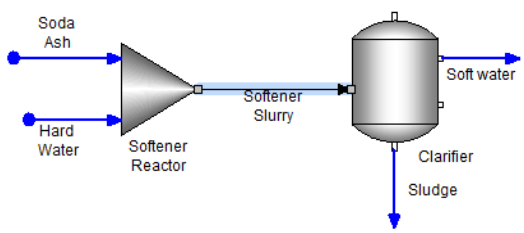


Figure 1-1 – Adiabatic mixing of Hard water with Soda Ash and separating the solids from the liquid

You will build this case in two steps. The first step is to create the chemistry model and the second is to build the streams and process blocks.

Creating a Chemistry Model

The Chemistry Model is one of two core modules in any ESP calculation. The other core module is the Process Case. The Chemistry Model module contains all the inflows, dissolved species, solids, gases and oils that are to be used in a case. The Model also contains the thermodynamic properties so that the reaction equilibrium constants and species properties can be computed.

The procedure for creating a chemistry model are explained in the following steps.

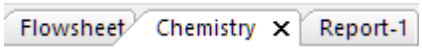
- Choose the database and thermodynamic framework to use.
- Enter the inflow components.
- Edit the solid phases that will be included or excluded from the case.
- Add customized equations, kinetics and surface reactions.

Once completed, the process can be designed. A chemistry model can always be changed. It is a matter of returning to the model generation steps (above) and making the necessary modifications.

Introduction to the Chemistry Model tabs

Creating a Chemistry Model can be as complex as the case requires. The chemistry is simple in this example. It contains a few components and no modifications to the default settings.

Selecting the thermodynamic method and databases to be used in the Model

- ✓ Click on the Chemistry tab - 

The Chemistry section contains five sub-tabs: Inflows, Databanks, Phases, Redox, and Kinetics. New cases default to the Databanks tab. This tab contains the thermodynamic framework and specialized any databases to be included.

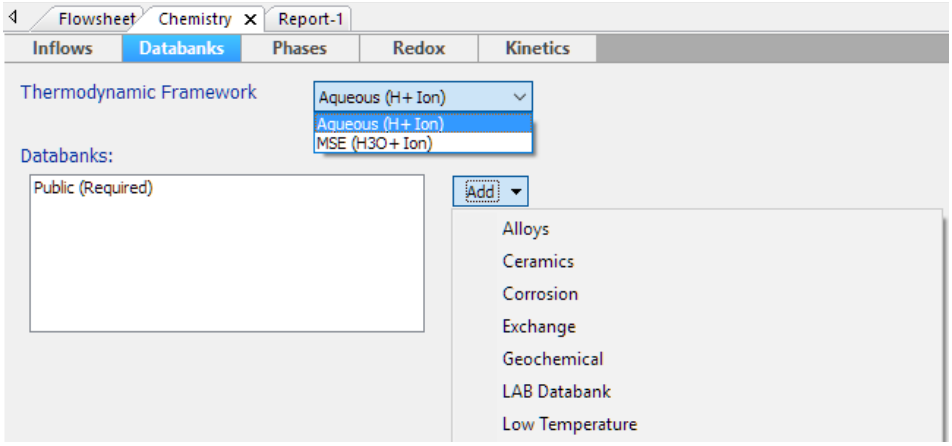


Figure 1-2 - The available framework and databases installed with the software

OLI uses two thermodynamic frameworks, Aqueous (H+ ion) and MSE (H3O+). MSE stands for Mixed Solvent Electrolyte. The available databases (note the Add button) include the required Public database, OLI-installed private databases and client-specific private databases.

- ✓ Use the default settings of Aqueous (H+) and no private databases.

Adding the chemical inflows to the model

The inflows tab contains the grid for adding molecular inflows, assays, pseudocomponents and other optional inflows.

- ✓ Click on the Inflows tab to access the grid for adding inflows.
- ✓ Type the following Inflows to the grid:

NaCl
CaCl2
MgCl2
Na2CO3

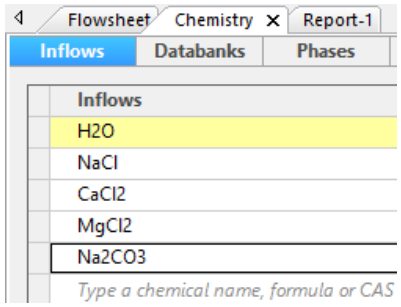


Figure 1-3 – entering the molecular inflows.

Editing the Solid Phases in the Model

- ✓ Click on the Phases tab.

This screen is the Phase Editor. Here the user can exclude solid phases if they feel that these solids will not form within the timeframe of the process. All solids are "on" by default, so when the case is run precipitation of any phase is possible.

- ✓ Click on the "+" sign adjacent to the All section

This action exposes the complete phase list in the Chemistry Model. There are nearly thirty potential solid phases. This solids list is based on any combination of Ca^{+2}, Mg^{+2}, Na^{+1}, CO_3^{-2}, and H_2O. Whether or not one or more forms depends on the solution composition and conditions. Users can prevent any solid from precipitating by unchecking the individual box.

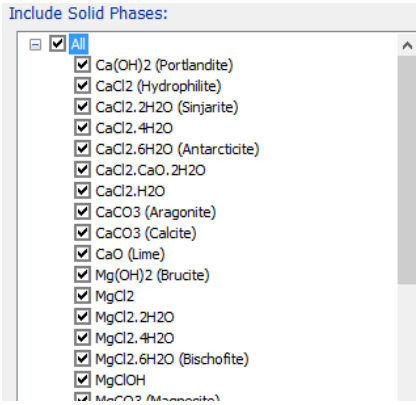


Figure 1-4 – Selecting the phases to be included-excluded in the case

All phases will be allowable in this case and so no action is required.

Review the REDOX and Kinetics options

- ✓ Click on the Redox tab.

The Redox screen contains toggle boxes to enable or disable oxidation-reduction reactions. The default setting is for Redox reactions to be off. If Redox chemistry is included, then the user selects which elements will be included, and also which oxidation states within the particular element is included.

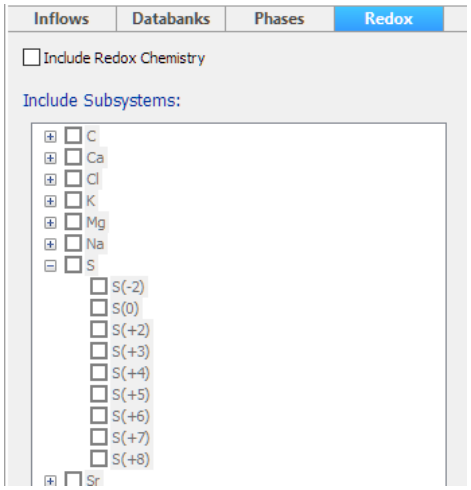


Figure 1-5 – Include or exclude Oxidation-Reduction reactions and select which element and oxidation state will be allowed

- ✓ Use the default settings for the Redox tab.
- ✓ Click on the Kinetics tab.

The Kinetics tab is where users can construct rate-limiting equations for one or more reactions. A template of species is available to create the kinetic model. Creating kinetic reactions will be explained in later chapters.

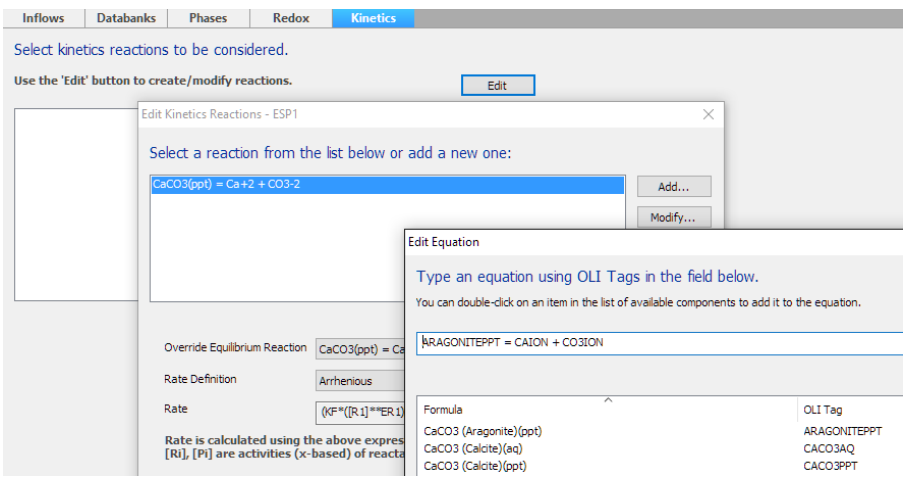


Figure 1-6 – Selecting reactions that will be undergo rate-limiting kinetics

- ✓ You will not create any reactions.

This completes the basic introduction of the Chemistry Model Build step. There are additional options, but they are not germane to the first example.

Building the Softening Process

Quick introduction to the Flowsheet screen

The procedure building a process is straightforward. Each form/screen asks for the required information, as do the Block screens.

✓ Click on the Flowsheet tab.

The main flowsheet screen contains a center workspace, support panels, and a toolbar. The workspace is blank, and becomes filled with streams and units. The support panels include Navigator, Library, Properties, and a general Output section (errors, trace, monitor, and output). The toolbar contains various actions that are described below.

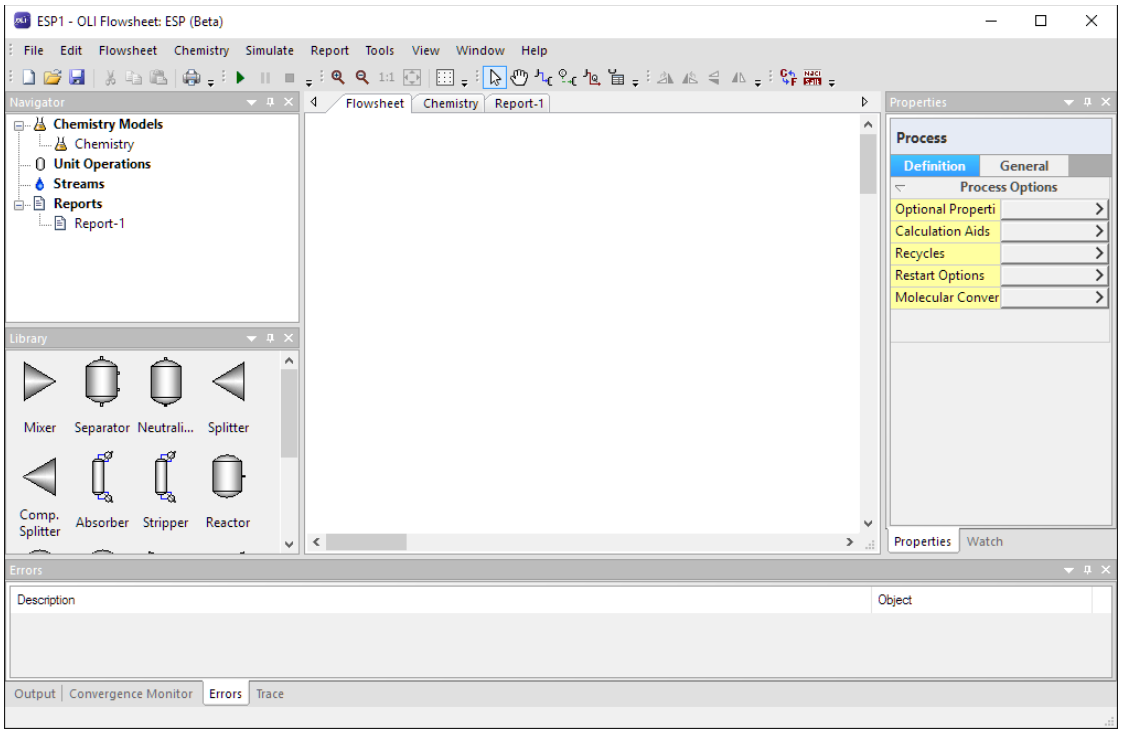
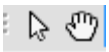


Figure 1-7 – Flowsheet tab showing the blank process screen and the five default support panels

- The Navigator panel contains the complete list of objects that are part of the file. This includes all chemistry models, streams, unit operations and reports.
- The Library panel contains the available units and unit operations. Objects in the library panel are brought into the workspace using drag and drop.
- The Properties panel contains the settings for a unit, the molecular composition of a stream, or the properties of the flowsheet. The panel view will therefore change, depending on what object or stream is in focus on the worksheet. There are tabs at the bottom and top of the panel that display input and output composition and settings.
- The general output panel at the bottom of the screen contains several sub panels. The Convergence Monitor contains a graph that shows the progress of converging recycle streams (Tear streams) and controller settings. The Errors panel contains the list of problems that need to be corrected either before running the case or problems found after the case is run. The Trace and Output tabs contain detailed information on the calculation. These are intended for more advanced users.
- The toolbar contains several action buttons:
    - Start, Pause, and Stop
    - Zoom and centering

- Object select and move 
- Add Streams, Signals and Energy buttons
- An add Callout Table button
- Rotate objects buttons
- Names and Units Manager buttons

✓ Start by saving the case file. Give it a name that you can recognize quickly because this file will be used in the next several chapters.

Adding the Softener Reactor and Inlet Streams

This example contains a mixer, a separator, two inlet streams, and two outlet streams. You will start by creating the Mixer block with the two inlet streams.

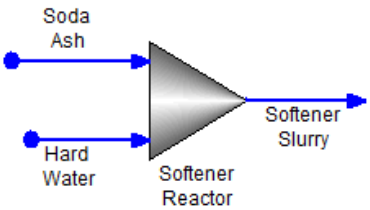


Figure 1-8 Adiabatic mixing of two liquids

The mixer is an adiabatic (by default) block that can accept a single stream to over twenty inlet streams. It calculates all reactions to equilibrium, which is the case for most Flowsheet ESP blocks. Its output is a single stream.

Each of these panels and toolbar action items will be used to varying degrees in the first several chapters of this manual.

✓ Click on the Mixer object in the Library (lower left of the screen) and drag it onto the Worksheet.

✓ **Double click** on the new block to change its name to Softener Reactor.

You will notice that the right Properties panel displays the settings for this mixer.

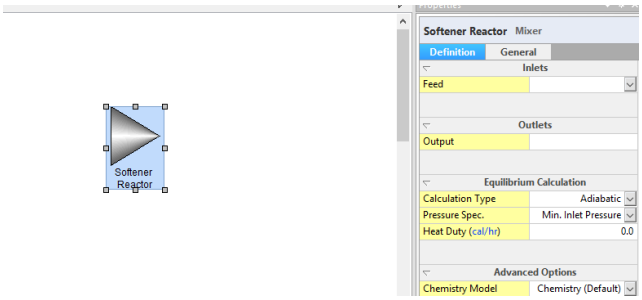


Figure 1-9 - The Mixer block and the Properties Panel (Definition tab)

- ✓ Click on the Add Stream button in the Toolbar.

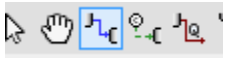


Figure 1-10 - The Add Stream button in the toolbar

- ✓ Create an inlet stream to the mixer by clicking on the flowsheet to the left of the mixer and dragging the mouse to the mixer. Unclick and click again when the + symbol appears on the cursor.

Notice that a separate click is needed to anchor the stream to the unit.

- ✓ Create a second inlet stream the same way.
- ✓ Lastly, create an outlet stream.
- ✓ Press the ESC key to deactivate the Add Stream button.

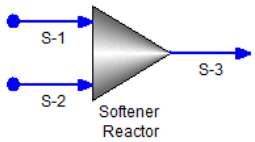
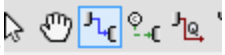


Figure 1-11- A mixer containing two inlet steams and one outlet stream

The Add stream mode stays active until the ESC key is pressed, or the arrow button is selected , or if the Add Stream button is clicked a second time 

- ✓ Double click on the first stream and label it Soda Ash.
- ✓ Label the second stream Hard Water
- ✓ Label the outlet stream Softener Slurry.

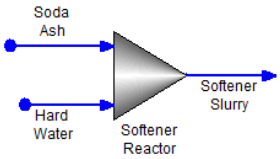


Figure 1-12- Names added to the mixer block

Entering the Stream compositions

- ✓ Click on the Hard Water to access the Properties panel for the stream.

The Properties panel on the right has the Definition tab active. This tab is the inflow composition grid where you enter the conditions (T,P), flow rate (called Stream Amount), Composition (called Inflows), and Specialized settings for the stream.

- ✓ Enter the composition shown in the table below for the Hard Water.

	Soda Ash	Hard Water
Temperature (C)	25	25
Pressure (atm)	1	1
Stream Amount (mole/hr)	1	100

H2O	0	55
NaCl	0	1
CaCl2		0.1
MgCl2	0	0.1
Na2CO3	1	

Table 1-1 – Process Stream and Acid Waste stream compositions

✓ Click on the Soda Ash stream and enter the composition.

The row labeled Stream Amount is the Flow Rate. The units in this case are 100 moles/hr. At the bottom of the grid is a Total value. This is the sum of inflows entered, which in this case is 56.2 mol/hr. Each inflow component therefore, is multiplied internally (by 100/56.2=1.779) to achieve the total flow rate.

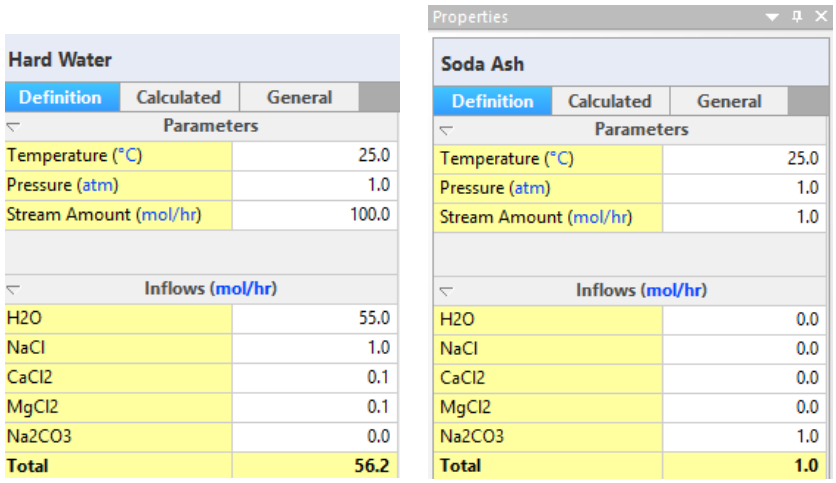


Figure 1-13 - The mixer block with the completed Process Stream and Acid Waste

The Soda Ash stream is 100% Na2CO3. In this case, both are entered as 1 mol/hr and so it does not require renormalization.

Viewing the Mixer properties

✓ Click on the Softener Reactor object to view its Properties panel.

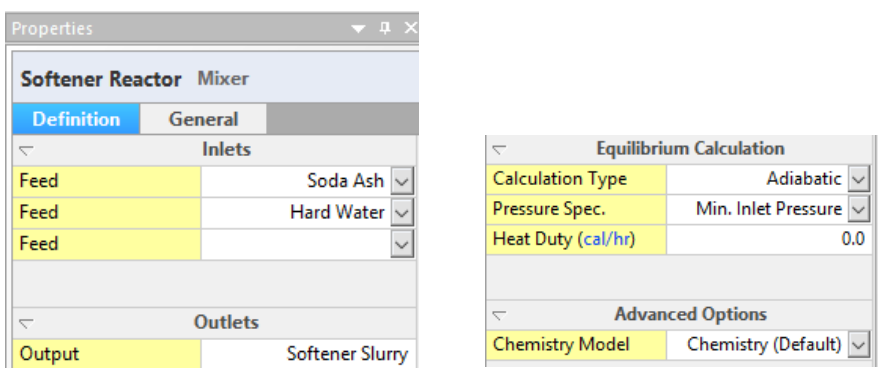


Figure 1-14 - The Mixer block with the completed Acid Waste stream

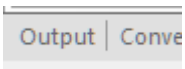
The top of the panel contains the inlet and outlet streams names. The default calculation type is Adiabatic (mix of inflows) and the default pressure setting is the lowest value pressure of any inlet stream. In this case the inlet stream pressures are both 1atm, and so this will be the outlet pressure. There is an option that allows the user to change the Chemistry Model. This is an advanced setting described later in the manual.

There are no changes to make on this panel.

Calculate the case and view the results

✓ Press the Calculate button.

The software will generate the chemistry model, initialize the process, calculate the properties of the two each inlet streams and, lastly, calculate the mixer block. This progress is displayed in the Output tab at the bottom of the screen.

✓ Click on the Output tab at the bottom of the screen. 

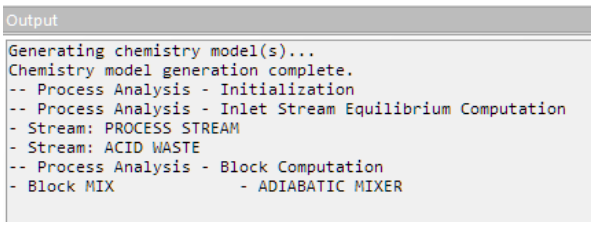


Figure 1-15 - The Output tab displaying the simulation progress

When the simulation is complete, a popup window will appear in the lower right of the screen.

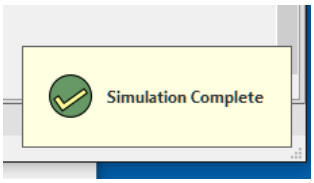
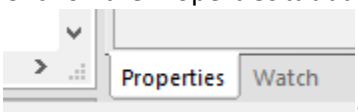


Figure 1-16 - The Simulation Complete popup

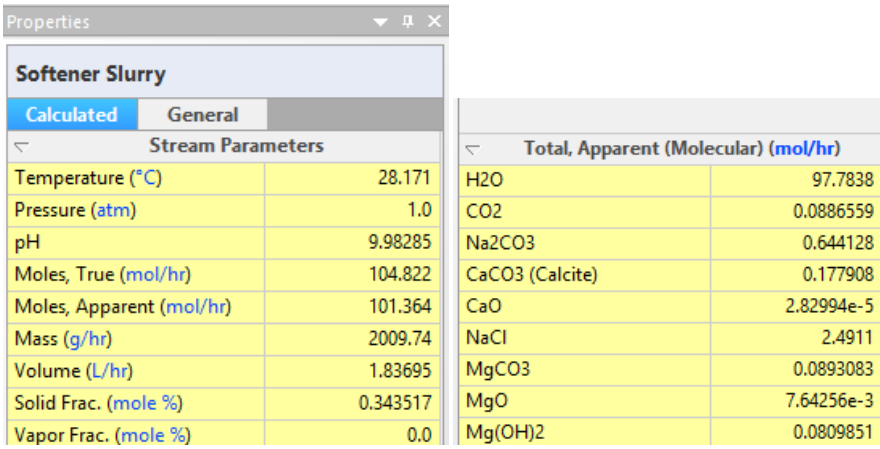
✓ Click on the Softener Slurry stream to access the Properties panel.

The resulting composition and properties of this outlet stream are displayed in the Properties panel.

✓ Click on the Properties tab at the bottom of the panel if this tab is not yet highlighted.



.

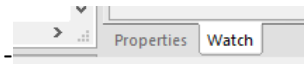


Stream Parameters	
Temperature (°C)	28.171
Pressure (atm)	1.0
pH	9.98285
Moles, True (mol/hr)	104.822
Moles, Apparent (mol/hr)	101.364
Mass (g/hr)	2009.74
Volume (L/hr)	1.83695
Solid Frac. (mole %)	0.343517
Vapor Frac. (mole %)	0.0

Total, Apparent (Molecular) (mol/hr)	
H2O	97.7838
CO2	0.0886559
Na2CO3	0.644128
CaCO3 (Calcite)	0.177908
CaO	2.82994e-5
NaCl	2.4911
MgCO3	0.0893083
MgO	7.64256e-3
Mg(OH)2	0.0809851

Figure 1-17 - The Properties panel containing the Softener slurry stream

The Calculated tab of the Properties panel contains two tables: Stream Parameters (pH, volume, mass, etc.) and apparent molecular flow. Its purpose is to provide a brief summary of the stream. The slurry temperature is 28C, which is 3C higher than the feed streams due to heats of reaction. The pH is 10, which is an indication that excess carbonate (CO_3^{-2}) is present. The slurry flow rate is 1.8 L/hr and of this, 34% (on a mole basis) are solids.

✓ Click on the Watch tab at the bottom of the Properties panel - 

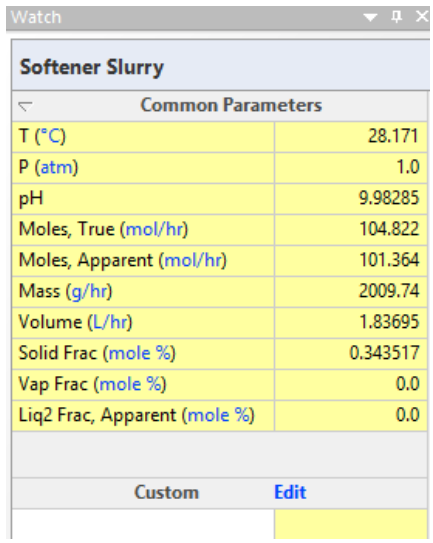


Figure 1-18 - The Softener Slurry Watch tab containing the Common Parameters and Custom variables section

This panel displays the same grid as the Properties panel, but it also includes a lower panel called Custom. This Custom panel enables users to select variables to be viewed quickly, eliminating the need to look at the complete report. The Edit button is the access to this variable list. Our interest is the dissolved calcium and magnesium concentration remaining in the water. So, you will add these two variables.

✓ Click on the Edit button.

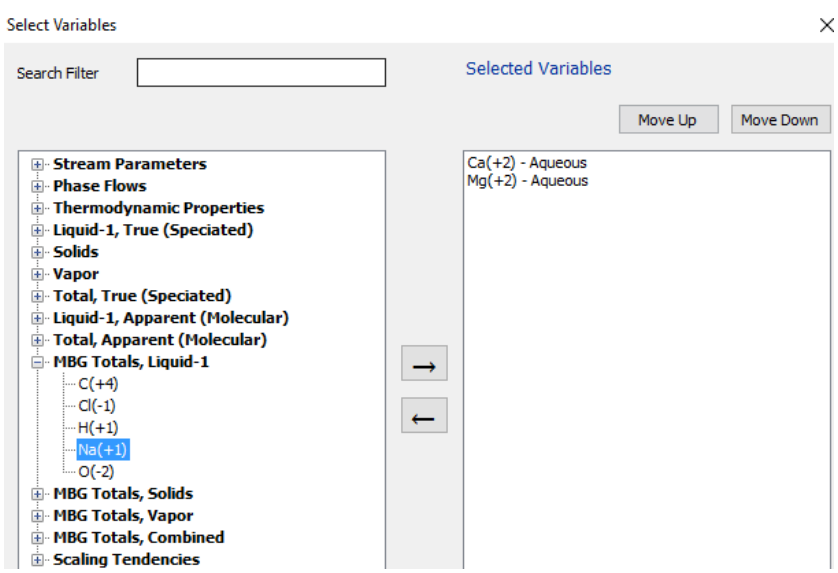


Figure 1-19 - The Select Variable window for adding variables to the Custom grid on the Properties panel.

The Select Variables window that appears contains several categories. The category we are interested in is the MBG Totals, Liquid-1. The abbreviation MBG is Material Balance Group, and it represents the sum of all that material in the liquid phase. Therefore, total dissolved calcium and magnesium is captured in the variable Ca(+2) and Mg(+2) MBG.

- ✓ Expand the MBG Totals Liquid 1 category.
- ✓ Double-click on the Ca(+2) and Mg(+2) variables so they are moved to the right panel.
- ✓ Close the window.

Custom	Edit
Ca(+2) Aq (mol/hr)	2.82994e-5
Mg(+2) Aq (mol/hr)	7.64256e-3

Figure 1-20 - The moles of total dissolved calcium and magnesium in the Softener slurry

The grid now contains the total dissolved calcium and magnesium. However, the units are not convenient. They are in moles and not concentration. Therefore, we need to change units before proceeding with the data interpretation.

- ✓ Click on the mol/hr hyperlink unit adjacent to either the Ca(+2) or Mg(+2) variable.

This action activates the Units editor. You will change the Aqueous composition units from moles to concentration.

- ✓ Change the Basis for the Aqueous Composition from moles to Concentration.

Edit Units - Softener Slurry

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Stream Amount	Moles	mol/hr
Inflows	Moles	mol/hr
Output variables		
Aqueous Composition	Concentration	mg/L
Vapor Composition	Moles	mol/hr
Solid Composition	Moles	mol/hr
2nd Liquid Composition	Moles	mol/hr

Figure 1-21 – The Edit Units window for the Softener Slurry stream. The Aqueous Composition is set to Concentration

- ✓ Press OK to close the window

Custom	Edit
Ca(+2) Aq (mg/L)	0.62117
Mg(+2) Aq (mg/L)	101.733

Figure 1-22 – The updated panel showing the dissolved calcium and magnesium in concentration units

According to the calculations, calcium concentration is less than 1mg/l, but the dissolved magnesium is above 100 mg/l. Consequently, the goal of 10 mg/l combined for both was not achieved. Changes to this scenario or additional processing will be needed.

Taking action to reduce total Ca+2 and Mg+2 to below 10 mg/l

The simplest task to meet our target concentration is to adjust an inflow or a condition. For instance, soda ash can be increased to raise the pH, or temperature can be increased to reduce solubility. You will do the latter.

The solubility of magnesium hydroxide decreases exponentially with temperature. This is shown in the plot below.

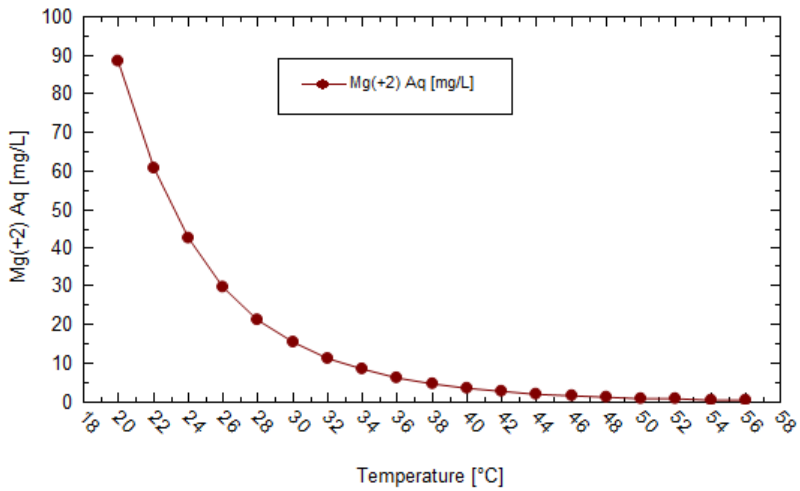
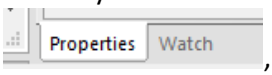


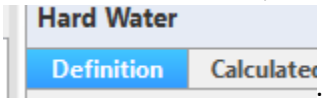
Figure 1-23 – Plot of the calculated solubility of Mg(OH)2, brucite, in pure water between 20 and 56C. The plot was generated in OLI Studio V9.3.2.

Therefore, a significant performance improvement can be achieved by raising the feed temperature of the hard water. To do this we will simply change the feed temperature from 25 to 50C. We will assume that a heating process is present upstream of the softener reactor.

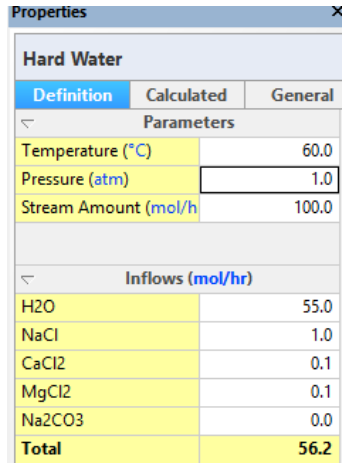
- ✓ Click on the Hard water stream to access the Properties panel.

The panel view will probably be the Watch tab. You need to be in the Definition subtab of the Properties tab.

- ✓ You may need to Click the Properties tab at the bottom of the panel - 

, and then click on the Definition sub tab at the top of the panel - 

. This places you on the Stream Input editor where you can change the temperature.
- ✓ Change the Temperature from 25 to 60C.



Properties

Hard Water

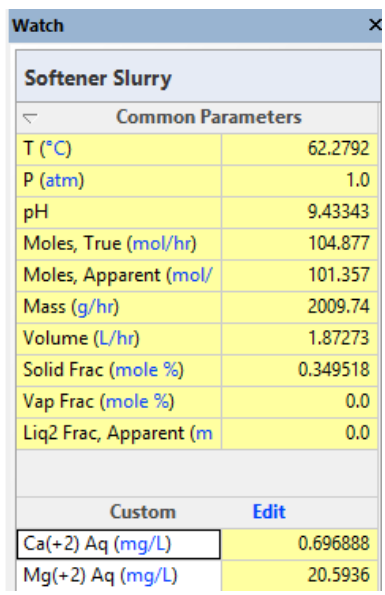
Definition	Calculated	General

Parameters	
Temperature (°C)	60.0
Pressure (atm)	1.0
Stream Amount (mol/h	100.0

Inflows (mol/hr)	
H2O	55.0
NaCl	1.0
CaCl2	0.1
MgCl2	0.1
Na2CO3	0.0
Total	**56.2**

Figure 1-24 - The Hard Water composition with the updated temperature

- ✓ Recalculate the case.
- ✓ Click on the Softener Slurry stream and then click on the Watch tab (bottom of the panel).



Watch

Softener Slurry

Common Parameters	
T (°C)	62.2792
P (atm)	1.0
pH	9.43343
Moles, True (mol/hr)	104.877
Moles, Apparent (mol/	101.357
Mass (g/hr)	2009.74
Volume (L/hr)	1.87273
Solid Frac (mole %)	0.349518
Vap Frac (mole %)	0.0
Liq2 Frac, Apparent (m	0.0

Custom	Edit
Ca(+2) Aq (mg/L)	0.696888
Mg(+2) Aq (mg/L)	20.5936

Figure 1-25 - The updated Softener Slurry composition and properties. The Mg+2 concentration decreased by 80%

Raising the inlet temperature decreased the dissolved magnesium by about 80%. It is tempting to raise the temperature further, and this can be done. However, in the interest of this example, we will combine the temperature increase with a higher dose of soda ash.

- ✓ Click on the Soda Ash stream to access the Properties panel.
- ✓ Change the panel view so that the Properties-Definition tab is visible.
- ✓ Change the soda ash Stream Amount from 1 to 2 mol/hr.

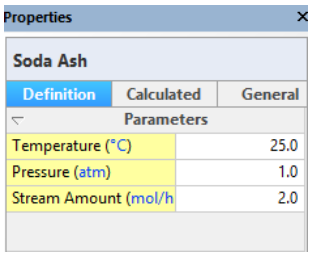


Figure 1-26 - The updated Soda Ash flow rate of 2 moles/hr.

- ✓ Calculate.
- ✓ Click on the Softener slurry and view the total dissolve calcium and magnesium in the Watch panel.

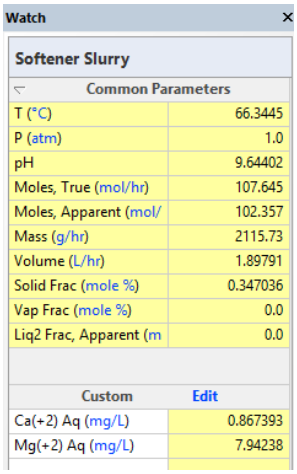


Figure 1-27 - The updated Softener Slurry stream. The Total dissolved calcium and magnesium is now less than 10 mg/l.

The combination of higher temperatures and soda ash flow rates results in a slurry with total dissolved calcium and magnesium less than 10 mg/l. Thus, our target has been met. This may not be the most efficient/economical approach, but it does meet product limits.

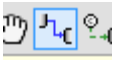
- ✓ Save the file. If you have not saved the case file yet, then name it something that you can find quickly because it will be used in the next several chapters.

Adding the Clarifier block

If the first part of the case converges properly, then the work on the clarifier block can begin. It is not required that the first section be run to add the new block. However, for diagnostic reasons it is sometimes easier to create and calculate incrementally so that it's easier to find any errors.

- ✓ Click on the Separator block in the Library and drag it to the right of the Softener reactor.

- ✓ Name this object Clarifier.
- ✓ Click on the Softener Slurry stream to activate it. Link it to the inlet of the Clarifier.

- ✓ Activate the Add Stream action 
- ✓ Add two streams to the outlet of the Clarifier. Add one to the Liquid outlet (upper right) and add another to the solids outlet (bottom).
- ✓ Label the liquid stream Soft water and the solid stream Sludge.

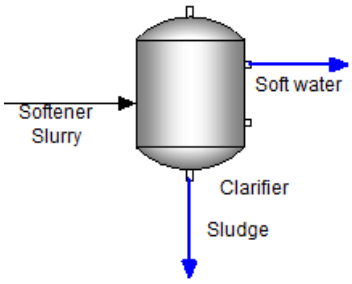


Figure 1-28 - The schematic for the Separator/Clarifier unit

Calculate and review the results

- ✓ Press the Calculate button.
- ✓ When complete, click on the Soft water stream to access the Properties panel.
- ✓ Then look at the Sludge stream.

Properties

Soft water

Calculated | General

Stream Parameters	
Temperature (°C)	66.3445
Pressure (atm)	1.0
pH	9.64402
Moles, True (mol/hr)	101.504
Moles, Apparent (mol/hr)	96.5003
Mass (g/hr)	1974.99
Volume (L/hr)	1.7852

Watch

Sludge

Common Parameters	
T (°C)	66.3445
P (atm)	1.0
pH	
Moles, True (mol/hr)	0.355214
Moles, Apparent (mol/hr)	0.355214
Mass (g/hr)	28.1463
Volume (L/hr)	0.010937
Solid Frac (mole %)	100.0
Vap Frac (mole %)	0.0
Liq2 Frac, Apparent (mole	0.0

Figure 1-29 - The Properties panel for Soft Water and Sludge. The Soft water is 100% liquid and the Sludge is 100% solids.

The panel displays the calculated results. The final pH is about ~10 and the software water is 100% liquids; all the solids are in the sludge stream. Note that the sludge stream is 100% solids and there is no water present. Thus the separator block "separates" phases completely. There is no entrainment or suspension assumed. This can be done in the next section.

Modifying the Separator so that the sludge and soft water streams are more realistic

There are Entrainment settings in the Separator object used to mix phase in exit streams. The default separator setting is for 100% of the liquid and solids to separate into their respective outputs. This does not allow for suspended solids in the liquid or for entrained water in the solids (i.e., sludge). You will use these settings to make the Clarifier sludge 80% water and 20% solids. This is a liquid to solid ratio of 4:1.

✓ Click on the Clarifier block to access the Properties panel.

There is an Entrainment row at the bottom of the Equilibrium Calculation section on the Properties tab. This section contains the various phase entrainment options.

✓ Set the Liquid in Solid ratio to 4 g/g. This is a 4:1 mass ratio or 80% liquid.

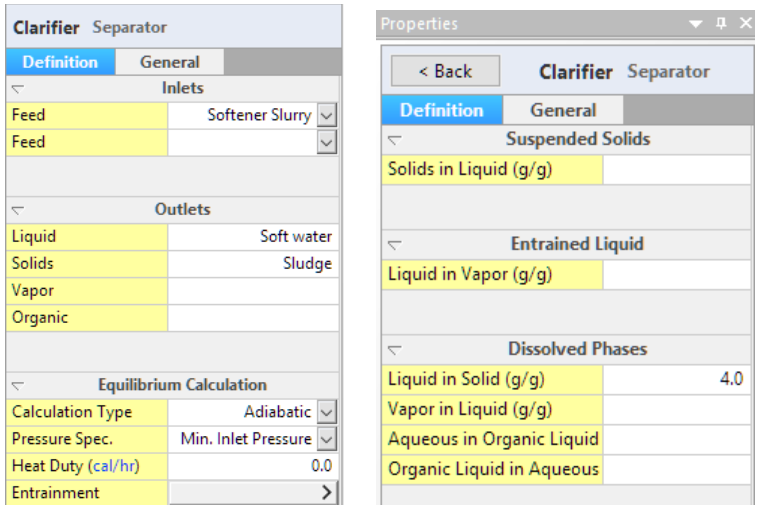


Figure 1-30 – The Entrainment option in the Clarifier unit. The Liquid to solid ratio is 4:1, or an 80 wt% sludge

✓ Calculate.

✓ Click on the Sludge stream to view the calculated results.

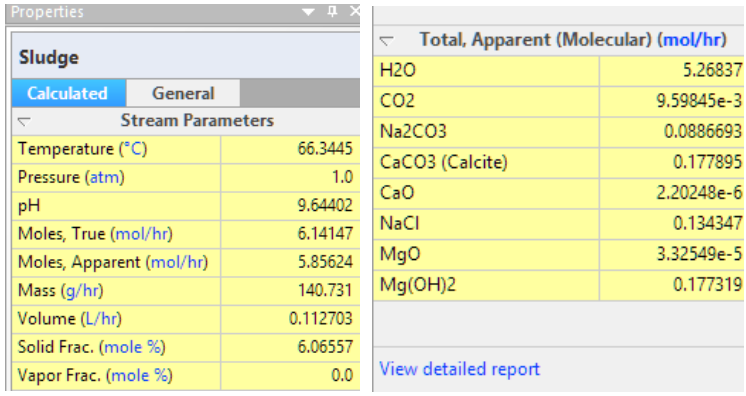
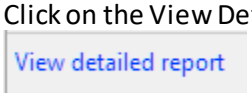


Figure 1-31 - The Sludge properties panel containing 80% water

The sludge stream now contains 6.1 mole% solids. This converts to 20 wt% solids defined in the Entrainment. The software does not have a wt% solids variable, so to see this you need to view the detailed report.

✓ Click on the View Detailed Report link at the bottom of the Sludge panel -



This link activates a Stream Report tab. The report contains the Sludge properties and compositions. View the Phase flow section, specifically the Mass. Total mass is 140.7 g/hr. The solid mass is 28.1 g/hr, or 20% of the total flow.

Sludge				
Stream Parameters				
Temperature (°C)	66.3445			
Pressure (atm)	1.0			
pH	9.64402			
Solid Frac. (mole %)	6.06557			
Vapor Frac. (mole %)	0.0			
Phase Flows	**Liquid-1**	**Solids**	**Vapor**	**Total**
Moles, True (mol/hr)	5.78626	0.355214	0.0	6.14147
Moles, Apparent (mol/hr)	5.50102	0.355214	0.0	5.85624
Mass (g/hr)	112.585	28.1463	0.0	140.731
Volume (L/hr)	0.101766	0.010937	0.0	0.112703

Figure 1-32 - The Stream report generated by the View detailed report button. The phase flow section contains the phase distribution of the stream

Summary

We have completed the first case. It presents the basic mechanics of building and converging a steady-state simulation. In the next chapter, you will expand this case to include additional blocks and chemistry.

Chapter 2 A simple Absorption Column

The Application

There are several types of multi-stage, or column, blocks in Flowsheet ESP. The simplest is the Absorber column. This column consists of a minimum two equilibrium stages, and two inlet and two outlet streams. Figure 2-1 is an example column. It is a four-stage flue gas scrubber. Combustion gas contains various pollutants (SO2, SO3, HCl, H2S, and Hg), which are absorbed into a high pH washing solution.

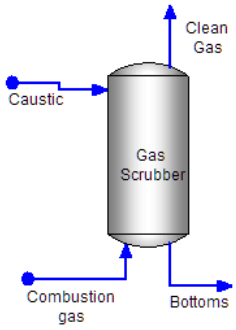


Figure 2-1 – Absorption column for removing pollutants from combustion gases

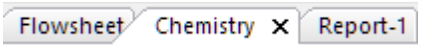
You will build this case in the same two steps as the previous chapter. Step 1 is to create the chemistry model and the step 2 is to build the process.

- ✓ Start the Software.
- ✓ Confirm that a blank case is on the screen.
- ✓ Save this blank case as Section1 – Chapter2 - Absorption Tower.

Creating a Chemistry Model

As explained in the previous chapter, the chemistry model is one of two modules required for the case.

Selecting the thermodynamic method and databases to be used in the Model

- ✓ Click on the Chemistry tab - 

The start tab for all new cases is the Databanks. This tab contains the thermodynamic framework and specialized database.

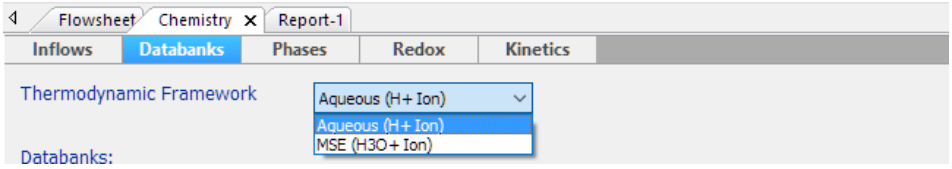


Figure 2-2 - The available framework and databases installed with the software

You will use the Aqueous (H+ ion) framework and will not add any specialized databases to this case.

✓ Keep the existing framework and add no private databases.

Adding the chemical inflows to the model

✓ Click on the Inflows tab to access the grid for adding inflows.

This inflows tab contains the grid for adding the chemical components used in the case. The software will automatically generate the aqueous species, gases and solids from this list.

✓ Type the following Inflows to the grid.

N2	SO2
CO2	SO3
O2	HCl
Ar	NaOH

The grid should look like the following screen

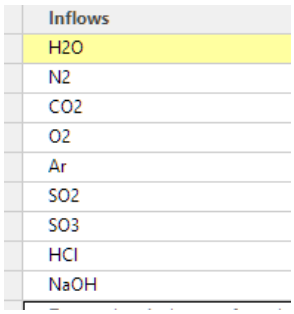


Figure 2-3 – Entering the molecular inflows.

✓ Click on the Chemistry icon in the Navigator panel and press F2 to change its name. Name it Combustion Gas.

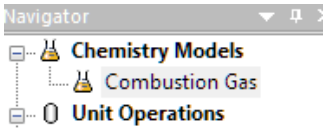


Figure 2-4 – Renaming the Chemistry model

This completes the Chemistry Model Build step. There are additional options, but they are not germane to this example.

Building the Scrubber Process

Adding the Absorber block

The first step is to create the block. It is a simple procedure.

- ✓ Click on the Flowsheet tab.
- ✓ Click on the Absorber object in the Library (lower left of the screen) and drag it onto the Worksheet.

- ✓ **Double click** on the new block to change its name to Gas Scrubber.

You should notice that the right Properties panel displays the settings for this column.

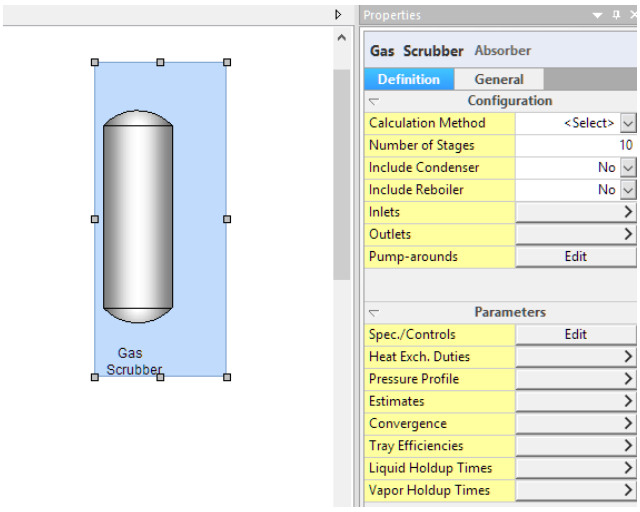


Figure 2-5 - The Absorber block and its Properties Panel (Definition tab)

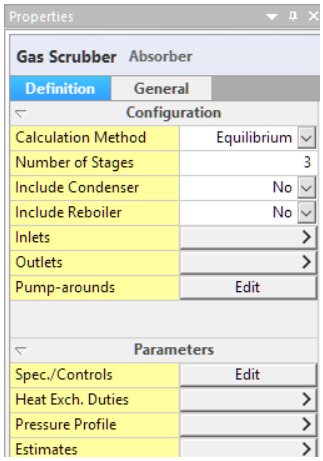
- ✓ Change the Calculation Method to Equilibrium.

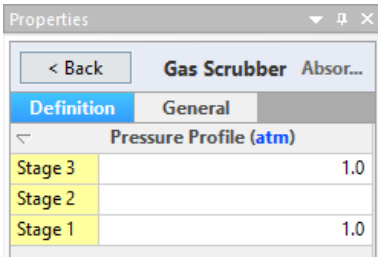
This instructs the software that each column stage will calculate to equilibrium; that there will be no mass-transfer limitations.

- ✓ Change the Number of Stages from 10 to 3.

This action instructs the software that there are three theoretical stages in the column.

- ✓ Click on the Pressure Profile and enter 1 atm in the stage 3 and stage 1 row.





Adding the Inlet and Outlet streams

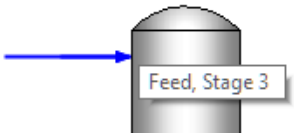
- ✓ Click on the Add Stream button in the Toolbar.

Figure 2-6 - The Add Stream button in the toolbar

- ✓ Create an inlet stream to the Absorber. Add it to the upper left side.

Notice that a separate click is needed to anchor the stream to the unit.

- ✓ Create a second inlet stream to the bottom of the column.



- ✓ Lastly, create two outlet streams, on at the top and one at the bottom of the column.

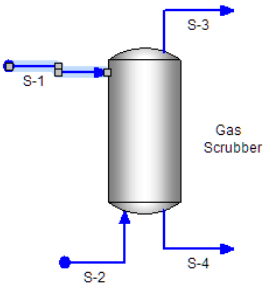
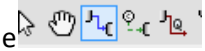


Figure 2-7- the column with the two inlet steams and two outlet streams

- ✓ Press the ESC key to deactivate the Add Stream button.

The Add stream mode stays active until the ESC key is pressed, or the arrow button is selected , or if the Add Stream button is clicked a second time 

- ✓ Name the streams as follows

Top inlet	Caustic
Lower inlet	Combustion gas
Top outlet	Clean Gas
Bottom outlet	Bottoms

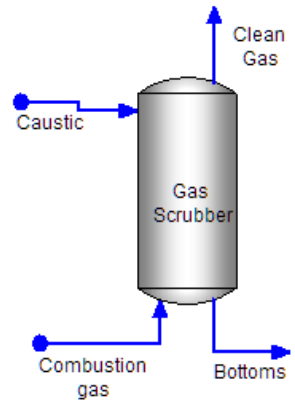


Figure 2-8- Names added to the absorber block

Entering the Stream compositions

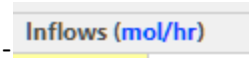
The table below contains the compositions for the two inlet streams. The combustion gas contains the standard air and combustion components. There are several other combustion components missing, like NOx and Hg. These components are not included so that the simulation calculates easily. You will change this value later in the chapter.

	Combustion Gas	**Caustic**
Temperature (C)	100	25
Pressure (atm)	1	1
Stream Amount	100 m3/hr	100 L/hr
H2O	8 mole%	90 mass%
N2	73	
CO2	11	
O2	6	
Ar	0.8	
SO2	0.2	
SO3	0.01	
HCl	0.005	
NaOH		10

✓ Click on the Combustion Gas stream to access its Properties panel

Review the composition shown in the table below. Note that the Flow rate is m3/hr and the composition is mole%. You will need to modify units before adding the information

Table 1-1 – Process Stream and Acid Waste stream compositions

✓ Click on the units link in the Inflows section head - 

. This opens the Units Editor

✓ Make the following changes. Note that the bottom section (Basis Options) is where you change the specific units set.

Stream Amount	Volume	m3/hr

Inflows	Mole Fraction	Mole%
Vapor Composition	Mole Fraction	Mole%
Volume		m3/hr
Mole Fraction		Mole%

Edit Units - Combustion gas

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Stream Amount	Volume	m3/hr
Inflows	Mole Fraction	mole %
Output variables		
Aqueous Composition	Moles	mol/hr
Vapor Composition	Mole Fraction	mole %
Solid Composition	Moles	mol/hr
2nd Liquid Composition	Moles	mol/hr
Total Composition	Moles	mol/hr
Basis options		
Moles		mol/hr
Mass		g/hr
Volume		m3/hr
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		mass %
Mole Fraction		mole %

- ✓ Click OK to close the Edit Units window.
- ✓ Enter the composition and conditions for the Combustion Gas.

The composition will not sum to 100%. Therefore, you will use the Normalization option labeled Makeup with Water to set it to 100%.

- ✓ Change the Normalization Type to Makeup with water - Normalization: Type — Makeup wit... .

Inflows (mole %)	
H2O	8.935
N2	73.0
CO2	11.0
O2	6.0
Ar	0.8
SO2	0.2
SO3	0.01
HCl	5.0e-3
NaOH	0.0
Total	99.95

Normalization: Type — Prorate; Normalize

Inflows (mole %)	
H2O	8.985
N2	73.0
CO2	11.0
O2	6.0
Ar	0.8
SO2	0.2
SO3	0.01
HCl	5.0e-3
NaOH	0.0
Total	**100.0**

Normalization: Type — Makeup with Water

The software adjusts the water content to create the 100% composition.

- ✓ Click on the Caustic stream to access the Properties panel.
- ✓ Edit its units in the same way, click on one of the linked units in the panel to open the Units Editor window.
- ✓ Make the following changes:

Stream Amount	Volume	L/hr

Inflows	Mass Fraction	Mass%
Aqueous Composition	Mass Fraction	Mass%
Volume		L/hr
Mass Fraction		Mass%

The Units Editor should look like this when complete

Edit Units - Caustic

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Stream Amount	Volume	L/hr
Inflows	Mass Fraction	mass %
Output variables		
Aqueous Composition	Mass Fraction	mass %
Vapor Composition	Moles	mol/hr
Solid Composition	Moles	mol/hr
2nd Liquid Composition	Moles	mol/hr
Total Composition	Moles	mol/hr
Basis options		
Moles		mol/hr
Mass		g/hr
Volume		L/hr
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		mass %
Mole Fraction		mole %

✓ Close the Edit Units window and enter the composition.

Properties

Caustic

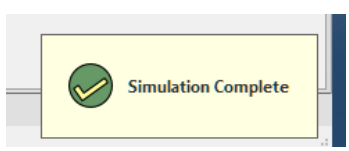
Definition | Calculated | General

Parameters	
Temperature (°C)	25.0
Pressure (atm)	1.0
Stream Amount (L/hr)	100.0

Inflows (mass %)	
H2O	90.0
N2	0.0
CO2	0.0
O2	0.0
Ar	0.0
SO2	0.0
SO3	0.0
HCl	0.0
NaOH	10.0
Total	**100.0**

✓ Press the Calculate button to calculate the case

✓ When complete, a Simulation Complete pup-up window appears in the lower right of the window.



Reviewing the resuls

✓ Click on the Clean Gas stream to access the Properties panel.

The Properties panel contains a Calculated tab, which is the default view after the simulation converges. It contains two sections - Stream Parameters and Total Apparent flow.

Properties

Clean Gas

Calculated | General

Stream Parameters	
Temperature (°C)	57.4744
Pressure (atm)	1.0
pH	
Moles, True (mol/hr)	3329.37
Moles, Apparent (mol/hr	3329.37
Mass (g/hr)	91098.3
Volume (m3/hr)	90.2732
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	100.0

Total, Apparent (Molecular) (mol/hr)	
H2O	570.399
CO2	152.62
Ar	26.1286
H2SO4	5.37357e-44
HCl	1.70344e-29
N2	2384.26
O2	195.965
SO2	2.48863e-22
SO3	1.27582e-50

The vent temperature has decreased to 57C and the measured volume decreased to 90 m3/hr.

The Total Apparent units will probably show mol/hr. These are the default software units. They, however, do not help interpretation, and so you will change them.

- ✓ Click on the Units link in the Total Apparent header Total, Apparent (Molecular) (mol/hr) to open the Units Editor.
- ✓ Make the following changes to this panel.

Stream Amount	Volume	m3/hr
Inflows	Mole Fraction	Mole%
Vapor Composition	Mole Fraction	Mole%
Total Composition	Mole Fraction	Mole%
Volume		M3/hr
Mole Fraction		Mole%

Edit Units - Clean Gas

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Stream Amount	Volume	m3/hr
Inflows	Moles	mol/hr
Output variables		
Aqueous Composition	Moles	mol/hr
Vapor Composition	Mole Fraction	mole %
Solid Composition	Moles	mol/hr
2nd Liquid Composition	Moles	mol/hr
Total Composition	Mole Fraction	mole %
Basis options		
Moles		mol/hr
Mass		g/hr
Volume		m3/hr
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		mass %
Mole Fraction		mole %

- ✓ Close the Units window and view the Clean Gas composition in the panel again.

Total, Apparent (Molecular) (mole %)	
H2O	17.1324
CO2	4.58405
Ar	0.784791
H2SO4	1.61399e-45
HCl	5.11639e-31
N2	71.6129
O2	5.88594
SO2	7.47476e-24
SO3	3.83203e-52

The SO_2 and SO_3 acids are virtually all removed from the gas. This is due in part because we added excess NaOH. You can confirm this by reviewing the bottoms stream pH.

✓ Click on the Bottoms stream and view the calculated pH.

Properties

Bottoms

Calculated | General

Stream Parameters	
Temperature (°C)	51.6827
Pressure (atm)	1.0
pH	8.72109
Moles, True (mol/hr)	5704.12
Moles, Apparent (mol/hr	5676.74
Mass (g/hr)	1.13978e5
Volume (L/hr)	101.926
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	0.0

The pH is nearly nine, significantly above the pH needed to remove SO2 gas. A more reasonable pH would be 7.2. Another potential problem with this high pH is the formation of NaHCO3 solids. Caustic solutions absorb CO2, converting it to NaHCO3. To see whether NaHCO3 may form, you need to view the report table for this stream. It is accessible by selecting the View detailed report link.

✓ Click on the View detailed report link at the bottom of the Bottoms panel.

View detailed report

This action creates a Report (Report-2) that contains the detailed information about the Bottoms stream. The table contains four results columns, for the separate phases and the total. The report contains the sections: Parameters, Flow rates, Thermodynamic properties, Composition, Material Balance groups (element concentration) and lastly Scaling Tendencies.

The Scaling tendencies is the table of interest. It contains the driving force to precipitation caused by increasing concentrations. Any value above one means that solids will form. Two solids, Na_2SO_4 and $NaHCO_3$ have values greater than 1. Both may potentially form.

Scaling Tendencies	
Row filter applied: only show rows with value greater than 1.0e-4	
Na2SO4	6.37945
NaHCO3 (Nahcolite)	1.18545
Na2CO3.NaHCO3.2H2O	0.175452
Na2CO3.3NaHCO3 (Wegscheiderite)	0.0925419
Na2CO3.1H2O (Thermonatrite)	0.0348179
Na2CO3 (Natrite)	0.0136027
Na2CO3.7H2O	0.0106414

Optimizing the Caustic inflow rate

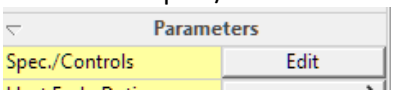
The goal is to add sufficient caustic to removed SO2 to the target limits and minimize excess flow. To do this we need to define a target SO2 limits then control the caustic flow accordingly. According to an excerpt from the document below, the SO2 limits are 180 ng/J energy output, or a flat 95% reduction.

The SO_2 emission limit for new electric utility steam generating units is 180 ng/J (1.4 pound per megawatt hour (lb/MWh)) gross energy output or 95 percent reduction regardless of the type of fuel burned with one exception. The SO_2 emission limit for new electric utility steam generating units that burn over 75 percent coal refuse (by heat input) is 180 ng/J (1.4 lb/MWh) gross energy output or 94 percent reduction.

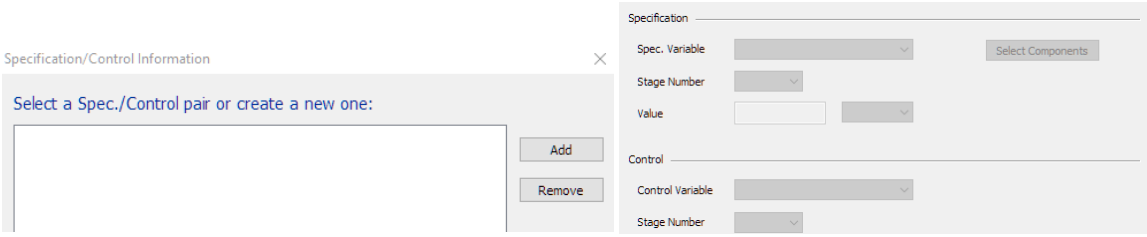
9868 **Federal Register** / Vol. 71, No. 38 / Monday, February 27, 2006 / Rules and Regulations

Since this example does not consider energy generated, the target will be the 95% reduction. The SO 2 in this combustion gas is 2000 ppmV. Therefore, the 95% reduction converts to 100 ppmV SO2 in the clean gas. You will enter this 100 ppmV values into the column's Spec/Control window, and instruct the column to adjust the caustic inflow to meet these specifications.

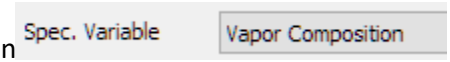
- ✓ Return to the Flowsheet tab and click on the Gas Scrubber to access the Properties Panel.
- ✓ Click on the Spec./Controls Edit button in the Parameters section.

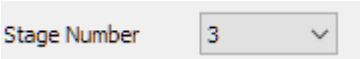


The Specification/Control Information window that opens contains the instruction settings for optimizing a tower function.



You can set several types of target specifications, and control several forms of dependent variables. In this case, you will set the SO2 vapor concentration (Specification), and adjust the Caustic flow into the column (Control). They are always set in pairs (i.e., one fixed and one free variable).

- ✓ Click on the Add button in the upper right.
- ✓ Change the Spec. Variable to Vapor Composition 

- ✓ Change the Stage number to 3 

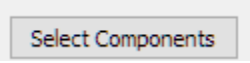
.

Stage 3 is the tope stage and is the location of the Clean Gas stream outlet.

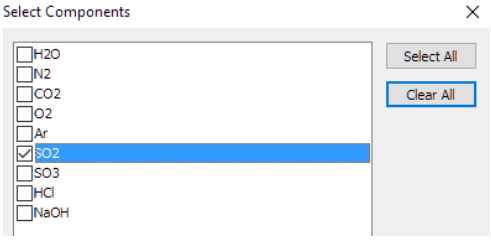
- ✓ Change the Value units to mole% and set the value to 0.01 mole% (equals 100ppmV)

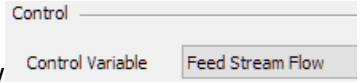
When you press Enter, the Select Components window will open. If it does not, then open it.

- ✓ Click on the Select Components button if the window does not open automatically.



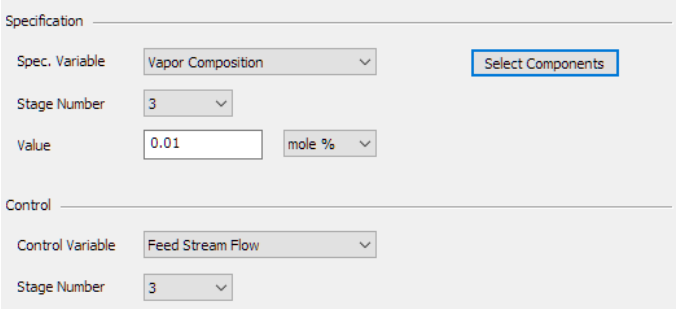
- ✓ Check the SO2 box and close the window



- ✓ Change the Control Variable option to Feed Stream Flow 

- ✓ Set the Stage Number to 3 (the stage where the Caustic enters)

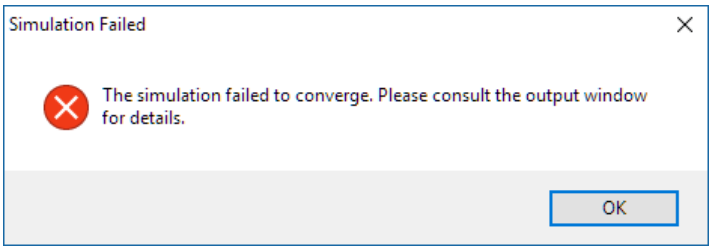
When finished your screen should look like the following:



- ✓ Close the window and calculate.

----------THE SIMULATION WILL FAIL----------

When complete, you will receive an ERROR stating that the simulation failed.



This is a common occurrence, and it occurs for several reasons. In this case, it occurred because the 10% Caustic feed is too concentrated. The software cannot find a flow rate that sets the SO2 vapor to 100ppmV. As the Caustic flow decreases (to allow more SO2 to remain in the vapor), it reaches a value where all the liquid added evaporates. A column cannot be all vapor, or it fails to converge.

This is an easily remedied problem; use a less concentrated caustic solution.

- ✓ Click on the Caustic stream to access the Properties panel.
- ✓ Change the Normalization type from Prorate to Makeup with water

Normalization	
Type	Makeup with .

- ✓ Change the NaOH content to 0.5%.
- ✓ Recalculate.

Now the simulation converges quickly.

- ✓ Click on the Clean Gas stream to access the Properties panel.
- ✓ View the Total Apparent section, specifically the SO2 value.

Total, Apparent (Molecular) (mole %)	
H2O	9.36804
CO2	10.9755
Ar	0.798455
H2SO4	1.5564e-39
HCl	1.53032e-26
N2	72.8596
O2	5.98842
SO2	0.01
SO3	1.69474e-46

The target SO2 is 0.01 mole%, per design.

- ✓ Click on the Caustic stream to access the Properties panel.
- ✓ Click on the Calculated tab and view the Volume row.

Caustic

Definition | Calculated | General

Stream Parameters	
Temperature (°C)	25.0
Pressure (atm)	1.0
pH	12.9879
Moles, True (mol/hr)	3085.8
Moles, Apparent (mol/hr)	3078.84
Mass (g/hr)	55619.2
Volume (L/hr)	55.4816

The calculated volume is 55 L/hr of a 0.5% caustic solution. Had the 10% been kept, approximately 3 L/hr would be required, but the software was unable to converge the tower with this small of a caustic flow rate. This is because the liquid evaporated completely in at least one of the three stages, and the tower will not converge unless water exists at every stage of the tower.

- ✓ Click on the Bottom stream to review the pH.

The computed pH is 4.0. If this is lower than expected, it is because the target SO2 vapor composition was set to 100 ppmV. Were the target specification set lower, then the bottoms pH would have increased.

- ✓ If you want, change the target Specification SO2 value to 10ppmV and review the results again.

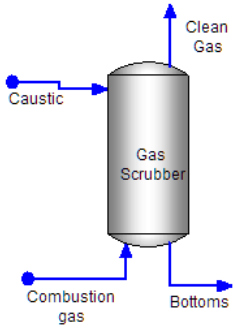
Summary

We have completed the first case. It presents the basic mechanics of building and converging a steady-state simulation. In the next chapter, you will expand this case to include additional blocks and chemistry.

Chapter 3 A simple absorption column

The Application

There are several types of multi-stage, or column, blocks in Flowsheet: ESP. The simplest is the **Absorber** column. This column consists of a minimum two equilibrium stages, and two inlet and two outlet streams. The figure below is an example of this type of column. It is a 3-stage flue gas scrubber. Combustion gas contains various pollutants (SO_2, SO_3, HCl, H_2S, and Hg), which are absorbed into a high pH washing solution.

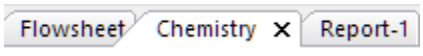


You will build this case in the same two steps as the previous chapter. **Step 1** is to create the **chemistry model** and the **step 2** is to **build the process**.

- ✓ Start the Software.
- ✓ Confirm that a blank case is on the screen.
- ✓ Save this blank case as Chapter02 – A simple absorption column.

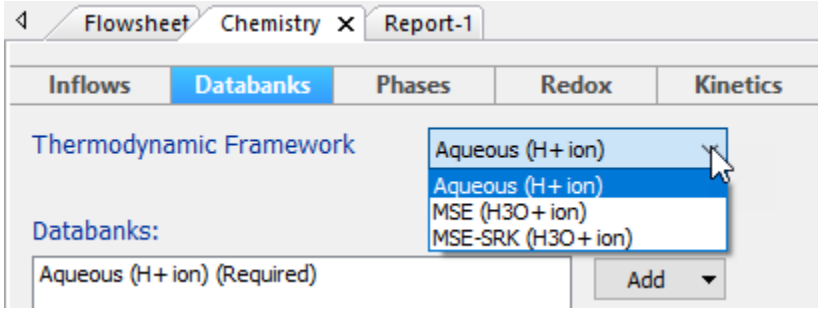
Creating a Chemistry Model

As explained in the previous chapter, the chemistry model is one of two modules required for the case.

- ✓ Click on the **Chemistry** tab - 

Selecting the thermodynamic framework and additional databases to be used in the model

The start tab for all new cases is the **Databanks**. This tab contains the thermodynamic framework and specialized database.



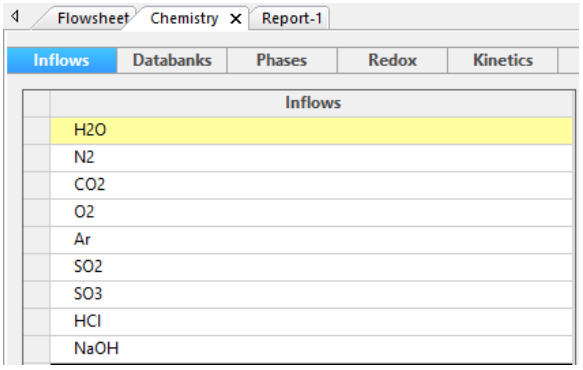
- ✓ **Select** the Aqueous (H+ ion) thermodynamic framework
- ✓ Keep the existing framework and add no private databases.

Adding the chemical inflows to the model

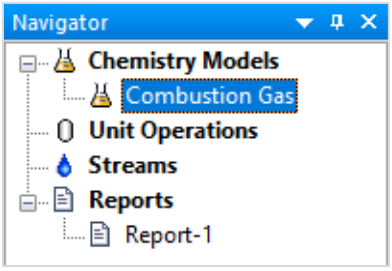
- ✓ Click on the **Inflows** tab to access the grid for adding inflows.

This inflows tab contains the grid for adding the chemical components used in the case. The software will automatically generate the aqueous species, gases and solids from this list.

- ✓ Type the following Inflows to the grid:



- ✓ Click on the **Chemistry** icon in the **Navigator panel** and press **F2** to change its name.
- ✓ Name it **Combustion Gas**



This completes the Chemistry Model Build step. There are additional options, but they are not germane to this example.

Building the Scrubber Process

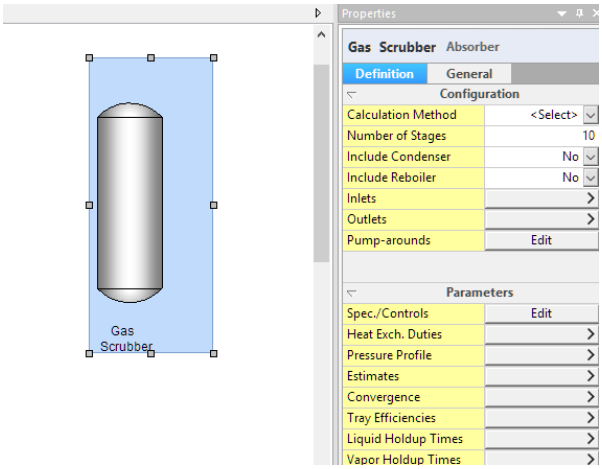
Adding the Absorber block

The first step is to create the block.

- ✓ Click on the **Flowsheet** tab.
- ✓ Click on the **Absorber** object in the **Library** (lower left of the screen) and drag it onto the Worksheet.

- ✓ **Double click** on the new block to change its name to **Gas Scrubber.**

You should notice that the right Properties panel displays the settings for this column.



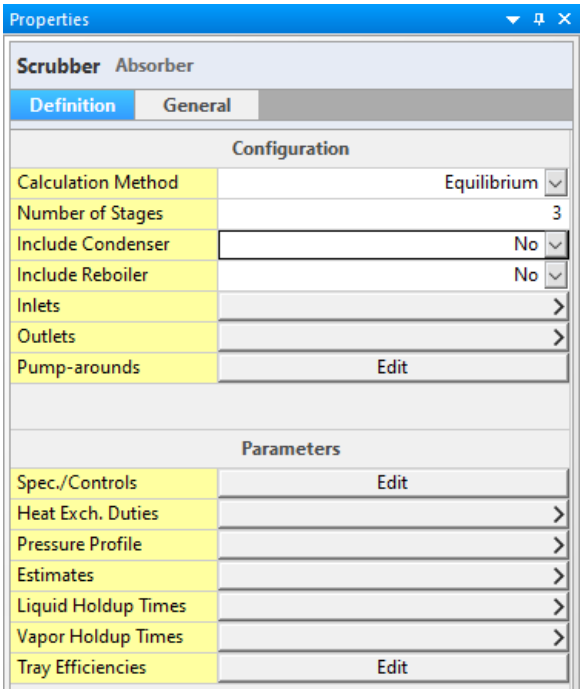
- ✓ Change the **Calculation Method** to **Equilibrium**.

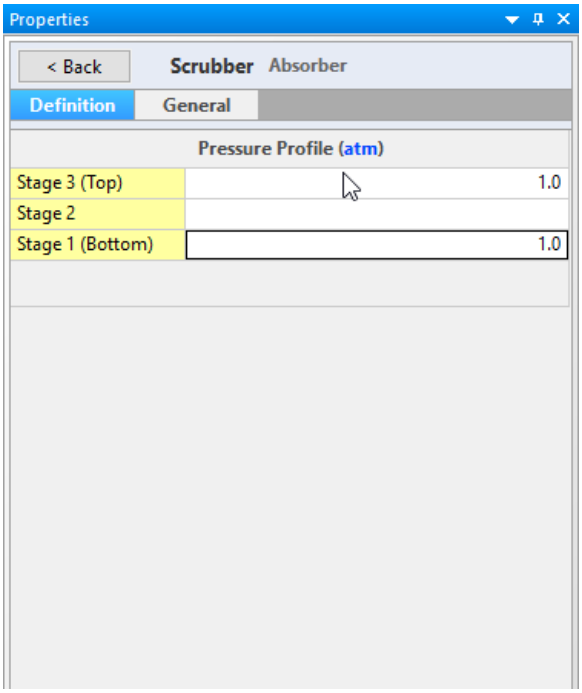
This instructs the software that each column stage will calculate to equilibrium; that there will be no mass-transfer limitations.

✓ Change the **Number of Stages** from 10 to 3.

This action instructs the software that there are three theoretical stages in the column.

✓ Click on the **Pressure Profile** and enter 1 atm in the stage 3 and stage 1 row.



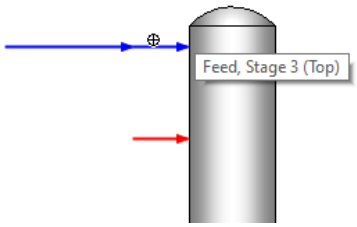


Adding the Inlet and Outlet streams

✓ Click on the **Add Stream** button in the Toolbar.

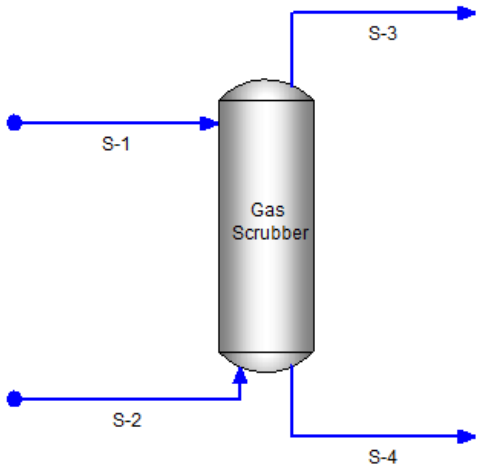
✓ Create an **inlet** stream to the **Absorber**. Add it to the upper left side.

Notice that a separate click is needed to anchor the stream to the unit.



✓ Create a **second inlet** stream to the bottom of the column.

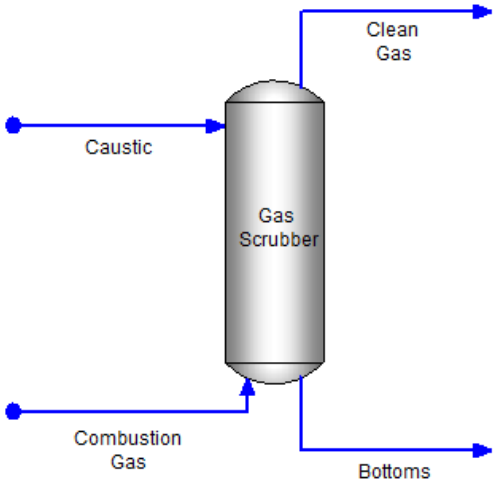
✓ Lastly, create two outlet streams, on at the top and one at the bottom of the column.



✓ Press the **ESC** key to deactivate the **Add Stream** button.

The Add stream mode stays active until the ESC key is pressed, or the arrow button is selected
, or if the Add Stream button is clicked a second time

✓ Name the streams as shown on the image below



Entering the Stream compositions

The table below contains the compositions for the two inlet streams. The combustion gas contains the standard air and combustion components. There are several other combustion components missing, like NOx and Hg. These components are not included so that the simulation calculates easily. You will change this value later in the chapter.

	Combustion Gas	Caustic
Temperature (C)	100	25
Pressure (atm)	1	1
Total Flow	100 m3/hr	100 L/hr
H2O	8 mole%	90 mass%
N2	73 mole%	
CO2	11 mole%	
O2	6 mole%	
Ar	0.8 mole%	
SO2	0.2 mole%	
SO3	0.01 mole%	
HCl	0.005 mole%	
NaOH		10 mass%

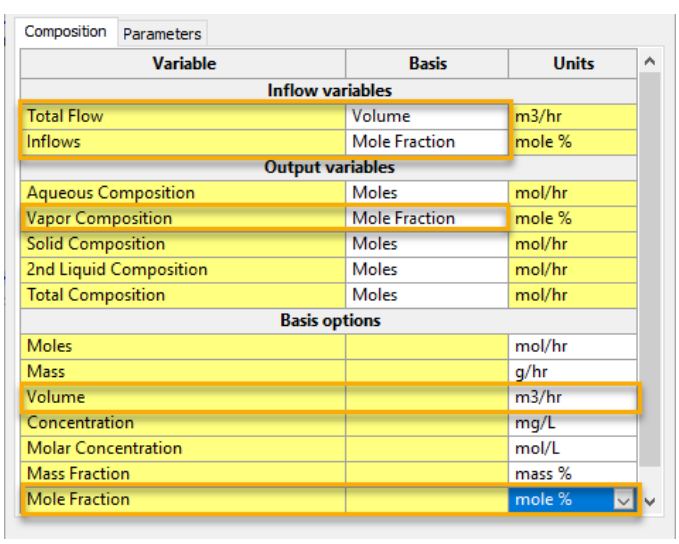
✓ Click on the **Combustion Gas** stream to access its **Properties** panel

Review the composition shown in the table above. Note that the flow rate is given in m3/hr and the composition is mole%. You will need to modify units before adding the information

✓ Click on the units link in the **Inflows** section head - Inflows (mol/hr). This opens the Units Manager

✓ Make the following changes. Note that the bottom section (Basis Options) is where you change the specific units set.

Inflow and Output Variables		
Total Flow	Volume	
Inflows	Mole Fraction	
Vapor Composition	Mole Fraction	
Basis Options		
Volume		m3/hr
Mole Fraction		mole%



✓ Click **OK** to close the Edit Units window.

✓ Enter the composition and conditions for the **Combustion Gas**.

Properties

Combustion Gas

Definition | Calculated | General

Show Ionic Input Options

Parameters	
Temperature (°C)	100.0
Pressure (atm)	1.0
Total Flow (m3/hr)	100.0

Inflows (mole %)	
H2O	8.0
N2	73.0
CO2	11.0
O2	6.0
Ar	0.8
SO2	0.2
SO3	0.01
HCl	5.0e-3
NaOH	0.0
Total	99.015

The composition will not sum to 100%. Therefore, you will use the **Normalization** option labeled **Makeup with Water** to set it to 100%.

✓ Change the Normalization Type to Makeup with water

Normalization	
Normalize Fractions Using	Makeup with Water

The software adjusts the water content to create the 100% composition.

Inflows (mole %)	
H2O	8.985
N2	73.0
CO2	11.0
O2	6.0
Ar	0.8
SO2	0.2
SO3	0.01
HCl	5.0e-3
NaOH	0.0
Total	**100.0**

Normalization	
Normalize Fractions Using	Makeup with Water

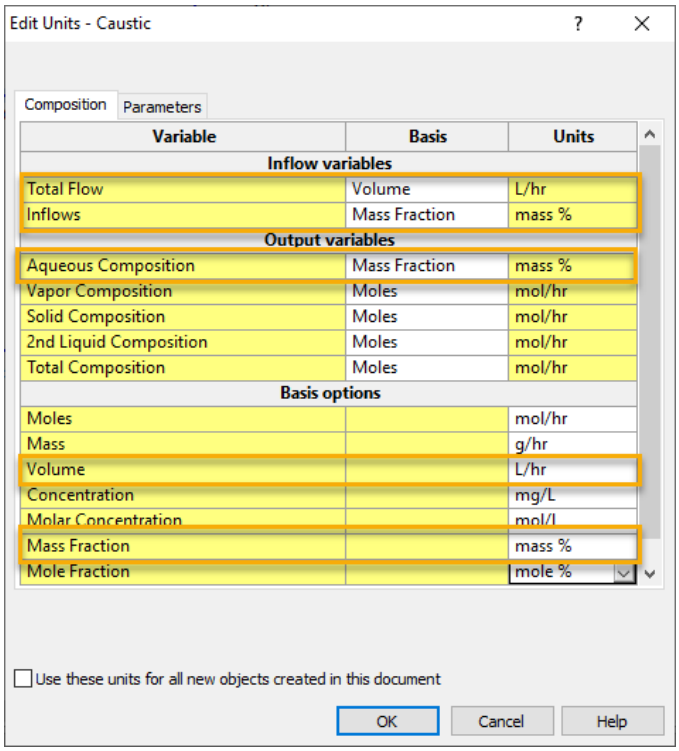
✓ Click on the **Caustic** stream to access the **Properties** panel.

✓ Edit its units in the same way, click on one of the linked units in the panel Inflows (mol/hr) to open the Units Editor window.

✓ Make the following changes:

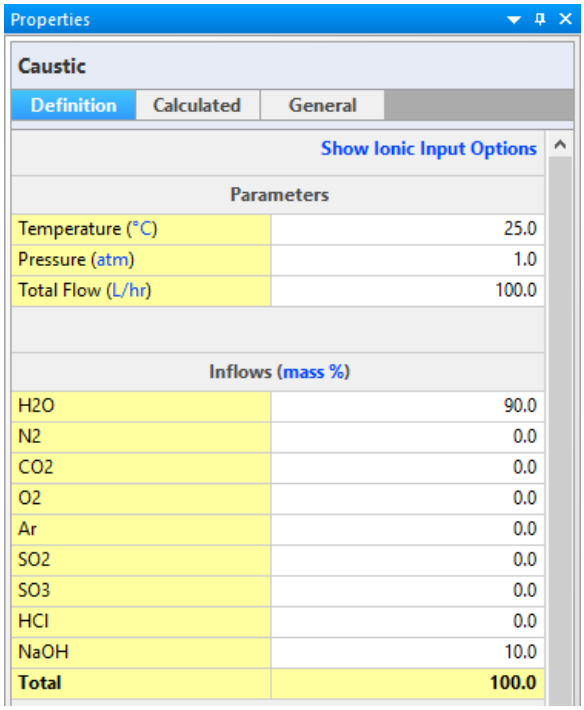
Inflow and Output Variables		
Stream Amount	Volume	
Inflows	Mass Fraction	
Aqueous Composition	Mass Fraction	
Basis Options		
Volume		L/hr
Mass Fraction		mass%

The Units Editor should look like this when complete



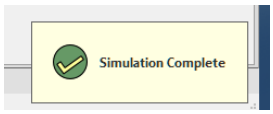
✓ Click **OK** to close the Edit Units window

✓ Enter the following conditions and composition:



✓ Press the **Run** button to calculate the case

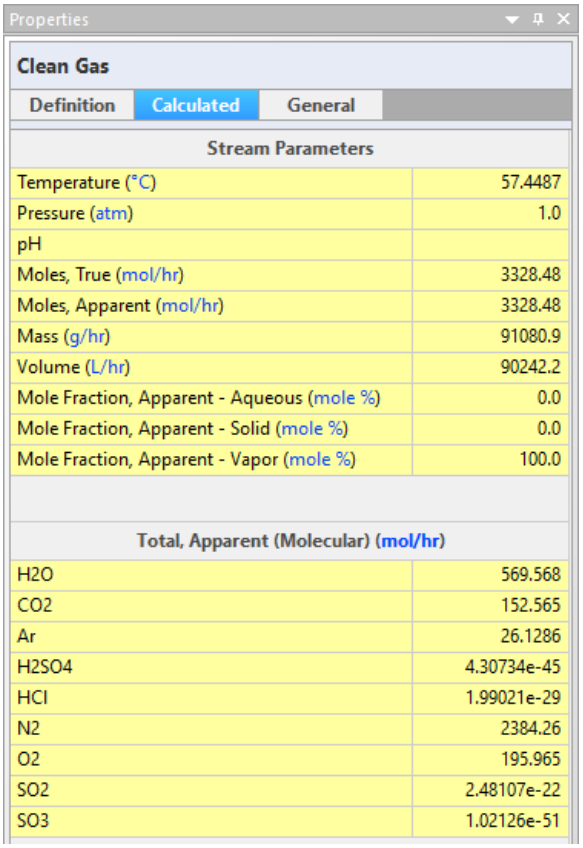
✓ When complete, a Simulation Complete pop-up window appears in the lower right of the window.



Reviewing the results

✓ Click on the **Clean Gas** stream to access the **Properties** panel.

The Properties panel contains a **Calculated** tab, which is the default view after the simulation converges. It contains two sections - **Stream Parameters** and **Total Apparent** flow.



Properties

Clean Gas

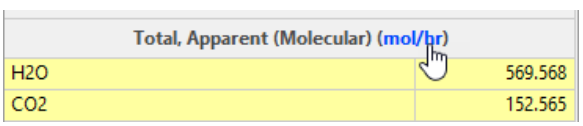
Definition | Calculated | General

Stream Parameters	
Temperature (°C)	57.4487
Pressure (atm)	1.0
pH	
Moles, True (mol/hr)	3328.48
Moles, Apparent (mol/hr)	3328.48
Mass (g/hr)	91080.9
Volume (L/hr)	90242.2
Mole Fraction, Apparent - Aqueous (mole %)	0.0
Mole Fraction, Apparent - Solid (mole %)	0.0
Mole Fraction, Apparent - Vapor (mole %)	100.0

Total, Apparent (Molecular) (mol/hr)	
H2O	569.568
CO2	152.565
Ar	26.1286
H2SO4	4.30734e-45
HCl	1.99021e-29
N2	2384.26
O2	195.965
SO2	2.48107e-22
SO3	1.02126e-51

The volume will probably show in **L/h** and the Total Apparent units will probably show **mol/hr**. These are the default software units. They, however, do not help interpretation, and so you will change them.

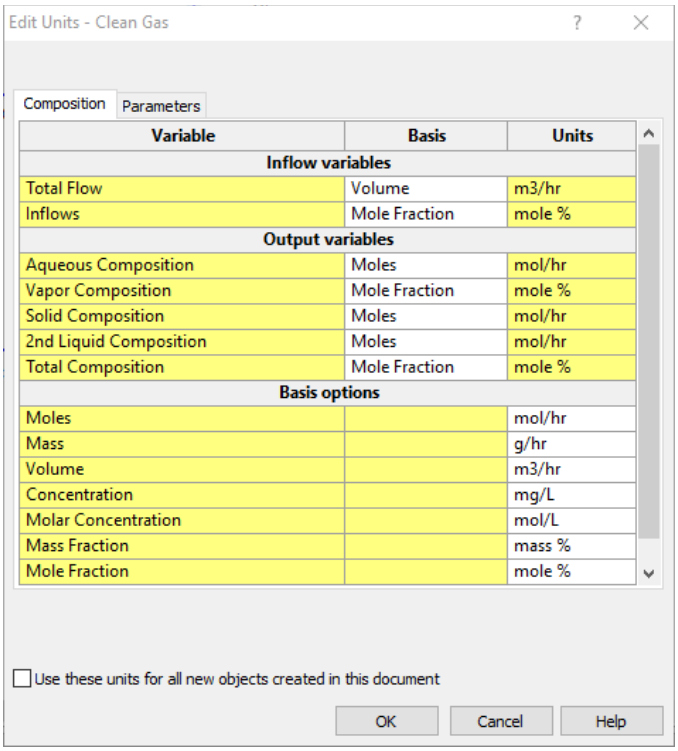
✓ Click on the Units link in the **Total Apparent** header to open the Units Manager.



Total, Apparent (Molecular) (mol/hr)	
H2O	569.568
CO2	152.565

✓ Make the following changes to this panel.

Inflow and Output Variables		
Total flow	Volume	m3/hr
Inflows	Mole Fraction	mole%
Vapor Composition	Mole Fraction	mole%
Total Composition	Mole Fraction	mole%
Basis Options		
Volume		m3/hr
Mole Fraction		mole%



✓ Click **OK** to close the Edit Units window

✓ Now we can interpret the results of the **Clean Gas** stream.

Clean Gas

Definition | Calculated | General

Stream Parameters	
Temperature (°C)	57.4487
Pressure (atm)	1.0
pH	
Moles, True (mol/hr)	3328.48
Moles, Apparent (mol/hr)	3328.48
Mass (g/hr)	91080.9
Volume (m3/hr)	90.2422
Mole Fraction, Apparent - Aqueous (mole %)	0.0
Mole Fraction, Apparent - Solid (mole %)	0.0
Mole Fraction, Apparent - Vapor (mole %)	100.0

Total, Apparent (Molecular) (mole %)	
H2O	17.1119
CO2	4.58361
Ar	0.785
H2SO4	1.29408e-46
HCl	5.97932e-31
N2	71.6319
O2	5.88751
SO2	7.45405e-24
SO3	3.06824e-53

✓ The vent temperature has decreased to 57.5 C and the measured volume decreased to 90 m3/hr.

The SO_2 and SO_3 acids are virtually all removed from the gas. This is due in part because we added excess NaOH. You can confirm this by reviewing the bottoms stream pH.

✓ Click on the **Bottoms** stream and view the calculated **pH**.

Bottoms

Definition | Calculated | General

Stream Parameters	
Temperature (°C)	51.6848
Pressure (atm)	1.0
pH	8.72122
Hardness (mg/L of Mg+2 and Ca+2)	0.0
Moles, True (mol/hr)	5706.28
Moles, Apparent (mol/hr)	5678.9
Mass (g/hr)	1.1402e5
Volume (L/hr)	101.967
Mole Fraction, Apparent - Aqueous (mole %)	100.0
Mole Fraction, Apparent - Solid (mole %)	0.0
Mole Fraction, Apparent - Vapor (mole %)	0.0

The pH is nearly nine, significantly above the pH needed to remove SO2 gas. A more reasonable pH would be 7.2. Another potential problem with this high pH is the formation of NaHCO3 solids. Caustic solutions absorb CO2, converting it to NaHCO3. To see whether NaHCO3 may form, you need to view the report table for this stream. It is accessible by selecting the View detailed report link.

✓ Click on the **View detailed report** link at the bottom of the **Bottoms** panel. View detailed report

This action creates a Report (Report-2) that contains the detailed information about the Bottoms stream. The table contains four results columns, for the separate phases and the total. The report contains the sections: Parameters, Flow rates, Thermodynamic properties, Composition, Material Balance groups (element concentration) and lastly Scaling Tendencies.

The Scaling tendencies is the table of interest. It contains the driving force to precipitation caused by increasing concentrations. Any value above 1, i.e. ST>1.0, means that solids will form.

✓ Scroll down to the **Scaling Tendencies** table

$NaHCO_3$ solid have a value greater than 1. It may potentially form.

Scaling Tendencies	Post-scale
Row filter applied: only show rows with value greater than 1	
TRange filter applied: only show solids in active TRange	
NaHCO3 (Nahcolite)	1.18522
Na2CO3.NaHCO3.2H2O	0.175327
Na2CO3.1H2O (Thermonatrite)	0.0348005
Na2SO3	3.3435e-3
Na2SO4 (Thenardite)	4.53015e-4

Optimizing the Caustic inflow rate

The goal is to add sufficient caustic to remove SO2 to the target limits and minimize excess flow. To do this we need to define a target SO2 limits then control the caustic flow accordingly. According to an excerpt from the document below, the SO2 limits are 180 ng/J energy output, or a flat 95% reduction.

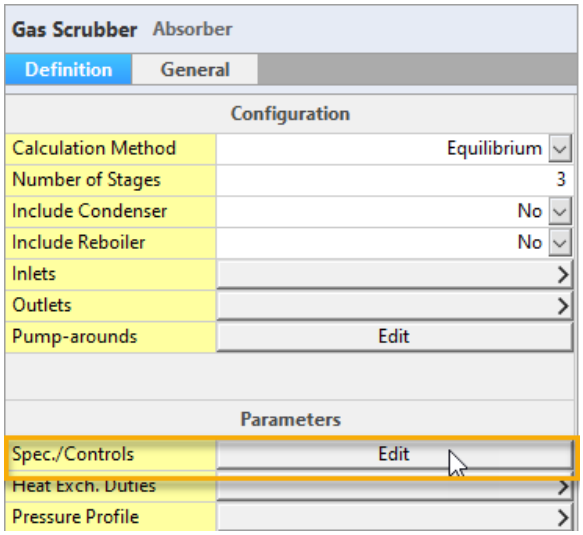
The SO_2 emission limit for new electric utility steam generating units is 180 ng/J (1.4 pound per megawatt hour (lb/MWh)) gross energy output or 95 percent reduction regardless of the type of fuel burned with one exception. The SO_2 emission limit for new electric utility steam generating units that burn over 75 percent coal refuse (by heat input) is 180 ng/J (1.4 lb/MWh) gross energy output or 94 percent reduction.

9868 **Federal Register** / Vol. 71, No. 38 / Monday, February 27, 2006 / Rules and Regulations

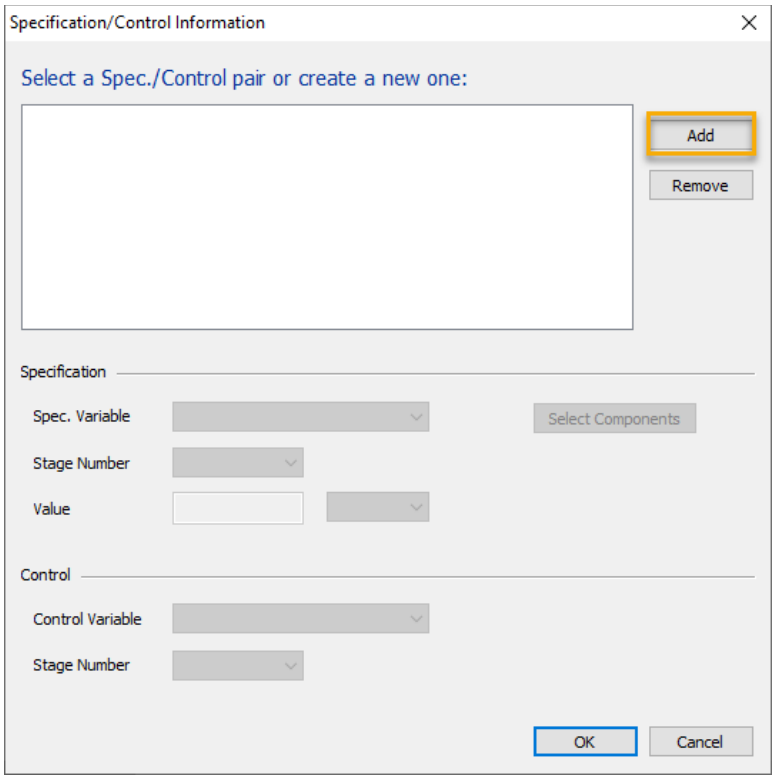
Since this example does not consider energy generated, the target will be the 95% reduction. The SO2 in this combustion gas is 2000 ppmV. Therefore, the 95% reduction converts to 100 ppmV SO2 in the clean gas. You will enter this 100 ppmV values into the column's **Spec/Control** window, and instruct the column to adjust the caustic inflow to meet these specifications.

✓ Return to the **Flowsheet** tab and click on the **Gas Scrubber** to access the **Properties** Panel.

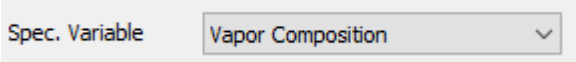
✓ Click on the Spec./Controls Edit button in the Parameters section.

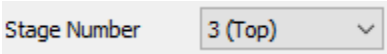


The Specification/Control Information window that opens contains the instruction settings for optimizing a tower function.

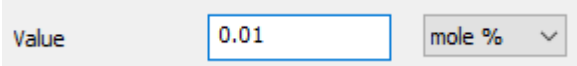


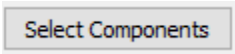
You can set several types of target specifications, and control several forms of dependent variables. In this case, you will set the SO2 vapor concentration (Specification), and adjust the Caustic flow into the column (Control). They are always set in pairs (i.e., one fixed and one free variable).

- ✓ Click on the **Add button** in the upper right.
- ✓ Change the **Spec. Variable** to **Vapor Composition** 

- ✓ Change the **Stage Number** to **3(Top)** 

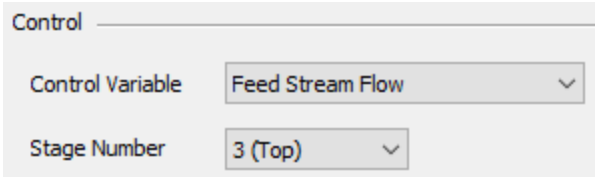
Stage 3 is the top stage and is the location of the **Clean Gas** stream outlet.

- ✓ Change the **Value** units to **mole%** and set the value to 0.01 mole% (equals 100ppmV)


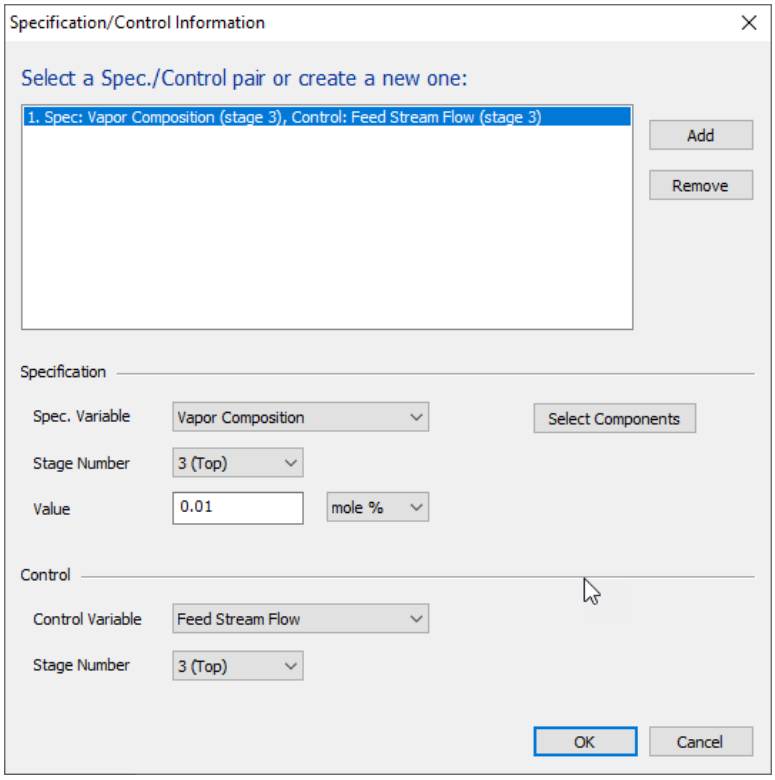
- ✓ Click on the **Select Components** button if the window does not open automatically.


- ✓ Check the SO2 box

and click OK to close the window
- ✓ Change the **Control Variable** option to **Feed Stream Flow**
- ✓ Set the **Stage Number** to 3(Top) (the stage where the Caustic enters)



When finished your screen should look like the following:

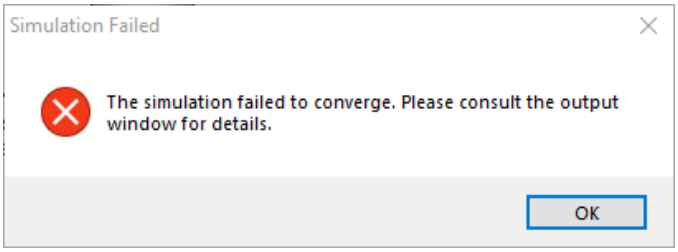


✓ Click OK to close the window

✓ **Run** the simulation

----------THE SIMULATION WILL FAIL----------

When complete, you will receive an ERROR stating that the simulation failed.



This is a common occurrence, and it occurs for several reasons. In this case, it occurred because the 10% Caustic feed is too concentrated. The software cannot find a flow rate that sets the SO2 vapor to 100ppmV. As the Caustic flow decreases (to allow more SO2 to remain in the vapor), it reaches a value where all the liquid added evaporates. A column cannot be all vapor, or it fails to converge.

This is an easily remedied problem; use a less concentrated caustic solution.

- ✓ Click OK to close the error message
- ✓ Click on the **Caustic** stream to access the **Properties** panel
- ✓ Change the **Normalization** type from Prorate to **Makeup with Water**

Normalization	
Normalize Fractions Using	Makeup with Water

- ✓ Change the **NaOH** content to **0.5 mass%.**
- ✓ **Rerun** the simulation

Now the simulation converges quickly.

- ✓ Click on the **Clean Gas** stream to access the **Properties** panel.
- ✓ View the **Total Apparent** section, specifically the **SO2** value.

Total, Apparent (Molecular) (mole %)	
H2O	9.3816
CO2	10.9738
Ar	0.798335
H2SO4	5.87508e-38
HCl	7.02266e-27
N2	72.8487
O2	5.98752
SO2	0.01
SO3	6.40882e-45

The target SO2 is 0.01 mole%, per design.

- ✓ Click on the **Caustic** stream to access the **Properties** panel.
- ✓ Click on the **Calculated** tab and view the **Volume** row.

Caustic

Definition | Calculated | General

Stream Parameters	
Temperature (°C)	25.0
Pressure (atm)	1.0
pH	12.9865
Hardness (mg/L of Mg+2 and Ca+2)	0.0
Moles, True (mol/hr)	3085.78
Moles, Apparent (mol/hr)	3078.83
Mass (g/hr)	55619.0
Volume (L/hr)	55.4848
Mole Fraction, Apparent - Aqueous (mole %)	100.0

The calculated volume is 55 L/hr of a 0.5% caustic solution. Had the 10% been kept, approximately 3 L/hr would be required, but the software was unable to converge the tower with this small of a caustic flow rate. This is because the liquid evaporated completely in at least one of the three stages, and the tower will not converge unless water exists at every stage of the tower.

✓ Click on the **Bottom** stream to review the pH.

The computed pH is ~ 4.0. This is lower than expected. This is because the target SO2 vapor composition was set to 0.01 mole%. Were the target specification set lower, then the bottoms pH would have increased.

Bottoms

Definition | Calculated | General

Stream Parameters	
Temperature (°C)	49.7247
Pressure (atm)	1.0
pH	3.97153
Hardness (mg/L of Mg+2 and Ca+2)	0.0
Moles, True (mol/hr)	3072.49

✓ If you want, change the target Specification SO2 value to 10ppmV and review the results again.

Summary

We have completed our second case. It presents the basic mechanics of building an absorber and converging it, and how to set up a column specification.

Chapter 4 Sour Water Stripper

The Application

There are multiple references to corrosion occurring in equipment processing sour water. The purpose of this case file is to study the chemical composition of the gas and fluid phases flowing through the separation unit. This case will use both the Flowsheet ESP and OLI Studio software. The Flowsheet software is used to create the stripping process and to compute the composition in each stream and on each column stage. The corrosion engineer or material scientist can then use the computed results, plus their knowledge of corrosion, to determine if the existing process is at risk.

The image below is the process flowsheet that we will study. It represents a generic stripping column in which heated sour water is injected into the fourteenth stage of a of a twenty-stage tower. Tower overheads are cooled and the liquid reflux returned to the top of the column. The remaining gas exits the process.

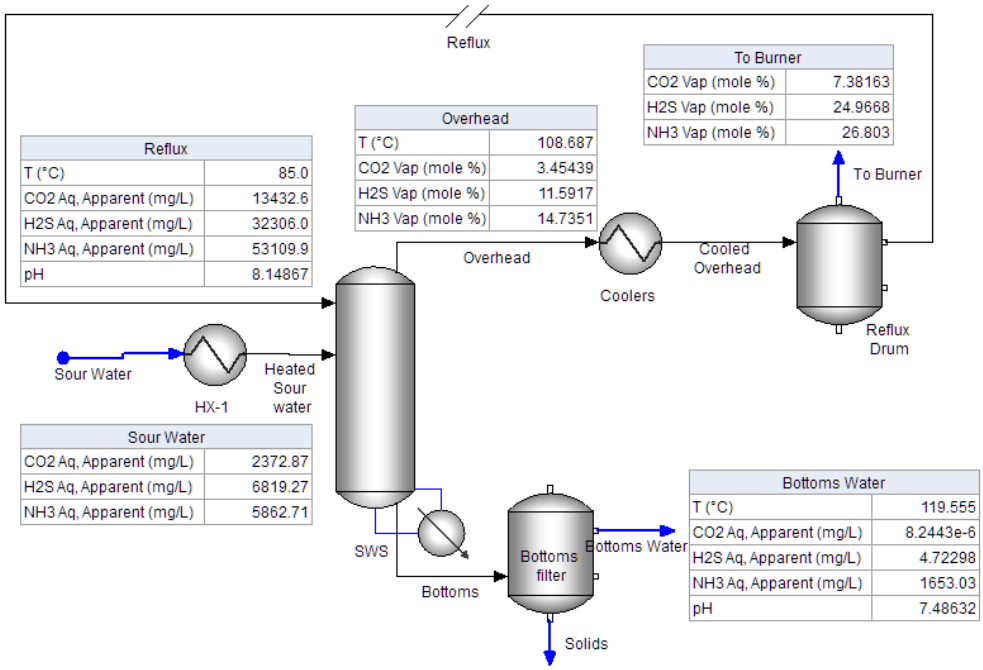


Figure 4-1 – Basic sour water stripper process

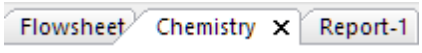
You will build this case in the same two steps as the previous chapter. Step 1 is to create the chemistry model and the step 2 is to build the process.

- ✓ Start the Software.
- ✓ Confirm that a blank case is on the screen.
- ✓ Save this blank case as Chapter 4 – Sour Water Stripper.

Creating a Chemistry Model

The chemistry model is one of two modules required for the case. This was described in previous chapters. The other module is the process.

Selecting the thermodynamic method and databases used in the Model

- ✓ Click on the Chemistry tab - 

The starting sub-tab for all new cases is the Databanks. This tab contains the thermodynamic framework and specialized database. You will use the Aqueous (H+ ion) framework and will not add any specialized databases to this case.

- ✓ Keep the existing framework and add no private databases.

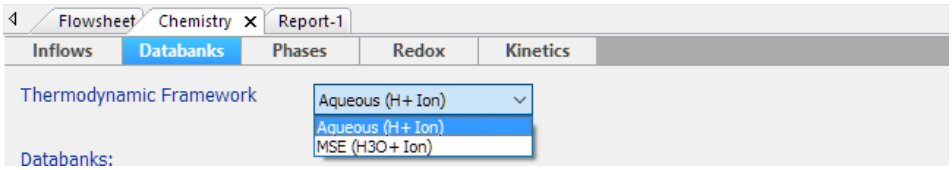


Figure 4-2 - The available framework and databases installed with the software

Adding the chemical inflows to the model

- ✓ Click on the Inflows sub-tab to access the grid for adding inflows.

This inflows sub-tab contains the chemical component grid. The software generates the complete chemistry model: aqueous species, gases, oils, solid phases, etc. from this list.

- ✓ Type the following Inflows to the grid.

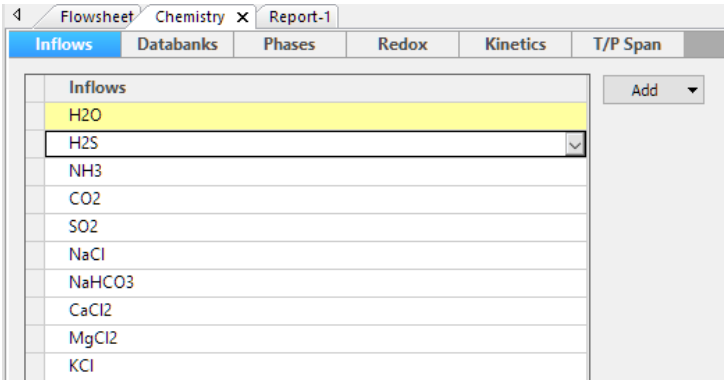


Figure 4-3 – Entering the molecular inflows.

- ✓ Click on the Chemistry icon in the Navigator panel and press F2 to change its name. Name it Sour Water.

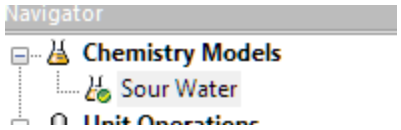
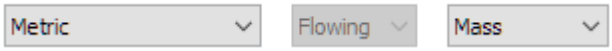
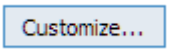


Figure 4-4 – Renaming the Chemistry model

This completes the Chemistry Model Build step. There are additional options, but they are not germane to this example.

Changing Units

- ✓ Click on the Units manager button in the toolbar -
- ✓ Set the units to Metric-Flowing-Mass - 

- ✓ Click on the Customize button to edit the existing units - 

- ✓ Make the following changes to the units, there are several:

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Total Flow	Mass	kg/hr
Inflows	Mass Fraction	ppm (mass)
Output variables		
Aqueous Composition	Concentration	mg/L
Vapor Composition	Mole Fraction	mole %
Solid Composition*	Concentration	mg/L
2nd Liquid Composition	Mole Fraction	mole %
Total Composition	Moles	mol/hr
Basis options		
Moles		mol/hr
Mass		kg/hr
Volume		m3/hr
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		ppm (mass)
Mole Fraction		mole %

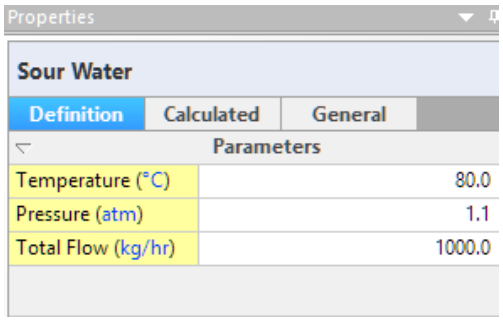
Building the Scrubber Process

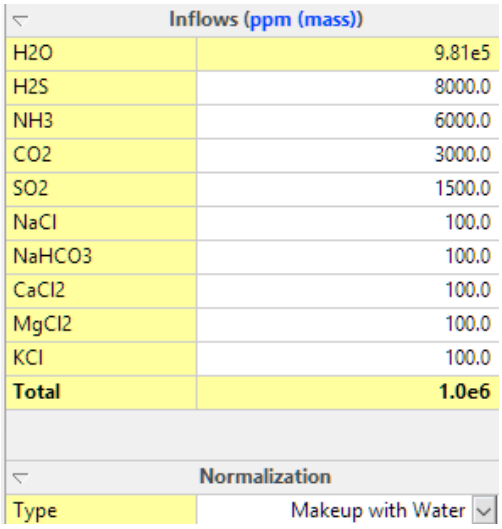
Adding the Sour Water stream

- ✓ Click on the Flowsheet tab and then the Add Stream button from the toolbar -
- ✓ Create a stream and label it Sour Water.
- ✓ Unclick the Add Stream, button -
- ✓ Double-click on the new stream you created to enable the name editor and change the name to Sour Water.

Next you will enter the Sour water composition in the Properties panel.

- ✓ Enter the conditions and compositions shown in the image below. Confirm that your Total flow units are kg/hr and Inflow units are ppm(mass).

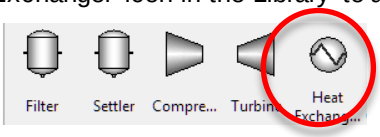




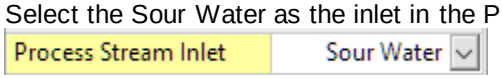
Set the Normalization to Makeup with Water – in that way the H2O is entered automatically.

Adding the Heat Exchanger

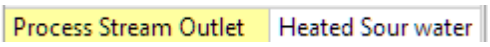
- ✓ Double-click on the Heat Exchanger icon in the Library to add it to the process.



- ✓ Select the Sour Water as the inlet in the Properties Panel -



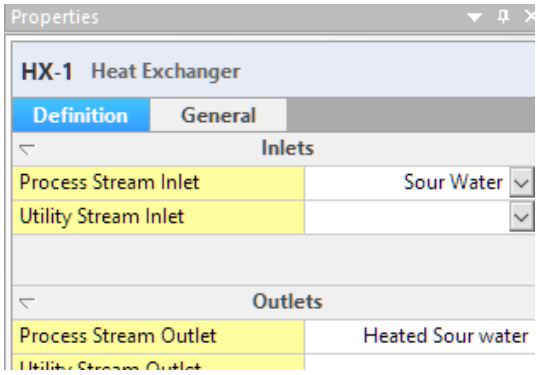
- ✓ Type in the outlet name, Heated Sour Water -

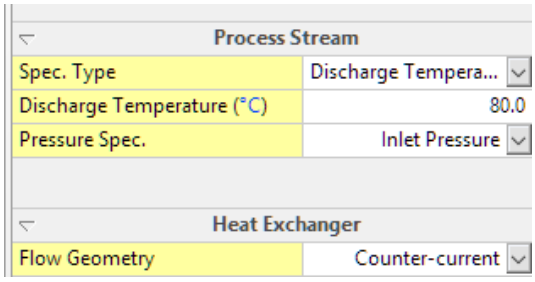


- ✓ Set the Process Stream Spec. type to Discharge Temp -

- ✓ Set the Discharge T to 80 C.

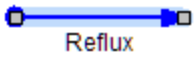
The Properties panel should look like the one below when finished:





Add a Reflux stream to be used in the Stripper

- ✓ Click on the Add Stream button and create a new stream.

- ✓ Label it Reflux - 

- ✓ Enter the following initial guess to the reflux composition:

Properties

Reflux

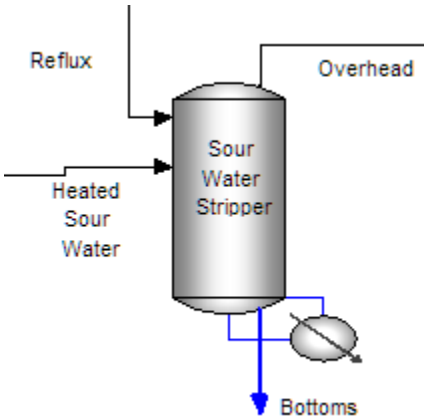
Definition	Calculated	General

Parameters	
Temperature (°C)	85.0
Pressure (atm)	1.3
Total Flow (kg/hr)	20.0

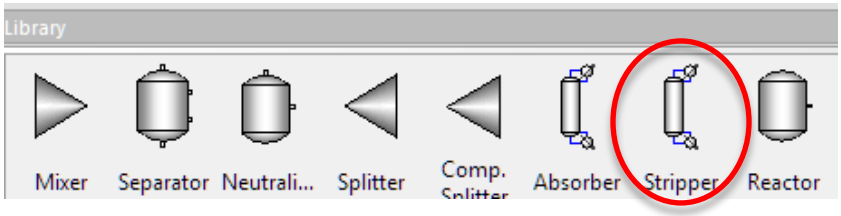
Inflows (ppm (mass))	
H2O	9.0e5
H2S	20000.0
NH3	60000.0
CO2	20000.0

This composition is an initial guess, because it will be the outlet of the reflux drum and will become an internal (calculated) stream, once the case is finished.

Add the Stripper column



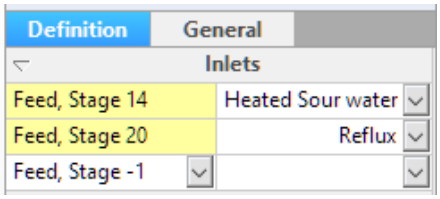
The stripper object contains a number of settings, so make sure that you complete each step.



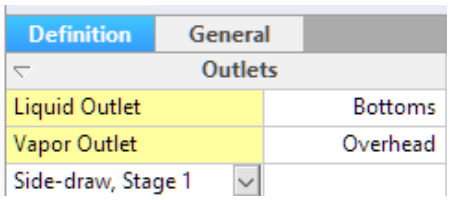
- ✓ Double-click on the Stripper object in the Library panel and add it to the process.
- ✓ Name it Sour Water Stripper.
- ✓ Move to the Properties panel and make the following changes.
- ✓ Set the Calculation method to Equilibrium.
- ✓ Set the Number of stages to 20.
- ✓ Set Include condenser to No.

Calculation Method	Equilibrium
Number of Stages	20
Include Condenser	No
Include Reboiler	Yes

- ✓ Open the Inlets window.
- ✓ Use the down arrows to add the Heated Sour Water to Stage 14 and the Reflux stream to stage 20.

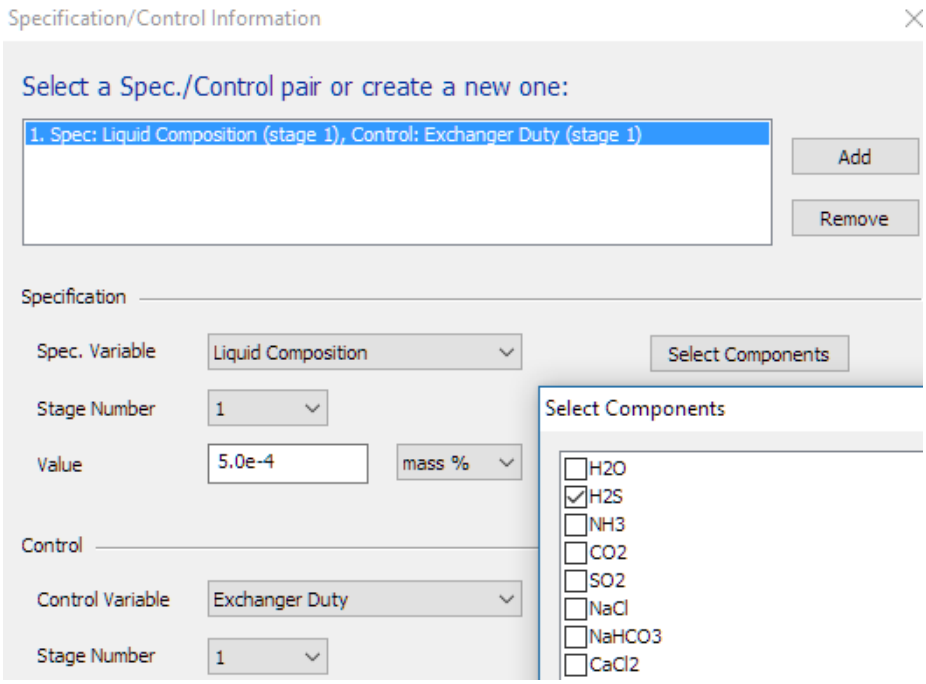


- ✓ Click on the Outlets window.
- ✓ Enter the name Bottoms to the Liquid Outlet and Overhead to the Vapor Outlet.



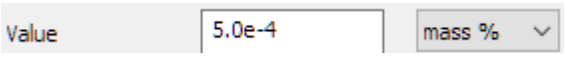
- ✓ Open the Spec./Controls Editor window.
- ✓ Click on the Add button to create a new tower Specification.

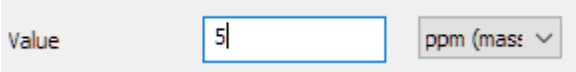
You will recreate the specifications shown in this image using the instructions below.



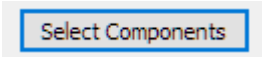
Specification section:

- ✓ Select Liquid Composition for Spec. Variable.
- ✓ Set the stage # to 1.
- ✓ Set the value to 5e-4 mass%. If mass% is not available, then use 5 ppm.





- ✓ Select the component H2S from the popup window that appears.

If the component popup window does not appear after pressing Enter, then click on the Select Components button 

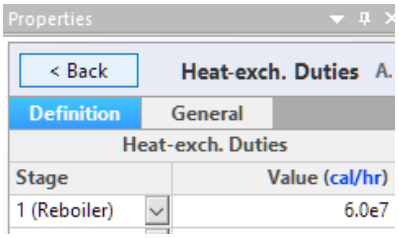
Control section:

- ✓ Select Exchanger duty.
- ✓ Select Stage 1.

Your windows should look like the one above:

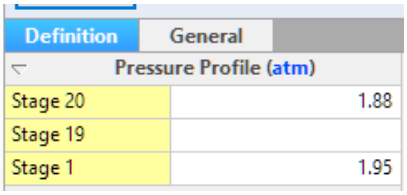
- ✓ Close the Specifications window.
- ✓ Click on the Heat Exch. Duties editor button -

- ✓ Set the initial guess for the Stage 1 (Reboiler) heat duty to 6e7 cal/hr.

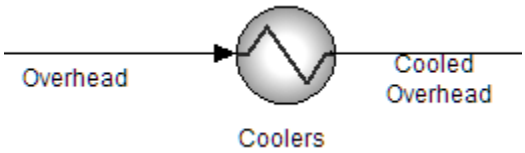


- ✓ Click on the Pressure Profile editor button -

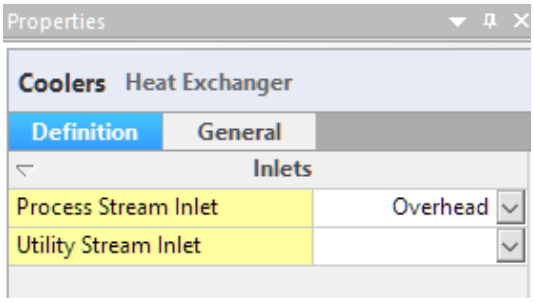
- ✓ Set Stage 20 to 1.88 atm and stage 1 to 1.95 atm.

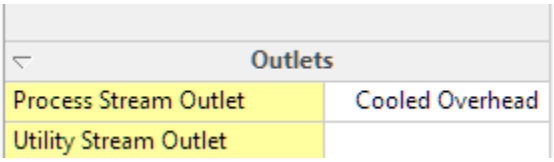


Add the Overhead Coolers



- ✓ Add another Heat Exchanger object and name it Coolers.
- ✓ Use the Properties panel to link the Overhead stream to the Process Stream Inlet field.
- ✓ Type the name Cooled Overhead in the Process Stream outlet field.

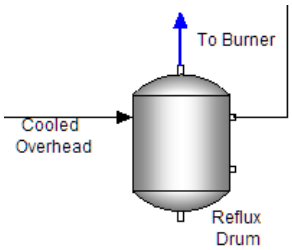




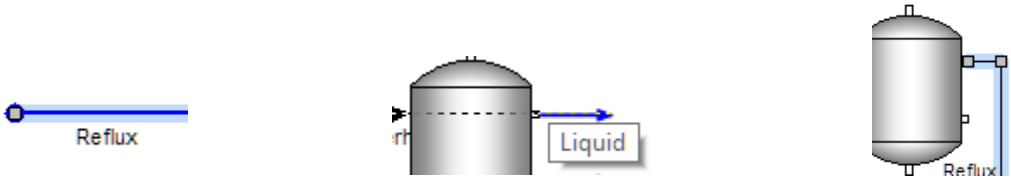
- ✓ Set the Process Stream Spec. Type to Discharge Temperature.
- ✓ Set the discharge Temperature to 85C.
- ✓ Set the Pressure Spec. to Absolute Pressure.
- ✓ Set the Pressure to 1.3 atm.

Process Stream	
Spec. Type	Discharge T...
Discharge Temperature (°C)	85.0
Pressure Spec.	Absolute Pre...
Pressure (atm)	1.3

Add the Reflux Drum



- ✓ Add a Separator object to the case and label it Reflux Drum.
- ✓ Use the Properties panel to select the Cooled Overhead as the Inlet stream.
- ✓ Click on the front-end of the Reflux stream and drag it to the liquid outlet of the Reflux drum.



- ✓ Type the name To Burner in the Vapor Outlet.
- ✓ Keep the existing Equilibrium Calculation Properties

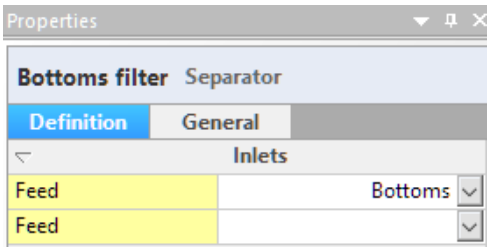
Outlets	
Liquid	Reflux
Solids	
Vapor	To Burner
Organic	

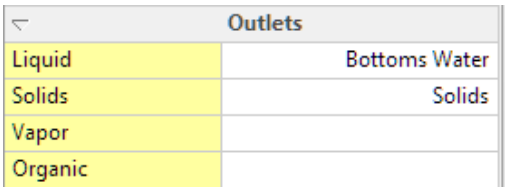
Equilibrium Calculation	
Calculation Type	Adiabatic
Pressure Spec.	Min. Inlet Pressure
Heat Duty (cal/hr)	0.0
Entrainment	

At this point, you may want to rearrange the blocks and streams to keep the flowsheet organized.

Add the Bottoms Filter

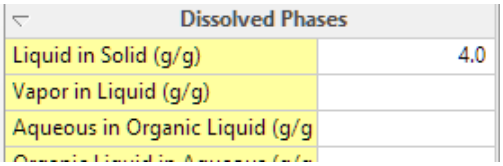
- ✓ Add another Separator block and label it Bottoms Filter.
- ✓ Link the Bottoms stream to the Inlet.
- ✓ Create two outlet streams – Bottoms Water in the Liquid outlet and Solids in the Solids outlet.





- ✓ Open the Entrainment editor -

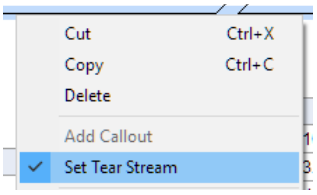
- ✓ Set the Liquid to Solid ratio in the Solids stream to 4.



This action will add four grams of liquid to every gram of solids that flow. It is essentially a solids slurry containing 80% water.

Set the Reflux stream as the Recycle/Tear stream

- ✓ Right mouse-click anywhere along the Reflux stream to activate the drop-down menu.
- ✓ Select the Set Tear option.

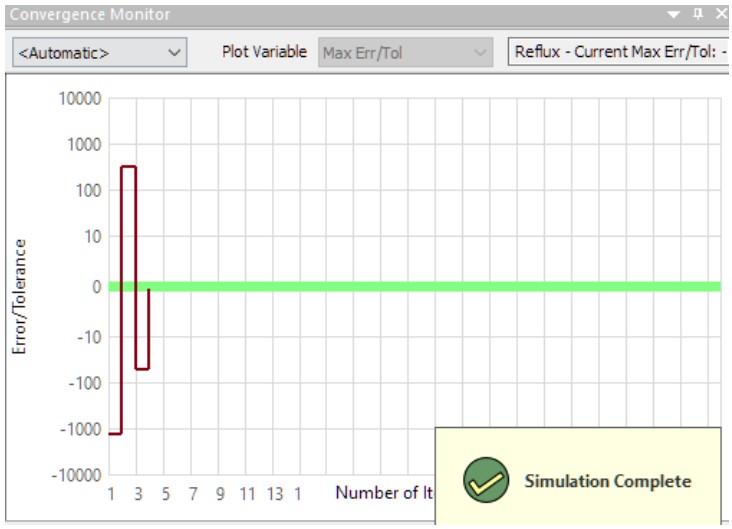


- ✓ Save the file – label it Stripper-Sour Water.

Calculate the Case

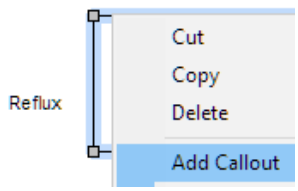
- ✓ Press the Calculate button -
- ✓ View the Convergence monitor. It will provide a quick view of the calculation progress.

It may take many iterations before the process converges. The monitor will show if the existing error is decreasing or increasing (calculation unstable).



Reviewing the calculation results

- ✓ Right-mouse-click on the Reflux stream and select Add Callout.



- ✓ Double-click on the callout table that appears to edit the variables.
- ✓ Remove the pressure from the existing variable list.
- ✓ Expand the Liquid-1, Apparent field and select CO2, H2S, and NH3.

Reflux	
T (°C)	85.0
pH	8.14867
CO2 Aq, Apparent (mg/L)	13432.8
H2S Aq, Apparent (mg/L)	32305.9
NH3 Aq, Apparent (mg/L)	53110.1

According to the calculation, this is the concentration of sour components in the reflux stream. Use these data, plus the pH, to evaluate whether corrosion is possible at these conditions.

- ✓ Add other callout tables where you think that corrosion may be a problem in your process and review the composition at these locations.

Summary

The purpose of this case is to obtain the steady-state composition and conditions at various points in a sour water stripper unit. A chemical corrosion assessment is then performed using these results and other relevant factors.

Chapter 5 Water Treatment - Getting Started

The Application

The simplest ESP calculation is an adiabatic mix of two streams. We will use this calculation to see ESP's general workings. Figure 5-1 is a process diagram containing two inlet streams, one mixer, and one outlet.

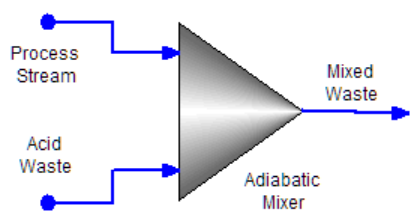


Figure 5-1 – Adiabatic mixing of two liquids

Before building this process, we will create Chemistry Model.

Creating a Chemistry Model

Creating and saving the file

Before starting the Flowsheet work you will save this blank case file. This file will be open several time in the upcoming chapters.

✓ Save the file with the name Water Treatment Softening Process

Setting up the Chemistry model for a new Case

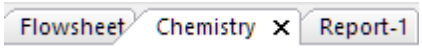
The chemistry model is the core of any ESP calculation. It instructs the solver to use specific chemistry (e.g., NaCl, CO_2, H_2S, etc.) and properties (e.g., precipitate certain solids, include kinetics, etc.). The procedure for creating a chemistry model has the following steps:

- Choosing the database and thermodynamic framework to use.
- Selecting the inflow components.
- Selecting which phases to allow (this is a two-step procedure).
- Adding equations, kinetics, and surface reactions.

Once completed, we can build the process and run the calculation.

A chemistry model can always be changed. It is a matter of returning to the model generation steps (above) and making the necessary modifications.

Introduction to the Chemistry Model tabs

- ✓ Click on the Chemistry tab - 

The Chemistry section contains five sub-tabs, Inflows, Databanks, Phases, Redox, and Kinetics. New cases default to the Databanks tab. This tab contains the thermodynamic framework and specialized database.

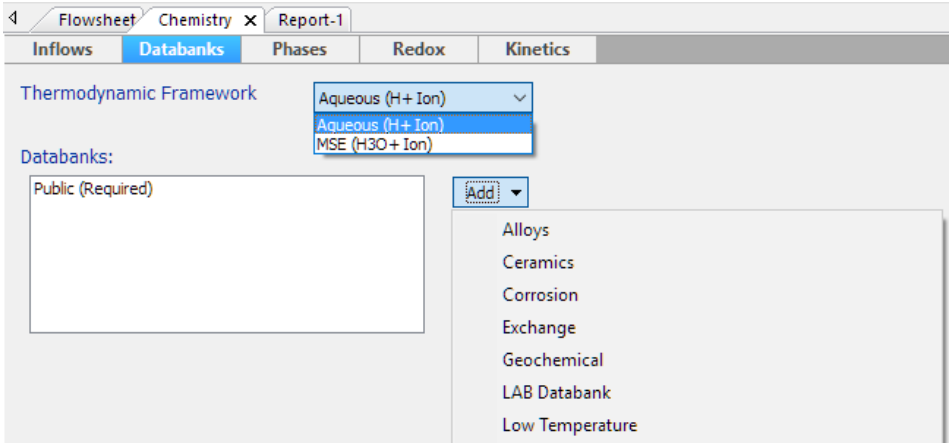


Figure 5-2 - The available framework and databases installed with the software

OLI uses two thermodynamic frameworks, Aqueous (H+ ion) and MSE (H3O+). MSE stands for Mixed Solvent Electrolyte. The available databases (note the Add button) include the required Public database, OLI-installed private databases, and client-specific private databases.

- ✓ Use the default settings of Aqueous (H+) and no private databases.
- ✓ Click on the Inflows tab.

Adding the chemical inflows to your case file

The inflows tab contains the grid for adding molecular inflows, assays, pseudocomponents, and other optional inflows.

- ✓ Enter the following inflows, NaCl, KCl, CaCl2, MgCl2, SrCl2, NaHCO3, Na2SO4, CO2, H2SO4, HCl, FeCl3, and AlCl3

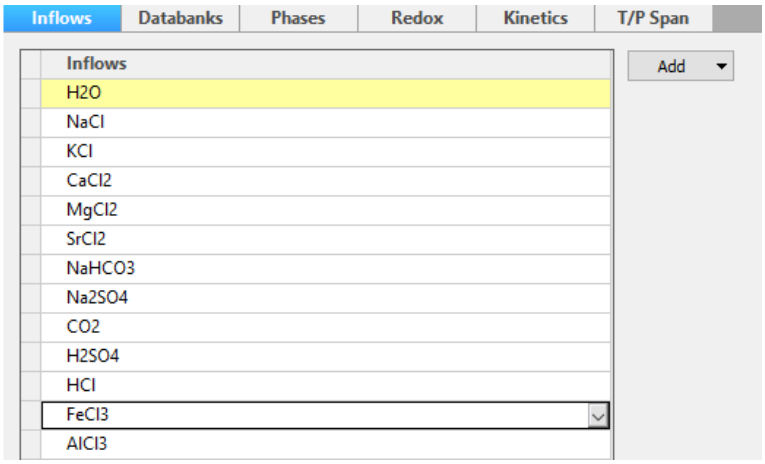


Figure 5-3 – entering the molecular inflows. The Assay and pseudocomponent entry down-arrow is shown on the right

- ✓ Click on the Phases tab.

This screen contains the options for including or excluding phases from the simulation. This includes each of the solid phases that the software determines may exist based, on the inflows you entered. This case contains sixty-seven solid phases that will be considered for precipitation. Whether or not they form depends on the solution composition. Users can prevent solid from forming by unchecking th e individual box.

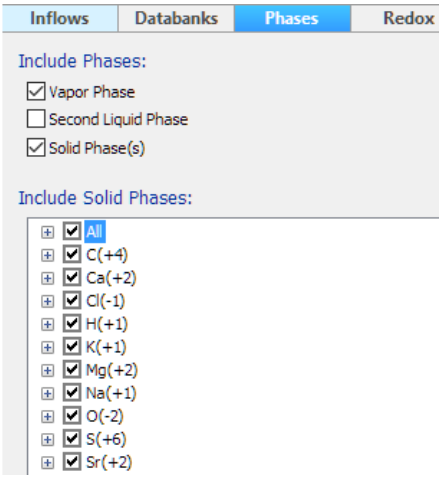


Figure 5-4 – Selecting the phases to be included-excluded in the case

- ✓ Use the default settings for the Phases tab.
- ✓ Click on the Redox tab.

The Redox screen contains toggle boxes to enable or disable oxidation-reduction reactions. The default setting is for Redox reactions to be off. If Redox chemistry is included, then the user selects which elements will be included, and also which oxidation states within the particular element is included.

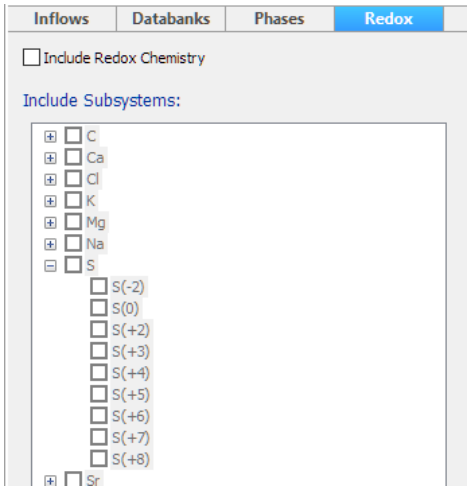


Figure 5-5 – Include or exclude Oxidation-Reduction reactions and select which element and oxidation state will be allowed

- ✓ Use the default settings for the Redox tab.
- ✓ Click on the Kinetics tab.

The Kinetics tab is where users can construct rate-limiting equations for one or more reactions. A template of species is available to create the kinetic model. Creating kinetic reactions will be explained in later chapters.

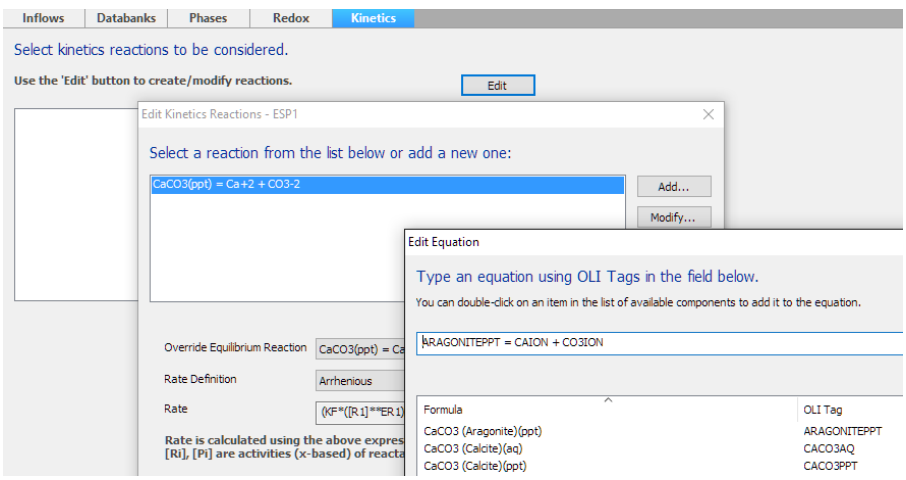


Figure 5-6 – Selecting reactions that will be undergo rate-limiting kinetics

- ✓ You will not create any reactions.

This completes the basic introduction of the Chemistry Model Build step. There are additional options that but they are not germane to the first example.

Building the Process

Our simple example contains one mixer, two inlet streams, and one outlet. We will run the mixer adiabatically, or heat-isolated from the environment. This way, we can observe temperature changes that may occur upon mixing.

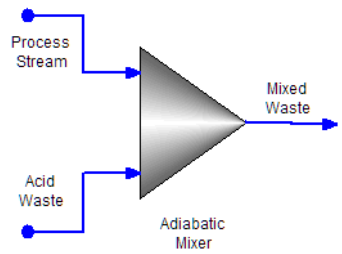


Figure 5-7 Adiabatic mixing of two liquids

Creating a New Process Block

✓ Click on the Flowsheet tab.

The main flowsheet screen contains a center workspace, support panels, and a toolbar. The workspace is blank, and becomes filled with streams and units. The support panels include Navigator, Library, Properties, and a general Output section (errors, trace, monitor, and output). The toolbar contains various actions that are described below.

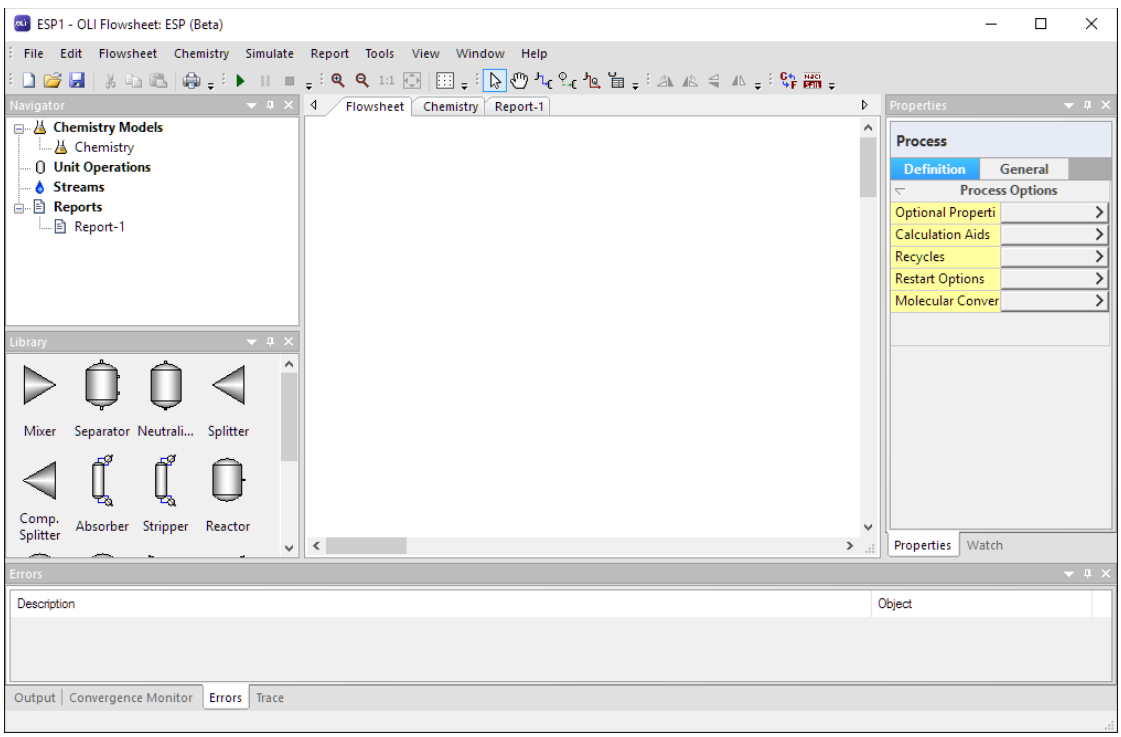


Figure 5-8 – Flowsheet tab showing the blank process screen and the five default support panels

- The Navigator panel contains the complete list of objects that are part of the file. This includes all chemistry models, streams, unit operations, and reports.
- The Library panel contains the available units and unit operations. Objects in the library panel are brought into the workspace using drag and drop.
- The Properties panel contains the settings for a unit, the molecular composition of a stream, or the properties of the flowsheet. The panel view will therefore change, depending on

what object or stream is in focus on the worksheet. There are tabs at the bottom and top of the panel that display input and output composition and settings.

- The general output panel at the bottom of the screen contains several sub panels. The Convergence Monitor contains a graph that shows the progress of converging recycle streams (Tear streams) and controller settings. The Errors panel contains the list of problems that need to be corrected either before running the case or problems found after the case is run. The Trace and Output tabs contain detailed information on the calculation. These are intended for more advanced users.
- The toolbar contains several action buttons:
  - Start, Pause, and Stop
  - Zoom and centering
  - Object select and move
  - Add Streams, Signals and Energy buttons
  - An add Callout Table button
  - Rotate objects buttons
  - Names and Units Manager buttons

Each of these panels and toolbar action items will be used to varying degrees in the first several chapters of this manual.

✓ Click on the Mixer in the Library and drag it onto the Worksheet.

✓ Double click on the new block to change its name to Adiabatic Mixer.

You will notice that the right Properties panel displays the settings for this mixer.

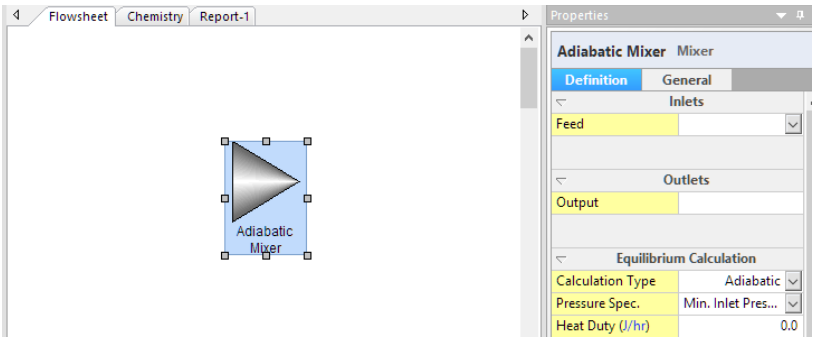


Figure 5-9 - The Mixer block and the unit settings (Definition tab)

✓ Click on the Add Stream button in the Toolbar.

Figure 5-10 - The Add Stream button in the toolbar

✓ Create an inlet stream to the mixer by clicking on the flowsheet to the left of the mixer

and dragging the mouse to the mixer. Unclick and click again when the + symbol appears on the cursor.

Notice that a separate click is needed to anchor the stream to the unit.

- ✓ Create a second inlet stream the same way.
- ✓ Lastly, create an outlet stream.
- ✓ Press the ESC key to deactivate the Add Stream button.

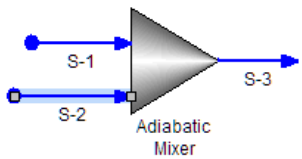
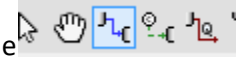


Figure 5-11- A mixer containing two inlet steams and one outlet stream

The Add stream mode stays active until the ESC key is pressed, or the arrow button is selected , or if the Add Stream button is clicked a second time 

- ✓ Double click on the first stream and label it Process Stream.
- ✓ Label the second stream Acid Waste.
- ✓ Label the outlet stream Mixed Waste.

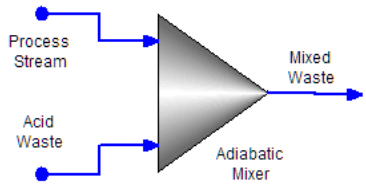


Figure 5-12- Names added to the mixer block

- ✓ Click on the Process stream and enter the composition shown in the table below.

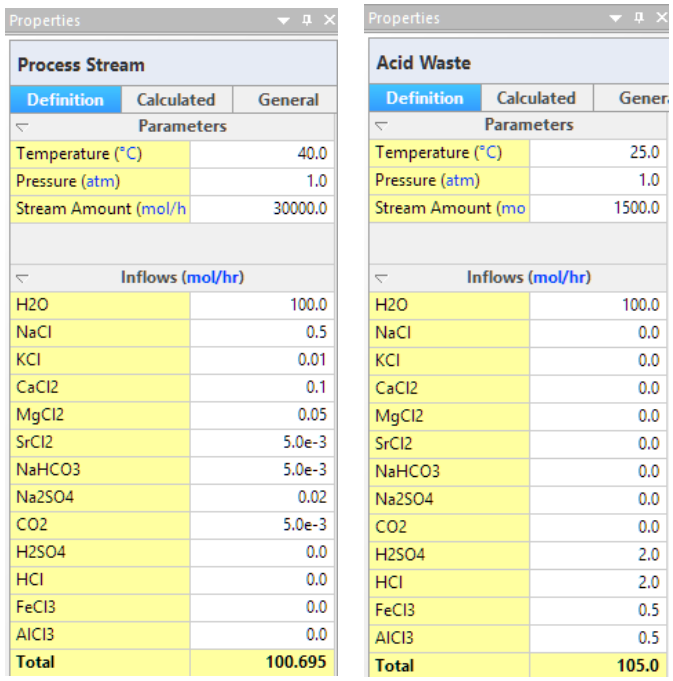
	Process Stream	Acid Waste
Temperature (C)	40	25
Pressure (atm)	1	1
Stream Amount (mole/hr)	30000	1500
H2O	100	100
NaCl	0.5	0
KCl	0.01	0
CaCl2	0.1	0
MgCl2	0.05	
SrCl2	0.005	
NaHCO3	0.005	
Na2SO4	0.02	
CO2	0.005	
H2SO4		2
HCl		2
FeCl3		0.5

AlCl3		0.5

Table 1-1 – Process Stream and Acid Waste stream compositions

✓ Click on the Acid Waste stream and enter the composition.

The Stream Amount row is its Overall flow rate, in this case with units of moles/hr. At the bottom of the grid is a second Total value. This total composition is the sum of the inflows. The Process stream is comprised of 100.695 moles. Its flow rate is 30,000 mol/hr. The composition is multiplied internally to produce the total flow of each component.



Properties

Process Stream

Definition | Calculated | General

Parameters	
Temperature (°C)	40.0
Pressure (atm)	1.0
Stream Amount (mol/h	30000.0

Inflows (mol/hr)	
H2O	100.0
NaCl	0.5
KCl	0.01
CaCl2	0.1
MgCl2	0.05
SrCl2	5.0e-3
NaHCO3	5.0e-3
Na2SO4	0.02
CO2	5.0e-3
H2SO4	0.0
HCl	0.0
FeCl3	0.0
AlCl3	0.0
Total	**100.695**

Properties

Acid Waste

Definition | Calculated | Gener

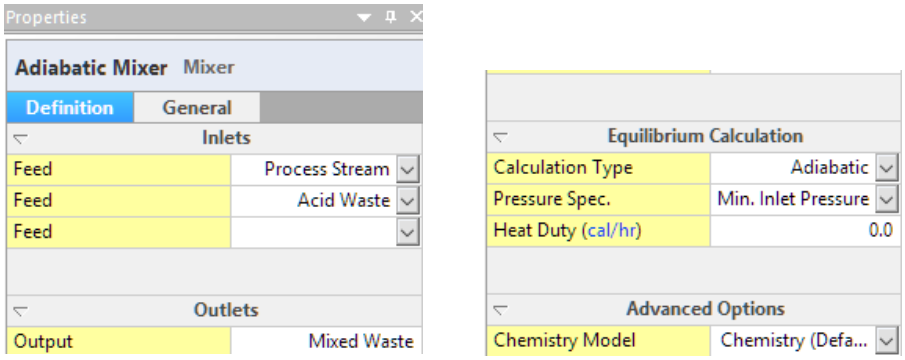
Parameters	
Temperature (°C)	25.0
Pressure (atm)	1.0
Stream Amount (mo	1500.0

Inflows (mol/hr)	
H2O	100.0
NaCl	0.0
KCl	0.0
CaCl2	0.0
MgCl2	0.0
SrCl2	0.0
NaHCO3	0.0
Na2SO4	0.0
CO2	0.0
H2SO4	2.0
HCl	2.0
FeCl3	0.5
AlCl3	0.5
Total	**105.0**

Figure 5-13 - The mixer block with the completed Process Stream and Acid Waste

✓ Click on the Adiabatic Mixer block.

The Properties panel displays the Mixer settings. There are two feed streams and one outlet stream. The default calculation type is Adiabatic (mix of inflows) and the default pressure setting is the lowest value pressure of any inlet stream. In this case the inlet stream pressures are both 1atm, and so this will be the outlet pressure. There is an option that allows the user to change the Chemistry Model. This is an advanced setting described later in the manual.



Properties

Adiabatic Mixer Mixer

Definition | General

Inlets	
Feed	Process Stream
Feed	Acid Waste
Feed	

Outlets	
Output	Mixed Waste

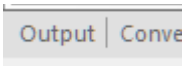
Equilibrium Calculation	
Calculation Type	Adiabatic
Pressure Spec.	Min. Inlet Pressure
Heat Duty (cal/hr)	0.0

Advanced Options	
Chemistry Model	Chemistry (Defa...

Figure 5-14 - The Mixer block with the completed Acid Waste stream

✓ Press the Calculate button.

The software will generate the chemistry model, initialize the process, calculate the properties of the two each inlet streams, and lastly, calculate the mixer block. This progress is displayed in the Output tab at the bottom of the screen.

✓ Click on the Output tab at the bottom of the screen. 

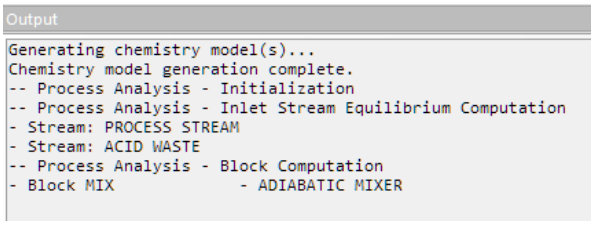


Figure 5-15 - The Output tab displaying the simulation progress

When the simulation is complete, a popup window will appear in the lower right of the screen.

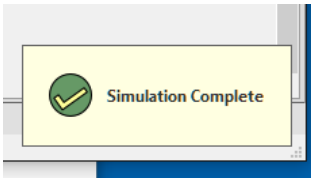


Figure 5-16 - The Simulation Complete popup

✓ Click on the Mixed Waste stream.

The resulting composition and properties of this outlet stream are displayed in the Properties panel.

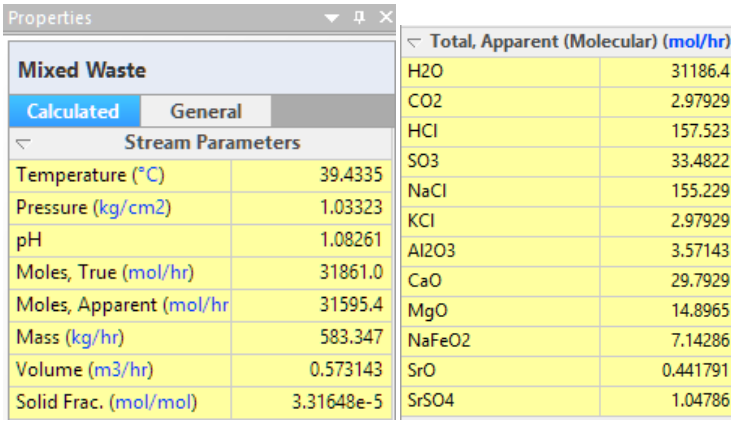


Figure 5-17 - The Properties panel containing the calculated Mixed waste stream

The contents of the Calculated tab of the Properties panel include the tables, Stream Parameters (pH, volume, mass, etc.) and apparent molecular flow. Its purpose is to provide a brief summary of the stream. The detailed information on each stream is provided in the Report section.

✓ Click on the Process Stream and select the Calculated Tab in the Properties Panel. Do the same for the Acid Waste stream.

Properties

Process Stream

Definition	Calculated	Gen

Stream Parameters	
Temperature (°C)	40.0
Pressure (atm)	1.0
pH	5.90622
Moles, True (mol/hr)	30254.9
Moles, Apparent (m	30052.8
Mass (g/hr)	5.51656e5
Volume (L/hr)	545.165
Solid Frac. (mole %)	2.90607e-3
Vapor Frac. (mole %)	0.0

Total, Apparent (Molecular) (mol/	
H2O	29754.2
CO2	2.97929
HCl	78.9513
SO3	5.08523
NaCl	162.372
KCl	2.97929
CaO	29.7929
MgO	14.8965
SrO	0.616293
SrSO4	0.873354

Properties

Acid Waste

Definition	Calculated	Genera

Stream Parameters	
Temperature (°C)	25.0
Pressure (atm)	1.0
pH	-0.585679
Moles, True (mol/hr)	1603.06
Moles, Apparent (m	1532.14
Mass (g/hr)	31691.2
Volume (L/hr)	28.32
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	0.0

Total, Apparent (Molecular) (mol/hr)	
H2O	1435.71
HCl	71.4286
SO3	17.8571
Al2O3	3.57143
Fe2(SO4)3	3.57143

Figure 5-18 - The Properties panel containing the calculated Inlet streams

The inlet streams have respective pH's of 5.9 (at 40C) and -0.6 (at 25C). The mixed-stream pH is 1.1 (at 39.4C).

- ✓ Click on the Adiabatic Mixer object and then click on the Watch tab located at base of the Properties panel

Watch

Adiabatic Mixer Mixer

Common Parameters	
Heat Duty (cal/hr)	0.0
Total Inlet Mass (g/hr)	5.83347e5
Total Outlet Mass (g/hr)	5.83347e5
Total Inlet Energy (cal/hr	-2.1614e9
Total Outlet Energy (cal/	-2.1614e9

Custom Edit

Figure 5-19 - The watch view of the Adiabatic Mixer Properties panel.

- ✓ Save the file. If you have not saved the case file yet, then name it something that you can find quickly because it will be used in the next several chapters.

The panel displays the energy and mass balance across the mixer. Since mixing is isolated and adiabatic, no energy or mass is gained or lost. Therefore, the inlet-outlet values should be identical. Users can view additional properties by clicking on the Edit link in the Custom section at the bottom of the panel.

Summary

We have completed the first case. it presents the basic mechanics of building and converging a steady-state simulation. In the next chapter, you will expand this case to include additional blocks and chemistry.

Chapter 6 Water Treatment – Lime Softeners

The Application

This chapter expands the mixing process presented in Chapter 1. The Mixed Waste is sent to a softener to remove Ca, Mg, Fe, and Al. The remaining liquid is neutralized.

Formulating the Process

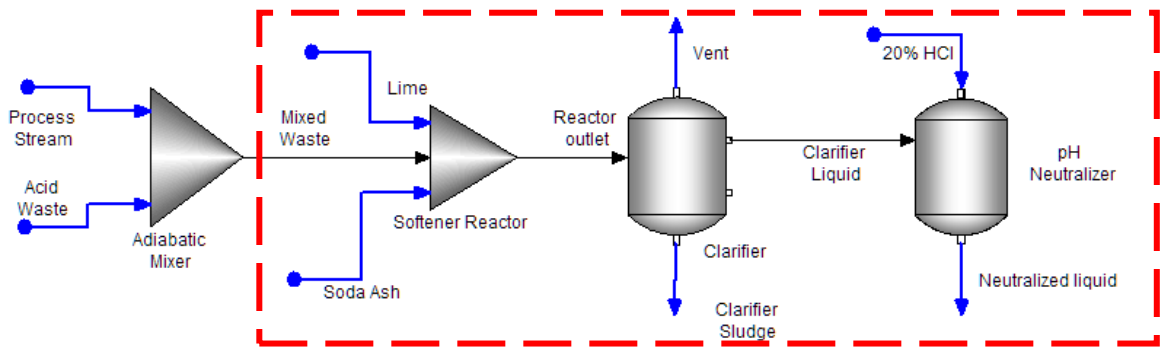


Figure 6-1- Softening and Neutralization Process

The Mixed Waste stream contains a water, solid, and gas phase. It flows into a reaction tank with lime and soda ash that are used to raise pH and to increase the carbonate concentration. The higher pH and carbonate results in $CaCO_3$, $Mg(OH)_2$, $Al(OH)_3$, and $Fe(OH)_3$ precipitation. These solids are removed in the clarifier unit. The remaining liquid is neutralized for and sent to a downstream process.

The required procedure is to expand the chemistry model to include the lime and soda ash additives. Then the additional units and streams are added.

Chemistry Model

Open the existing Case file

The work on this case started in Chapter 1. You were instructed to save the file. Open it now.

- ✓ Open the file, Water Treatment Softening Process

Adding additional components to the model

The first step is to add lime (CaO) and soda ash (Na2CO3) to the chemistry model.

- ✓ Click on the Chemistry tab.
- ✓ Enter CaO and Na2CO3 to the list.

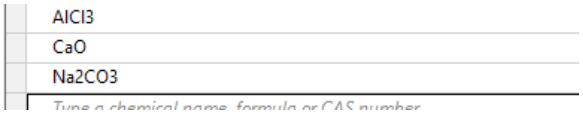


Figure 6-2 – Adding CaO and Na2CO3 to the Chemistry Inflows List

- ✓ Return to the flowsheet view.

Building the Process

The following instructions are designed to take us on a tour through some of the interesting features of the ESP Process Analysis facilities.

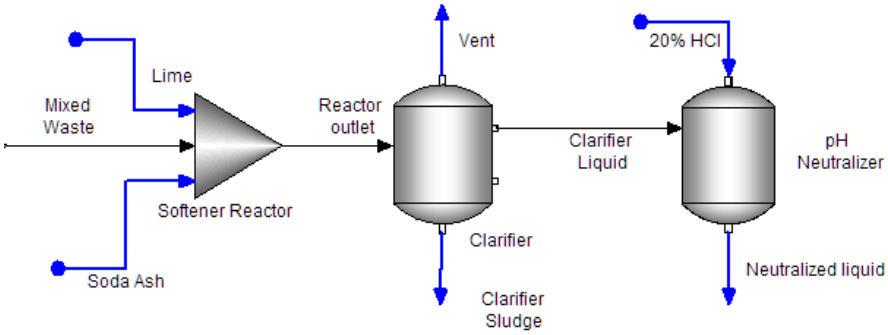


Figure 6-3 - The Water Softening process created in this chapter

Adding new process blocks

Start by adding the new unit operations:

- ✓ Click on the Mixer object in the library, and drag it to the right of the Adiabatic mixer.
- ✓ Label it Softener Reactor.
- ✓ Next, click on the Separator object in the library and drag it to the right of the Softener reactor.
- ✓ Label it Clarifier.
- ✓ Next, click on the Neutralizer object and drag it to the right of the Settler.
- ✓ Label it pH Neutralizer.

Adding new streams

Next, add link existing stream and add new ones.

- ✓ Link the Mixed Waste stream to the inlet side of the Softener Reactor block.
- ✓ Click on the Add Stream button in the menu and add two streams to the Softener Reactor (mixer) inlet.

- ✓ Add a stream to the Softener reactor outlet and link it to the Clarifier (separator) inlet.
- ✓ Add three streams to the Clarifier outlet; vapor, solid and liquid. Link the liquid stream to the pH neutralizer (Neutralizer) inlet.
- ✓ Add a streams to the neutralizer inlet top and one to the bottom.
- ✓ Press the ESC key or click the Add stream button a second time to deactivate the action.

Labeling and Editing the new streams

- ✓ Label the eight streams as follows. Use the above screenshot for identification

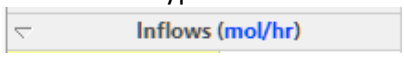
Lime	Soda Ash	Reactor Outlet	Clarifier Liquid
Vent	Clarifier Sludge	20% HCl	Neutralized Liquid

Entering the Lime stream data

- ✓ Click on the Lime stream.
- ✓ Enter a Stream Amount of 80 mol/hr.

The lime stream composition is based on mass fraction, and so the Inflow units need to be changed from mol/hr to mass fraction. This is done through the Units Manager window.

- ✓ Click on the hyperlinked units at the header of the Inflows category.



.

- ✓ Change the Inflows units from Moles to Mass Fraction. Press OK.

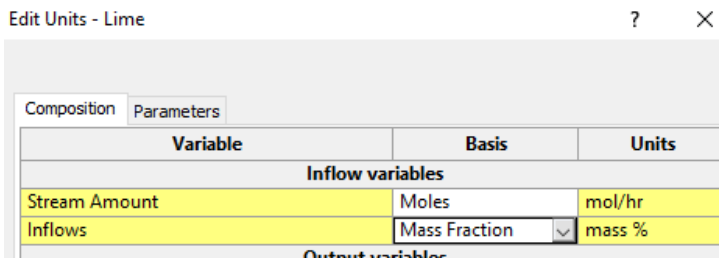


Figure 6-4 Changing the units of the Lime stream

- ✓ Enter a CaO value of 100 mass %.

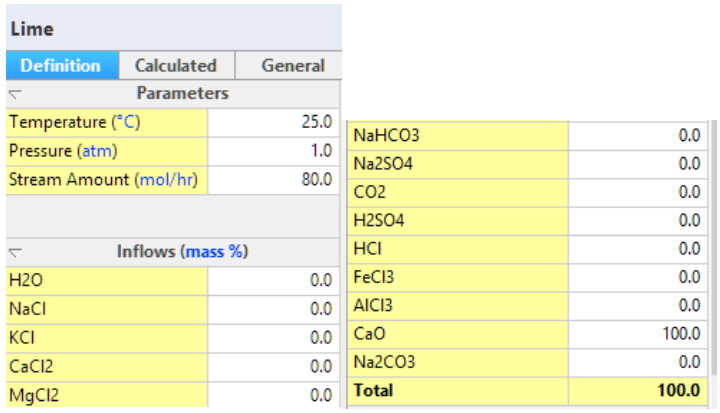
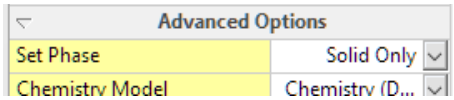


Figure 6-5 The Lime Stream Composition. Note the inflow units are changed to Mass%

- ✓ Change the Set Phase setting to Solid Only. This is in the Advanced Options section at

the bottom of the Lime stream Properties panel.



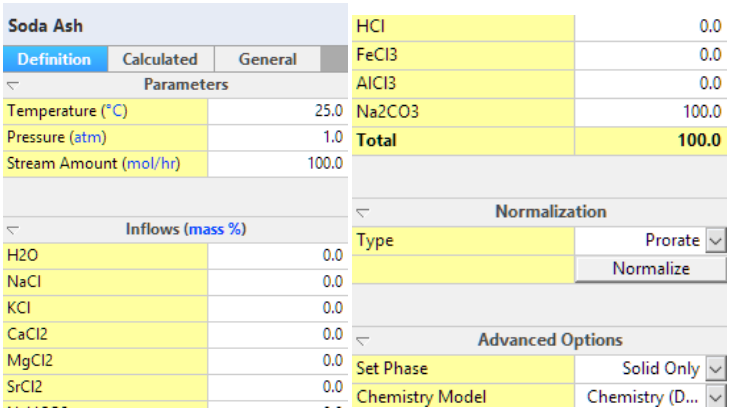
Advanced Options	
Set Phase	Solid Only
Chemistry Model	Chemistry (D...

Figure 6-6 Entering the Lime Inflow rate

By changing the Set Phase to Solid only, the software will compute the stream's total enthalpy and heat capacity, but will not attempt to compute any phase properties. This change ensures that the calculation proceed without any problems.

Soda Ash inflow stream

- ✓ Click on the Soda Ash stream.
- ✓ Enter a Stream Amount of 100 mol/hr.
- ✓ Change the inflow units to Mass Fraction (mass %).
- ✓ Enter a Na2CO3 value of 100 mass %.
- ✓ Change the Set Phase setting to Solid Only.



Soda Ash	
Definition / Calculated / General	
Parameters	
Temperature (°C)	25.0
Pressure (atm)	1.0
Stream Amount (mol/hr)	100.0
Inflows (mass %)	
H2O	0.0
NaCl	0.0
KCl	0.0
CaCl2	0.0
MgCl2	0.0
SrCl2	0.0
HCl	0.0
FeCl3	0.0
AlCl3	0.0
Na2CO3	100.0
Total	**100.0**
Normalization	
Type	Prorate
	Normalize
Advanced Options	
Set Phase	Solid Only
Chemistry Model	Chemistry (D...

Figure 6-7 Entering the Soda Ash composition and inflow rate

The soda ash stream has similar setting to the lime stream. In many instances, lime and soda ash are slaked with process water before entering the reactor. We will look into that scenario in a later chapter.

20% HCl Inflow stream

- ✓ Click on the 20% HCl stream entering the pH Neutralizer.
- ✓ Enter a Stream Amount of 50 mol/hr.
- ✓ Change the Inflow units from moles to mass fraction (mass %).
- ✓ Enter 80% H2O and 20% HCl.

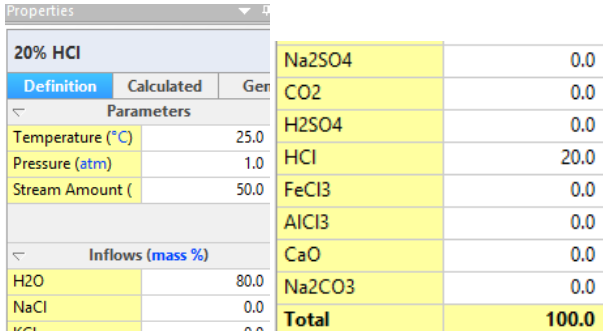


Figure 6-8 Entering the 20% HCl composition and inflow rate

Reviewing the Clarifier settings

✓ Click on the Clarifier block to access its Properties panel.

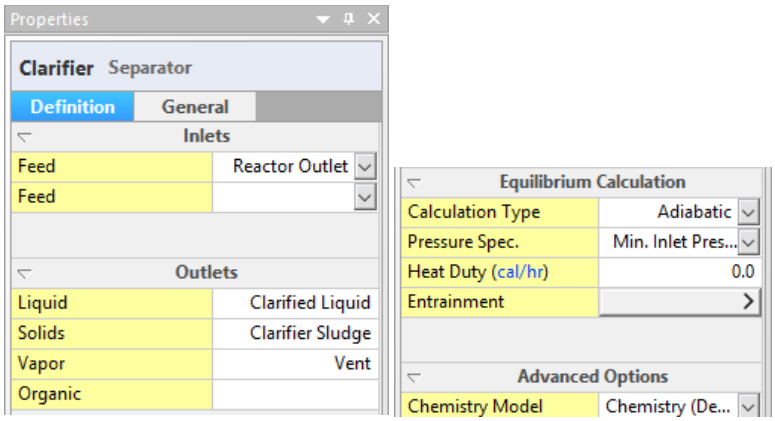


Figure 6-9 The Clarifier Properties panel. It contains four sections, Inlets, Outlets, Equilibrium calculations and Advanced options

The Properties panel contains four sections. The Inlets and Outlets section display the streams attached to the block. The Equilibrium Calculation section contain the calculation settings. The Advanced Options section contains the Chemistry model selection (to be explained in later chapters).

There are three outlet streams, and each outlet will contain a single phase. This means that the vapor will not contain mist or dust, the liquid will not contain gas bubbles or suspended solids, and the solids will not be wet. Also, the Clarifier is set to run adiabatically.

There are no properties/settings to adjust in this block.

Changing the pH Neutralizer Block settings

✓ Click on the pH Neutralizer block to access its Properties panel.

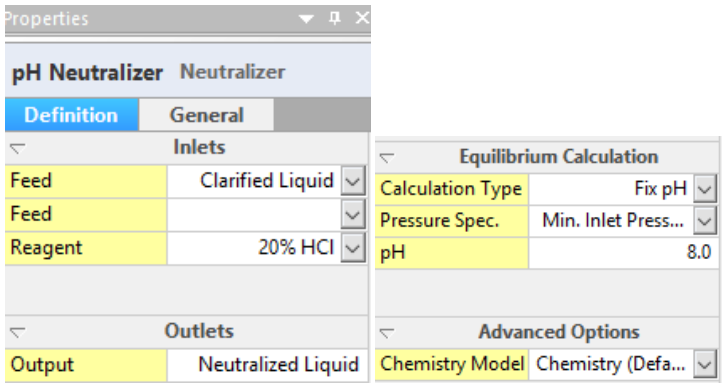


Figure 6-10 The pH Neutralizer Properties panel. It contains the same four sections as the Clarifier

The purpose of this block is to add sufficient quantities of the 20% HCl stream to set the Neutralized liquid output stream pH=8. The 50 moles of you entered when creating the 20% HCl stream, is therefore an initial guess. This Neutralizer block will adjust this value until the target pH of 8 is achieved. This block, therefore, acts as a mixer, a pH controller and as an HCl valve.

- ✓ Click on the Calculation Type option in the Equilibrium Calculation section and change to Fix pH.
- ✓ Enter a pH of 8.0.

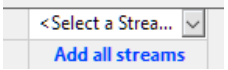
Calculate and Review

The flowsheet is ready for calculation. This is also a good time to save the file.

- ✓ Save your file.
- ✓ Press the Calculate button

The calculation should complete within seconds. If you receive an Error warning, please look at the Error tab located at the bottom of the window. It will tell you what step you may have missed.

There are now eleven streams in the process. With that number it is easier to review the results using the Report or by using the Callout tables. You will start by reviewing the reports.

- ✓ Click on the Report-1 tab. This is the default report.
- ✓ Click on the Add all streams action link - 

The table that appears contains the properties and composition of each stream.

	Process Stream	Acid Waste	Lime	Soda Ash	Mixed Waste	Clarifier Liquid	Vent	Clarifier Sludge	Settler Liquid	Settler solids	Filtrate	Reactor outlet	Filter Cake	Neutralized liquid	20% HCl
	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove
Stream Parameters															
Temperature (°C)	40.0	25.0	25.0	25.0	39.4423	46.0059	46.0059	46.0059	46.0059	46.0059	46.0059	46.0059	46.0059	46.0155	25.0

Unnecessary or redundant streams, namely the lime, soda ash, 20% HCl and vent are removed in a manner similar to adding streams.

- ✓ Review the 20% HCl inflow stream, look at the Apparent moles and the volume.

	20% HCl
	Remove
Stream Parameters	
Temperature (°C)	25.0
Pressure (atm)	1.0
pH	-1.43284
Moles, True (mol/hr)	5.65347
Moles, Apparent (mol/hr)	5.0935
Mass (g/hr)	102.091
Volume (L/hr)	0.093198

Figure 6-11 The 20% HCl inlet stream

Review the Moles, Apparent row; 196.4 moles of acid were added, and not the 50 moles that you entered earlier. Notice that there are two Moles values: Moles, True and Moles, Apparent. The Moles, True sums the cations (H+) and anions (Cl-, OH-) separately. By comparison the Moles Apparent is simply the molecular HCl and H2O. Thus the True moles is always equal or greater than the apparent moles (it can be equal if there is no ionization – for example when dissolving carbon monoxide in water).

	Process Stream	Acid Waste	Mixed Waste	Clarifier Liquid	Clarifier Sludge	Reactor outlet	Neutralized liquid
	Remove	Remove	Remove	Remove	Remove	Remove	Remove
Stream Parameters							
Temperature (°C)	40.0	25.0	39.4423	46.0059	46.0059	46.0059	46.0155
Pressure (atm)	1.0	1.0	1.0	1.0	1.0	1.0	1.0
pH	5.83608	-0.585679	1.05727	9.29576	9.29576	9.29576	8.0
Moles, True (mol/hr)	30401.9	1603.06	32008.1	25931.5	6293.18	32224.7	32001.3
Moles, Apparent (mol/hr)	30052.6	1532.14	31595.2	25523.2	6196.16	31719.4	31497.6
Mass (g/hr)	5.57593e5	31691.2	5.89284e5	4.7814e5	1.26229e5	6.04369e5	5.9017e5
Volume (L/hr)	545.46	28.32	573.521	465.219	115.176	580.395	574.131
Solid Frac. (mole %)	2.39998e-3	0.0	3.13618e-3	0.0	2.12778	0.415648	3.5844e-3

Figure 6-12 The Stream Parameters section of the Report

You will now reduce the size of the report to make it easier to review.

- ✓ Click the Remove link Remove on the 20% HCl, Lime, Soda Ash, and Vent columns to remove them.

This reduces the table size, and leaves only the seven streams. Values to be reviewed include the sludge flow rate and the pH of each stream. Note also Clarifier Liquid and Sludge temperature. It has increased to 46C.

One purpose of the softening unit is to remove total calcium and magnesium (hardness) from the water as solids (sludge). You can review the extent of Mg and Ca removal from the process, including the amount that still remains in the Neutralized liquid. These results are in a section called MBG Totals, Combined, located towards the bottom of the report. The term, MBG is Material Balance Group, or the element with a specific oxidation state. The section, **MBG Totals, Combined** contains the *total amount of each element that is in the stream.* By comparison, the section, **MBG Totals, Solids** contains the elements that make up the solids phase of that stream.

- ✓ Remove all the streams except for the Reactor Outlet, Clarifier Sludge, and Neutralized Liquid.
- ✓ Scroll down the report to the MBG Totals, Combined section.
- ✓ Compare the Ca(+2) and Mg(+2) flow of the Mixed Waste and neutralized liquid.

The reactor outlet stream is a mixed phase, containing water, solids, the clarifier sludge is all solids, and the neutralized liquids is nearly all liquid.

	Reactor outlet	Clarifier Sludge	Neutralized liquid
	Remove	Remove	Remove
Na(+1)	509.798	97.8734	508.232
Cl(-1)	462.752	88.8413	461.891
Ca(+2)	109.646	104.224	7.82006
C(+4)	102.965	102.942	1.15942
S(+6)	34.5006	7.57368	33.2353
Mg(+2)	14.8229	13.7154	1.51423
Al(+3)	7.14286	7.13561	0.0873434
Fe(+3)	7.14286	7.14257	0.0788466
K(+1)	2.96457	0.569153	2.95547
Sr(+2)	1.48229	1.23467	0.31843

Figure 6-13 – Comparing total dissolved Hardness (Ca^{+2} + Mg^{+2}) before and after the lime softener unit

The Mg^{+2} is converted to $Mg(OH)_2$ by raising the mixed waste pH to 9.3 using CaO. Adding CaO increases the Ca^{+2} content. Thus, Na_2CO_3 is added to remove the existing and added Ca^{+2} as $CaCO_3$. The total dissolved Ca^{+2} decreases from 129.8 mol/hr to 7.8 mol/hr and the and the dissolved Mg^{+2} decreases from 14.9 mol/hr to 1.5 mol/hr. The optimum amount of CaO and Na2CO3 is investigated in the next chapter.

- ✓ Save your file.

Including entrained water in the sludge and settling it out

The sludge stream is 100% solids. It contains no entrained water. This does not exist in practice, since clarifier sludge may contain up to 90% water. The Separator unit, where the sludge and supernatant were separated, can accept instructions to entrain water in the solids, thereby creating a more representative sludge product. This will be performed now.

Setting the Separator Entrainment value

- ✓ Click on the report tab and view the sludge stream. It is currently 100% solids.

	Clarifier Sludge
	Remove
Stream Parameters	
Temperature (°C)	46.0059
Pressure (atm)	1.0
pH	
Moles, True (mol/hr)	131.841
Moles, Apparent (mol/hr)	131.841
Mass (g/hr)	12622.9
Volume (L/hr)	4.63964
Solid Frac. (mole %)	100.0

Figure 6-14 – Stream parameters of the Clarifier sludge stream

- ✓ Return to the flowsheet and select the Clarifier unit.
- ✓ Select the Entrainment arrow button - Entrainment >
- ✓ Set the Liquid in Solid (g/g) value to 9 - Liquid in Solid (g/g) 9.0

This instructs the software to set the water to Sludge ratio to 9:1, that is, to make the Clarifier Sludge stream 90% water.

- ✓ Calculate and view the Phase flows section of the Clarifier Sludge in the report.

	Clarifier Sludge
	Remove
Phase Flows	
Moles, True - Aqueous (mol/hr)	6161.34
Moles - Solid (mol/hr)	131.841
Moles - Vapor (mol/hr)	0.0
Moles, Apparent - Aqueous (mol/hr)	6064.32
Mass - Aqueous (g/hr)	1.13606e5
Mass - Solid (g/hr)	12622.9
Mass - Vapor (g/hr)	0.0
Volume - Aqueous (L/hr)	110.536
Volume - Solid (L/hr)	4.63964

Figure 6-15 – Phase flow results for the Clarifier Sludge stream

There is now 114 kg/hr process water entrained with the sludge. This is about 20% of the total liquids, and it needs to be separated from the solids and returned to the process. In water treatment operations, a significant fraction of the liquid can be separated using coagulating and settling. The software contains a settler block that can mimic this step. Please note, that this block does not compute the physical-chemical process of coagulation, settling, and separation. Rather it separates based on user-entered separation values, and these values are presumed to be obtained from plant performance data.

Adding a Settler block

The purpose of a settler block is to separate a process stream into a liquid and solid streams with a fixed fraction of liquids remaining with the solids a fixed fraction of solids flowing with the liquid as suspended solids. In this scenario, you will split 100% of the solids to the "Solids" stream and split 80% of the liquids to the "Liquid" stream. Thus, 80% of the liquids entering the settler will decant.

- ✓ Click on the Settler block in the Library and drag it below and to the right of the Clarifier unit.
- ✓ Label the block "Sludge Settler".
- ✓ Link the Clarifier Sludge stream to the inlet.
- ✓ Click on the New Stream button in the Toolbar - and add two outlet streams to the sludge settler.
- ✓ Label the liquid stream "Settler Liquid".
- ✓ Label the solid stream "Settler Solids".
- ✓ Link the Settler Liquid stream to the inlet of the pH Neutralizer.

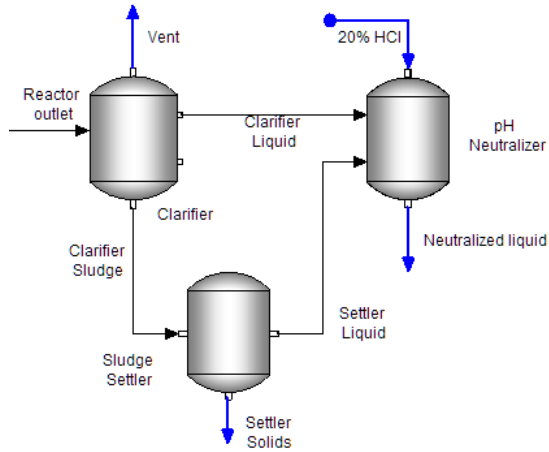
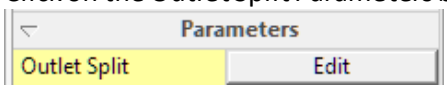
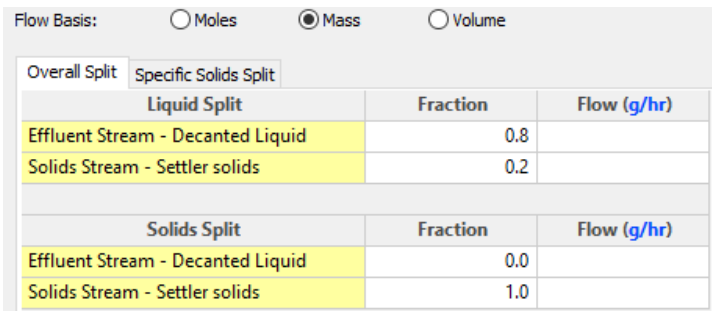


Figure 6-16 – Clarifier sludge is processed in a Sludge Settler

- ✓ Click on the Sludge Settler object.
- ✓ Click on the Outlet Split Parameters button in the Properties panel.



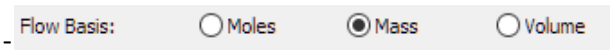
The window that appears contains two splits, Liquid phase and Solid phase. Each phase can split to two outlets.



Liquid Split	Fraction	Flow (g/hr)
Effluent Stream - Decanted Liquid	0.8	
Solids Stream - Settler solids	0.2	

Solids Split	Fraction	Flow (g/hr)
Effluent Stream - Decanted Liquid	0.0	
Solids Stream - Settler solids	1.0	

Figure 6-17 – Sludge Settler Parameters

The split flows can be set to volume, mass, or moles - 

. In this case, 100% of the solids go with the Solids stream outlet (Settler Solids), and 80% of the liquid goes with the Effluent stream outlet (Decanted Liquid).

- ✓ Set the Flow Basis: to Mass.
- ✓ Set the fractions in the settler to match the values shown in the image above.
- ✓ Recalculate.
- ✓ Click on the Report. Change the stream selection to display the Reactor Outlet, Settler Solids, Neutralized Liquid, vent, and 20% HCl.

These streams represent the mass balance around the clarifier, settler, and neutralized liquid.

- ✓ Review the Phase Flow section and then MBG Totals, Combined section.

There is 563 kg/hr liquid exiting the neutralization tank and 24 kg/hr liquid exiting with the Settler solids. The settler solids stream is now about 60% liquid.

	Reactor outlet	Settler solids	Neutralized liquid	20% HCl
	Remove	Remove	Remove	Remove
Phase Flows				
Moles, True - Aqueous (mol/hr)	32092.9	1232.27	32000.2	5.65347
Moles - Solid (mol/hr)	131.841	130.522	1.129	0.0
Moles - Vapor (mol/hr)	0.0	0.0	0.0	0.0
Moles, Apparent - Aqueous (mol/hr)	31587.5	1212.86	31496.5	5.0935
Mass - Aqueous (g/hr)	5.91746e5	22721.2	5.90057e5	102.091
Mass - Solid (g/hr)	12622.9	12496.7	112.661	0.0
Mass - Vapor (g/hr)	0.0	0.0	0.0	0.0
Volume - Aqueous (L/hr)	575.755	22.1072	574.09	0.093198
Volume - Solid (L/hr)	4.63964	4.59324	0.0409456	0.0

Figure 6-18 – Flow balance around the clarifier, settler, and neutralizer.

Adding a filter press to recover remaining liquid

The last part of this scenario is to recover the remaining water. It is performed using a filter press. The Filter object in Flowsheet ESP is very similar to the Settler. It differs in that it does not contain the individual solid phase split option that is part of the settler.

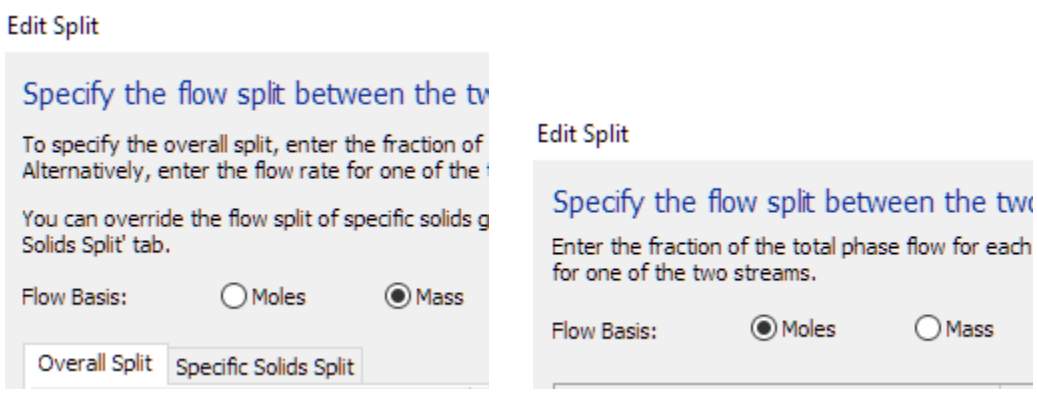


Figure 6-19 – The left image is the Settler parameter window, and the right is the Filter parameter window. There is no Specific Solids Split in the Filter.

- ✓ Click on the Filter object in the Library and drag it below and to the right of the Settler block.
- ✓ Label the object Filter Press.
- ✓ Drag the Settler Solids stream to the filter Press inlet.
- ✓ Click on the Add Stream button and add a stream to the Filter press liquid and solid exits.
- ✓ Label the liquid stream Filtrate. Label the solids stream Filter Cake.

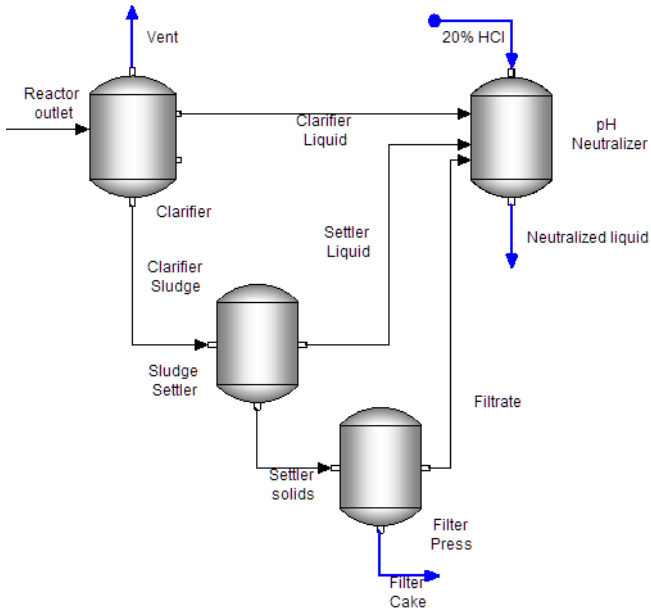


Figure 6-20 – Filter press is added to the solid-liquid separation section

- ✓ Click on the Filter Press object and click on the Outlet Split Edit button.

Parameters	
Outlet Split	Edit

- ✓ Change the Flow Basis: to Mass.
- ✓ Set the Liquid split settings to 0.92 (filtrate stream) and 0.08 (Solids stream).
- ✓ Set the Solids Split to 0 and 1.

Flow Basis: ○ Moles ◉ Mass ○ Volume

Liquid Split	Fraction	Flow (g/hr)
Filtrate Stream - Filtrate	0.92	
Solids Stream - Filter Cake	0.08	
Solids Split	**Fraction**	**Flow (g/hr)**
Filtrate Stream - Filtrate	0.0	
Solids Stream - Filter Cake	1.0	

Figure 6-21 – The Parameters screen for the Filter block.

As with the Settler, the final water content in the filter cake is computed from these settings. If the filter cake water content is known, then a separator can be used instead of the filter.

- ✓ Calculate and view the Results tab.
- ✓ Change the columns to display the Reactor Outlet, Filter Cake, and Neutralized liquid.

	Reactor outlet	Filter Cake	Neutralized liquid
	Remove	Remove	Remove
Phase Flows			
Moles, True - Aqueous (mol/hr)	32092.9	98.5815	32000.2
Moles - Solid (mol/hr)	131.841	130.392	1.129
Moles - Vapor (mol/hr)	0.0	0.0	0.0
Moles, Apparent - Aqueous (mol/hr)	31587.5	97.0292	31496.5
Mass - Aqueous (g/hr)	5.91746e5	1817.7	5.90057e5
Mass - Solid (g/hr)	12622.9	12484.2	112.661
Mass - Vapor (g/hr)	0.0	0.0	0.0
Volume - Aqueous (L/hr)	575.755	1.76858	574.09
Volume - Solid (L/hr)	4.63964	4.58865	0.0409456

Figure 6-22 – Stream results following the addition of a filter press. Nearly all the water is returned to the process

The filter cake flows at 12.5 kg/hr solid and 1.8 kg/hr liquid; ~13% liquid in the filter cake. Now, a small fraction of the liquid is lost to disposal.

✓ Save the file. It will be used in the next chapter.

Summary

This chapter expanded on the water treatment process with the addition of a softening/clarifier unit, a pH neutralizer, and filtration. The lime and soda ash inlet rates were set manually, by reviewing the results and adjusting the Stream Amount cell. This action can be performed automatically by using controllers and manipulating (valve) units. You will add these units in the next chapter.

Chapter 7 Water Treatment Lime and Soda Ash Controllers

The Application

This chapter introduces the controller objects that enable users to meet target specifications without requiring the user to manually adjust a concentration, flowrate, or condition. There are three target specifications in the existing process, pH of the Clarifier Liquid, dissolved calcium in the Clarifier Liquid, and water content in the Filter Cake.

Formulating the Process

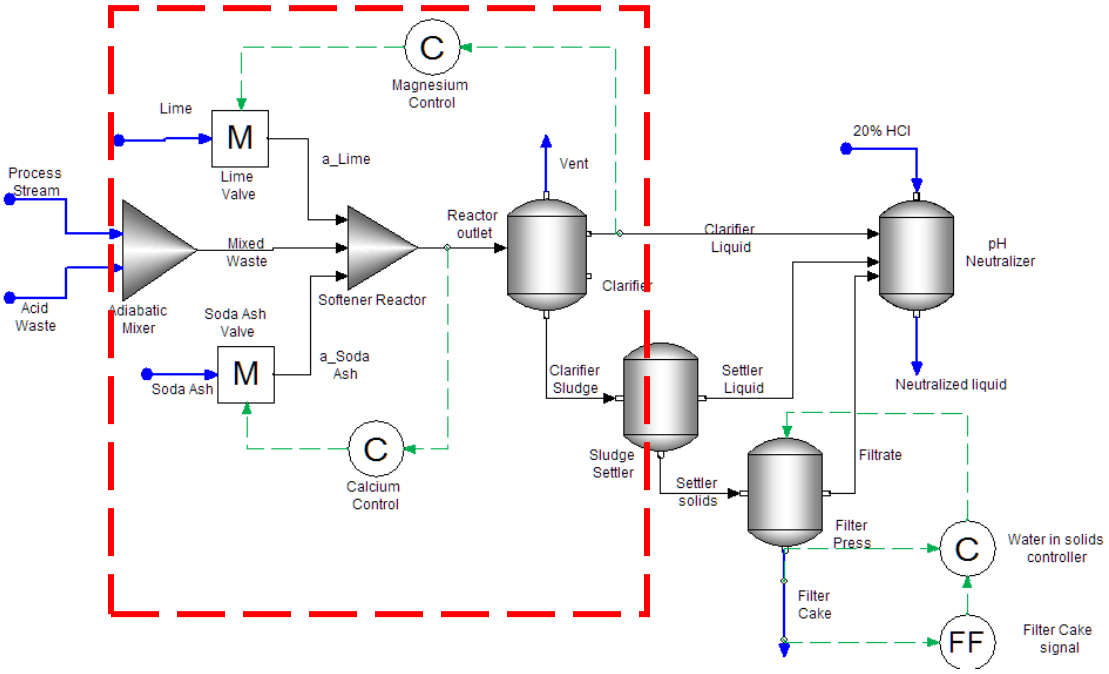


Figure 7-1- Softening and Neutralization Process

You are continuing with the process created in Chapter 1 and 2. At this point in the training, you will have completed the front end of the softening process. If you have not completed this section, then return to Chapters 1 and 2.

Total hardness, Ca^{+2} & Mg^{+2}, is removed from the water by adding soda ash and lime. This was discussed in Chapter 2. The exact amount of soda ash and lime added was not determined in that chapter. Rather, a specific value was entered that seemed to produce a good result. In this chapter you will set a target concentration for total dissolved Ca^{+2} and Mg^{+2}, and instruct the software to adjust the soda ash and lime automatically to achieve these target values. You will do this using two new objects, a Feedback Controller and a Manipulator.

The water fractions in the filter press and the settler were also set using values that were not based on any specific condition. Solids removal efficiency and dewatering varies depending on the process environment and the type of solids formed. Therefore, the simulation would be more useful if process specifications were entered that represented plant operations. This will also be done in this chapter using two blocks; Feed Forward Controller and Feedback Controller.

Chemistry Model

Opening an existing Case file

You create a case file in Chapter 1 and used it again in Chapter 2. This is the starting point for Chapter 3. Open this file now.

- ✓ Open your case file, Water Treatment Softening Process.

There are no chemistry change in this step.

Building the Process

Adjusting the Front-end of the Process

You will start by optimizing the lime and soda ash addition. To do this, a valve and controller need to be added to both inflow streams. A valve is defined in the software by the Manipulate block. The manipulate block receives information from the control block and adjusts the inflow rate accordingly.

Adding the Manipulate block

- ✓ Click on the Manipulate object in the Library and drag it adjacent to the Lime stream.

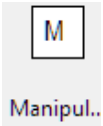


Figure 7-2 - The manipulate object

- ✓ Label it Lime Valve.
- ✓ Click on the Manipulate object a second time and drag it adjacent to the soda ash stream.
- ✓ Label it Soda Ash Valve.
- ✓ Disconnect the Lime stream from the Softener Reactor block and attach it to the Lime Valve.
- ✓ Disconnect the Soda Ash stream and attach it to the Soda Ash Valve.

At this point, you may want to reorganize the stream and blocks so that it is easier to recognize the various objects.

- ✓ Click on the Add Stream button in the Toolbar.
- ✓ Add a stream between the Lime valve and the Softener Reactor.
- ✓ Add a stream between the Soda Ash valve and the Softener Reactor.
- ✓ Label the first a_Lime (adjusted lime). Label the other a_Soda Ash.
- ✓ Click on the Lime valve – view the Factor, Flow.
- ✓ Click on the Soda Ash valve and view the Factor Flow.

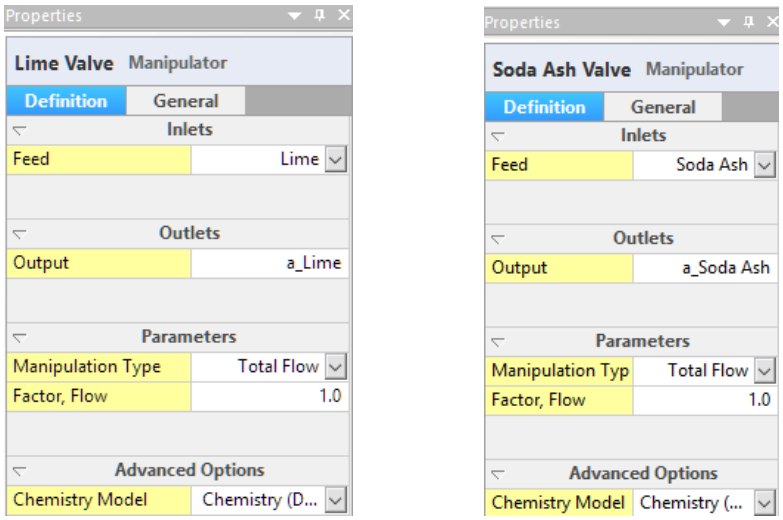


Figure 7-3 - The Properties panel for the Manipulate object

The factor flows for each valve is set to 1 by default. Thus 100% of the inflow stream is sent to the Softener Reactor.

- ✓ Calculate.

The results are identical to the previous run. This is because the Factor, Flow values of 1 in the Manipulate blocks have not changed the inflow rates of either lime or soda ash. When the controller is added then this factor flow value will change to meet the dissolved calcium and magnesium specifications.

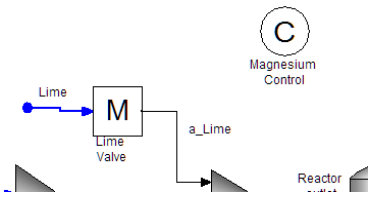
Adding the Magnesium Controller

This Magnesium Controller block will measure the dissolved magnesium concentration, compare it to the target magnesium concentration, and adjust the lime flow rate (via the factor flow value) until this value is achieved. The controller will require several iterations to find the optimum factor flow value.

- ✓ Click on the Feedback Controller object in the Library and drag it above and to the right of the Lime Valve.

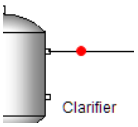
Figure 7-4 - The Feedback Controller object in the library

✓ Label it Magnesium Control.



✓ Click on the Signal button in the toolbar.

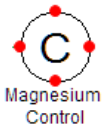
Figure 7-5 – The Signal button in the toolbar. It links controllers to streams and objects



✓ Mouse over the Clarifier Liquid stream. Red dots appear on the stream.

✓ Click on one of the red dots to link the signal line to the stream.

✓ Mouse over the right edge of the Magnesium controller until a red dot appears.



✓ Click on one of them to link the other side of the signal stream.

✓ Next, link the Magnesium controller to the Lime Valve using a second signal stream.

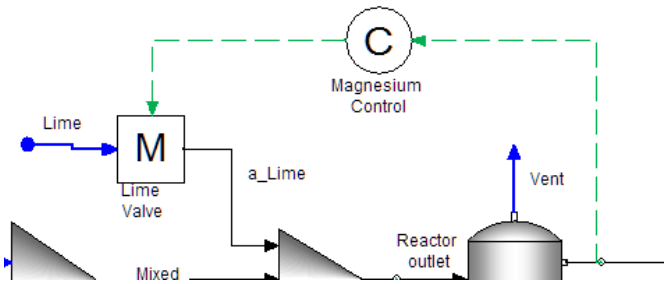


Figure 7-5 - The Feedback Controller is linked to the process stream and to the manipulate block

Adding the Calcium Controller

You will repeat the steps taken for the Magnesium controller with the Calcium controller. The calcium controller compares the dissolved calcium concentration to the target specification and adjusts the soda ash valve Factor flow.

✓ Select the Feedback Controller again and drag it below and to the right of the Soda Ash valve.

✓ Label it Calcium Control.

✓ Click on the Signal button in the toolbar.

✓ Link the signal from the Reactor Outlet stream to the Calcium Control block.

✓ Add another signal from the Calcium control to the Soda Ash Valve.

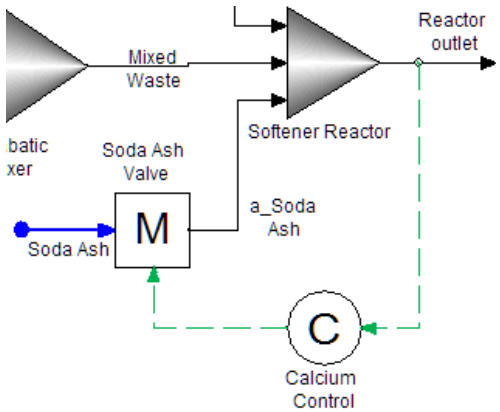


Figure 7-6 - The Calcium Feedback Controller linked to the soda ash valve

Assigning Settings to the Magnesium Feedback Controllers

✓ Click on the Magnesium Controller to access the Properties panel.

The main panel contains three sections: Target Specifications, Control Parameters and Options. A fourth section, Convergence Option, is hidden because it contains optional settings.

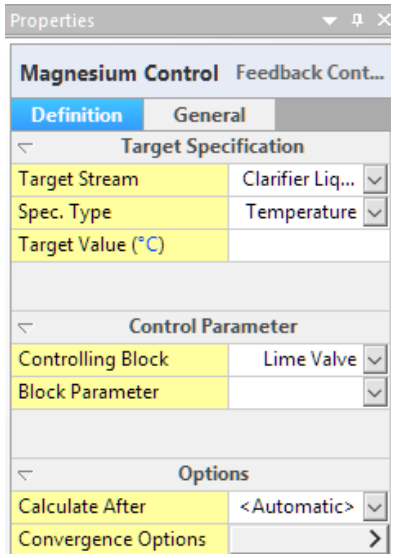


Figure 7-7 - The Magnesium Feedback Controller Panel

The target specification section instructs the controller to measure the value of a user-specified variable. This variable can be temperature, pressure, phase flow rates, concentrations or component flow rates. The Control Parameter section instructs the controller to adjust a variable continuously until the measured value meets the target value.

✓ Change the Spec. Type from the default Temperature to Mat'l balance Group composition.

Spec. Type	Mat'l Balanc...

✓ Click on the Edit button on the Mat'l Balance Group row.

Mat'l Balance Groups	Edit

✓ Check the box for Mg(+2) and press OK close the window.

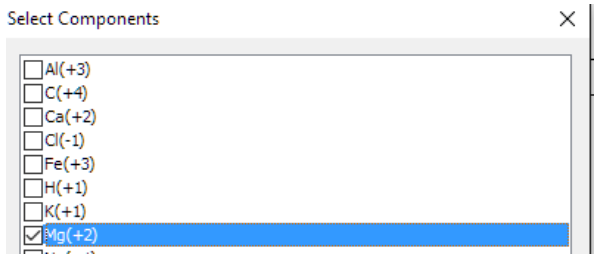


Figure 7-8 - Selecting the Mg+2 material balance group in the controller

Figure 7-9 –Click on the Phase cell and select Aqueous Only. Phase | Aqueous Only

- ✓ Click on the Basis cell and select Concentration. Basis | Concentrati...
- ✓ Enter a Target value of 5 mg/l. Target Value (mg/L) | 5.0
- ✓ Click on the Block Parameter in the Control Parameter section – Change to Factor, Flow. Block Parameter | Factor, Flow

The panel should look like this when done.

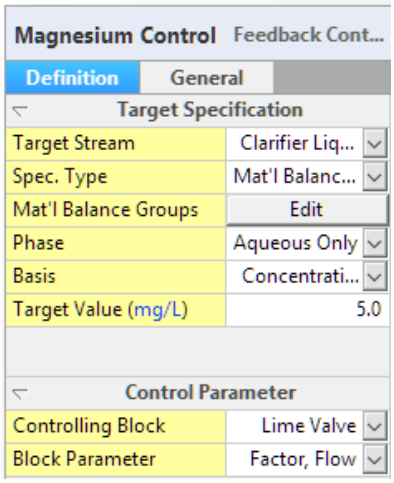


Figure 7-9 - The completed Magnesium Feedback Controller Panel

Assigning Settings to the Calcium Feedback Controller

- ✓ Select the Calcium Control object to access the Properties panel.
- ✓ Change the Spec Type in the Properties panel to Mat'l Balance Group. Spec. Type | Mat'l Balanc...
- ✓ Open the Edit button on the Mat'l Balance Groups row and select Ca(+2).

- ✓ Change the Phase to Aqueous. Phase | Aqueous Only
- ✓ Change the Basis to Concentration. Basis | Concentrati...

- ✓ Change the Target Value to 10 mg/l.

Target Value (mg/L)	10.0

- ✓ Click on the Block Parameter row and select Factor, Flow.

Block Parameter	Factor, Flow

Your Calcium Control Parameters panel should look like this:

Calcium Control	Feedback Controller
Definition	General
Target Specification	
Target Stream	Reactor outlet
Spec. Type	Mat'l Balanc...
Mat'l Balance Groups	Edit
Phase	Aqueous Only
Basis	Concentrati...
Target Value (mg/L)	10.0
Control Parameter	
Controlling Block	Soda Ash Va...
Block Parameter	Factor, Flow

Figure 7-10 - The completed Calcium Feedback Controller Panel

Reviewing the Controller results

- ✓ Calculate the case.
- ✓ When completed, click on the Lime valve and select the Watch tab at the base of the panel.
- ✓ Look at the Factor, Flow value.

The software multiplied the Lime Stream flow rate by 1.015. The Lime flow is 80 mol/hr. Therefore, the actual flow is 81.27 mol/hr. This can be confirmed by reviewing the a_Lime flow rate.

- ✓ Click on the a_Lime stream and review the Moles, True row in the Properties Panel.

Moles, True (mol/hr)	81.2714

Next, you will confirm that the magnesium concentration is 5 mg/l. You will look for this in the Report section.

- ✓ Click on the Report-1 tab.
- ✓ Change one of the columns to Clarifier Liquid.
- ✓ Scroll down to the MBG Totals, Liquid-1 section (near the bottom of the report).
- ✓ Click on the mol/hr units. MBG Totals, Liquid-1 (mol/hr)
- ✓ Change the Aqueous Composition Basis from moles to concentration.

Output variables		
Aqueous Composition	Concentration	mg/L

- ✓ Close the Units Manager window. Find the Mg(+2) concentration.

Mg(+2)	5.0

- ✓ Review the calcium concentration – it should be 10 mg/l.

Ca(+2)	10.0

- ✓ Next change the stream columns in the Report to show a_Lime and a_Soda Ash.
- ✓ Scroll to the top of the table and view the Stream Parameters section.

The target Mg^{+2} and Ca^{+2} concentrations exiting the Reactor are achieved. The controllers computed that 81.4 mol/hr lime and 109.9 moles soda ash were required. Our initial inputs of 80 and 115 were good, but the controller optimized it within seconds.

The purpose of this example is to illustrate how the controller works with the multiplier and target stream to achieve the desired value. The number of iterations/passes, that the controller required to meet the specification can be observed in the Convergence Monitor.

Using the convergence monitor

The Panel at the bottom of the software contains several tabs, including Output, Errors, Trace, and Convergence Monitor. The Convergence monitor tab is a graphic representation of the progress for controllers and recycle streams.

- ✓ Click on the Convergence Monitor tab.

The default variable view is <Automatic>

- ✓ Click on the Automatic button and select Magnesium Control.

It took seven iterations for the Magnesium controller to achieve its target specification.

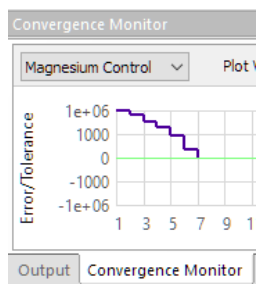


Figure 7-11 – The Convergence monitor output for the magnesium controller

- ✓ Change the view from Magnesium to Calcium control

By comparison, the calcium controller took about forty iterations to converge on the right concentration.

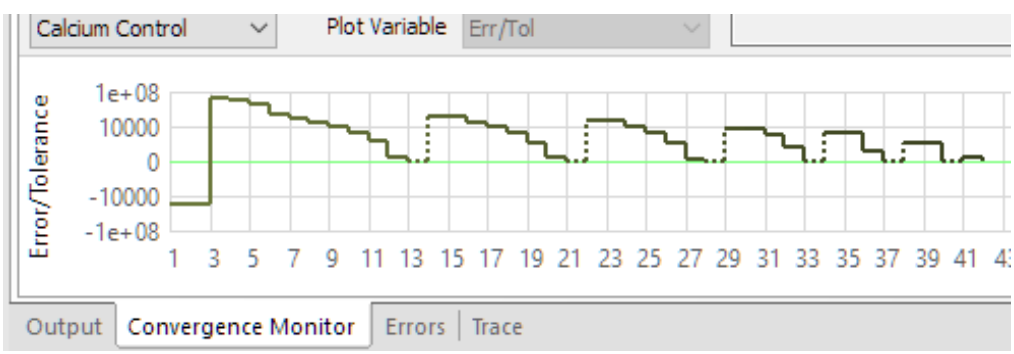


Figure 7-12 – The Convergence monitor output for the calcium controller

Updating the controller settings

It is possible to start subsequent calculations at this converged setting. The Software contains a tool called Restart, which updates a number of converged settings, including controllers. It is also relatively easy to access.

- ✓ Click anywhere on the flowsheet, so that nothing is selected to access the Flowsheet Properties panel.

When no stream or unit is selected, the Properties panel displays the Flowsheet Process Options (settings)

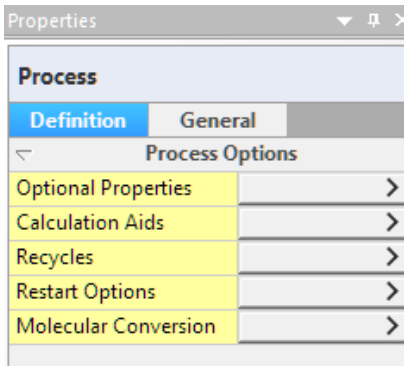
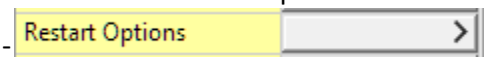
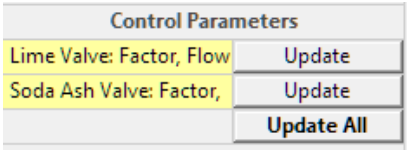


Figure 7-13 – The Flowsheet (Process) options panel

There are presently five options categories. The one of interest is the Restart Options.

- ✓ Click on the Restart Options button - 

- ✓ Click on the Update All button in the Control Parameters section -



A window appears stating that settings for some objects were updated.

- ✓ Press OK and Calculate.
- ✓ View the Convergence Monitor.

The monitor should now be empty, because the controllers converged in the first iteration.

- ✓ Save your file.

Setting the Water content in the filter cake

The water content in the filter cake is currently based on a split value entered into the filter block settings. This is a fixed/static value, and should the liquid or solids rate change, the water content will differ; the fixed values entered are not robust. It is, therefore, not a function of the filter press efficiency. To convert this setting to one that is automatic, a controller is needed. This controller would read the mass of solids exiting in the filter cake and adjust the water mass so that a target water fraction in the solids cake is achieved. A water content of 9wt% for example would be reasonable. Thus the water to solids ratio would be 1:10.

Adding this setting requires two controllers, a feedback controller to signal the water flow rate, and a feed forward (FF) controller that reports to the feedback (FB) controller how much solids are being produced. The image below illustrates how these objects should look when you are done.

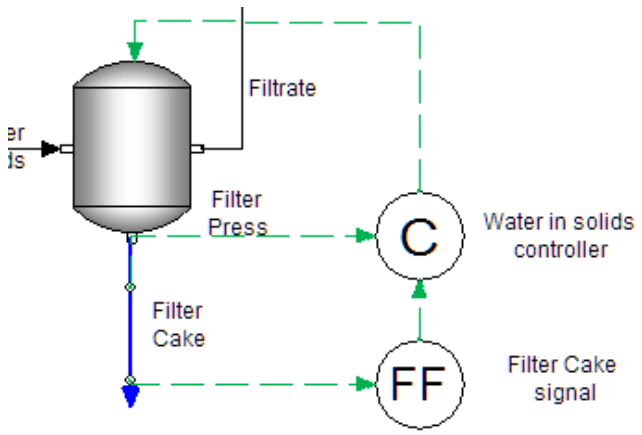


Figure 7-14 – The filter press linked to a Feed Forward and Feedback controller so that the water content in the filter cake is fixed at 9%.

Add the objects

- ✓ Click on the FF Controller object in the Library and drag it to the lower right of the Filter press.
- ✓ Label the FF controller, Filter Cake Signal.
- ✓ Click on the FB Controller object and drag it above the FF controller.
- ✓ Label the FB controller Water in Solids Controller.

Link the signals to the objects

- ✓ Next, click on the Signal button in the toolbar – you will add four signals.
- ✓ Link the Filter cake stream to the FF controller (Filter Cake Signal).
- ✓ Link the FF Controller to the FB Controller (Water in solids controller).
- ✓ Link the Filter Cake to the Feedback controller (there are two signal lines from the filter cake).
- ✓ Link the Feedback controller to the Filter Press.

This is how the four signal lines and the controllers operate:

- The first signal line (Filter Cake stream to FF controller) sends to the FF controller the current solids flow rate (kg/hr).
- The second signal line (FF controller to FB controller) sends the FB controller how much liquid mass needs to be in the Filter cake stream (0.1*solids flow rate, kg/hr).
- The third signal line (Filter Cake stream to FB controller) sends to the FB controller the current liquid mass in the cake (kg/hr).
- The fourth signal line (FB Controller to Filter Press) instructs the filter press to change the water flow fraction to the Filter Cake stream so as to achieve the proper water mass in the filter cake.

Assigning Settings to the Feed Forward controller

You will adjust the properties panel for this controller. When completed, it should look like this:

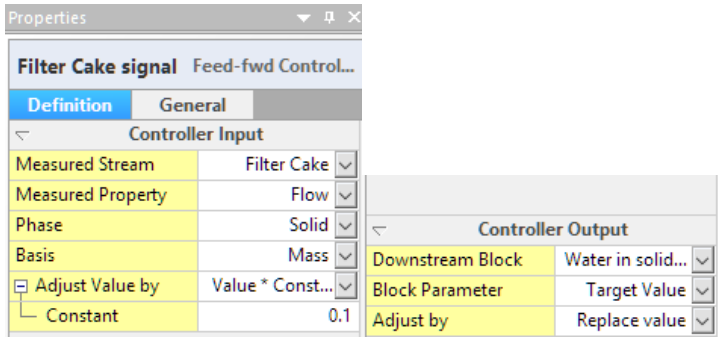


Figure 7-15 - The completed Properties panel for the Filter Cake signal

- ✓ Click on the FF controller, now called Filter Cake Signal.
- ✓ The Measured stream should be Filter Cake. If not change it.
- ✓ Change the Controller Input settings to the following:

  Measured Property = Flow
  Phase = Solid
  Basis = Mass
  Adjust Value by = Value * Constant
  Constant = 0.1

- ✓ Change the Controller Output settings to the following:

  Downstream Block = Water in Solids
  Block Parameter = Target Value
  Adjusted by = Replace Value

You have instructed the FF controller to do the following: Measure the solid mass flow rate in the filter cake. This mass is multiplied by 0.1 and that value is sent to the Feedback controller. In this case, there is 13.33 kg/hr of solids exiting the Filter press. The FF controller will send this 1.333 kg/hr value to the Feedback controller.

Assigning settings to the Feedback controller

The feedback controller will measure the filter cake liquid flow rate, and adjust the "liquid in Solid" split so that 1.333 kg/hr liquid exits with the filter cake. This is how the feedback controller will look when you have completed the following steps.

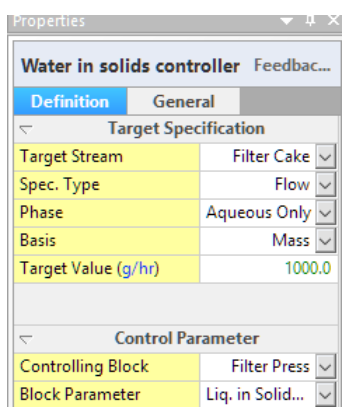


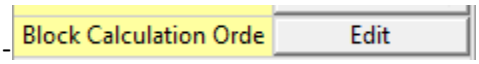
Figure 7-16 - The completed Properties panel for the Water in Solids controller

- ✓ Click on the Water in Solids controller.
- ✓ The Target stream should be Filter Cake – if not change it.
- ✓ Change the settings to the following:

  Spec Type = Flow
  Phase = Aqueous Only
  Basis = Mass
  Target Value = 1000 (g/hr)
  Controlling Block = Filter Press
  Block Parameters = Liquid in Solid

Setting the calculation order so that the Feed Forward controller calculates before the Feedback controller

The last step is to instruct the software to calculate the FF controller before the Feedback controller. This is because the FF needs to sends the required liquid mass to the FB controller before the FB controller is calculated.

- ✓ Click anywhere on the white section of the Flowsheet (to activate the Process properties).
- ✓ Click on the Block Calculation Order Edit button- 

- ✓ Locate the Filter Cake Signal and ensure that it is before the Water in solids controller. If not highlight it and move it up.

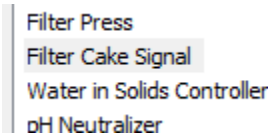


Figure 7-17 – Changing the order of the Filter cake signal so that it is calculated before the Water in Solids controller

- ✓ Press OK to leave the window, and Calculate.
- ✓ Click on the Convergence Monitor tab and select the Water in solids controller.

The controller took five iterations to converge. The final water content in the filter cake should be 9%.

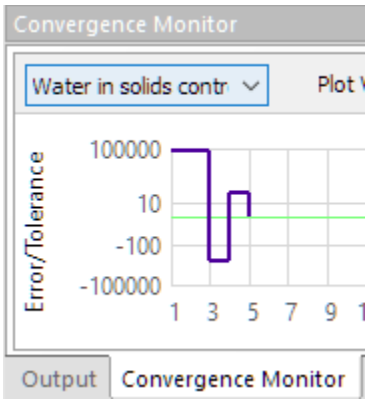


Figure 7-18 - The Convergence Monitor showing the progress of the Water in solids controller

- ✓ Click on the Report-1 tab and change the first column to show the Filter Cake

✓ Review the Liquid and solid mass in the Phase Flow section

	Filter Cake
	Remove
Phase Flows	
Moles, True - Aqueous (mol/hr)	73.636
Moles - Solid (mol/hr)	141.493
Moles - Vapor (mol/hr)	0.0
Moles, Apparent - Aqueous (mol/hr)	72.7696
Mass - Aqueous (g/hr)	1350.44
Mass - Solid (g/hr)	13504.4
Mass - Vapor (g/hr)	0.0
Volume - Aqueous (L/hr)	1.32606
Volume - Solid (L/hr)	4.97195

Figure 7-19 - The Phase Flow section of the Filter Cake. The Water mass is 1/10th the solids mass as designed

The water content in the filter cake is 9% as designed in the controllers. These controllers took five iterations to converge, and with this additional automation a more robust model is created. What-if scenarios can now be run, in which the stream flow rates or target Ca^{+2} and Mg^{+2} concentrations are changed, and the filter press will continue to produce a cake with 9 wt% water.

Now that the software converged on the target specification for water, the settings can be updated so that in future calculations the converged case will be the restart point.

✓ Click anywhere on the flowsheet (off any block or stream) so that the Flowsheet Properties panel in the panel.

✓ Select the Restart Options and then click the Restart All button.

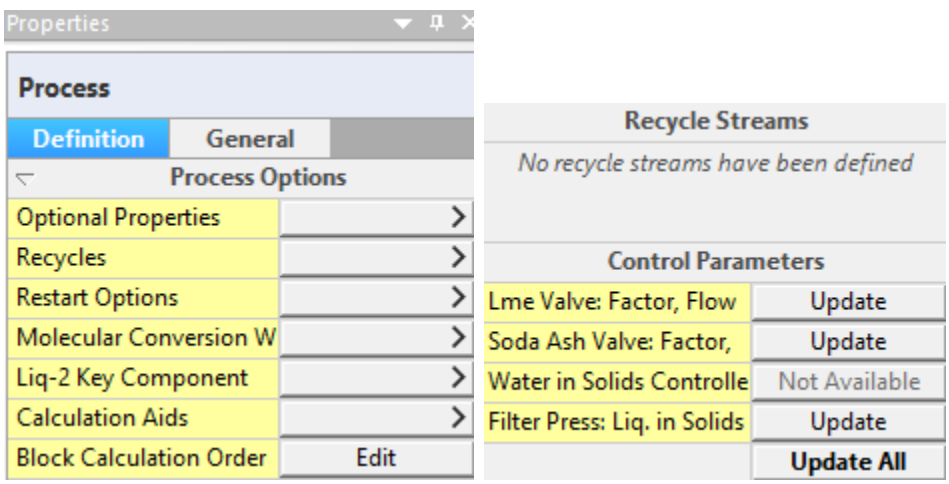


Figure 7-20 – Updating all the controllers so that the next time the calculation is run it starts at the converged case

The settings for filter press controllers are now updated. The last thing we will do is review the Filter Press fractions to see how the controller modified them.

✓ Click on the Filter Press to access the Properties panel.

✓ Click on the Edit button and review the updated Liquid splits.

In order to achieve the 9 wt% waster target, the software rerouted 5.4% of the liquid to the filter Cake stream, with the balance exiting the filtrate.

- ✓ Save your file. It will be used in the next chapter.

Summary

This chapter introduces controllers and multipliers. Multiplier blocks were added to the lime and soda ash streams to represent flow valves. Each multiplier was controlled by a Feed Back controller that measured the dissolved calcium and magnesium concentrations and adjusted the lime and soda ash flow rates, respectively. Then, the water content in the filter cake was controlled using a Feed Forward controller and a Feedback controller in series.

Chapter 8 Water Treatment – Adding Reverse Osmosis

The Application

This chapter introduces the flow Splitter and the component splitter objects. The flow splitter separates stream by mass or volume, with each stream having an identical composition. The Component splitter separates elements, molecular flows, and solid phases, creating streams with different compositions.

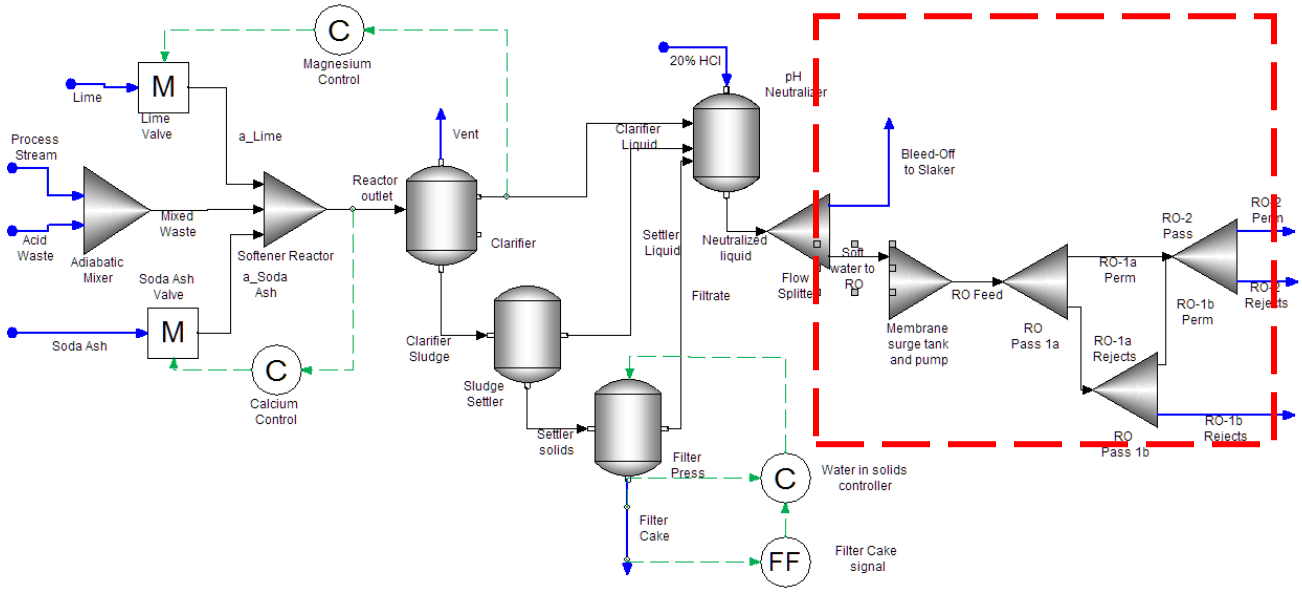


Figure 4-1- Softening and Neutralization Process

The softener and clarifier operation created in Chapters 1 - 3 is continued in this chapter. The softened water exiting the Neutralization tank is split to two streams. The first stream, representing 95% of the total, flows to the RO process for further purification. The remainder flows to a lime slaker.

The RO process is comprised of three units: Pass 1a, Pass 1b and Pass 2, laid out in a semi-parallel configuration. The neutralized liquid flows into Pass 1a. Pass 1a permeate flows to Pass 2 and the rejects flow to Pass 1b. Pass 1b permeate flows to Pass 2 and the rejects exit and are sent for further processing. Pass 2 rejects are also sent downstream for further processing.

The membranes will be modeled using component split blocks. These blocks contain settings that e nable component, molecular and phase separation. The supporting units in a plant RO system (booster pumps, mixing points, permeate tanks, filters) are ignored or consolidated in these split blocks.

The neutralized liquid has a dissolved solids concentration of ~30,000 mg/l, which is roughly the salinity of seawater. Consequently, the membrane performance is impacted by the back-pressure generated on the concentrate side of the membrane. We will assume in this example, that the maximum operating pressure is 75 atm.

Adding the Chemistry

Open the existing case file

The case described in this chapter builds on the water treatment case file saved previously. Open that case file now. If you do not have the case file, and have already completed the work, contact AQSim for a copy. If you have not run Chapters 1 - 3 yet, then close this chapter and complete those chapters first.

- ✓ Open the case file, Water Treatment Softening Process

There are no chemistry changes in this step.

Building the Process

Adding a Flow split for the Lime Slaker

- ✓ Click on the Splitter object in the Library and drag it the lower-right of the pH Neutralizer.

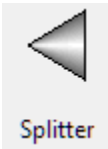


Figure 4-2 - The Flow Splitter object

- ✓ Label it Slaker Bleed-off valve.
- ✓ Link the Neutralized Liquid to the inlet of the Slaker Bleed-off valve.
- ✓ Click on the Add Stream button in the Toolbar.
- ✓ Add two streams to the outlet of this block.
- ✓ Label the top one Bleed-off to Slaker.
- ✓ Label the lower one Soft Water to RO.

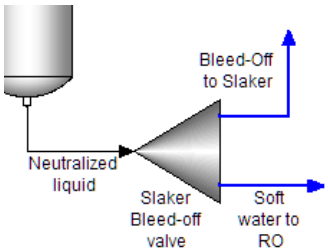


Figure 4-3 - The configuration for the Slaker bleed-off valve (splitter)

- ✓ Click on the Splitter object to access the Properties panel.

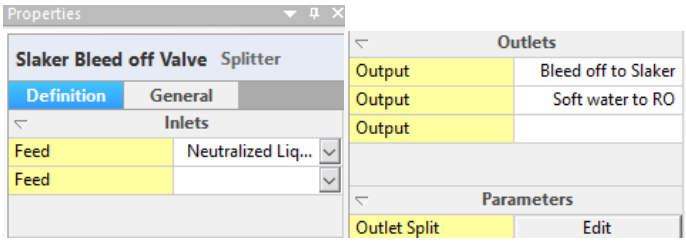


Figure 4-4 - The Properties panel for the Splitter object

- ✓ Click on the Edit button in the Parameters section.
- ✓ Change the Flow basis to Volume.
- ✓ Set the fraction to the Bleed-off to Slaker to 0.05 and the fraction to the Soft water to RO to 0.95. Press OK to close.

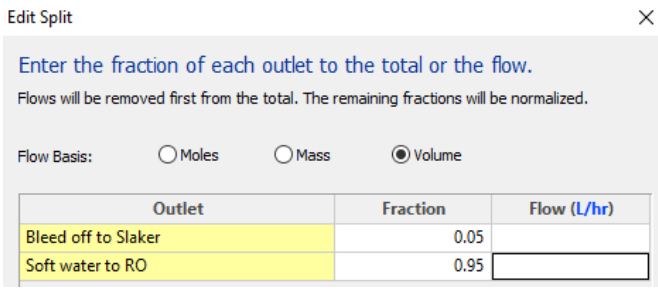


Figure 4-5 - The Edit Split window showing the fraction of flow for each outlet stream

Adding the Membrane Surge Tank and Pump

A single mixer block will represent the surge tank and booster pump. The mixer parameters contain a setting to fix temperature and pressure. So, the outlet pressure of the booster pump will be set in this block.

- ✓ Click on the Mixer object in the Library and drag it to the lower-right of the Slaker Bleed-off valve.
- ✓ Label it Membrane Surge Tank and Pump.
- ✓ Link the Soft Water to RO stream to the mixer inlet.
- ✓ Click on the Add Stream button in the Toolbar.
- ✓ Add a stream to the Outlet of the mixer.
- ✓ Label the stream RO Feed.

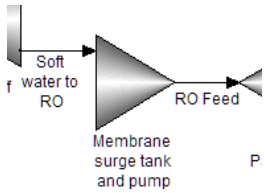


Figure 4-6 – The Membrane surge tank and pump (mixer) inlet and outlet configuration

- ✓ Click on the mixer.
- ✓ Change the Pressure Spec. to Absolute Pressure.
- ✓ Set the pressure to 50 atm.

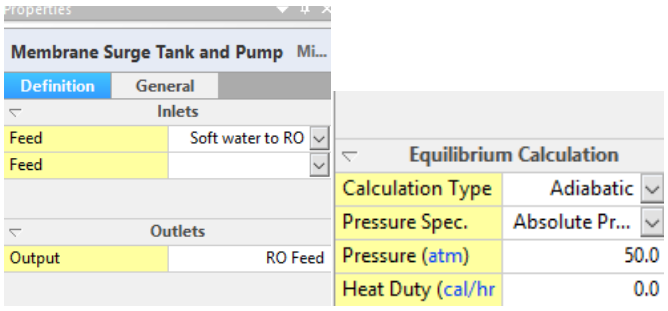


Figure 4-7 – Using the mixer's Pressure Specifications to simulate a booster pump

- ✓ Calculate.
- ✓ Review the flow rates for the Neutralized liquid, Bleed-off to Slaker and the RO Feed stream.

	Neutralized Liq...	Bleed off to Sla...	RO Feed
	Remove	Remove	Remove
Stream Parameters			
Temperature (°C)	46.1045	46.1045	45.0521
Pressure (atm)	1.0	1.0	50.0
pH	8.0	8.0	7.98972
Moles, True (mol/hr)	31887.7	1594.38	30293.0
Moles, Apparent (mol/hr)	31512.6	1575.63	29936.9
Mass (g/hr)	5.84807e5	29240.4	5.55567e5
Volume (L/hr)	574.26	28.713	544.224

Figure 4-8 – Mass balance around the Bleed-off valve and Membrane Surge Tank/Pump

The neutralized liquid is split into the RO Feed and Bleed of to Slaker. The RO Feed is pressurized to 50 atm and is slightly cooler. This is an artifact of using an adiabatic pressure increase rather than a pump (the latter emitting heat). The Bleed off to Slaker stream is one twentieth the flow of the RO Feed by design.

- ✓ Save your file.

Adding RO Pass 1a

This next step will be the template for adding the three RO blocks. It is more involved than the previous blocks in that there are multiple entries to set the RO rejection rates for each dissolved element.

- ✓ Click on the Comp. Splitter object in the Library, and drag it to the right of the Membrane Surge Tank and Pump.

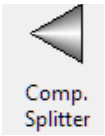


Figure 4-9 - The Component Splitter object in the library

- ✓ Label the object RO Pass 1a.

- ✓ Link the RO Feed stream to the RO Pass 1a inlet.
- ✓ Click on the Add Stream button in the Toolbar.
- ✓ Add two streams to the Outlet side of the RO Pass 1a object.
- ✓ Label the top stream RO-1a Permeate and the bottom stream RO-1a Rejects.

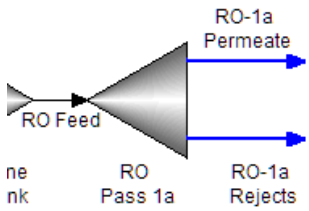


Figure 4-10 – The RO Pass 1a flow configuration

- ✓ Click on the RO Pass 1a block to access the Properties panel.
- ✓ Change the Outlet Pressure Spec to Specified Pressure Drop.
- ✓ Enter a Pressure drop of 45 atm.

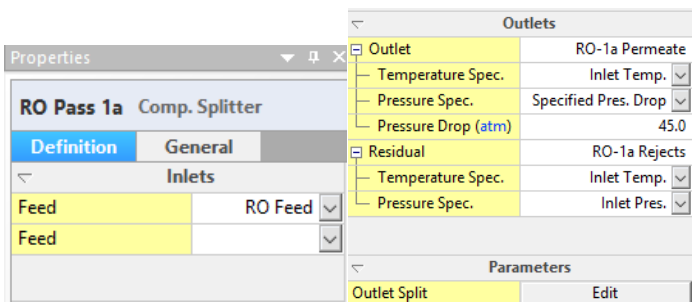


Figure 4-11 – The RO Pass 1a Properties panel. The Pressure drop is set for the Permeate Outlet stream

The purpose of this 45 atm pressure drop is to create the physical pressure differential (Delta-P) required for water to flow through the membrane. It is not a field-validated value; such a value would be provided by the plant operators or from RO simulation software. This pressure drop is provided for descriptive purposes.

The next step in creating the RO unit is to define the rejection rates of the dissolved species and the flux of water through the membrane. This is done using the Component Split function in this block.

- ✓ Click on the Edit button in the Parameters section.

This opens a window containing multiple rows. Each row represents either an element or a molecular flow, depending on the split option selected. The default split option is Inflow species. This option contains molecular representations of the species are part of the process stream that enters this RO-1a block.

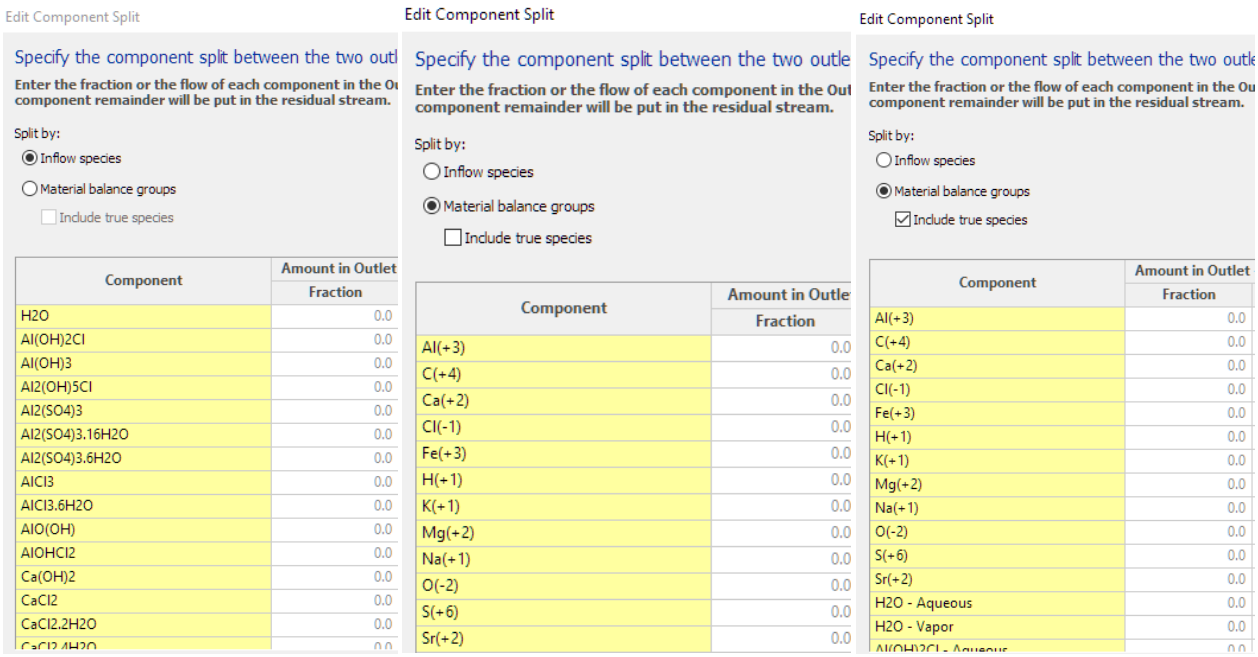


Figure 4-12 – The three component split options; Inflow species, which provide the list of molecular species that make up the inlet stream, Material Balance Group, which provide the list of elements (plus oxidation state), and Material balance group plus true species, which add all the species (cations, anions, neutrals) that make up the stream.

The component split block attempts to provide sufficient flexibility to enable compositional changes of various forms. This is because the Component Split block is used for many process design applications, such as defining the required purity of a reagent stream, or simulating an extraction process.

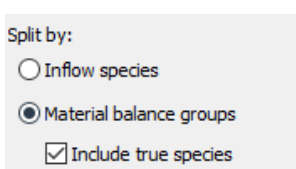
For example, the *Inflow Species* setting is useful when simulating a vacuum swing adsorption Oxygen generator, where oxygen is split from air.

The *Material balance group (MBG)* setting is useful for simulating membrane and ion exchange processes. Specific material balance group like Ca(+2) or Glucose(0) can be assigned rejection rates. With this setting, rejection (or retention) of all MBG-containing species can be set with a single value. For example, if a value is set for Ca(+2), then all Ca-containing species (e.g., Ca^{+2}, $CaCO_3^{o}$, $CaHCO_3^{+1}$) are modified by the same proportion. This is because the *MBG Ca(+2)* is an aggregate of all calcium-containing species in a stream. This simplifies the input for RO and Ion Exchange units.

The *Material balance group (MBG)* setting plus the Include true species option adds the full speciation to the list. This setting is useful for ion-selective resins or rejection-specific membranes. Examples include resins that are specific for exchanging radioactive Cs^{+1} or membranes that reject SO_4^{-2} preferentially.

You will use the last option; *Material balance groups plus Include true species* in this example case.

- ✓ Click on the check boxes for the Spit by options: Material balance group plus Include true species.



- ✓ Enter fractions of 0.01 for all elements except for H(+1) and O(-2).

The 0.01 value represents the fraction of each material balance group that exits with the RO-1a Permeate stream. This is shown in the table header.

Component	Amount in Outlet - RO-1a Permeate	
	Fraction	Flow (mol/hr)
Al(+3)	0.01	
C(+4)	0.01	

Figure 4-13 – The table header shows the stream to which the fraction entered is directed. The 0.01 value means that 1% of that MBG will flow with the RO-1a Permeate. The remaining 99% of that component exits with the reject stream

- ✓ Enter a fraction of 0.33 for the H2O – Aqueous.

The significance of this H_2O fraction is that 33% of the H_2O will passes through the membrane. This is the H2O flux. The actual flux is a function of osmotic pressure (salinity), the membrane type, and the pressure differential across the membrane. The H2O fraction of 33% is arbitrary for this case.

H2O - Aqueous	0.33	
H2O - Vapor	0.0	

Figure 4-13 – The fraction of H2O molecules that pass through the membrane at steady-state is 33%. The remaining 67% flows with the reject stream.

Based on these settings, 33% of the water and 1% of the dissolved species will pass through the membrane.

Component	Amount in Outlet - RO-1a Permeate	
	Fraction	Flow (mol/hr)
Al(+3)	0.01	
C(+4)	0.01	
Ca(+2)	0.01	
Cl(-1)	0.01	
Fe(+3)	0.01	
H(+1)	0.0	
K(+1)	0.01	
Mg(+2)	0.01	
Na(+1)	0.01	
O(-2)	0.0	
S(+6)	0.01	
Sr(+2)	0.01	
H2O - Aqueous	0.33	
H2O - Vapor	0.0	
Al(OH)2Cl - Aqueous	0.0	

Figure 4-13 – The Edit Component Split fractions for RO Pass 1a. The membrane rejects all species at the same fraction of 99% (e.g., 1% pass through).

- ✓ Calculate.
- ✓ Create a new Report window by clicking on the Report item in the menu ulate Report Toc and select Add Multi-Stream Report.
- ✓ Add the following streams to this new report, RO Feed, RO-1a Permeate, and RO-1a Rejects.
- ✓ Review the Total Pressure and the Osmotic pressure for each stream. The Osmotic pressure is found in the Thermodynamic Properties table.

	RO Feed	RO-1a Permeate	RO-1a Rejects
	Remove	Remove	Remove
Stream Parameters			
Temperature (°C)	45.0521	45.0521	45.0521
Pressure (atm)	50.0	5.0	50.0
pH	7.98972	4.20955	8.28256
Moles, True (mol/hr)	30293.0	9776.13	20518.0
Moles, Apparent (mol/hr)	29936.9	9772.5	20164.4
Mass (g/hr)	5.55567e5	1.76217e5	3.79349e5
Volume (L/hr)	544.224	177.791	366.93
Osmotic Pressure (atm)	33.5118	1.07017	50.2334

Figure 4-14 – The thermodynamic properties table for the RO Pass 1a inlet and outlet streams.

The property osmotic pressure is the chemical pressure differential imposed on the concentrate side of the membrane by the permeate side. It is therefore a back-pressure. This back-pressure is the difference between the osmotic pressures of the concentrate and permeate and in this case is 50.2-1.1=40.1 atm. The delta P across the membrane is 50 atm pump pressure -5 atm permeate stream pressure, or 45 atm (you set this differential in the RO-Pass 1a block). Thus the delta P exceeds the osmotic back pressure by 4.9 atm, making this scenario feasible. If Delta-P<40.1 atm, then the osmotic pressure differential would force water back to the concentrate side, and the 33% H_2O fraction across the membrane would not be achieved. The fraction would be something less than this value.

- ✓ Rename this report "RO-1a Input-Output". Do this by right-mouse-clicking on the Report icon in the Navigator Panel, and selecting Rename.

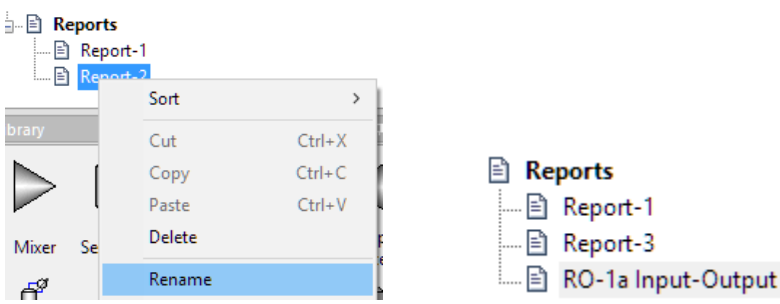


Figure 4-15 – Renaming the Report object that contains the RO-1a input and output streams

- ✓ Save your file

Adding the RO-1b booster pump and membrane unit

A booster pump will be needed between RO-1a and RO-1b because the osmotic pressure of the RO-1a rejects is already 50 atm and concentrating it further in RO-1b will require a larger Delta-P, in order to achieve meaningful H2O flux. The booster pump will once again be modeled using a Mixer object. The mixer object can be configured to run isothermally with a specific outlet pressure.

- ✓ Click on the Mixer in the Library.
- ✓ Drag it to the lower right of the RO-1a unit.
- ✓ Label it RO-1b Booster Pump.

- ✓ Link the RO-1a Rejects stream to the inlet.
- ✓ Add an Outlet stream and label it Feed to RO-1b.

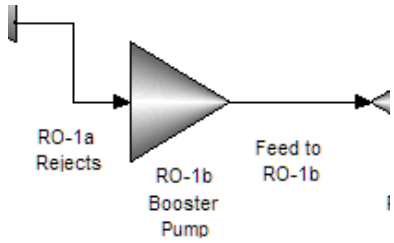


Figure 4-16 – The RO-1b Booster Pump configuration

- ✓ Click on the RO-1b Booster Pump (mixer) to access the Properties panel.
- ✓ Change the Calculation type to Isothermal.
- ✓ Change the Pressure Spec to Absolute Pressure.
- ✓ Enter 80 atm in the pressure cell below.
- ✓ Enter 40C in the Temperature cell below that.

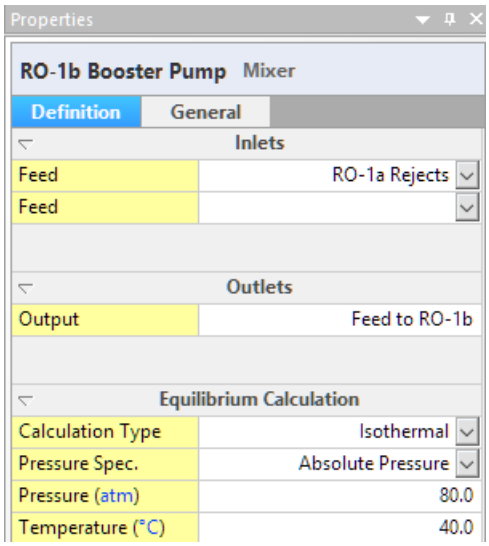


Figure 4-17 – The RO-1b Booster pump outlet settings

Adding the RO-1b membrane

- ✓ Click on the Comp. Splitter object in the Library, and drag it to the right of the RO-1b booster pump.

Figure 4-18 - The Component Splitter object in the library

- ✓ Label the object RO Pass 1b.

- ✓ Link the Feed to RO-1b stream to the RO Pass 1b inlet.
- ✓ Click on the Add Stream button in the Toolbar.
- ✓ Add two streams to the Outlet side of the RO Pass 1b object.
- ✓ Label the top stream RO-1b Permeate and the bottom stream RO-1b Rejects.

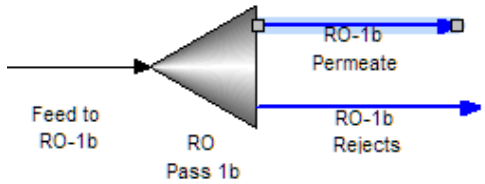


Figure 4-19 – The RO-1b Booster pump outlet settings

The RO Pass 1b configuration will be similar to the 1a settings. The difference will be the amount of H_2O flowing across the membrane and also the pressure drop.

- ✓ Click on the RO Pass 1b block to access its Properties Panel.
- ✓ Change the Outlet Pressure Spec to "Specified Pres. Drop".
- ✓ Enter the value of 65 atm.

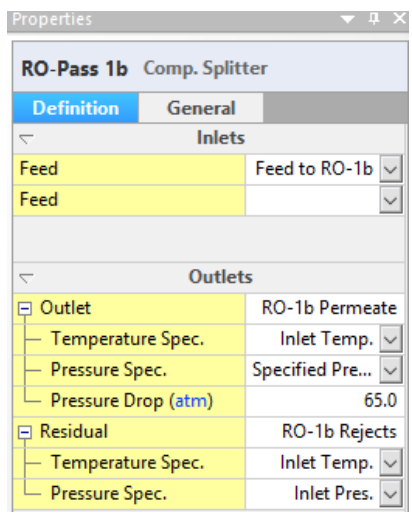


Figure 4-20 – RO-Pass 1b Properties. The 65 atm Pressure drop is set for the Permeate Outlet stream

The pressure drop (Delta-P) is set to 65 atm. Therefore, at steady-state, the osmotic pressure differential across the membrane must be less 65 atm. Otherwise a 25% H2O flow target (read below) will not be achieved.

- ✓ Click on the Edit button.
- ✓ Change the Split By to: Material Balance Group with Include True Species.
- ✓ Set the Fractions for each Material Balance Group (element) as shown below.

Split by:

- ○ Inflow species
- ◉ Material balance groups
  - ☑ Include true species

Component	Amount in Outlet - Fraction
Al(+3)	0.01
C(+4)	0.01
Ca(+2)	0.01
Cl(-1)	0.01
Fe(+3)	0.01
H(+1)	0.0
K(+1)	0.01
Mg(+2)	0.01
Na(+1)	0.01
O(-2)	0.0
S(+6)	0.01
Sr(+2)	0.01
H2O - Aqueous	0.25

Figure 4-21 – The Edit Component Split fractions for RO Pass 1b. The membrane rejects all species at the same fraction of 99% (e.g., 1% pass through). The water permeate to reject ratio is 1:3 or 25%.

- ✓ Close the Edit window and Calculate.
- ✓ Create a new Multi-Stream Report.
- ✓ Rename the Report, RO-1b Input-Output.

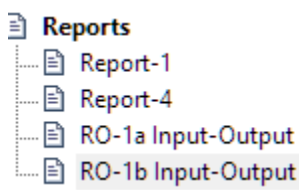


Figure 8-22 – A new multi-stream report is added and named RO-1b Input-Output.

- ✓ Add the streams Feed to RO-1b, RO-1b Permeate, and RO-1b Rejects.
- ✓ Compare the total pressure and Osmotic pressures in each stream.

	Feed to RO-1b	RO-1b Permeate	RO-1b Rejects
	Remove	Remove	Remove
Stream Parameters			
Temperature (°C)	40.0	40.0	40.0
Pressure (atm)	80.0	15.0	80.0
pH	8.32398	3.81217	8.55518
Moles, True (mol/hr)	20516.1	4965.49	15551.8
Moles, Apparent (mol/hr)	20164.4	4961.91	15202.5
Mass (g/hr)	3.79349e5	89551.5	2.89798e5
Volume (L/hr)	365.679	90.0574	275.978
Solid Frac. (mole %)	1.47834e-4	0.0	1.93437e-4

Thermodynamic Properties			
Density - Aqueous (g/ml)	1.03738	0.994382	1.05007
Density - Solid (g/ml)	2.47202	0.0	2.47222
Density - Vapor (g/ml)	0.0	0.0	0.0
Enthalpy (cal/hr)	-1.38886e9	-3.37776e8	-1.05122e9
Enthalpy - Aqueous (cal/hr)	-1.38886e9	-3.37776e8	-1.05121e9
Enthalpy - Solid (cal/hr)	-9098.85	0.0	-8975.32
Enthalpy - Vapor (cal/hr)	0.0	0.0	0.0
Osmotic Pressure (atm)	49.5914	2.02656	66.5978

Figure 4-23 – The Thermodynamic properties of the inlet and outlet streams of the RO-1b unit

The osmotic pressure differential between the Rejects and permeate is 66.6-2.0=64.6 atm. This compares to the Delta P of 65 atm. There is a 0.4 atm differential between the Delta-P and the osmotic pressure differential. Thus, the 25% water fraction is barely achieved.

- ✓ Save your file.

Adding the RO-2 Booster pump

You will now create the RO-Pass 2 unit. This is the polishing membrane that will take the dissolved ion concentrations down to very low levels. This extra pass will allow the permeate water to be used in processes that are sensitive to dissolved ions, like boiler units.

- ✓ Click on the Mixer in the Library.
- ✓ Drag it to the upper-right of the RO-1b unit.
- ✓ Label it RO-2 Booster Pump.
- ✓ Link the RO-1a Permeate and the RO-1b Permeate streams to the inlet.
- ✓ Add an Outlet stream and label it Feed to RO-2.

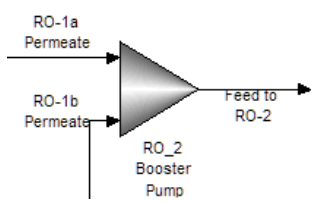


Figure 8-24 – The RO-1b Booster Pump configuration

- ✓ Click on the RO-2 Booster Pump (mixer) to access the Properties panel.
- ✓ Change the Calculation type to Isothermal.
- ✓ Change the Pressure Spec to Absolute Pressure.
- ✓ Enter 20 atm in the pressure cell below it.
- ✓ Enter 40C in the Temperature cell below that.

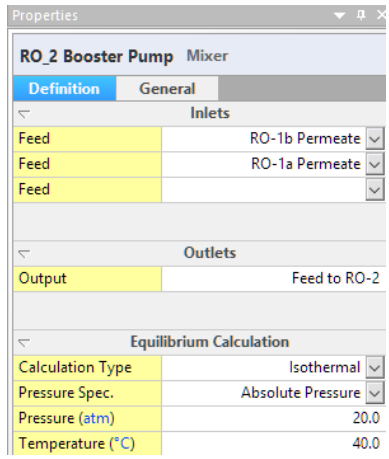


Figure 4-25 – The RO-1b Booster pump outlet settings

A lower booster pump pressure is needed now, because the permeate water salinity is quite low.

Adding the RO-2 membrane

- ✓ Click on the Comp. Splitter object in the Library, and drag it to the right of the RO-2 booster pump.
- ✓ Label the object RO Pass 2.
- ✓ Link the Feed to RO-2 stream to the inlet.
- ✓ Add two streams to the Outlet.
- ✓ Label the top stream RO-2 Permeate and the bottom stream RO-2 Rejects.

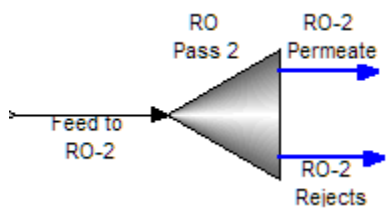


Figure 4-27 – The RO-2 Booster pump outlet settings

The RO Pass 2 configuration similar to the 1a and 1b settings. The differences are the amount of H2O passing through.

- ✓ Click on the RO Pass 2 block to access its Properties Panel.
- ✓ Change the Outlet Pressure Spec of the RO-2 Permeate to "Specified Pres. Drop".
- ✓ Enter the value of 17 atm.

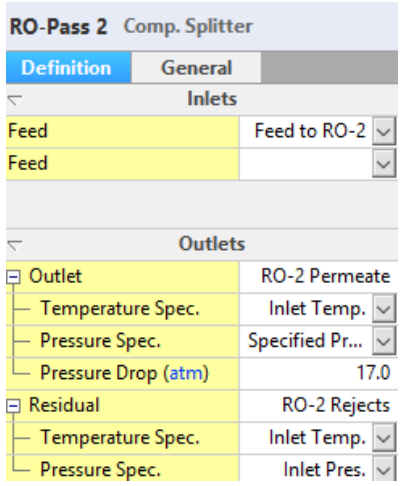
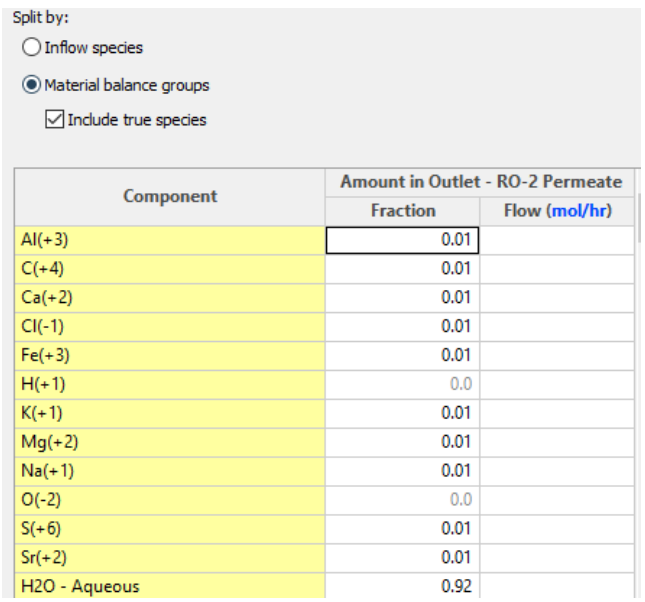


Figure 4-28 – RO-Pass 1b Properties. The 17 atm Pressure drop is set for the Permeate Outlet stream

This step instructs the software to create a 17 atm Delta-P across the membrane.

- ✓ Click on the Edit button.
- ✓ Change the Split By: to Material Balance Group with Include true Species.
- ✓ Set the Fractions for each Material Balance Group (element) as shown below:



Component	Amount in Outlet - RO-2 Permeate	
	Fraction	Flow (mol/hr)
Al(+3)	0.01	
C(+4)	0.01	
Ca(+2)	0.01	
Cl(-1)	0.01	
Fe(+3)	0.01	
H(+1)	0.0	
K(+1)	0.01	
Mg(+2)	0.01	
Na(+1)	0.01	
O(-2)	0.0	
S(+6)	0.01	
Sr(+2)	0.01	
H2O - Aqueous	0.92	

Figure 4-29 – The Edit Component Split fractions for RO Pass 2. The membrane rejects all species at 99% (e.g., 1% pass through). The water flux ratio is 92%.

- ✓ Close the Edit window and Calculate.
- ✓ Create a new Multi-stream Report.
- ✓ Rename the Report, RO-2 Input-Output.

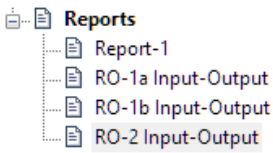


Figure 4-30 – A new multi-stream report is added and named RO-1b Input-Output.

- ✓ Add the following streams to this report, Feed to RO-2, RO-2 Permeate, and RO-2 Rejects
- ✓ Compare the total pressure and Osmotic pressures in each stream

	Feed to RO-2	RO-2 Permeate	RO-2 Rejects
	Remove	Remove	Remove
Stream Parameters			
Temperature (°C)	40.0	40.0	40.0
Pressure (atm)	20.0	3.0	20.0
pH	4.02216	5.68833	3.15928
Moles, True (mol/hr)	14741.6	13549.6	1191.86
Moles, Apparent (mol/hr)	14734.4	13549.6	1184.84
Mass (g/hr)	2.65769e5	2.44103e5	21665.8
Volume (L/hr)	267.374	246.044	21.5051
Osmotic Pressure (atm)	1.3855	0.016076	16.2575

Figure 4-31 – The Thermodynamic properties of the inlet and outlet streams of the RO-2 unit

The Delta P is fixed at 17 atm in the RO-Pass 2 Membrane block the Osmotic back pressure is 16.3-0.02=16.3 atm. Thus, the Delta-P exceeds the osmotic back pressure by 0.7 atm, and so sufficient physical pressure exist to enable 92% of the water to pass through the membrane.

- ✓ Save your case file. It will be used in the next Chapter.

Summary

This chapter introduced the component splitter block which was used to simulate a reverse-osmosis membrane unit. The Component splitter separated material balance groups (MBG) for the cations and anions between the permeate and concentrate streams, and a flow fraction was used to simulate H2O transport through the membrane to the permeate side. In addition to the mechanics of setting up the block, attention was paid to the Delta-P across the membrane and the osmotic back pressure created by the membrane process. It was necessary to confirm that the Delta-P was always greater than the osmotic pressure. Otherwise, the specified water flow rate would not be achieved.

Chapter 9 Water Treatment – Adding Evaporators

The Application

This chapter introduces the heat exchanger block and the entrainment feature of the separator. The process objective is to evaporate the RO-1b rejects brine and to recover water. At this point in the process, all the salts are isolated into two streams, the filter cake and the RO-1b rejects brine. The filter cake is already stabilized as a solid phase. The RO-1b rejects water contains most of the remaining salts and the RO-2 reject stream contains the rest. The plan is to evaporate the RO-1b reject brine, recover the water as steam and dispose of the remaining liquid/solid slurry that forms.

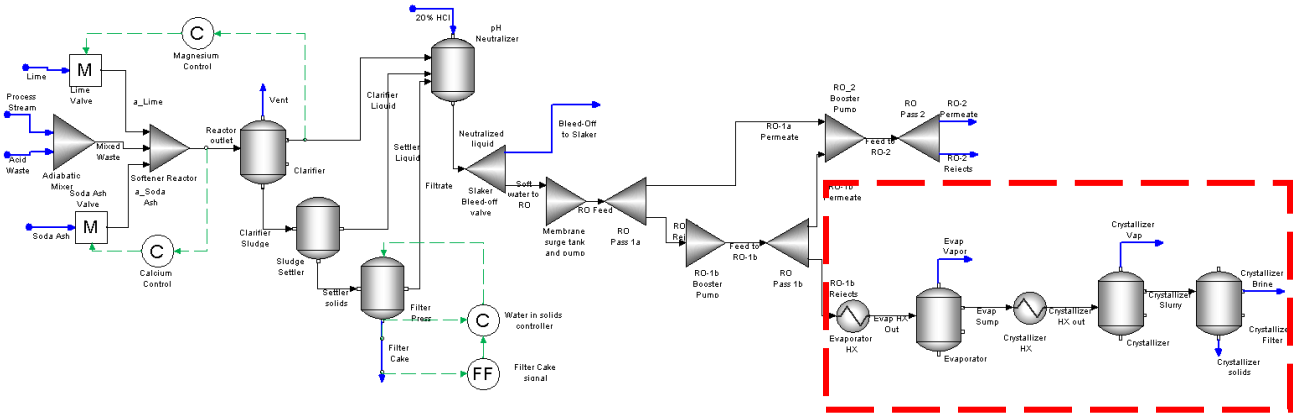


Figure 5-1- Focusing on the evaporation section of the process

The far right section of the schematic contains the new units. They include three separators and two heat exchangers. The separators were introduced in Chapter 2, and the instructions in this chapter introduce a few additional features. The heat exchangers are introduced in this chapter and two options for modeling the heat exchangers are presented.

Adding the Chemistry model

Opening the existing file

This case builds off of the case created in earlier Chapters. Therefore, you should have a file ready to use. If you do not have a completed file, then please contact AQSim to obtain it

- ✓ Open the file, Water Treatment Softening Process

Modifying the chemistry

There are no chemistry modifications in this step.

Building the Process

The evaporation section shown here is a linear process. The RO-1b Reject stream flows through each of the five units and is separated into two vapor streams, a brine stream, and a solids stream.

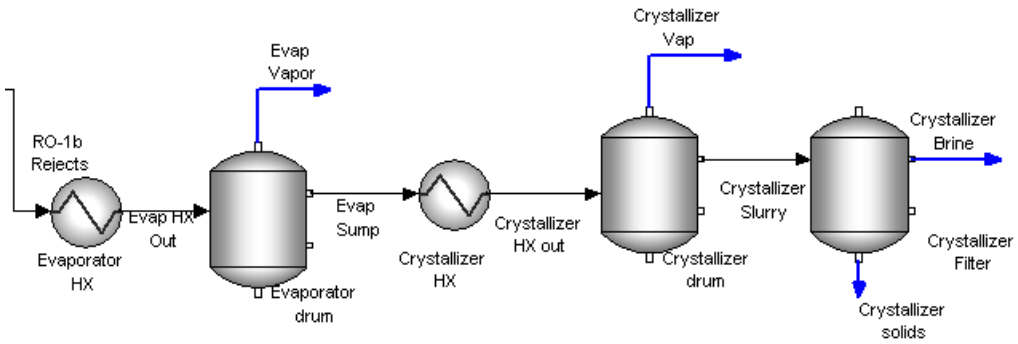


Figure 9-2- The evaporation section of the process. It contains two heat exchangers and three separator blocks. The flow is linear, with one inlet and four outlet streams.

The process' linearity is reflected in the instructions, as each object will be created in the order in which flow reaches it.

Adding the Evaporator Heat Exchanger

- ✓ Click on the Heat Exchanger object in the Library and drag it the lower-right of the RO Pass 1b unit.

Figure 9-3 - The Heat Exchanger object

- ✓ Label it Evaporator HX.
- ✓ Link the RO-1b Rejects stream to the inlet.
- ✓ Click on the Add Stream button in the Toolbar to activate the Add stream action.
- ✓ Add a streams to the heat exchanger outlet and label it Evap HX out.

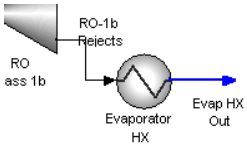


Figure 9-4 - The configuration of the Evaporator heat exchanger

- ✓ Click on the Evaporator HX object to access its Properties panel.

The Heat Exchanger Properties panel contains six sections: Inlets, Outlets, Process Stream specifications, Utility Stream specifications (not shown), Heat Exchanger specifications and Advanced Options. The number of settings is too varied and numerous to present in this chapter. Therefore, a simplified set of Heat Exchanger specifications will be used here.

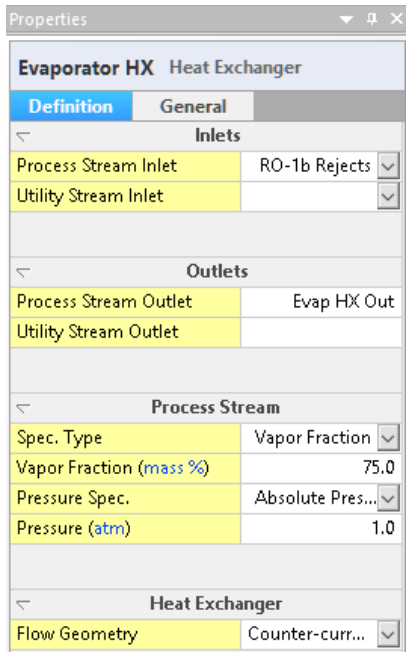


Figure 9-5 - The Properties panel of the Evaporator heat exchanger

- ✓ Change the Spec Type in the Process Stream section to Vapor Fraction.
- ✓ Enter a value of 75 mass%.
- ✓ Change the Pressure Spec to Absolute Pressure.
- ✓ Enter a value of 1 atm.

These settings instruct the software to calculate the heat requirements to evaporate 75% of the inlet stream at 1atm. The heat requirement is reported as the heat duty. The temperature at this final state is then calculated.

Adding the Evaporator body

The evaporated liquid enters the flash separation drum. Where the phases are separated. The vapor is sent to a heat recovery unit (not modeled here), and the remaining liquid is sent to a crystallizer for further evaporation.

- ✓ Click on the Separator object in the Library and drag it to the right of the Evaporator HX block.
- ✓ Label it Evaporator drum.
- ✓ Link the Evap HX Out stream to the inlet.
- ✓ Add a stream to the separator top (this is the vapor outlet).
- ✓ Add a stream to the upper outlet on the right (this is the Aqueous liquid outlet).

✓ Label the top stream Evap Vapor and label the other stream Evap Sump.

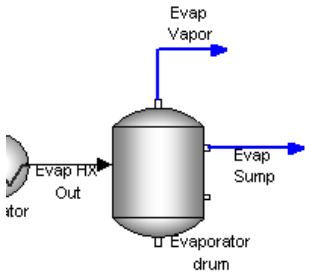


Figure 9-6 – The Evaporator drum containing a vapor and aqueous liquid outlet. Two other outlets, solids and organic liquid are not used.

✓ Click on the block to access the Properties Panel.

✓ Make no changes to the panel.

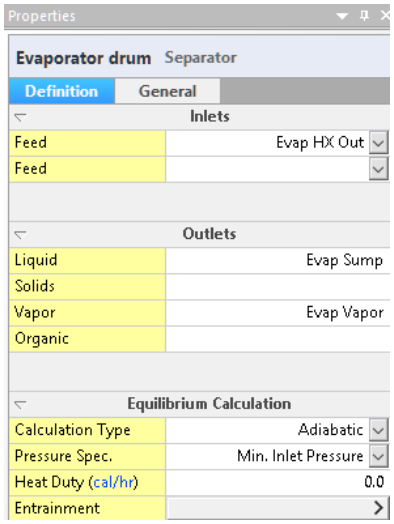
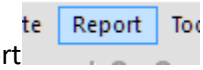
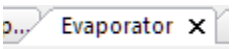


Figure 9-7 – The properties panel of the Evaporator.

The Separator block default settings are adiabatic mix of inflows and pressure set to the lowest inflow stream pressure. In this case, there is one inlet stream, and the outlet pressure is set to the inlet stream pressure. Since there is no pressure drop, the vapor-liquid fraction, and the temperature, will be identical to the outlet of the heat exchanger.

✓ Calculate.

✓ Create a new Multi-stream report 

and name it Evaporator.


✓ Add the following streams to the report Evap HX Out, Evap Vapor, and Evap Sump.

✓ Review the Temperature and the flow rates for each phase.

	Evap HX out	Evap Vapor	Evap Sump
	Remove	Remove	Remove
Stream Parameters			
Temperature (°C)	108.365	108.365	108.365
Pressure (atm)	1.0	1.0	1.0
pH	8.7856		8.7856
Moles, True (mol/hr)	15552.9	12064.2	3488.65
Moles, Apparent (mol/hr)	15202.3	12064.2	3138.07
Mass (g/hr)	2.89798e5	2.17349e5	72449.2
Volume (L/hr)	3.74773e5	3.74712e5	61.6137
Solid Frac. (mole %)	0.024276	0.0	0.117605
Vapor Frac. (mole %)	79.3579	100.0	0.0
Phase Flows			
Moles, True - Aqueous (mol/hr)	3484.96	0.0	3484.96
Moles - Solid (mol/hr)	3.69052	0.0	3.69052
Moles - Vapor (mol/hr)	12064.2	12064.2	0.0
Moles, Apparent - Aqueous (mol/hr)	3134.38	0.0	3134.38
Mass - Aqueous (g/hr)	71937.3	0.0	71937.3
Mass - Solid (g/hr)	511.899	0.0	511.899
Mass - Vapor (g/hr)	2.17349e5	2.17349e5	0.0
Volume - Aqueous (L/hr)	61.4224	0.0	61.4224
Volume - Solid (L/hr)	0.191351	0.0	0.191351
Volume - Vapor (L/hr)	3.74712e5	3.74712e5	0.0

Figure 9-8 – Mass balance around the evaporator

The calculated water temperature is 108.4 C at 1atm and the remaining water contains about 0.7 wt% solids.

✓ Scroll down the Report to find the Solids table.

Solids (mol/hr)			
Row filter applied: only show non-zero rows			
Na2SO4 (Thenardite)	3.43164	0.0	3.43164
Mg(OH)2 (Brucite)	0.109498	0.0	0.109498
CaCO3 (Calcite)	0.0908584	0.0	0.0908584
SrSO4 (Celestine)	0.0441941	0.0	0.0441941
AlO(OH) (Bohmite)	0.014326	0.0	0.014326

Figure 9-9 – Solids content in the evaporator

Five solid phases are computed to form in the evaporator. The dominant phase is sodium sulfate. On a molar basis, it constitutes over 90% of the solids formed. The current units, mol/hr, can be changed by selecting the unit link adjacent to the "Solids" table title. You will not do that now; since managing units is part of a later chapter, and we are not concerned with the solid phases in this block.

✓ Save your file.

Creating the Crystallizer section

The evaporator section is designed to reduce the brine's water content without producing too many solids. The crystallizer on the other hand, is designed to evaporate the brine with the purpose of producing significant amounts of solid.

The crystallizer section will be created in the same way as the evaporator section, with a heat exchanger followed by a separator. The difference in this case, is that two separators will be used. The first, called the crystallizer includes a pressure drop of 0.3 atm and will separate vapors. The second separator, called Crystallizer Filter, will contain a solids outlet plus a setting for water entrainment in the solids.

Adding the crystallizer heat exchanger

- ✓ Click on the Heat Exchanger object in the Library and drag it to the right of the Evaporator block.

Figure 9-10 - The Heat Exchanger object

- ✓ Label it Crystallizer HX.
- ✓ Link the Evap Sump stream to the inlet.
- ✓ Add a stream to the outlet and label it Crystallizer HX out.

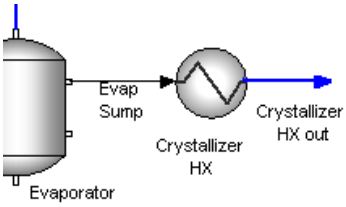


Figure 9-11 - The configuration of the Crystallizer heat exchanger

- ✓ Click on the Crystallizer HX object to access the Properties panel.

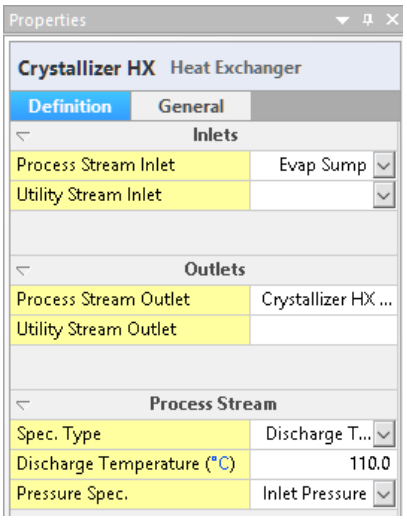


Figure 9-12 - The Properties panel for the Crystallizer heat exchanger

- ✓ Change the Spec Type to Discharge Temperature.
- ✓ Enter a value of 110 C.
- ✓ Keep the Pressure Spec set to Inlet Pressure.

In this exchanger, the target specification is temperature: the software fixes temperature and adjusts total enthalpy. It is different from the Evaporator exchanger above in which the phase amounts were fixed and the total enthalpy was computed. The temperature was then computed from the total enthalpy.

Adding the Crystallizer body

The crystallizer body unit is similar to the Evaporator body unit above, except that a pressure drop of 0.3 atm below the inlet stream pressure is set. This will create an additional adiabatic flash, that cools the input stream as additional liquid vaporizes.

- ✓ Click on the Separator object in the Library and drag it to the right of the Crystallizer HX block.
- ✓ Label it Crystallizer.
- ✓ Link the Crystallizer HX Out stream to the inlet.
- ✓ Add new streams to the top outlet and to the upper right outlet.
- ✓ Label the streams Crystallizer Vapor and Crystallizer Slurry.

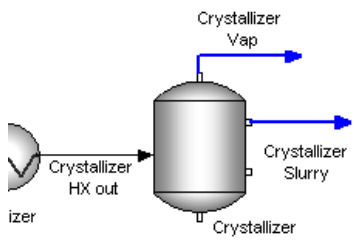


Figure 9-13 – The Crystallizer body containing a vapor and aqueous liquid outlet.

- ✓ Click on the block to access the Properties Panel.
- ✓ Change the Pressure specifications to Pressure Drop.
- ✓ Enter a pressure drop value of 0.3 atm

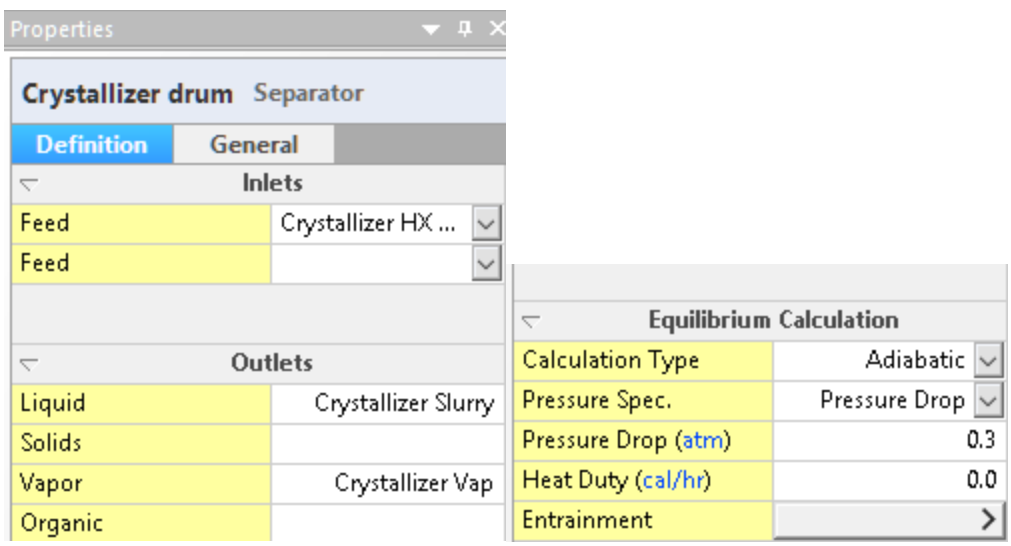
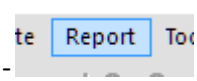
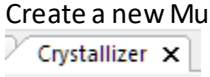


Figure 9-14 - The Properties panel for the Crystallizer object showing that there is a pressure drop of 0.3 atm

- ✓ Calculate.
- ✓ Create a new Multi-Stream Report tab - 

and name it Crystallizer. 

- ✓ Add the streams Crystallizer HX Out, Crystallizer Vapor, and Crystallizer slurry.
- ✓ Review the output temperature and the Phase Flows.

	Crystallizer HX ...	Crystallizer Vapor	Crystallizer Slurry
	Remove	Remove	Remove
Stream Parameters			
Temperature (°C)	110.0	99.5974	99.5974
Pressure (atm)	1.0	0.7	0.7
pH	9.92677		9.99382
Moles, True (mol/hr)	3164.86	2655.54	504.961
Moles, Apparent (mol/hr)	3138.05	2655.54	482.502
Mass (g/hr)	72449.2	47840.4	24608.8
Volume (L/hr)	81927.1	1.15356e5	12.5484
Phase Flows			
Moles, True - Aqueous (mol/hr)	238.205	0.0	199.976
Moles - Solid (mol/hr)	300.851	0.0	304.984
Moles - Vapor (mol/hr)	2625.81	2655.54	0.0
Moles, Apparent - Aqueous (mol/hr)	211.388	0.0	177.518
Mass - Aqueous (g/hr)	5030.85	0.0	4235.49
Mass - Solid (g/hr)	20113.5	0.0	20373.3
Mass - Vapor (g/hr)	47304.8	47840.4	0.0
Volume - Aqueous (L/hr)	4.19487	0.0	3.51011
Volume - Solid (L/hr)	8.9208	0.0	9.03827
Volume - Vapor (L/hr)	81914.0	1.15356e5	0.0

Figure 9-15 – Mass balance around the crystallizer body

The solids slurry stream is now about 83 wt% solids and 72% by volume. It is quite possible that this slurry will not flow. We have probably evaporated too much solid, and it will be necessary to limit evaporation or add additional liquid to reduce the solids-content of the stream. For now, we will leave the problem as is and correct it in the next chapter by adding liquid to this crystallizer by recycling some of the separated crystallizer liquid.

Add the Crystallizer filter

The last step in the process is to add a solids separation unit. The presumption is that the slurry exiting the crystallizer is filtered to recover the remaining brine. The solids are then discarded, used in another process, or sold.

- ✓ Click on the Separator object in the Library and drag it to the right of the Crystallizer block.
- ✓ Label it Crystallizer Filter.
- ✓ Link the Crystallizer Slurry stream to the inlet.
- ✓ Add a new stream to the Aqueous outlet on the upper-right and to the solids outlet on the bottom.
- ✓ Label the streams Crystallizer brine and Crystallizer solids.

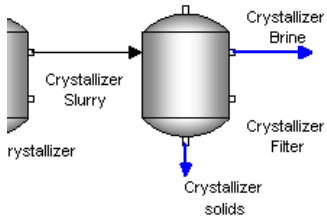


Figure 9-16 – The Crystallizer filter containing a liquid and solids outlet.

- ✓ Click on the block to access the Properties panel.
- ✓ Click on the Entrainment button.
- ✓ Enter a value of 0.15 (g/g) in the Liquid in Solids row.

This action instructs the software to add 0.15 grams of liquid per gram of solid. The solids stream thus contains 13% moisture ($\frac{0.15}{0.15+1}$).

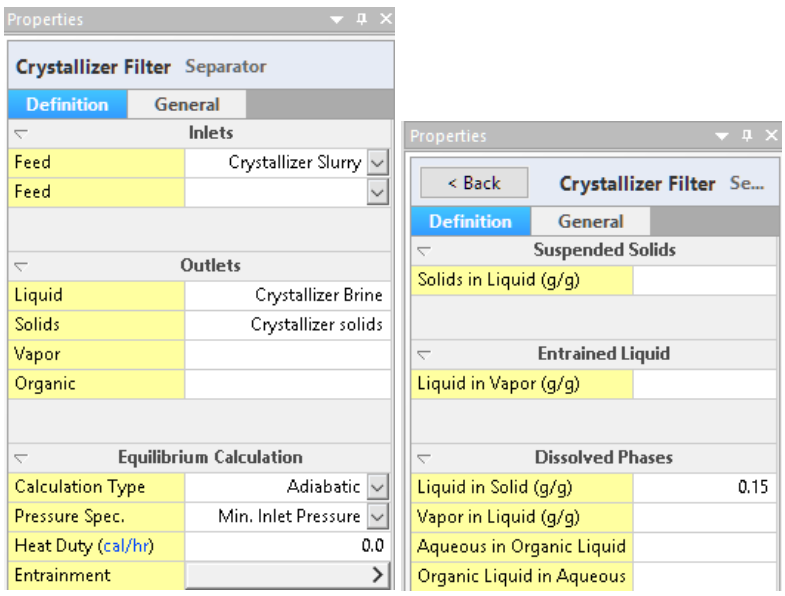


Figure 9-17 – The properties panel of the Crystallizer Filter including the entrainment window.

- ✓ Calculate.
- ✓ Return to the Crystallizer Report and add the Crystallizer Brine and Crystallizer solids streams. Review the volume of each stream and the Solids table.

	Crystallizer HX ...	Crystallizer Vapor	Crystallizer Slurry	Crystallizer brine	Crystallizer solids
	Remove	Remove	Remove	Remove	Remove
Stream Parameters					
Temperature (°C)	110.0	99.5974	99.5974	99.5974	99.5974
Pressure (atm)	1.0	0.7	0.7	0.7	0.7
pH	9.92677		9.99382	9.99382	9.99382
Moles, True (mol/hr)	3164.86	2655.54	504.961	55.6894	449.271
Moles, Apparent (mol/hr)	3138.05	2655.54	482.502	49.435	433.067
Mass (g/hr)	72449.2	47840.4	24608.8	1179.5	23429.3
Volume (L/hr)	81927.1	1.15356e5	12.5484	0.977495	11.5709
Solid Frac. (mole %)	9.58722	0.0	63.2089	0.0	70.4243

Mass - Aqueous (g/hr)	5030.85	0.0	4235.49	1179.5	3056.0
Mass - Solid (g/hr)	20113.5	0.0	20373.3	0.0	20373.3
Mass - Vapor (g/hr)	47304.8	47840.4	0.0	0.0	0.0
Volume - Aqueous (L/hr)	4.19487	0.0	3.51011	0.977495	2.53262
Volume - Solid (L/hr)	8.9208	0.0	9.03827	0.0	9.03827
Volume - Vapor (L/hr)	81914.0	1.15356e5	0.0	0.0	0.0
Solids (mol/hr)					
Row filter applied: only show non-zero rows					
NaCl (Halite)	270.421	0.0	274.345	0.0	274.345
Na2SO4 (Thenardite)	30.1411	0.0	30.3559	0.0	30.3559
Mg(OH)2 (Brucite)	0.109975	0.0	0.109975	0.0	0.109975
CaCO3 (Calcite)	0.103005	0.0	0.103007	0.0	0.103007
SrSO4 (Celestine)	0.0441975	0.0	0.0442231	0.0	0.0442231
CaSO4 (Anhydrite)	0.0157768	0.0	0.0177527	0.0	0.0177527
Al(OH)3 (Bayerite)	0.0	0.0	8.16566e-3	0.0	8.16566e-3
AlO(OH) (Bohmite)	0.0162439	0.0	0.0	0.0	0.0

Figure 9-18 – Solids present in the crystallizer and filter streams

The crystallizer brine volume rate is 0.98 L/hr. By comparison, 2.5 l/hr liquid leaves with the filtered solids. The crystallizer solids are 90 mole% NaCl, with the remaining 10% being sulfate salts of Na, Ca, and Sr. If the sulfates are removed upstream of the crystallizer or separated in a downstream process, then it may be possible to create a commercial grade NaCl product.

✓ Save your file. It will be used in the next chapter.

Summary

This chapter introduces heat exchangers and flash separators to the process. The purpose of these units are to process the rejects brine into a salt for disposal or sale and to produce low-grade vapor. This work is only partially complete, however, since the existing salt is not pure and the crystallizer slurry's solids content is too high. This cannot be fixed at this point because the control and calculation objects needed have yet to be introduced. They are presented next.

Chapter 10 Water Treatment – Adding Recycles

Flowsheet ESP – Adding a recycle stream to the crystallizer so that the slurry will flow

The Application

The previous chapter ended with a converged evaporator and crystallizer section, but the results were not practical because the software computed a crystallizer slurry containing >80wt% solids. This may cause pump problems. To resolve this potential problem, a slurry diluent is to be added. This diluent needs to be saturated with the crystallizer solids, otherwise the heat added to crystallize these solids is wasted. The diluent will be the crystallizer brine, which will be recycled upstream of the Crystallizer.

Formulating the Process

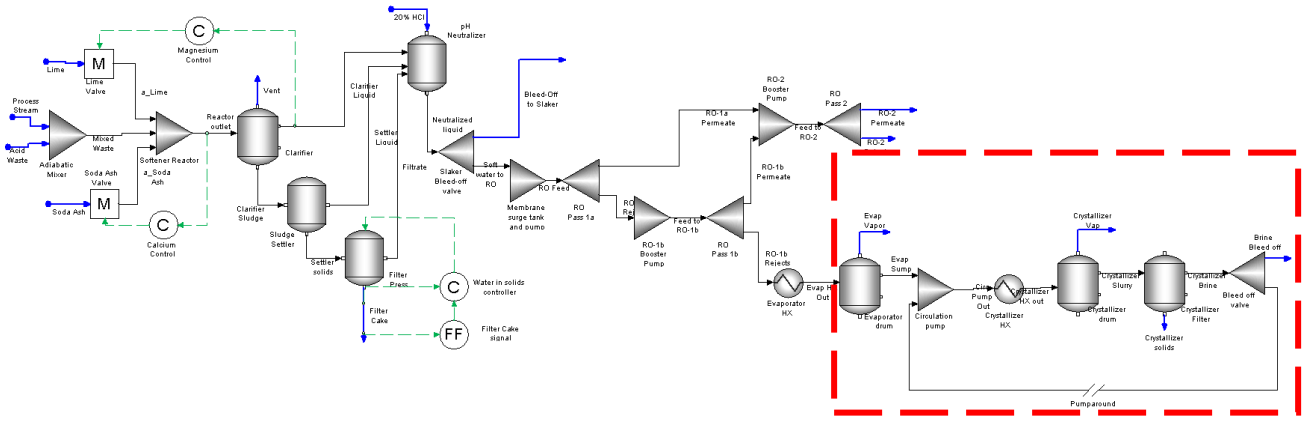


Figure 10-1- Focusing on the evaporation section of the process

You will update the far right section of the schematic as follows:

1) Add a mixer placed upstream of the crystallizer heat exchanger – labeled the Circulation Pump.
2) Add a flow split block downstream of the crystallizer filter – labeled the bleed-off valve.

3) Add a stream exiting the bleed off valve and entering the circulation pump – labeled Pumparound. This stream will be defined as the Tear/Recycle.

The Pumparound recycle stream is the primary training goal of this chapter. It is significant to solving the process, because it is an internal stream that must have a guessed composition in order to start the simulation. Eventually, the steady-state composition of this internal stream is computed. The better the guess entered for this stream's composition and properties. the easier and faster the software will converge the complete system.

Building the recirculation loop in the crystallizer

The enlarged image below is evaporator crystallizer section containing the new objects. The mixer is labeled Circulation pump and the splitter labeled Bleed off valve.

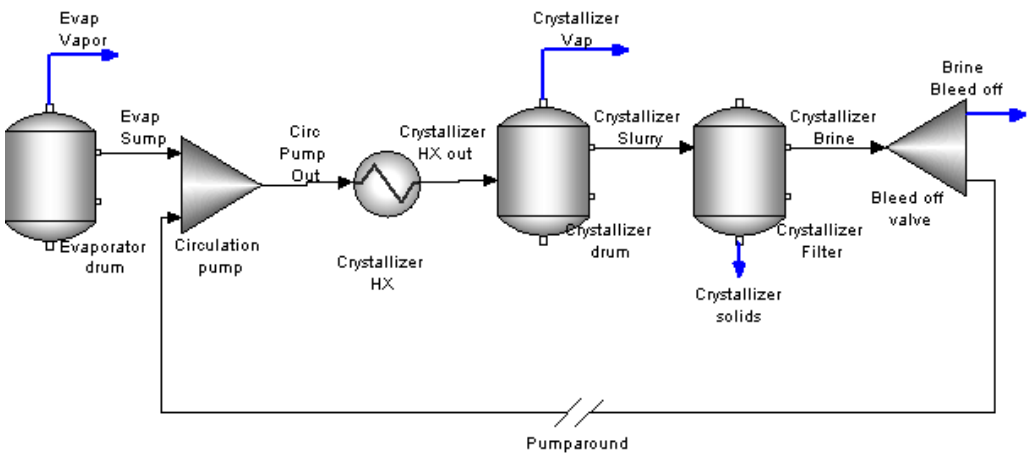


Figure 10-2- The evaporation section of the process. It contains two heat exchangers and three separator blocks. The flow is linear, with one inlet and four outlet streams.

Open existing work file used in Chapters 1 through 5

Inserting the Circulation Pump (mixer)

- ✓ Disconnect the Evap Sump stream from the Crystallizer HX.
- ✓ Highlight the three objects, Crystallizer HX, Crystallizer drum and Crystallizer Filter and drag them to the right to make room for the new block.

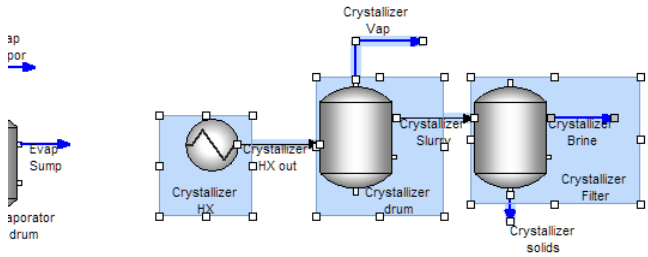


Figure 10-3 – Highlighting and moving several blocks at one time

- ✓ Click on the mixer object in the Library and drag it in between the Evaporator drum and the Crystallizer HX.
- ✓ Label it Circulation Pump.

- ✓ Link the Evap Sump stream to the inlet.
- ✓ Add a new stream outlet of the mixer and link it to the inlet of the Crystallizer HX.
- ✓ Label the new stream Circulation Pump Out (abbreviate it if you wish).
- ✓ Click on the Circulation pump object to access the Properties panel.
- ✓ Change the Pressure Spec. to Absolute.
- ✓ Set the exit pressure to 1atm.

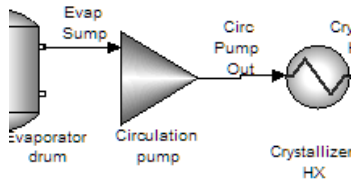


Figure 10-4 – Inserting the Circulation pump between the evaporator drum and crystallizer HX

Adding the Flow Splitter

- ✓ Click the Splitter block in the Library and drag it to the right of the Crystallizer filter.
- ✓ Label it Bleed-off valve.
- ✓ Link the Crystallizer brine stream to the inlet of the Bleed-off valve.
- ✓ Add two new streams to the Outlet of the bleed-off valve.
- ✓ Name the top stream Brine Bleed off and the bottom stream Pumparound.
- ✓ Link the Pumparound stream to the inlet of the Circulation pump.

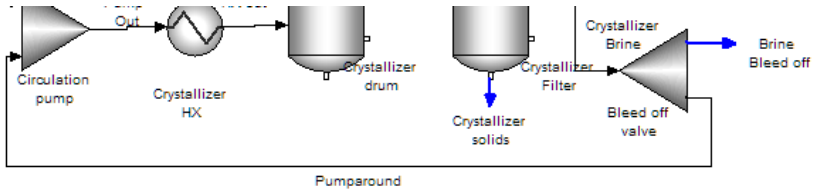


Figure 10-5 – The pumparound stream is linked back to the circulation pump

- ✓ Click on the Bleed-off valve block to expose the panel.
- ✓ Click on the Edit button in the Parameters.
- ✓ Change the Flow basis to Volume.
- ✓ Set the Brine Bleed off fraction to 5 (%) and the Pumparound fraction to 95 (%). The software will normalize it back to 1.
- ✓ Click OK to close the window.

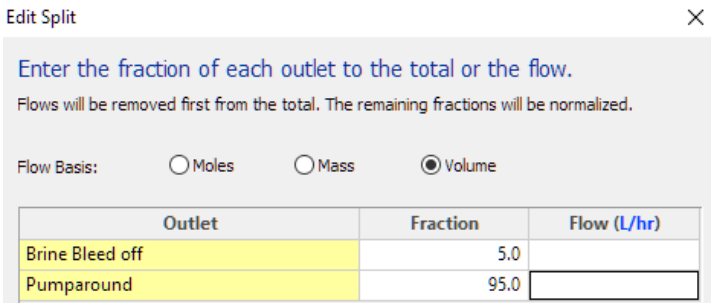


Figure 10-6 – The Split Fraction for the streams exiting the Bleed off valve. The recycle ratio is 20:1

Defining the Pumparound stream as the Recycle stream

- ✓ Click anywhere on the white area of the flowsheet to access the Process Properties panel.

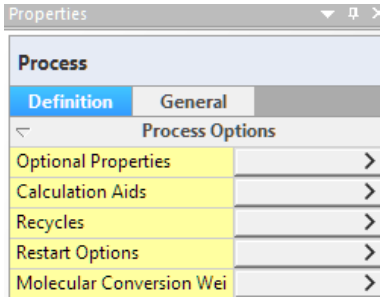


Figure 10-7 – The Properties panel of the overall Process

- ✓ Click on the Recycles button.

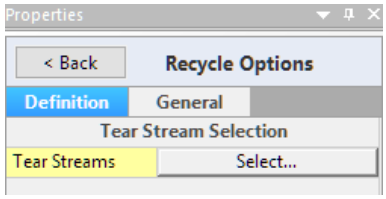


Figure 10-8 – The Tear Stream panel

- ✓ Click on the Tear Streams Select button.
- ✓ Highlight the Pumparound in the Suggested list then press OK to close the window.

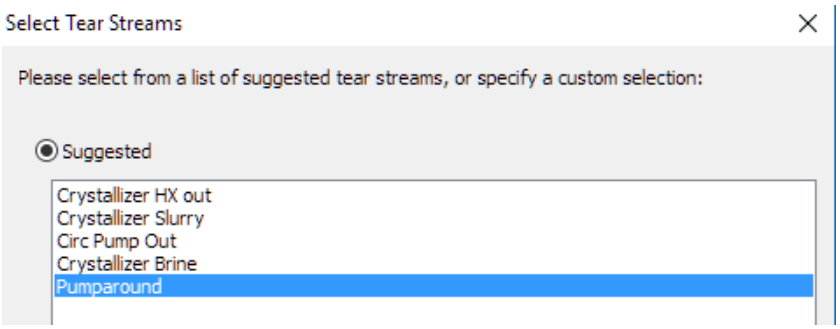


Figure 10-9 – The Tear Stream selection panel. The Pumparound stream is selected

When the window closes, a new section appears in the Recycle options panel. You use this section to create an initial guess composition for this stream.

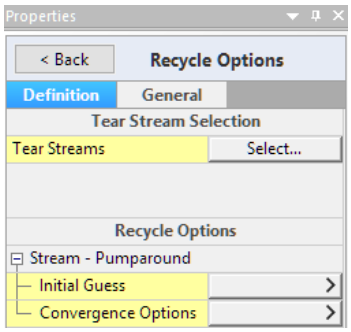


Figure 10-10 – The Recycle Options panel showing the Pumparound settings

✓ Click on the Initial Guess button.

The initial composition is empty. The simulation will converge faster if this stream contains some material.

✓ Enter 90C, 1 atm, and 100 mole/hr H2O (the software will compute the stream amount).

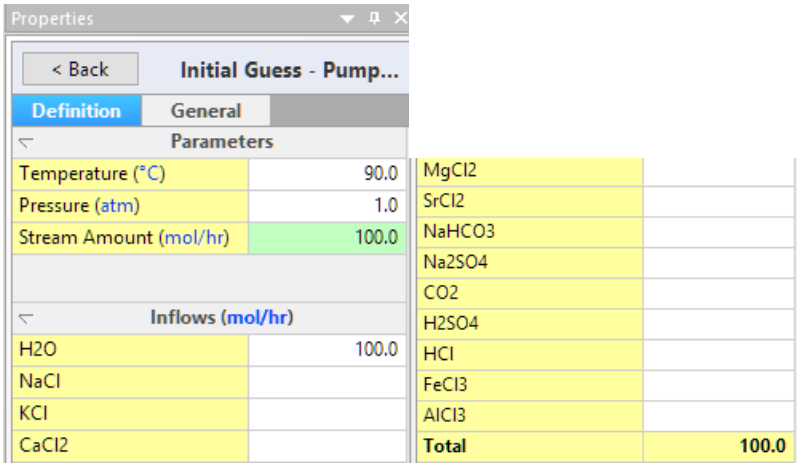
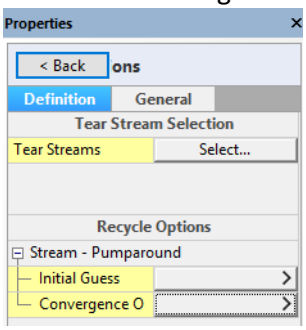


Figure 10-11 – The initial guess for the Pumparound stream

✓ Click on the Back button in the upper left of the Properties panel < Back

✓ Select the Convergence Options button below the Initial Guess



The Convergence Options panel contains settings that are used to speed up the recycle convergence or to make the convergence more stable. There are several convergence approaches and settings for each. In this scenario, we are simply going to increase the number of iterations that the software will attempt before giving up.

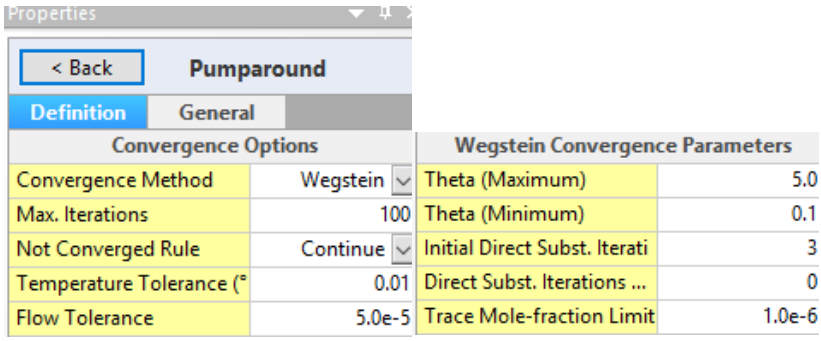


Figure 10-12 – The Convergence options panel for the Pumparound recycle. Each recycle in a simulation will have its own convergence option settings.

- ✓ Change the Iterations from 50 to 100

Converging the case with a Tear/Recycle stream and updating results

- ✓ Calculate.
- ✓ Save your file
- ✓ While calculating, click on the Convergence monitor at the bottom of the screen.

The Monitor is set to automatic and will eventually focus on the Pumparound convergence. It may take up to 40 iterations for the pumparound stream composition to converge to a steady state.

What is happening internally is that the software will use the composition you entered for the pumparound stream as the inlet to the circulation pump. The simulation will proceed and the bleed off valve will create a new pumparound stream composition. The software compares this new composition to your initial guess, make adjustment rerun the calculation loop. This loop will iterate multiple times until the adjustments become negligible relative to a tolerance level. This final updated pumparound composition represents the steady-state conditions.

The image below is the convergence monitor that shows how the convergence is progressing. The initial iterations have high error/tolerance levels and as the software updates the guessed pumparound composition, then the error decreases until it drops below 1.

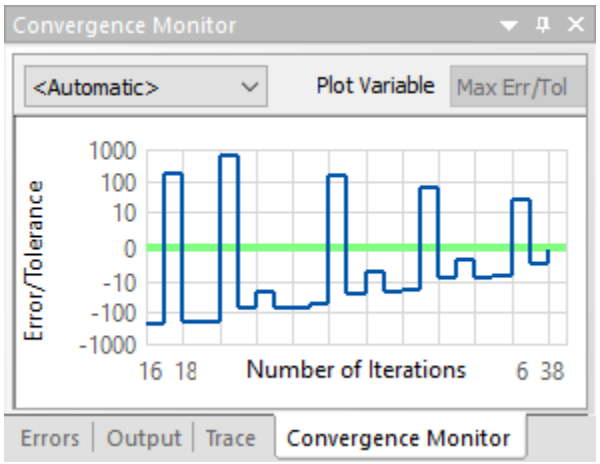


Figure 10-13 – The Convergence monitor showing the convergence progress of the recycle stream.

You will recalculate the case, but this time, instead of viewing the convergence monitor, view the Pumparound Properties panel.

- ✓ Click on the pumparound stream to access the properties panel.
- ✓ Click on the calculated tab – it will show the updated results.
- ✓ Recalculate the case and view this Calculated panel.

The software will erase the calculated values and start with your initial guess. After each iteration, it will update the composition. The changes become smaller with each iteration, provided that it is converging to a steady-state solution.

Properties

Pumparound

Definition | Calculated | Gene

Stream Parameters	
Temperature (°C)	99.5332
Pressure (atm)	0.7
pH	9.9292
Moles, True (mol/hr)	1623.07
Moles, Apparent (m	1442.07
Mass (g/hr)	34274.4
Volume (L/hr)	28.4772
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	0.0

Total, Apparent (Molecular) (mol/h	
H2O	1271.91
CO2	7.82254e-4
Na2SO4 (Thenardite)	13.1142
NaCl	137.223
KCl	19.6229
CaO	0.102254
Al2O3	0.0734099
MgO	6.72024e-6
Na2O	0.0163164
NaFeO2	7.12773e-3
SrO	2.08326e-4

Figure 10-14 – The converged Pumparound stream- this is its composition at steady-state

- ✓ Click on the Crystallizer Report and add the streams Pumparound and Brine Bleed Off.

The pumparound flow is ~28 L/hr and the Crystallizer slurry is now about 33% solids. The Crystallizer brine bleed off is 1.5L/hr and 2.5 L/hr brine is entrained in the crystallizers solids.

	Crystallizer Vapor	Crystallizer Slurry	Crystallizer brine	Crystallizer solids	Pumparound	Crystallizer Blee...
	Remove	Remove	Remove	Remove	Remove	Remove
Stream Parameters						
Temperature (°C)	99.5332	99.5332	99.5332	99.5332	99.5332	99.5332
Pressure (atm)	0.7	0.7	0.7	0.7	0.7	0.7
pH		9.9292	9.9292	9.9292	9.9292	9.9292
Moles, True (mol/hr)	2632.52	2154.0	1708.5	445.505	1623.07	85.4249
Moles, Apparent (mol/hr)	2632.52	1947.48	1517.97	429.513	1442.07	75.8986
Mass (g/hr)	47425.8	59295.3	36078.3	23217.0	34274.4	1803.92
Volume (L/hr)	1.14336e5	41.4474	29.976	11.4714	28.4772	1.4988
Solid Frac. (mole %)	0.0	15.5123	0.0	70.3352	0.0	0.0
Vapor Frac. (mole %)	100.0	0.0	0.0	0.0	0.0	0.0
Phase Flows						
Moles, True - Aqueous (mol/hr)	0.0	1851.9	1708.5	143.406	1623.07	85.4249
Moles - Solid (mol/hr)	0.0	302.099	0.0	302.099	0.0	0.0
Moles - Vapor (mol/hr)	2632.52	0.0	0.0	0.0	0.0	0.0
Moles, Apparent - Aqueous (mol/hr)	0.0	1645.39	1517.97	127.414	1442.07	75.8986
Mass - Aqueous (g/hr)	0.0	39106.6	36078.3	3028.31	34274.4	1803.92
Mass - Solid (g/hr)	0.0	20188.7	0.0	20188.7	0.0	0.0
Mass - Vapor (g/hr)	47425.8	0.0	0.0	0.0	0.0	0.0
Volume - Aqueous (L/hr)	0.0	32.492	29.976	2.51609	28.4772	1.4988
Volume - Solid (L/hr)	0.0	8.95532	0.0	8.95532	0.0	0.0
Volume - Vapor (L/hr)	1.14336e5	0.0	0.0	0.0	0.0	0.0

Figure 10-15 – The report of the crystallizer section containing the brine bleed-off pumparound stream and the updated Crystallizer slurry which now contains about 33wt% solids.

Updating the initial guess with the new results

You ran the calculation twice, and both cases took the same number of interactions to converge the pumparound stream. There is a way to update your initial guess with the final results, so that the next time the calculation is run, it starts at this converged state. This is done using the Restart option in the Flowsheet Process Options (properties panel)

- ✓ Return to the Flowsheet tab.
- ✓ Click anywhere on the white area to access the Process Properties panel.
- ✓ Click on the Restart Options button.

The panel opens into the Restart section that displays all the initial guesses that were used to create this case. There are Recycle streams and Controller settings. You will update the Pumparound Recycle stream.

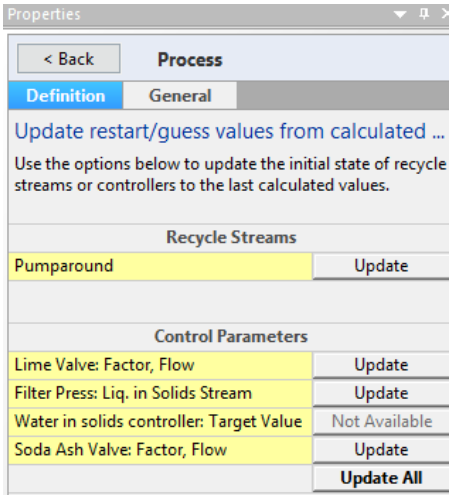


Figure 10-16 – The Restart section of the Process' Properties panel

- ✓ Click on the Update button for the Pumparound.

The software will make the changes and confirm it in a popup window.

- ✓ Recalculate.

The software will now converge much more quickly and in fewer iterations.

Summary

Chapter 6 introduces the Recycle, or Tear, stream feature. Recycle streams are part of all complex processes, and a method to compute its composition is presented. Key aspects to setting up a recycle stream include: selecting a stream that is part of a recycle loop, providing a reasonable initial composition, flow and conditions to that stream, and updating your stream guess with the calculated values using the Restart option.

Chapter 11 Simple Air Stripper Column

The Application

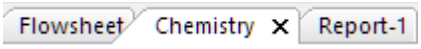
A common OLI Flowsheeting application is an electrolyte column. Cases such as stripping organics, stripping reactive acids, absorbing reactive gases following combustion, or product distillation are examples. In this chapter you will model an air stripping process in which BTEX (benzene, toluene, ethylbenzene, xylene) is stripped from contaminated groundwater.

This process contains a single column with two inlets; contaminated water entering the top of the column, and air entering the bottom. The column contains no reboiler nor condenser.

Creating a Chemistry Model

You created a chemistry model in Chapter 1, but did little else with it in the following five chapters. This is because typically once a chemistry model is built, there are a limited number of reasons to change it.

You will create a new, simple chemistry model for this case. It contains four organics, the components of air, and water.

- ✓ Open the software and start with a new case.
- ✓ Click on the Chemistry tab - 

The default view when creating a new chemistry model is the Databanks tab. It is here where the activity coefficient framework, Aqueous(H+) or MSE(H3O+) is selected plus any specialized databases.

- ✓ Keep the default settings of Aqueous (H+) and no private databases.
- ✓ Click on the Inflows tab.
- ✓ Enter the following components' benzene, toluene, ethylbenzene, o-xylene, N2, O2, Ar, and CO2.

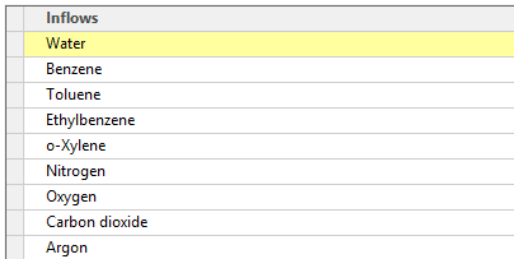


Figure 11-1 – The list of components to be used in the air-stripper example

The chemistry is kept simple so that the focus of the chapter is on the tower block. The tower is perhaps the most complex block in the Flowsheet ESP toolkit with many thermodynamic and mass transfer settings.

- ✓ Click on the Phases tab.

You will not make any changes to this screen, but notice that there is an unchecked second liquid phase. Were the BTEX contamination to the extent that an organic, NAPL (non-aqueous-phase liquid) was present, then it would be necessary to check this box. Otherwise the software would not form the organic phase and would overestimate the amount of BTEX in the water and vapor phase.

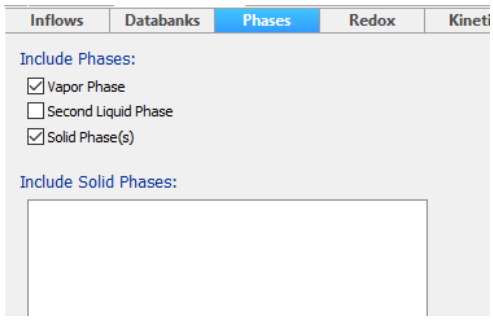


Figure 11-2 – The Phase-Selection tab. There are no solids to select, since this is a BTEX example. The second liquid would be selected if a NAPL phase was expected

- ✓ Use the default settings for the Phases tab.

The last step is optional. You will provide a name to this chemistry model.

- ✓ Click on the Model icon in the Navigator Panel.
- ✓ Use the F2 key to edit the name – Label it BTEX.

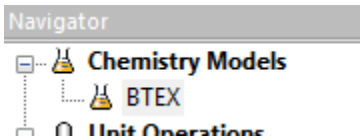


Figure 11-3 – The Location of the Chemistry model in the Navigator panel. The name can be changed for reference purposes.

The Chemistry Model build step is finished.

Building the Process

This process contains one multi-stage column, two inlet streams, and two outlet streams. There would be additional components in an actual unit, such as pumps, oil skimmers, and filters. They are not addressed in this chapter, because we want to focus on the column.

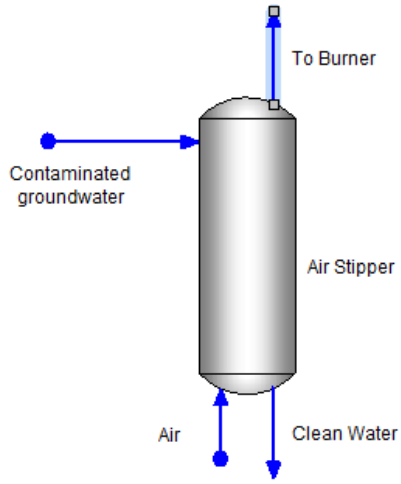


Figure 11-4 the Air stripper tower is comprised of two inlet and two outlet streams

Adding the Air Stripper and adjusting its default settings

The Flowsheet ESP library contains two tower objects Absorber and Stripper. They are essentially the same process block, except that the Absorber does not include have the reboiler or condenser on by default. Beyond that they are the same.

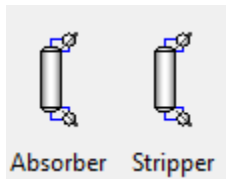


Figure 11-5 – The Absorber and Stripper icons in the Block Library. They differ in that the stripper includes a reboiler and condenser by default while these units are off by default in the absorber block.

- ✓ Click on the Absorber object in the Library and drag it onto the Worksheet.
- ✓ Double click on the new block and change its name to Air Striper.

You will notice that the Properties panel on the right side of the window displays the Air Stripper parameters.

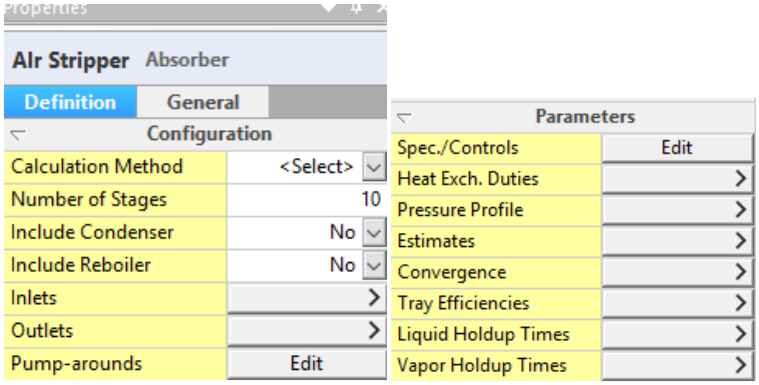


Figure 11-6 the properties panel for the Absorber block

The calculation method for the absorber is not defined initially. It can be defined as either equilibrium or mass transfer limited. The number of (theoretical) stages is set to 10 by default, with a range between 2 and 50+. The condenser and reboiler are off but can be switched on. The pressure profile of the column is not set.

- ✓ Change the calculation method to Equilibrium by clicking on the <Select> cell and activating the drop-down menu.
- ✓ Change the number of stages to 5.
- ✓ Click on the Pressure Profile button in the Parameters section of the panel

- ✓ Enter a value of 1 atm for both Stage 1 and Stage 5.

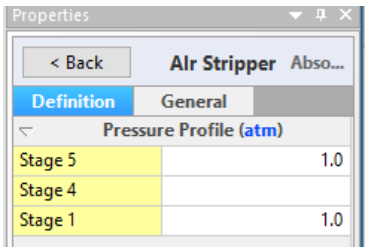


Figure 11-7 The pressure profile is set for absorber block. The air stripper is run at atmospheric pressure

Entering the same pressure at stage 1 and 5 results in a horizontal pressure profile across all stages. There will be no pressure gradient between the bottom and the top of the tower.

Adding the inlet and outlet streams

- ✓ Click on the Add Stream button in the Toolbar.

Figure 11-8 - The Add Stream button in the toolbar

- ✓ Place an inlet stream at the top left of the column by first clicking somewhere to the left of the tower and drag the stream to the right so that it links with the top input link on the tower. Click the mouse again to link the stream to the tower.

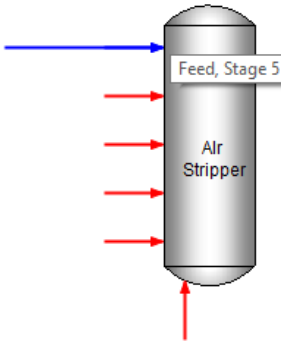


Figure 11-9 – Linking the inlet stream to the proper stage on the tower. This inlet stream is attached to Stage 5, the top stage. This inlet stream is the contaminated water.

The Add-stream action is still active, so this is a good opportunity to create the remaining streams

- ✓ Repeat the last step and add a stream to the very bottom inlet of the tower.

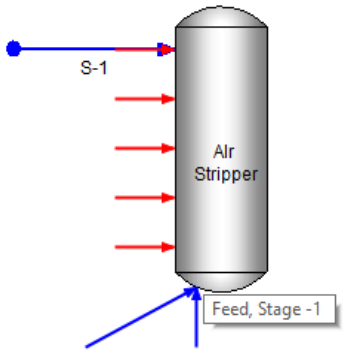


Figure 11-10 – Adding an inlet stream to the bottom of the tower. This is the Air inlet

Lastly, create the two outlet streams.

- ✓ With the Add Stream function still active, mouse over the top of the tower to activate the red arrows.
- ✓ Click on the tower top where the vertical red arrow is exiting. Click a second time somewhere above this location. This is the To Burner vent stream.

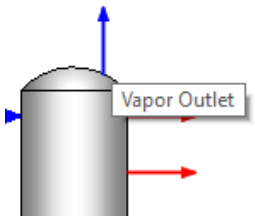


Figure 11-11-Adding the vent stream

- ✓ Lastly, mouse over the tower bottom section to activate the vertical-down arrow. Click at this point on the column and then again click below it. This creates the Clean Water stream.

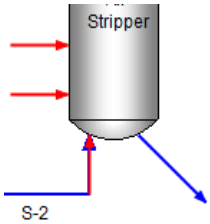


Figure 11-12- Adding the bottoms stream

- ✓ Press the ESC key to deactivate the Add Stream button.

The Add Stream mode stays active until the ESC key is pressed, or the arrow button is selected, or if the Add Stream button is clicked a second time.

- ✓ Double click on the first stream and label it Contaminated Water.

- ✓ Double-click on the bottom inlet stream and label it Air.
- ✓ Repeat this for the last two streams; label the top outlet To Burner and bottom outlet Clean water.

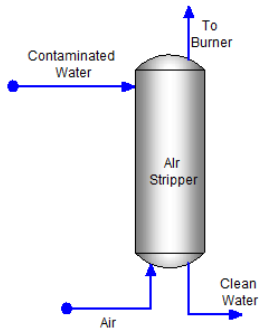


Figure 11-13- Names added to the stripper block

Modifying the unit set of the inlet streams before entering their compositions

The compositions of the two inlet streams are shown in the table below. Notice that each stream uses different inflow units (L/hr vs m3/hr) and composition basis (ppm vs. mole%). Therefore, before adding these compositions, the default stream units of moles needs to be modified.

	Contaminated Water	**Air**
Temperature (C)	13	20
Pressure (atm)	1	1
Stream Amount	670 L/hr	1500 m3/hr
H2O	999404 ppm	2.0 mole%
Benzene	350.0	
Toluene	180.0	
Ethylbenzene	40.0	
o-Xylene	26.0	
Nitrogen		76.46
Oxygen		20.6
Carbon dioxide		0.04
Argon		0.09

Table 1-1 – Process Stream and Acid Waste stream compositions

Changing the Contaminated Water units

- ✓ Click on the Contaminated Water stream to access its Properties panel.
- ✓ Click on the (mol/hr) units in the Stream Amount row. This will open the Units Manager.

You will make several changes to the Units manager window. They are to the Stream Amount, Inflows, Aqueous Composition, Vapor Composition, and Mass Fraction rows.

Edit Units - Contaminated Water

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Stream Amount	Volume	L/hr
Inflows	Mass Fraction	ppm (mass)
Output variables		
Aqueous Composition	Mass Fraction	ppm (mass)
Vapor Composition	Mole Fraction	mole %
Solid Composition	Moles	mol/hr
2nd Liquid Composition	Moles	mol/hr
Total Composition	Moles	mol/hr
Basis options		
Moles		mol/hr
Mass		g/hr
Volume		L/hr
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		ppm (mass)
Mole Fraction		mole %

Figure 11-14 – The Units Manager window for the Contaminated Water, after it has been modified. These will be the same units used for the Clean water outlet stream

- ✓ Change the Stream Amount Basis from Moles to Volume.
- ✓ Change the Inflows basis from moles to Mass Fraction.
- ✓ Change the Aqueous Composition Basis from moles to Mass Fraction.
- ✓ Change the Vapor composition basis from moles to Mole Fraction.
- ✓ Change the Mass Fraction Units from Mass% to ppm (mass).
- ✓ Press OK when done.

Changing the Air stream units

You will now change the units for the Air stream.

- ✓ Click on the Air stream to access the Properties panel.
- ✓ Repeat the steps from above; click on the Stream Amount unit (mol/hr) to open the Units Manager editor.
- ✓ Make the following changes to the window:

Parameter	Basis or unit
Stream Amount	Volume
Inflows	Mole Fraction
Vapor Composition	Mole Fraction
Volume units	m3/hr

Table 1-2 – the list of modifications made to the units for the Air stream

When completed, the Units Editor window should look like this:

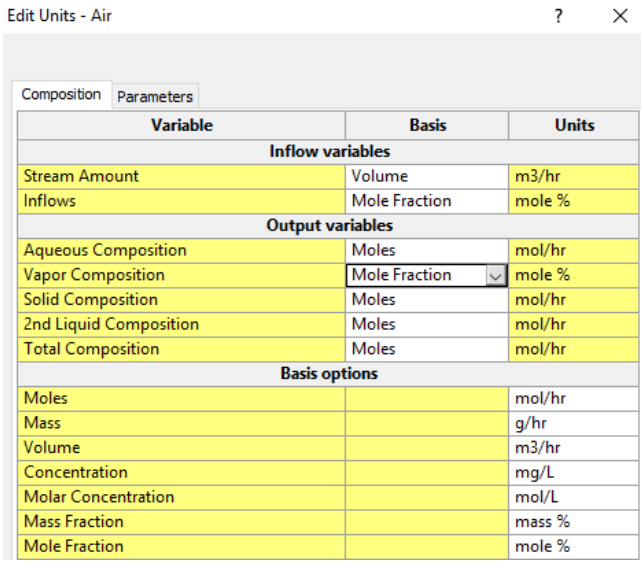


Figure 11-15 – The Units Manager window for the Air inlet stream after it has been modified. These will be the same units used for the To Burner outlet stream.

Changing the To Burner units

You also need to modify the To Burner stream units similar to the Air units; both are vapor phases. However, because the stream has yet to be calculated, there are no variables with units to click on. Therefore, the Units Editor must be accessed through the toolbar.

- ✓ Click on the To Burner stream.
- ✓ Click on the Units Manager button in the toolbar - .
- ✓ Select the Customize button to open the Units Manager Editor.

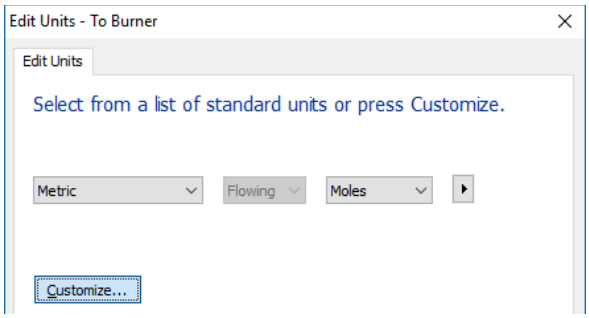


Figure 11-16 – The main Units Manager window accessed from the toolbar. The default Basis for Flowsheet ESP is Metric-Flowing-Moles. The Customize button allows the user to Edit the units for a stream, block, or Callout object.

- ✓ Make the following changes:

Parameter	Basis or unit
Stream Amount	Volume
Vapor Composition	Mole Fraction
Volume units	m3/hr

Table 1-3 – the list of modifications made to the To Burner units

When completed, the Units Editor window should look like this:

Edit Units - To Burner

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Stream Amount	Volume	m3/hr
Inflows	Moles	mol/hr
Output variables		
Aqueous Composition	Moles	mol/hr
Vapor Composition	Mole Fraction	mole %
Solid Composition	Moles	mol/hr
2nd Liquid Composition	Moles	mol/hr
Total Composition	Moles	mol/hr
Basis options		
Moles		mol/hr
Mass		g/hr
Volume		m3/hr
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		mass %
Mole Fraction		mole %

Figure 11-17 – The Units Manager window for the To Burner stream after it has been modified.

Changing the Clean Water units

Lastly, you will change the units of the Clean Water stream so that they match the Contaminated water units. Once again, to activate the units of an uncalculated stream, you need to open the Units Manager from the toolbar.

- ✓ Click on the Clean Water stream.
- ✓ Click on the Units Manager Button in the Toolbar.
- ✓ Click on the Customize button to open the Units Editor window.
- ✓ Make the following changes:

Parameter	Basis or unit
Stream Amount	Volume
Aqueous Composition	Mass Fraction
Total Composition	Mass Fraction
Mass Fraction units	ppm (mass)

Table 1-4 – the list of modifications made to the To Burner units

When completed, the Units editor window should look like this:

Edit Units - Clean Water

Composition | Parameters

Variable	Basis	Units
Inflow variables		
Stream Amount	Volume	L/hr
Inflows	Moles	mol/hr
Output variables		
Aqueous Composition	Mass Fraction	ppm (mass)
Vapor Composition	Moles	mol/hr
Solid Composition	Moles	mol/hr
2nd Liquid Composition	Moles	mol/hr
Total Composition	Mass Fraction	ppm (mass)
Basis options		
Moles		mol/hr
Mass		g/hr
Volume		L/hr
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		ppm (mass)
Mole Fraction		mole %

Figure 11-18 – The Units Manager window for the Clean Water stream after it has been modified.

Entering the composition of the contaminated water and the air streams

We are now ready to enter the conditions, flow rates, and compositions for the two inlet streams.

- ✓ Click on the Contaminated Water stream to access the Properties panel.
- ✓ Use the information in Table 1.1 above to enter the conditions, flow rate, and composition of the Contaminated Water.
- ✓ Repeat this for the Air stream.

When finished, the two Properties panels should look like the screenshots below:

Properties

Contaminated Water

Definition | Calculated | General

Parameters	
Temperature (°C)	13.0
Pressure (atm)	1.0
Stream Amount (L/hr)	670.0

Inflows (ppm (mass))	
H2O	9.99404e5
C6H6	350.0
C7H8	180.0
C8H10 (Ethylbenzene)	40.0
C8H10 (o-Xylene)	26.0
N2	0.0
O2	0.0
CO2	0.0
Ar	0.0
Total	**1.0e6**

Properties

Air

Definition | Calculated | General

Parameters	
Temperature (°C)	20.0
Pressure (atm)	1.0
Stream Amount (m3/hr)	10.0

Inflows (mole %)	
H2O	2.0
C6H6	0.0
C7H8	0.0
C8H10 (Ethylbenzene)	0.0
C8H10 (o-Xylene)	0.0
N2	76.46
O2	20.6
CO2	0.04
Ar	0.9
Total	**100.0**

Figure 11-19 – The Properties panel for the Contaminated water and the Air streams after their compositions are entered.

The tower is now ready to calculate.

✓ Press the Calculate button -

The tower should converge within seconds. When it does you will see a pop-up window in the lower right confirming this.

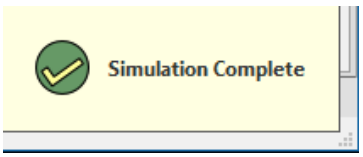


Figure 11-20 – The pop-up window indicating that the simulated converged.

✓ Click on the Clean Water stream and view the Calculated tab in the Properties Panel.

The Total Apparent flow should be present at the bottom of the panel. The units should be ppm (mass) that you modified previously.

Properties

Clean Water

Calculated | General

Stream Parameters	
Temperature (°C)	13.0069
Pressure (atm)	1.0
pH	5.5678
Moles, True (mol/hr	37155.7
Moles, Apparent (m	37155.7
Mass (g/hr)	6.69385e5
Volume (L/hr)	669.65
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %	0.0
Liquid-2 Frac., Appa	0.0

Total, Apparent (Molecular) (ppm (mass))	
H2O	9.99963e5
C6H6	5.37022
CO2	0.973858
C8H10 (Ethylbenzen	0.342357
Ar	0.620031
N2	16.897
O2	10.3922
C8H10 (o-Xylene)	0.0576762
C7H8	3.20829

Figure 11-21 – The Properties panel for the Clean Water stream showing the stream parameters and composition. Approximately 9 ppm BTEX remains in the water, including 5.4 ppm Benzene.

The calculated BTEX components in the Clean Water sum to ~9 ppm, inciding 5.4 ppm benzene. The inflow BTEX is 596 ppm, and so the removal is approximately 98.4%. According to a 2005 USEPA-NPDES permit document[1] however, the proposed BTEX effluent limits are 100 µg/l, nearly one-hundred times less than the calculated values.

> EPA's "Model NPDES Permit for Discharges Resulting From The Cleanup of Gasoline Released From Underground Storage Tanks;" (June 1989), recommends a BTEX limit of 100 ug/L. This limit is based on the typical removal efficiency of 99.5% or better for BTEX using a commercially available air stripper unit. Based on EPA's model permit and the observed performance of control equipment at historical or existing cleanup sites in New England, EPA-NE is setting a technology based limit for BTEX at 100 ug/L.

This existing tower simulation, therefore, does not meet discharge limits. Either more stripper air is needed, more separation trays are needed, or possibly a combination of both.

[1] https://www3.epa.gov/region1/npdes/remediation/RGP2010_FactSheet_AttachmentA.pdf. Fact Sheet Attachment A: 2005 Remediation General Permit Fact Sheet Excerpts. Page 14 of 50.

Modifying the process to remove additional BTEX from the water

The simplest way to increase BTEX removal is to increase the Air flow rate. You will do that first. Following this, you will use the tower's Target Specification function to compute the required flow needed to achieve the 100µg/L BTEX limit.

Increase the air flow to 100 m3/hr

The current air flow is 10 m3/hr. You will increase this to 100 m3/hr.

- ✓ Click on the Air stream.
- ✓ Change the Stream Amount value from 10 m3/hr to 100 m3/hr.
- ✓ Calculate.
- ✓ Click on the Clean water stream and review the Total Apparent (molecular) composition section at the bottom of the Properties panel.

Total, Apparent (Molecular) (ppm (mass)	
H2O	9.99972e5
C6H6	9.85316e-5
CO2	0.956966
C8H10 (Ethylbenzene)	5.60629e-6
Ar	0.61249
N2	16.7155
O2	10.2651
C8H10 (o-Xylene)	8.18262e-7
C7H8	6.05174e-5

Figure 11-22 – The molecular composition of the Clean Water stream when the air flow is increased to 100 m3/hr. The BTEX concentration is now less than 1 ppb.

Based on this calculation, the 100 m3/hr Air Flow decreased the BTEX concentrations to 0.2 ppb, much lower than the 100 µg/L target limits. The 100 m3/hr flow is too much air. The Air Flow rate can be adjusted further until a 100 µg/L BTEX concentration is obtained, but this manual approach is laborious and slow. Instead, the tower's Target Specifications function can be used to find the proper Air Flow rate.

Setting the Specs/Control in the Tower to calculate air requirements

Several target specifications can be calculated automatically in a Tower. Examples include the amount of air required to produce a clean water with 100 µg/L BTEX, or the reboiler duty required to strip 90% acid gases like H_2S and CO_2 from a sour water stream. This feature is very useful, and instructions for using it are presented here.

- ✓ Click on the Air Stripper block to access its Properties panel.
- ✓ Click on the Spec./Controls Edit button in the Parameters section to access the tower Specifications.
- ✓ Click on the Add button in the upper right of the window to add a new tower specification.

The first adjustable term is the Spec. Variable. The default setting is temperature.

- ✓ Click on the Spec Variable button to access the list.

There are seven general Spec. Variables. The temperature of a stage can be set by adjusting the heat duty of an exchanger. Likewise, the vapor flow rate at a given stage can be fixed and temperature, heat-duty, or

inlet flow rate can be adjusted to achieve this vapor rate. In this case, you will select liquid composition since that will enable you to fix the BTEX concentration in the liquid exiting the bottom of the column.

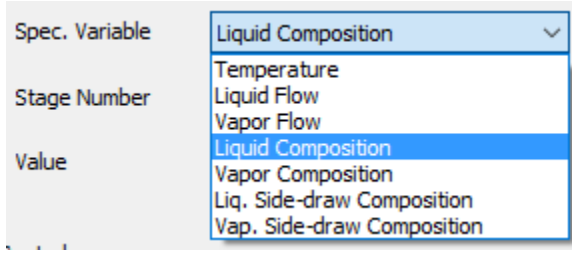


Figure 11-23 – The available Spec. variables in the tower block.

- ✓ Change the Spec variable to Liquid Composition.
- ✓ Confirm that the Stage Number is set to 1.
- ✓ Change the units to mass%.
- ✓ Enter a Value of 0.00001 (100 µg/L)

The Spec. Control window should look like this.

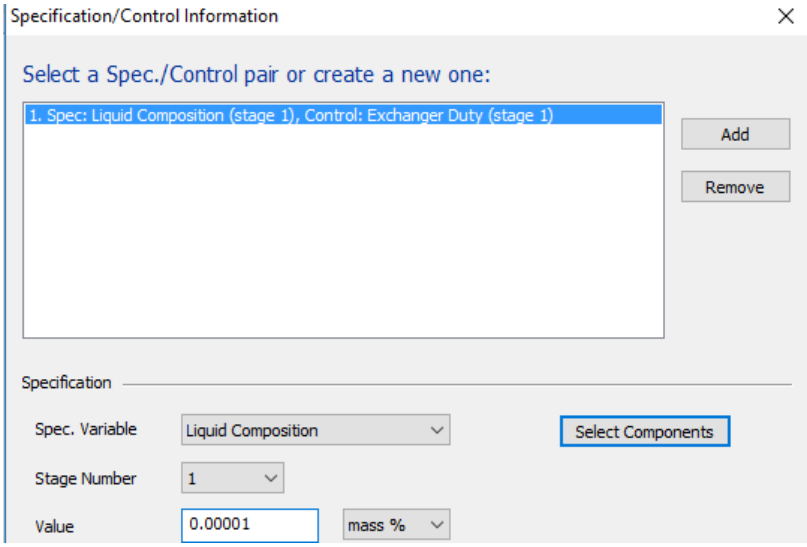


Figure 11-24 – The upper section of the Spec./Control window. The Liquid composition at stage 1 will be set to 0.00001 mass%. The specific species that will have a composition of 0.00001% has yet to be defined.

Upon pressing enter after entering the value, a Select Components window should open. It contains the list of components that will make up the 0.00001 mass%. In this case the components are the four BTEX organics.

If the Select Component window does not open automatically, then it can be opened using the Select Components button.

- ✓ Click on the Select Components button if a pop-up window does not appear. This window contains a list of dissolve aqueous components.
- ✓ Check the boxes for C6H6, C7H8, C8H10 (ethylbenzene), and C8H10 (o-xylene).

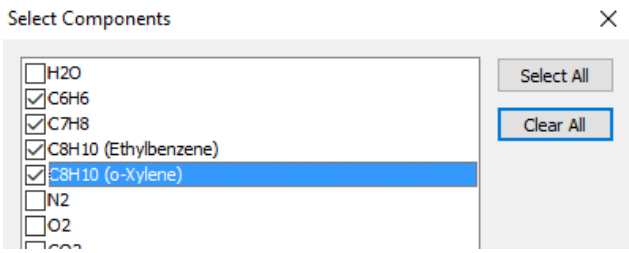


Figure 11-25 – The Select Components pop-up window. It contains the list of molecular species in the aqueous phase. The BTEX components are selected.

- ✓ Press OK to close the Select component window.

Once the target specifications are set, the adjustable variable can be selected. This is done in the lower half of the Spec./Control window.

- ✓ Change the Control variable to Feed Stream Flow.
- ✓ Change the Stage number to 1.

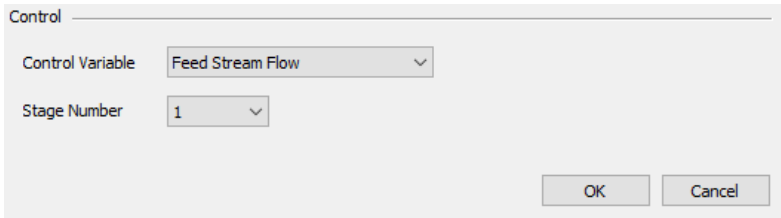


Figure 11-26 – The lower section of the Spec./Control window. The Air stream flow, which is the Feed Stream entering at stage 1 will be controlled to meet the 0.00001% target composition specification set in the upper section of this window.

The software now knows to adjust the inflow rate of the stream entering Stage 1 (the air stream) until the total composition of the four components selected, BTEX, amounts to 0.00001% (100 µg/L) in the liquid phase exiting stage 1 (Clean Water).

This is a good time to save the file.

- ✓ Save the file.

Calculate and review the results

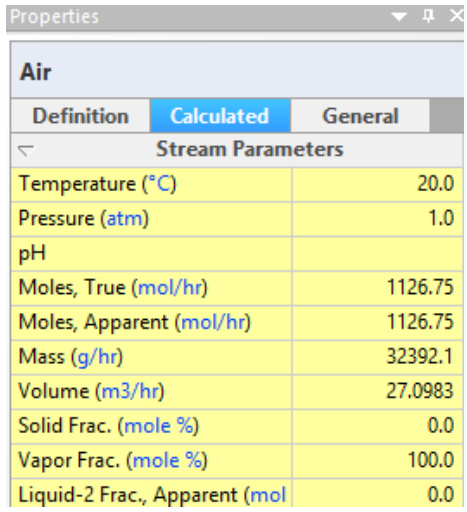
- ✓ Calculate.
- ✓ Click on the Clean Water stream to view the apparent molecular composition.

Total, Apparent (Molecular) (ppm (mass))	
H2O	9.99972e5
C6H6	0.0595219
CO2	0.970963
C8H10 (Ethylbenzene)	3.4892e-3
Ar	0.618775
N2	16.8673
O2	10.371
C8H10 (o-Xylene)	5.18132e-4
C7H8	0.0364707

Figure 11-27 – The lower section of the Properties panel for the Clean water stream after the tower specifications are set to fix the BTEX concentration in clean water to 100 µg/L. The target concentration for the BTEX organics is met.

The BTEX species sum up to 100 ppb in the clean water, meeting Target Specifications.

- ✓ Click on the Air stream and view the Calculated tab of the Properties panel.



Properties

Air

Definition | Calculated | General

Stream Parameters	
Temperature (°C)	20.0
Pressure (atm)	1.0
pH	
Moles, True (mol/hr)	1126.75
Moles, Apparent (mol/hr)	1126.75
Mass (g/hr)	32392.1
Volume (m3/hr)	27.0983
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	100.0
Liquid-2 Frac., Apparent (mol	0.0

Figure 11-28 – The Properties panel for the Air stream after the tower specifications are set to fix the BTEX concentration in clean water to 100 µg/L. The air flow requirement is 27.1 m3/hr.

The Air flow rate is 27.0983 m3/hr. The software adjusted this rate to its 4th decimal before converging on the target specification.

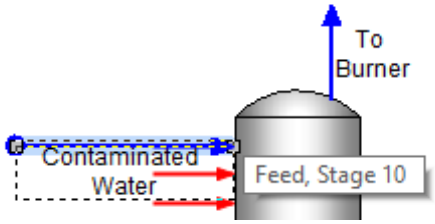
Increasing the Air flow rate is one way to meet discharge limits. This would require a larger air pump and higher electricity costs. By comparison, it may be possible to increase the number of tower stages and achieve the same discharge limits using less air. This may increase CapEx but may reduce long-term OpEx.

Increase the number of stages to improve BTEX-water separation

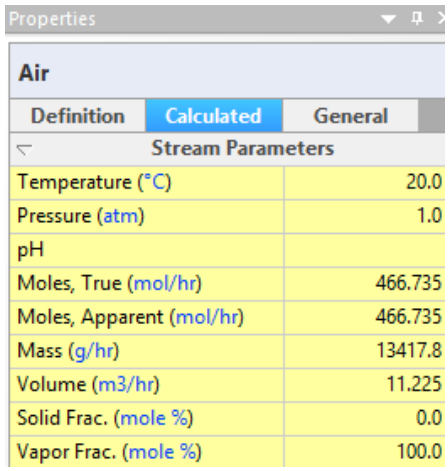
- ✓ Click on the Air stripper tower to access the Properties panel.
- ✓ Change the Number of stages to 10.

Now that the tower has ten stages, the contaminated water inlet is only half-way up the column. It needs to be reset.

- ✓ Reconnect the Contaminated water back to the top of the tower by delinking it from Feed Stage 5 and linking it to Feed Stage 10.



- ✓ Calculate.
- ✓ Click on the Air stream to view the updated air requirements.



Properties

Air

Definition | Calculated | General

Stream Parameters	
Temperature (°C)	20.0
Pressure (atm)	1.0
pH	
Moles, True (mol/hr)	466.735
Moles, Apparent (mol/hr)	466.735
Mass (g/hr)	13417.8
Volume (m3/hr)	11.225
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	100.0

Figure 11-29 - The Properties panel for the Air stream after the number of tower stages is increased to 10. The calculated air flow requirement is 11.2 m3/hr

The doubling of stages decreased the Air flow requirements by about 60%. Therefore, two potential approaches may be used to meet the discharge limits.

- ✓ Save the file. If you have not saved the case file yet, then name it something that you can find quickly because it will be used in the next several chapters.

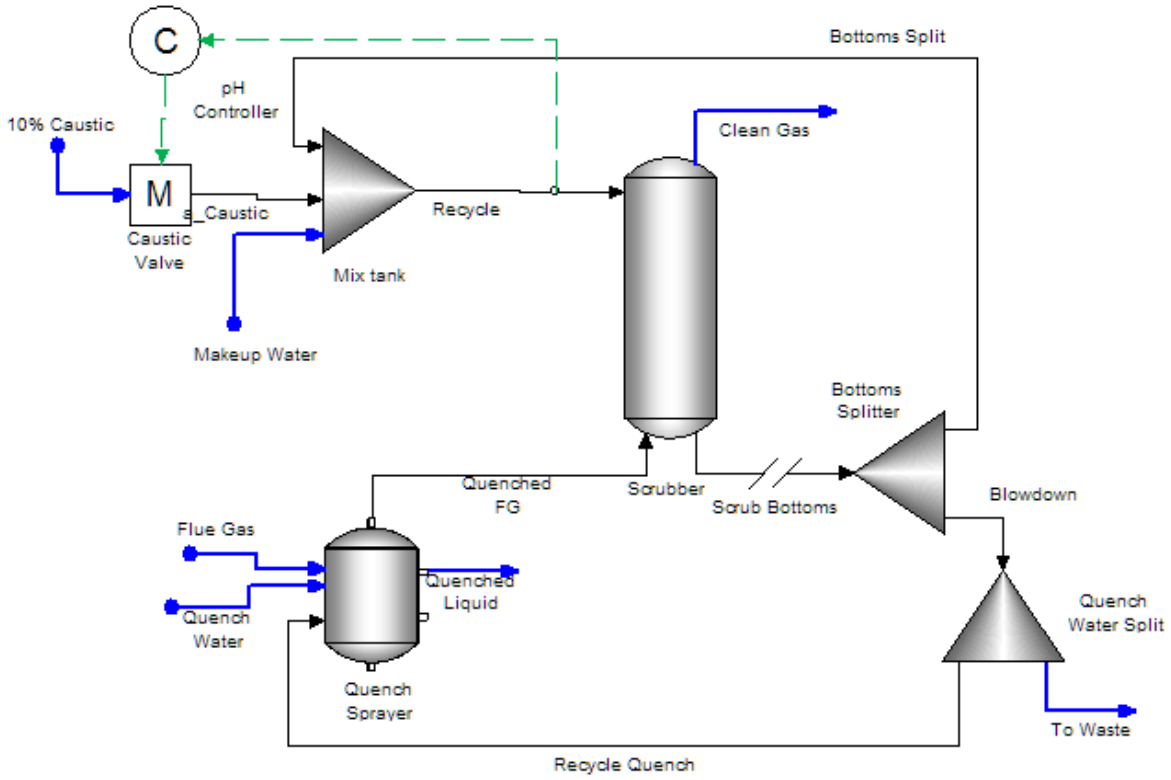
Summary

We have completed the first multi-stage tower case. This chapter presented the basic mechanics of building, converging and optimizing this block. In later chapters, more complex tower applications will be studied, including those linked to larger processes.

Chapter 12 Caustic Scrubber

The Application

The following case study is a caustic gas scrubber. It contains five units, the main scrubber, a quench sprayer, the caustic mix tank, and two flow splitters. This process removes reactive/acid components from a gas. The gas may be from combustion or from an industrial process. This example is for scrubbing a combustion gas that contains SO_2, HF, HCl, NO_2, and SO_3.

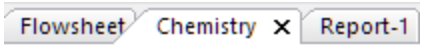


Creating a Chemistry Model

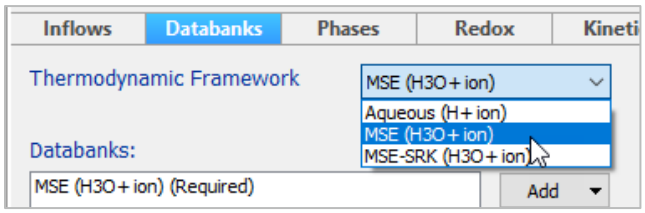
Creating and saving the file

Save the file with the name: Chapter12 Flue Gas Scrubber

Setting up the Chemistry model for a new Case

✓ Click on the **Chemistry** tab - 

✓ Select the MSE (H3O+ ion) and no private databases.



✓ Click on the **Inflows** tab.

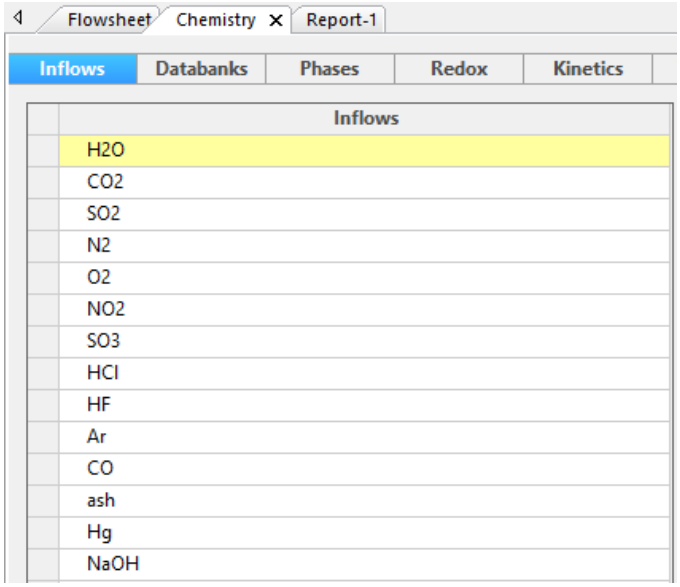
Adding the chemical inflows to your case file

✓ Enter the chemical components from the table below into the **Inflows** grid

Table 1 - Flue Gas Case study - Inlet Stream Compositions

Component	Flue Gas	Ash	Quench Water	10% Caustic	Makeup Water	Bottom Split
T, °C	170	170	25	25	25	50
P, barg	0.1	0.1	0.1	0	1	0
Total Flow	1.25E6 m3/hr	10000 kg/hr	30000 kg/hr	2 kg/hr	1 m3/hr	18000 kg/hr
Inflows	**mole%**	**mass, kg/h**	**mole%**	**mass%**	**mass%**	**mass, kg/h**
H2O	5.5225 (adjusted)		100	90	100	17000
CO2	11					
SO2	0.3					
N2	76					
O2	7					
NO2	0.06					
SO3	0.02					
HCl	0.001					
HF	0.0015					
Ar	0.09					
CO	0.005					
ash		10000				
Hg		0.1				
NaOH				10		1000

Your **inflows** should look like the image below

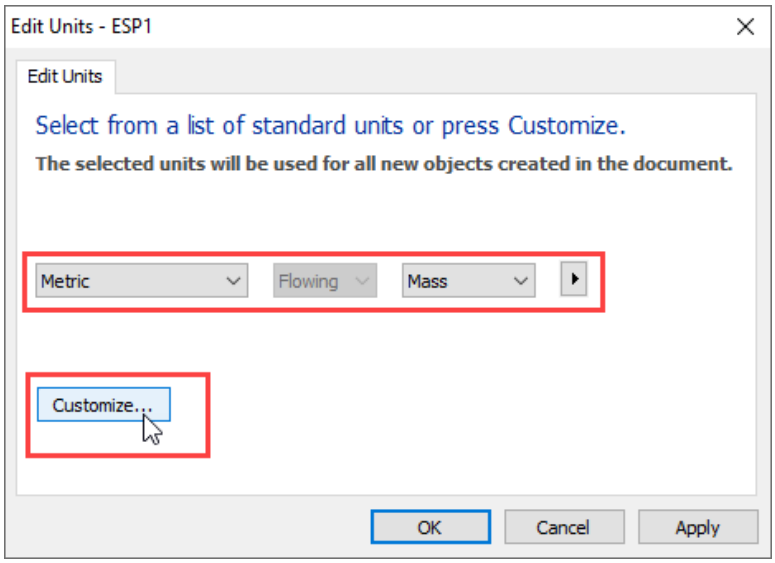


Set the Names and Units

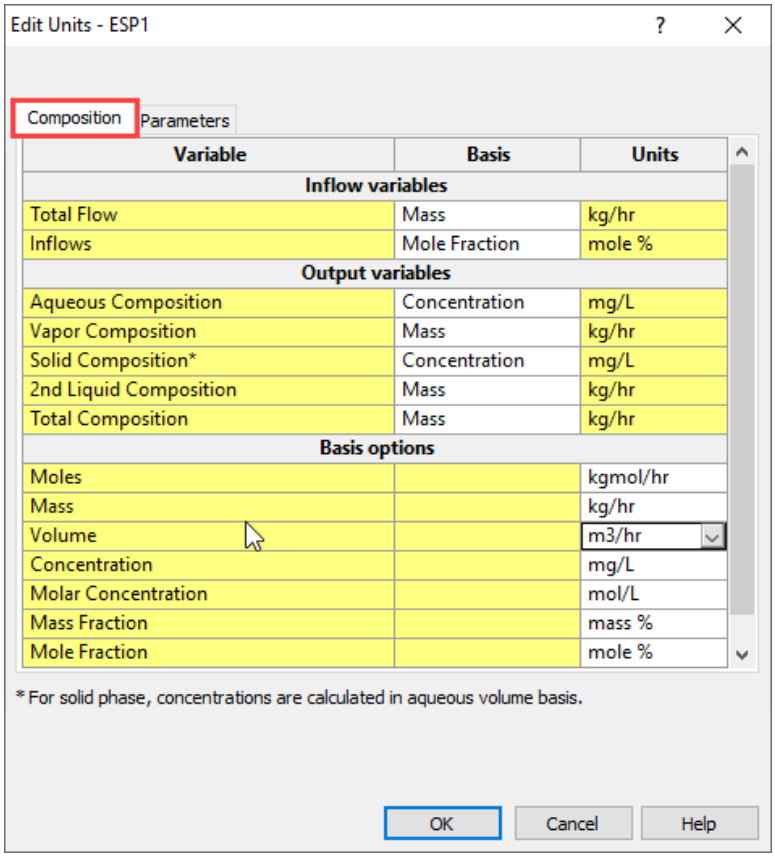
✓ Go to the **Flowsheet** tab

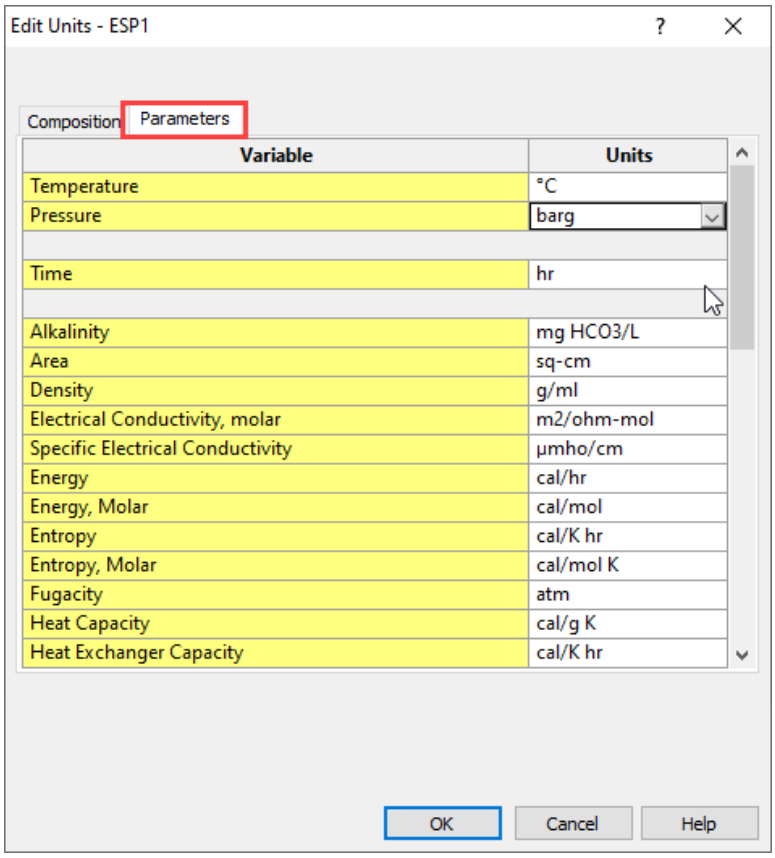
✓ Click on the names manager icon and set the Names to **Formula** view

✓ Click on the units manager icon and set the Units to Metric-Flowing-Mass



✓ Click on the **Customize** button and make the following changes


Edit Units - ESP1
Composition
Parameters
Variable
Basis
Units
Inflow variables
Total Flow
Mass
kg/hr
Inflows
Mole Fraction
mole %
Output variables
Aqueous Composition
Concentration
mg/L
Vapor Composition
Mass
kg/hr
Solid Composition*
Concentration
mg/L
2nd Liquid Composition
Mass
kg/hr
Total Composition
Mass
kg/hr
Basis options
Moles
kgmol/hr
Mass
kg/hr
Volume
m3/hr
Concentration
mg/L
Molar Concentration
mol/L
Mass Fraction
mass %
Mole Fraction
mole %
* For solid phase, concentrations are calculated in aqueous volume basis.
OK
Cancel
Help


Edit Units - ESP1
Composition
Parameters
Variable
Units
Temperature
°C
Pressure
barg
Time
hr
Alkalinity
mg HCO3/L
Area
sq-cm
Density
g/ml
Electrical Conductivity, molar
m2/ohm-mol
Specific Electrical Conductivity
µmho/cm
Energy
cal/hr
Energy, Molar
cal/mol
Entropy
cal/K hr
Entropy, Molar
cal/mol K
Fugacity
atm
Heat Capacity
cal/g K
Heat Exchanger Capacity
cal/K hr
OK
Cancel
Help

✓ Click **OK** to accept the changes and close the windows

Building the Process

Adding the Process Blocks

Adding the Quench Sprayer and the streams

✓ Click on the **Separator** object in the **Library** and drag it to the lower left of the window

✓ Label the object **Quench Sprayer**

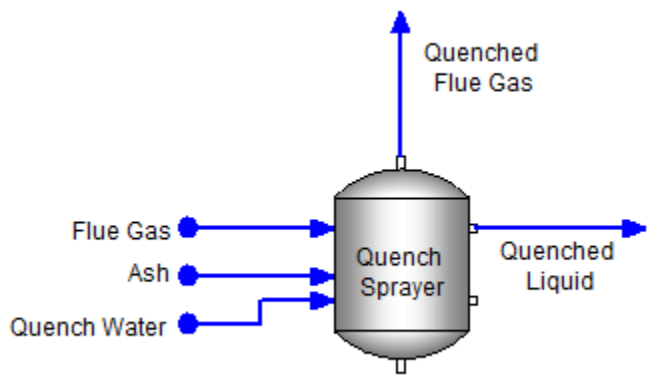
✓ Click on the **Add Stream** button -

✓ Add three **inlet** streams

✓ Add two **outlet** streams – the **vapor** and **liquid** outlet

✓ Label the three inlet streams **Flue Gas**, **Ash** and **Quench Water**

✓ Label the outlet streams, **Quenched Flue Gas** and **Quenched Liquid**



Quench Sprayer (separator) stream configuration

Entering the Quench Sprayer Specifications and the stream composition

✓ Click on the **Quench Sprayer**. Confirm that it is set to **Adiabatic** and **Min. Inlet Pressure**.

Equilibrium Calculation	
Calculation Type	Adiabatic
Pressure Spec.	Min. Inlet Pressure

Separator specifications

- ✓ Enter the **Flue Gas** composition from the table above. Be aware of the units
- ✓ Change the **Total Flow** units from kg/hr to m3/hr

Inflow variables		
Total Flow	Volume	m3/hr

- ✓ Normalize the **Flue Gas** stream using the **Makeup with Water** option

Normalization	
Normalize Fractions Using	Makeup with Water

Normalization of the gas phase to set total composition to 100%

Your stream should look like the image below

Flue Gas

Definition | Calculated | General

Show Ionic Input Options

Parameters	
Temperature (°C)	170.0
Pressure (barg)	0.1
Total Flow (m3/hr)	1.25e6

Inflows (mole %)	
H2O	5.5225
CO2	11.0
SO2	0.3
N2	76.0
O2	7.0
NO2	0.06
SO3	0.02
HCl	1.0e-3
HF	1.5e-3
Ar	0.09
CO	5.0e-3
ash	0.0
Hg	0.0
NaOH	0.0
Total	**100.0**

Normalization	
Normalize Fractions Using	Makeup with Water

- ✓ Enter the **Ash** composition.

✓ Change the **Inflows** units from **mole %** to **kg/hr**

Variable	Basis	Units
Inflow variables		
Total Flow	Mass	kg/hr
Inflows	Mass	kg/hr

✓ You will need to change the **Set Phase** option to **Solid only**

Advanced Options	
Set Phase	Solid Only

Set Phase to Solid Only so that the software can compute the water-free phase

Your stream should look like the image below

Ash

Definition | Calculated | General

Show Ionic Input Options

Parameters	
Temperature (°C)	170.0
Pressure (barg)	0.1
Total Flow (kg/hr)	10000.1

Inflows (kg/hr)	
H2O	0.0
CO2	0.0
SO2	0.0
N2	0.0
O2	0.0
NO2	0.0
SO3	0.0
HCl	0.0
HF	0.0
Ar	0.0
CO	0.0
ash	10000.0
Hg	0.1
NaOH	0.0
Total	**10000.1**

Advanced Options	
Set Phase	Solid Only
Chemistry Model	Chemistry (Default)

✓ Enter the **Quench Water** composition. No unit changes are needed.

Your streams should look like this

Quench Water

Definition | Calculated | General

Show Ionic Input Options

Parameters	
Temperature (°C)	25.0
Pressure (barg)	0.1
Total Flow (kg/hr)	30000.0

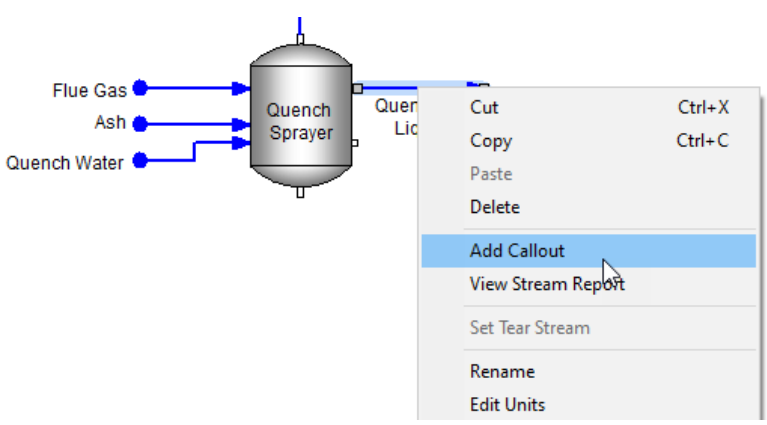
Inflows (mole %)	
H2O	100.0
CO2	0.0
SO2	0.0
N2	0.0
O2	0.0
NO2	0.0
SO3	0.0
HCl	0.0
HF	0.0
Ar	0.0
CO	0.0
ash	0.0
Hg	0.0
NaOH	0.0
Total	**100.0**

Inlet stream compositions and conditions

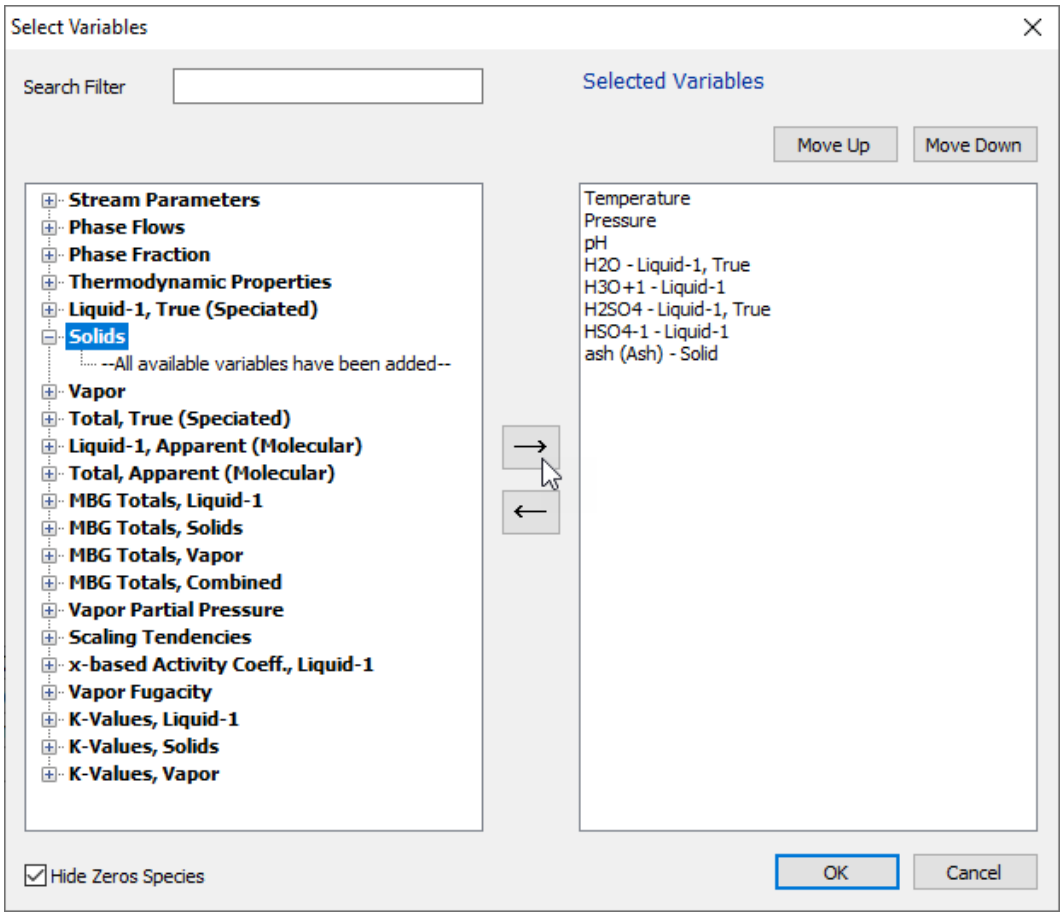
✓ **Run** the simulation

Adding Callout Tables

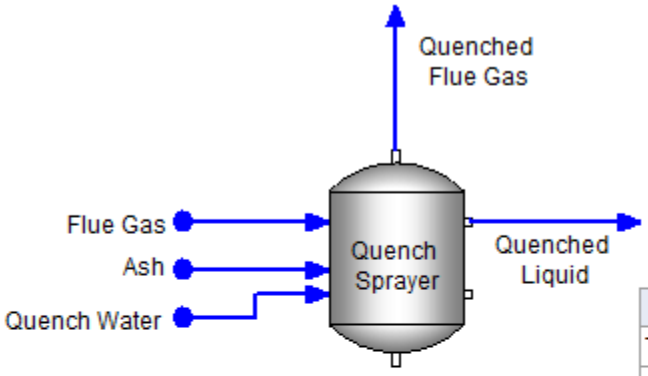
✓ Add a callout table to the **Quenched Liquid** stream (Right mouse click on the **Quenched Liquid** Stream – Select the **Add Callout** option)



- ✓ Double-click on the created table to open the variables list. This will open a new window
- ✓ Go to the **Phase Flows** category and expand it by using the '+' sign.
    - Select **Mass-Liquid-1.** Use the → to put them under the selected variables or simple double click.
- ✓ Go to the **Liquid-1, True (Speciated)**
    - Select H2O, H3O+1, H2SO4 and HSO4-1
- ✓ Go to the **Solids**
    - Select **Ash**



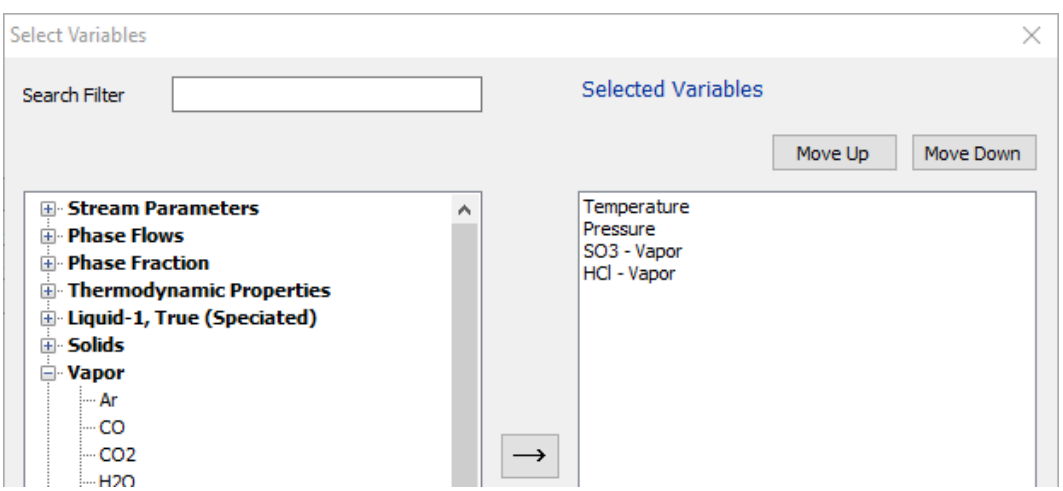
- ✓ Click **OK** to accept the changes and close the window



Quenched Liquid	
T (°C)	105.6
P (barg)	0.1
pH	-3.47596
Mass Liq1 (kg/hr)	1033.15
H2O Liq1, True (mg/L)	2.38458e5
H3O+1 Liq1 (mg/L)	2.07012e5
H2SO4 Liq1, True (mg/L)	54773.7
HSO4-1 Liq1 (mg/L)	1.01118e6
ash (Ash) (mg/L)	1.4847e7

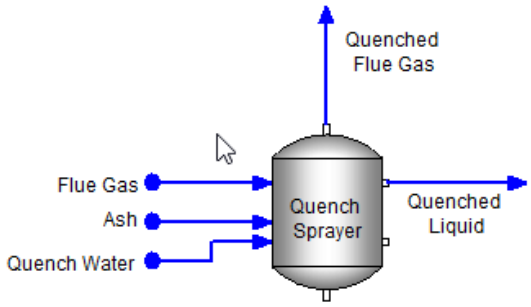
The quench water pH is negative, because of the high sulfuric acid concentration (about 80 wt%). SO_3 dissolved in water and hydrated to form H_2SO_4. There is another strong acid, HCl that is also being removed. The other reason is because nearly all the water evaporated during the quench. The flow is less than 1000 kg/hr (30,000 kg/hr quench water was added). This is the initial calculation output, and will not be the steady-state condition, because a portion of the quench water is recycled.

✓ Add a callout to the **Quenched Flue Gas** and bring in the variables **SO3** and **HCl** from the **Vapor** category and remove pH.



✓ Click **OK** to accept the changes and close the window

Quenched Flue Gas	
T (°C)	105.6
P (barg)	0.1
SO3 Vap (kg/hr)	3.72414e-5
HCl Vap (kg/hr)	13.7712



The SO3 is absorbed, but the HCl is still in the gas phase. Thus, the quench water flow and composition has not removed all the strong acids. For now, we can increase the quench water flow rate to see if the HCl can be absorbed.

✓ Change the **Quench Water** total flow to 50000 kg/hr and **recalculate**.

Quenched Flue Gas	
T (°C)	65.7563
P (barg)	0.1
SO3 Vap (kg/hr)	1.12574e-11
HCl Vap (kg/hr)	13.706

Quenched Liquid	
T (°C)	65.7563
P (barg)	0.1
pH	-1.70403
Mass Liq1 (kg/hr)	1615.55

This did not seem to help, why not. The short answer is this: nearly all the water evaporated, and the remaining water is insufficient to absorb the HCl. The positive is that now the quench flue gas temperature is down to 66 °C.

✓ Change the **Quench Water** total flow to 70000 kg/hr and **recalculate**

Quenched Flue Gas	
T (°C)	52.8697
P (barg)	0.1
SO3 Vap (kg/hr)	1.10098e-17
HCl Vap (kg/hr)	0.0799348

Quenched Liquid	
T (°C)	52.8697
P (barg)	0.1
pH	0.335337
Mass Liq1 (kg/hr)	15745.2

A threshold is passed. A substantial fraction of the input water remains a liquid, and the HCl vapor decreases by about 20x.

Add the Mix tank and caustic feed

✓ Add a **Manipulator** block and label it **Caustic Valve.** Place it above the **Quench Sprayer**.

✓ Add a **Mixer** and label it Mix tank

✓ Add four streams, label them as shown in the figure below.

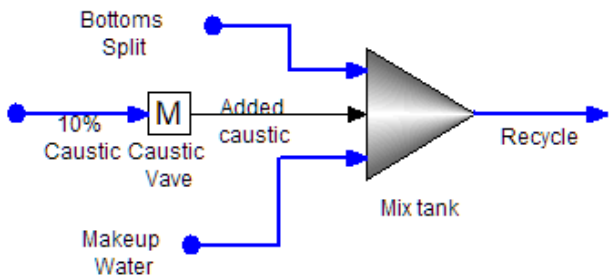


Figure 12-1- Caustic Mix section

Enter the stream compositions from the table below.

10% Caustic			Makeup Water			Bottoms Split		
Definition	Calculated	Ger	Definition	Calculated	Ger	Definition	Calculated	Gene
Parameters			Parameters			Parameters		
Temperature (°C)	25.0		Temperature (°C)	25.0		Temperature (°C)	25.0	
Pressure (barg)	0.1		Pressure (barg)	0.1		Pressure (barg)	0.1	
Total Flow (kg/hr	1.0		Total Flow (kg/hr	1.0		Total Flow (kg/hr	50000.0	
Inflows (mass %)			Inflows (mole %)			Inflows (kg/hr)		
H2O	90.0		H2O	100.0		H2O	50000.0	
CO2	0.0		CO2	0.0		CO2	0.0	
SO2	0.0		SO2	0.0		SO2	0.0	
N2	0.0		N2	0.0		N2	0.0	
O2	0.0		O2	0.0		O2	0.0	
NO2	0.0		NO2	0.0		NO2	0.0	
SO3	0.0		SO3	0.0		SO3	0.0	
HCl	0.0		HCl	0.0		HCl	0.0	
HF	0.0		HF	0.0		HF	0.0	
Ar	0.0		Ar	0.0		Ar	0.0	
CO	0.0		CO	0.0		CO	0.0	
ash	0.0		ash	0.0		ash	0.0	
Hg	0.0		Hg	0.0		Hg	0.0	
NaOH	10.0		NaOH	0.0		NaOH	0.0	
Total	**100.0**		**Total**	**100.0**		**Total**	**50000.0**	

Figure 12-2 - Stream Compositions for the caustic mixer section

Calculate

Add a callout to the Recycle stream and add the Mass Liq1 variable

Recycle	
T (°C)	25.0
P (barg)	0.1
pH	9.69044
Mass Liq1 (kg/hr)	50002.0

Add the scrubber

Add the Absorber block to the case, label it Scrubber

Enter the settings from the table below

Specifications	Scrubber
Calculation Method	Equilibrium
N. Stages	4
Condenser	No
Reboiler	No
Pressure – Stage 3	0.05 barg
Pressure – Stage 1	0.1 barg

Link the Recycle stream to Feed, Stage 4 inlet and Quench FG to the Feed, Stage -1 inlet

Add two additional streams, Clean Gas and Scrub Bottoms

Calculate

Add the Scrubber Bottoms callout, and show the Mass Liq1

Scrub Bottoms	
T (°C)	52.479
P (atm)	1.0987
pH	2.42924
Mass Liq1 (kg/hr)	51572.3

Add the Flow Splitters

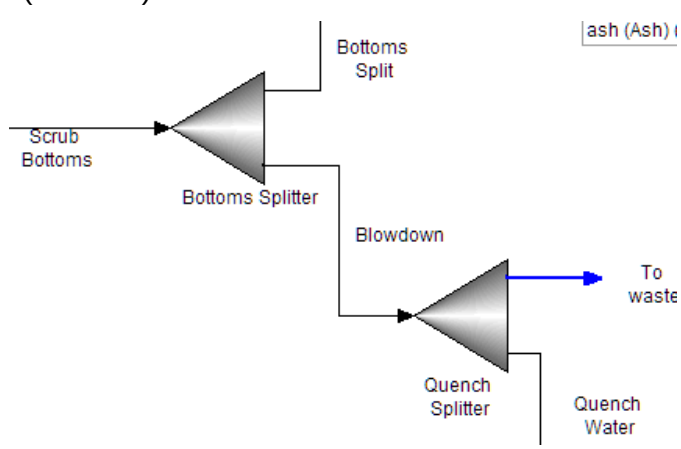
Add two splitters to the case, label them Bottoms Splitter and Quench Splitter

Link the scrubber bottoms to the splitter inlet.

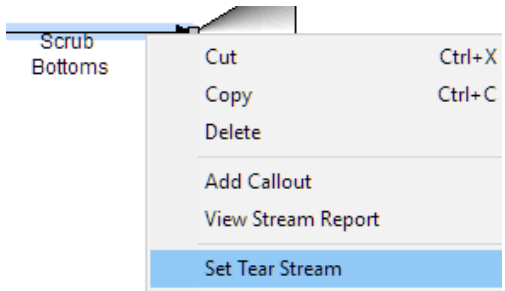
Link the Bottoms Split to the Bottom Splitter outlet

Link the Quench Water to the outlet of the Quench Splitter

Add two new streams, one linking the bottoms splitter to the quench splitter (label it blowdown), and the quench splitter outlet (to waste)



Set the Scrub Bottoms as the Tear stream: Right-mouse-click on the stream and select Set Tear



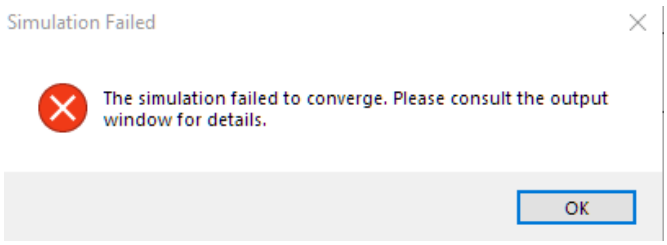
Set the split fractions for each unit. Use the following screens

Outlet	Fraction
Bottoms Split	0.92
Blowdown	0.08

Outlet	Fraction
Quench Water	0.9
To waste	0.1

Figure 12-3 - Split fractions for the Bottoms Splitter (left) and Quench Splitter (right)

Calculate



How to fix the simulation so that it converges

The case fails. The reason may not be clear, and so the first step is to investigate.

Add callout tables to Bottoms Split and Quench Water and include the Mass Liquid-1.

Bottoms Split	
T (°C)	52.479
P (barg)	0.100004
pH	2.42924
Mass Liq1 (kg/hr)	47446.5

Quench Water	
T (°C)	52.479
P (barg)	0.100004
pH	2.42924
Mass Liq1 (kg/hr)	3713.21

A few things to notice immediately:

- The quench water flow is <4000 kg/hr compared to the initial run of 50,000 kg/hr
- Consequently, the Quenched Liq pH is negative again.
- The tower failed on the first pass (see the Output tab for this). As a result, the simulation never got past the first pass
- Lastly, and most importantly, now that the Bottom's Split and Quench Water have been converted to internal streams, they are no longer an external source of water (80,000 kg/hr together).

Solutions:

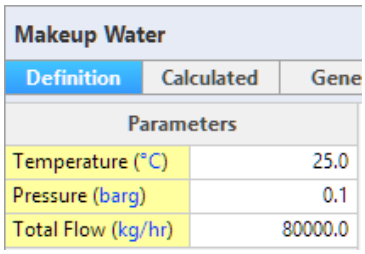
We converged the case before the recycles. It's not obvious what in the change caused the case to

fail, except that there is clearly no more water entering the system.

The first potential solution is to simply find a different external source for the 80,000 kg/hr water. The obvious choice is the makeup water stream.

The first step to resolving the problem is to increase the external flow rate.

Change the Makeup Water flow rate to 80000 kg/hr



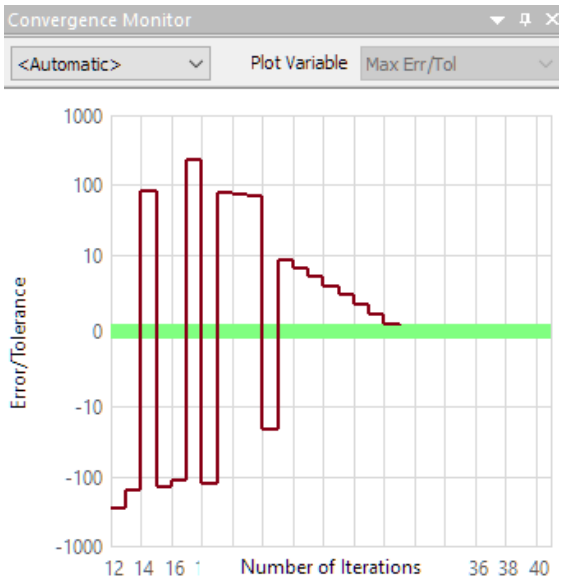
Makeup Water

Definition | Calculated | Gene

Parameters	
Temperature (°C)	25.0
Pressure (barg)	0.1
Total Flow (kg/hr)	80000.0

calculate

the case converges, in large part because an enormous amount of water is entering the tower. If you view the Convergence Monitor, you will see that many iterations were required to achieve final steady-state. Each iteration requires a column convergence, and so we can conclude in this case that adding excess water is a pathway to convergence.



We can also see that the Quenched FG contains a small amount of HCl, indicating that there is sufficient quench water available.

Add the Clean Gas callout and include the Vapor components, HF, Hg, NO2, and SO2 .

Change the vapor units to mole%

Clean Gas	
T (°C)	51.554
P (barg)	0.0500036
HF Vap (mole %)	1.14222e-4
Hg Vap (mole %)	1.21999e-6
NO2 Vap (mole %)	0.0555188
SO2 Vap (mole %)	0.277436

The SO2 concentration in the vapor is about 300 ppm, which is no different from the Flue gas. Thus, the purpose of the scrubber is not achieved. This is because the pH is too low, and molecular SO2 is not sufficiently soluble in water. It needs to be ionized to HSO3-1, which is achieved by adding an alkali, in this case NaOH.

Documenting and updating the existing convergence

There are several variables worth documenting before taking the next step. They provide a reference point for optimizing the process.

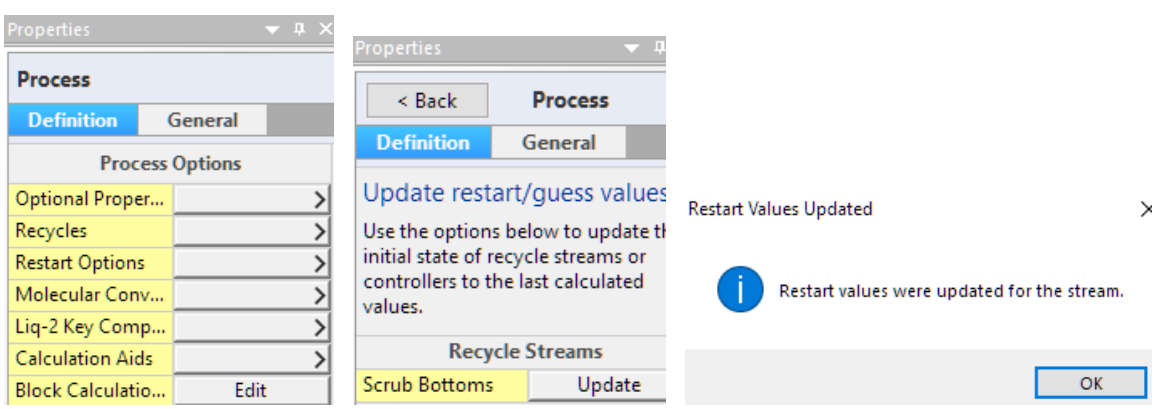
Document the following variables from your case

Stream	Variable		Value
Clean Gas	SO2 Vap	Mole%	0.28
Clean Gas	NO2 Vap	Mole%	0.056
Scrub Bottoms	pH		2.4
Quenched FG	HCl Vap	Kg/hr	0.069
Quenched Liq	pH		0.38
Recycle	pH		2.46
Recycle	Mass Liq1	Kg/hr	1.03e6
Quench Water	Mass Liq1	Kg/hr	7.47e4

The other step to take is updating the recycle streams so that the calculations proceeds more swiftly.

Access the Process panel by clicking on any white area in the flowsheet.

Select Restart Option and click on the Update button.



Adjusting the Caustic (NaOH) flow

Click on the Caustic valve and change the Factor, Flow to 10

Scan the documented variables, and see if there are substantial changes. Use the Clean Gas SO2

Vap or the Scrub Bottoms pH.

The changes are negligible, and so the NaOH increase was not sufficient
Change the Caustic Valve Factor, Flow to 100, and monitor the Clean Gas SO2 Vap for changes

There is still no change in the SO2 Vap but the Scrub bot pH is increasing.
Once again, change the Caustic Valve Factor, Flow to 1000, and if necessary 10000 and 100000

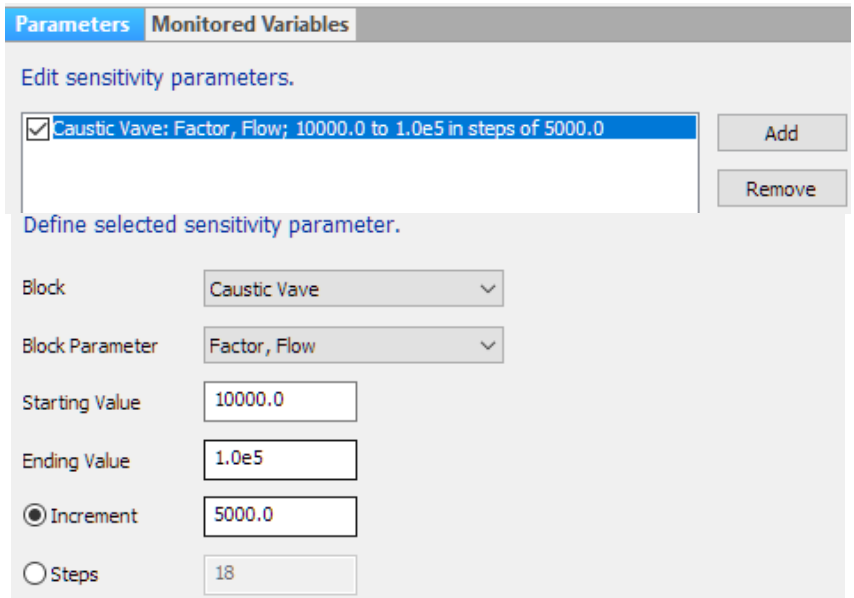
At 100000x the SO2 Vap reaches zero (effectively). The optimum multiplier, is somewhere 10000 and 100000 x.

Obtaining an optimum caustic addition

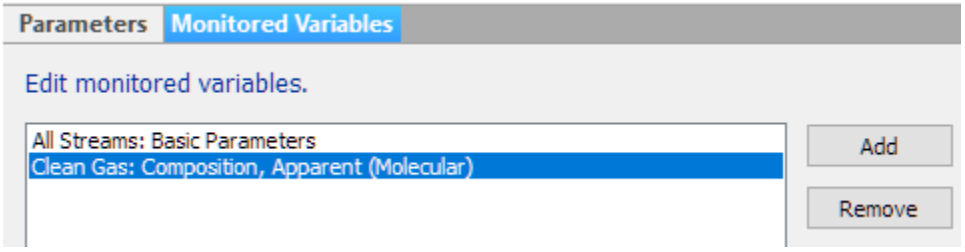
The continued manual changes to find an optimum is workable, but tedious. A better solution is to scan over this range. The Sensitivity Analysis is the best tool for this

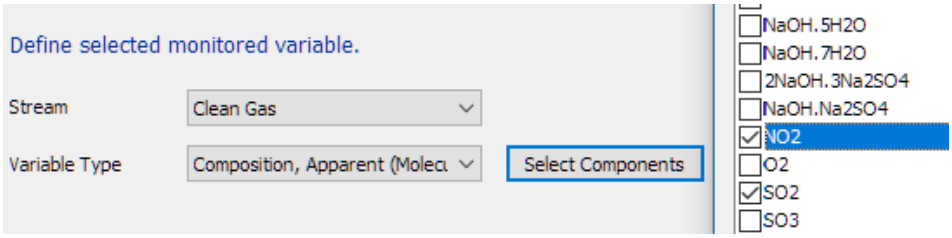
Add a Sensitivity Analysis from the Analysis menu item

Add a new sensitivity parameter with the following specs



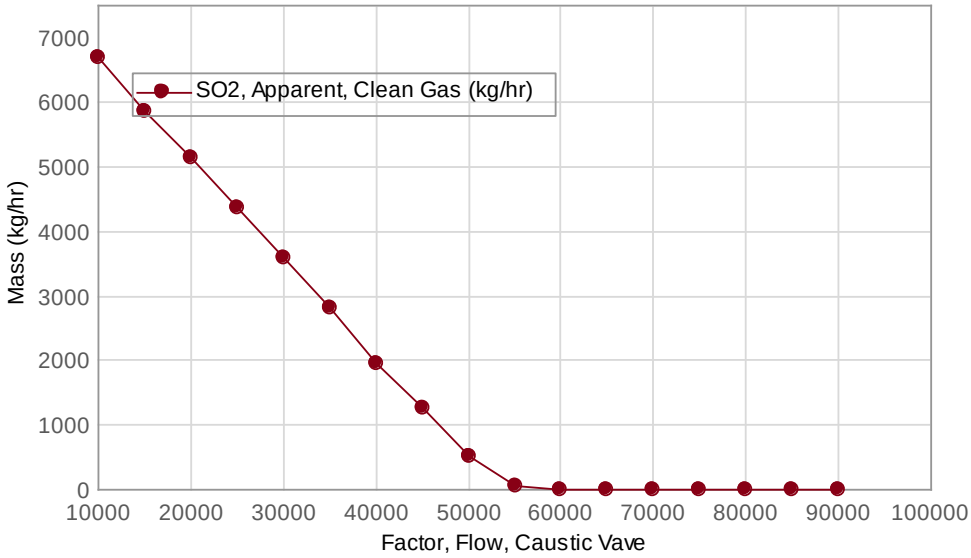
Set the monitored variables to the following (use the Select Components button to access the component list)





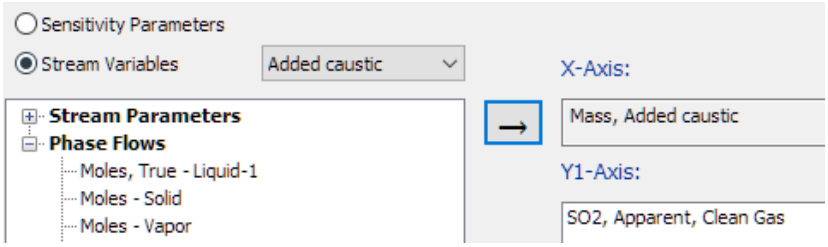
Calculate the case and view the SO2 exiting with the Clean Gas using the Plot tab

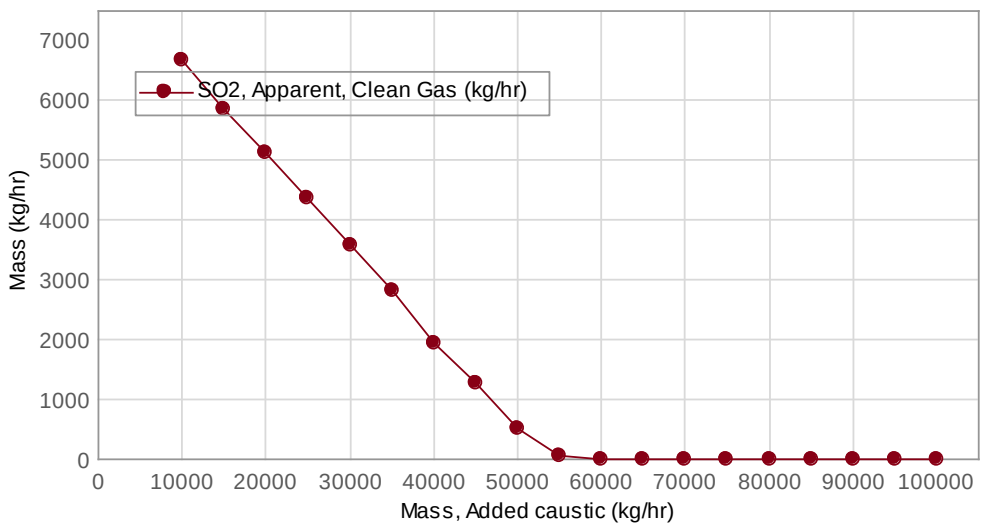
The SO2 decrease is linear with Caustic factor flow up to about 50000x. beyond this, the impact of additional caustic on SO2 removal decreases. Thus, it is reasonable first step to set the factor flow to 50,000x for now. It may not be the optimal, but it is at least the start for optimizing.



Factor Flow is directly related to the 10% Caustic rate, but there is no compelling reason to do the math. Instead, the rate of 10% caustic should replace this variable.

Click on the Select Data button, select the Added Caustic stream, and add the variable Mass to the x-axis (it reads Mass, Added caustic).





Testing for the optimal water content

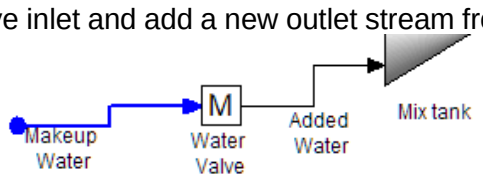
The Mass rate of 80000 kg/hr makeup water is based on getting the column to converge. It may not be the optimal rate. Once again, it is worth surveying over this variable to see if less water can be used while achieving the same SO2 removal.

Set the Caustic Valve Factor Flow to 50000 -

Parameters	
Manipulation Type	Total Flow
Factor, Flow	50000.0

Add a new Manipulate block to the case and label it Water Valve.

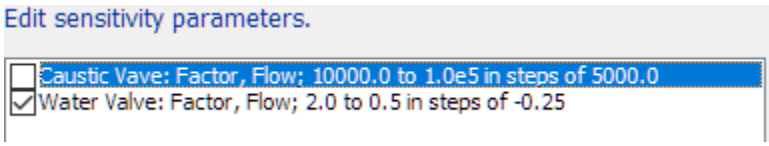
Link the Makeup water to the Water valve inlet and add a new outlet stream from the valve to the Mix tank. Label that stream Added Water -

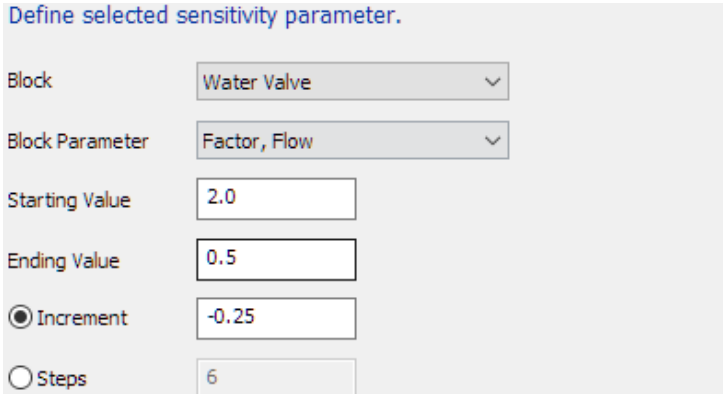


Return to the Sensitivity tab and uncheck the Caustic Valve box - Caustic Va. It's not needed for this next study.

add a new Sensitivity Parameter

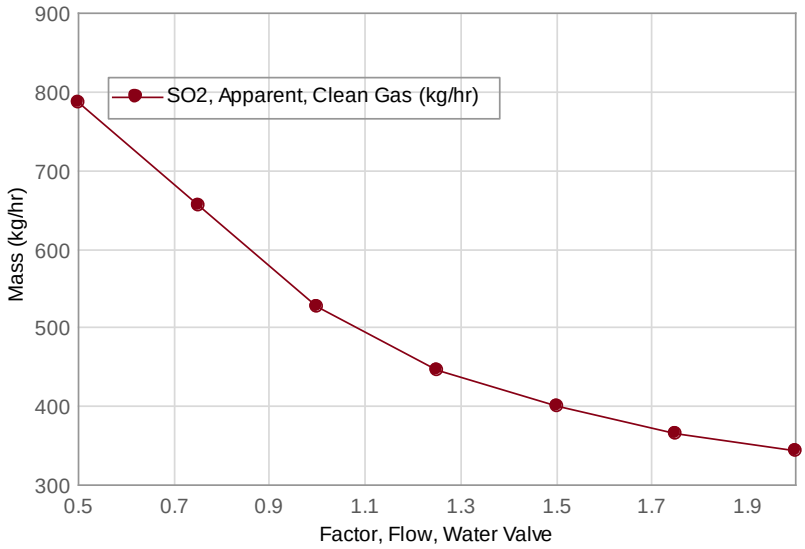
Set the parameter specifications to that shown in the images below





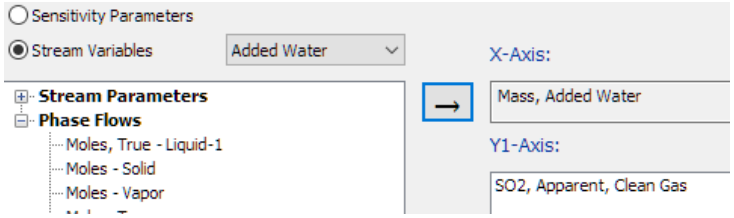
Calculate

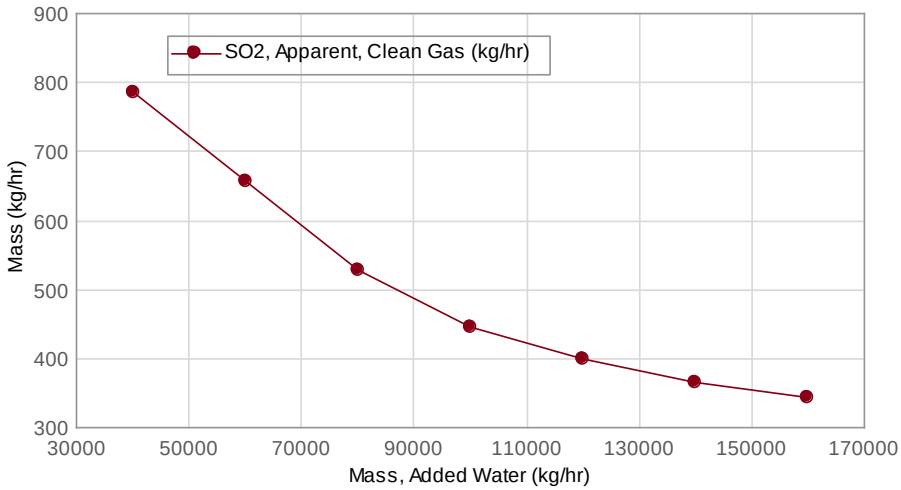
Notice that we're surveying in decreasing flow. This is because we're aware that excess water will not cause the column to fail, but insufficient water will. So, we're assured of seeing sufficient amount of results before. (in early versions of Flowsheet, the survey may proceed in increasing order).



Once again, factor flow is not the desired variable. The variable of interest is the added water.

Change the x-axis to be the Mass of the Added water stream.





The SO2 reduction is linear with the inlet water up to about 100,000 kg/hr. it decelerates more gradually beyond that.

Summary

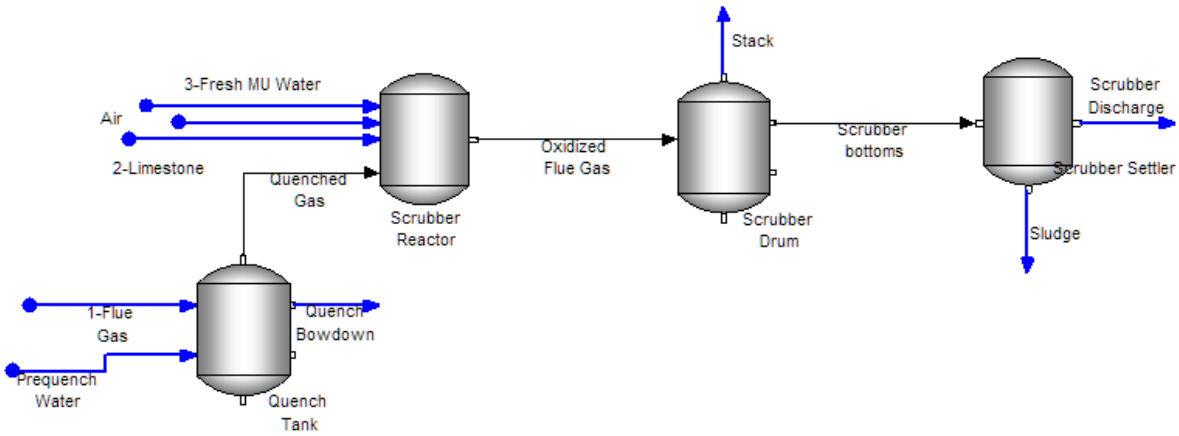
The purpose of this chapter was to describe how to create a scrubber unit, and how to troubleshoot it, if the case fails to converge. Lastly, by using the sensitivity analysis, a range of optimal conditions can be found. In this case, makeup water up to 90,000 kg/hr and up to 50,000 kg/hr of 10% Caustic would be sufficient to remove the SO2 and other acid gases from the flue.

The split fractions in the Bottoms splitter and the Quench splitter were not optimized. It is possible that the water and caustic use can be reduced by modifying these flow splits. The user is encouraged to look at these variables.

Chapter 13 Coal Boiler Flue Gas Scrubber

The Application

The following case study is a limestone flue gas scrubber. Coal-fired boiler flue gas is quenched and sent to the scrubber where it mixes with wet limestone and air. Sulfur dioxide is neutralized and oxidized to form sulfate, which precipitates as calcium sulfate. These solids are then separate in a settler.



This is the baseline case. It will be expanded to include additional solid-liquid separation units, process controllers, recycles and a more complex flue gas composition.

Creating the Chemistry Model

Creating and saving a new file

- ✓ Start Flowsheet ESP.

The software will open with an empty file.

- ✓ Save this empty file with the name: Coal boiler Flue Gas – Baseline Case.

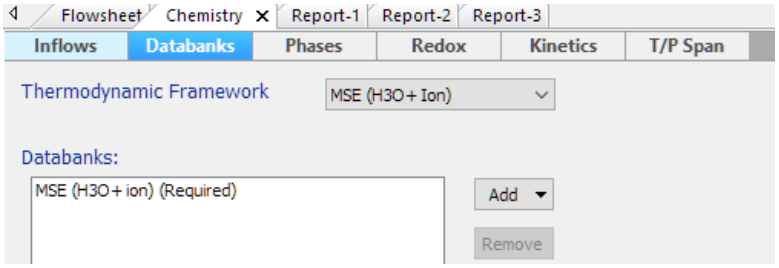
Adding Chemistry to the Model

When you start the software, the default view is the Flowsheet tab. Since this is a new case the first step is to create the chemistry model used in the case. Therefore, you need to start in the chemistry tab.

✓ Click on the Chemistry tab.

The Databanks sub-tab appears first for new case. This is because the thermodynamic framework (basis) and additional database(s) should be set before any components are added. This eliminates potential problems later.

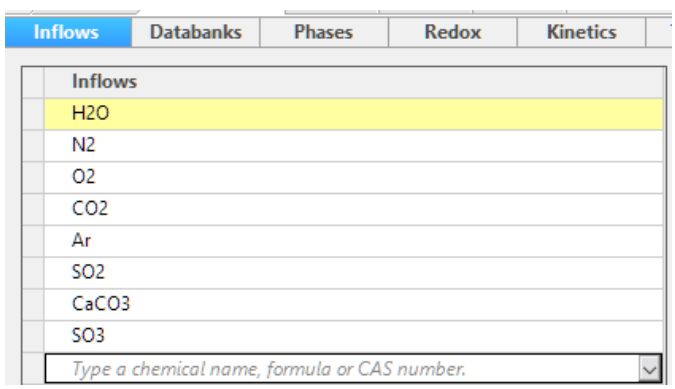
✓ Change the Thermodynamic framework to MSE(H3O+).



✓ Click on the Inflows sub tab.

✓ Enter the following seven components into the Inflows grid:

N2	SO2
O2	CaCO3
CO2	SO3
Ar	

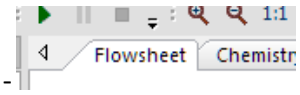


Building the process

Preparing the Flowsheet Units

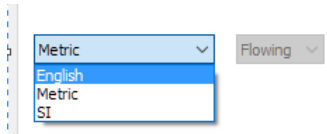
Changing the global units to English-Mass Fraction

The default Flowsheet ESP units are Metric-flowing-Moles. This particular case is a US coal-fired power plant that uses English units, and so the units require modification. The global units set will be changed from Metric to English and then specific units need to be changed, such as switching from hours to minutes.

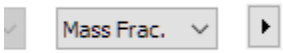
✓ Click on the Flowsheet tab - 

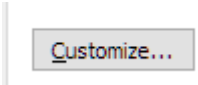
✓ Click on the Units Manager button in the Toolbar

✓ Change the Units set from Metric to English.



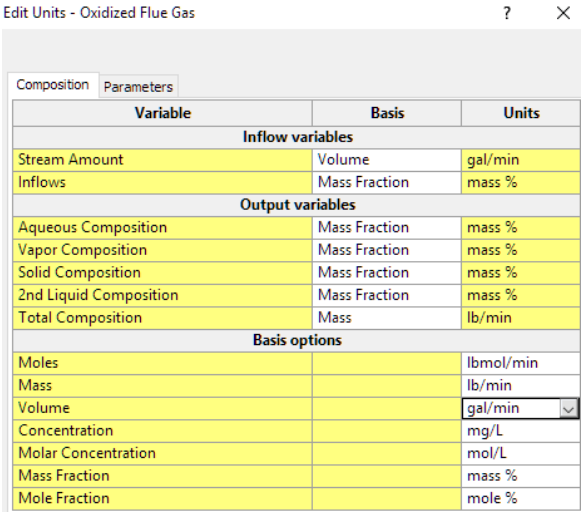
✓ Confirm that Mass Fraction is selected in the third drop down button. If not, then change it.



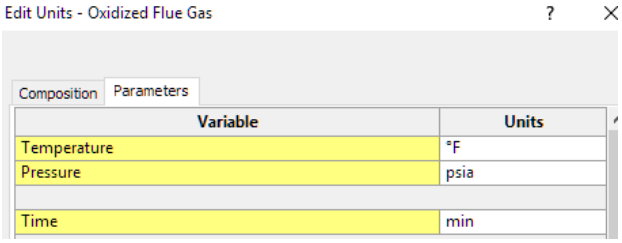
✓ Click on the Customize button to open the Units Editor. 

✓ Make the following changes.

Variable	Basis or Unit
Steam Amount	Volume
Total Composition	Mass
Volume	gal/
Mass Fraction	Mass%
Mole Fraction	Mole%
Time (Parameter tab)	min



Variable	Basis	Units
Inflow variables		
Stream Amount	Volume	gal/min
Inflows	Mass Fraction	mass %
Output variables		
Aqueous Composition	Mass Fraction	mass %
Vapor Composition	Mass Fraction	mass %
Solid Composition	Mass Fraction	mass %
2nd Liquid Composition	Mass Fraction	mass %
Total Composition	Mass	lb/min
Basis options		
Moles		lbmol/min
Mass		lb/min
Volume		gal/min
Concentration		mg/L
Molar Concentration		mol/L
Mass Fraction		mass %
Mole Fraction		mole %



Variable	Units
Temperature	°F
Pressure	psia
Time	min

Some streams are all vapor or all liquid, and several are mixed phase. Depending on the situation, vapor streams use both scfm & ppmV and liquid streams use both gal/hr & mg/l. The general changes you made here will require individual modifications later for specific streams.

✓ Press OK to close the Units Editor window and OK again to close the Units Manager.

External Inflows

Creating the external inflow streams

The baseline case contains five external streams representing the flue gas, quench water, oxidizing air, wet

limestone and makeup water. You will start the case by adding these streams. Then you will create the process blocks.

- ✓ Click on the Add Stream button in the Toolbar.
- ✓ Click anywhere on the flowsheet. This will activate the stream build action. Click a second time to set the end of the stream.

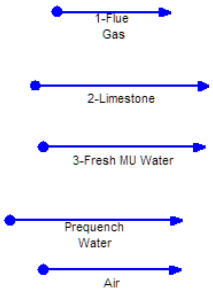
The Add Stream action remains active until the Esc key is pressed or another Toolbar button is selected. Since the Add Stream is still active, we can create the remaining streams.

- ✓ Create four more streams.
- ✓ Press the Esc key to deactivate the stream build action.
- ✓ Double-click on one of the streams to edit the Stream name.
- ✓ Label the first stream 1-Flue Gas.
- ✓ Label the remaining streams 2-Limestone, 3-Fresh MU Water, Prequench Water, and Air.

Entering the stream compositions

The table below contains the inflow composition for each of the five streams. *Notice that the units for flowrate and composition are different in some cases.* You will therefore edits the stream's units before entering the data.

Property	1-Flue Gas	2-Limestone	3-Fresh MU Water	Prequench Water	Air
Temperature (°F)	330	68	68	70	70
Pressure (psia)	14.696	14.696	14.696	14.696	14.696
Stream Amount	1280 Mft3/min	79.2 gal/min	105 gal/min	481.7 gal/min	34110 ft3/min
Inflows	mole %	mass %	mass %	mass %	mole %
H2O	10.53	66.6	100	100	2
N2	71.5				76.4
O2	10	0	0	0	20.6
CO2	7	0	0	0	0.04
Ar	0.9	0	0	0	0.9
SO2	0.0697	0	0	0	0
CaCO3	0	33.4	0	0	0
SO3	0	0	0	0	0



As you enter the stream compositions, you will see warnings about the composition not equaling 100%. This warning appears in the Error tab at the bottom of the screen and as red text in the Total row of the Properties panel. However, an exact 100% sum is not required and the software will function normally. The

warning is provided as a reminder to check the composition.

Flue Gas composition

- ✓ Click on the Flue Gas stream to access its Properties panel.
- ✓ Click on the Stream Amount units link to open the Units Editor.
- ✓ Change the Volume row from gal/min to Mft3/min.
- ✓ Change the Inflow row from Mass Fraction to Mole Fraction.
- ✓ Enter the data from the above table.

Properties

1-Flue Gas

Definition | Calculated | Gen

Parameters	
Temperature (°F)	330.0
Pressure (psia)	14.696
Stream Amount (Mft3/	1280.0

Inflows (mole %)	
H2O	10.53
N2	72.9
O2	8.6
CO2	7.0
Ar	0.9
SO2	0.0697
CaCO3	0.0
SO3	0.0
Total	99.9997

Remaining external streams

- ✓ Repeat this step for the remaining streams, remembering to modify units for Stream Amount or Inflows where necessary.

Properties

2-Limestone

Definition | Calculated | Ger

Parameters	
Temperature (°F)	68.0
Pressure (psia)	14.696
Stream Amount (g	79.2

Inflows (mass %)	
H2O	66.6
N2	0.0
O2	0.0
CO2	0.0
Ar	0.0
SO2	0.0
CaCO3	33.4
SO3	0.0
Total	**100.0**

Properties

3-Fresh MU Water

Definition | Calculated | Gen

Parameters	
Temperature (°F)	68.0
Pressure (psia)	14.696
Stream Amount (g	105.0

Inflows (mass %)	
H2O	100.0
N2	0.0
O2	0.0
CO2	0.0
Ar	0.0
SO2	0.0
CaCO3	0.0
SO3	0.0
Total	**100.0**

Properties

Prequench Water

Definition | Calculated | Gen

Parameters	
Temperature (°F)	70.0
Pressure (psia)	14.696
Stream Amount (g	481.7

Inflows (mass %)	
H2O	100.0
N2	0.0
O2	0.0
CO2	0.0
Ar	0.0
SO2	0.0
CaCO3	0.0
SO3	0.0
Total	**100.0**

Properties

Air

Definition | Calculated | Gen

Parameters	
Temperature (°F)	70.0
Pressure (psia)	14.696
Stream Amount (f	34110.0

Inflows (mole %)	
H2O	2.0
N2	76.4
O2	20.6
CO2	0.04
Ar	0.9
SO2	0.0
CaCO3	0.0
SO3	0.0
Total	99.94

Process Blocks

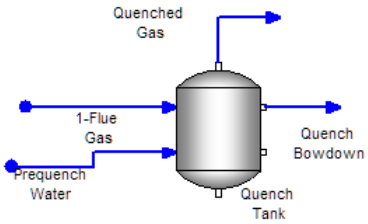
Adding a Quench Sprayer

There are four units in this baseline process: the Quench Sprayer, the scrubber (split into two units) and the settler. These units are linked in series and will therefore be created in flow order.

The Quench Sprayer is simulated using an adiabatic gas-liquid separator. There are two inlets, the flue gas and the quench water. The separator simulates the complete mixing of gas and liquid in a single stage.

- ✓ Click on the Separator object in the library and drag it to the lower left of the window.

- ✓ Label the object Quench Tank.
- ✓ Connect the 1-Flue Gas and Prequench Water streams as feeds to the tank.
- ✓ Click on the Add Stream button to activate the Stream action.
- ✓ Add new streams to the Quench vapor and Liquid outlets (the liquid outlet is at the upper right).
- ✓ Deactivate the Add Stream action using the Esc key.
- ✓ Double-click on each stream individually to rename them Quenched Gas and Quench Blowdown as shown.



Calculate and review results using Callouts

- ✓ Calculate the case – it should converge in seconds.
- ✓ You will see a pop-up with several warnings. Press OK to close this window.

You will use the Callout tables to review the results. These are customizable tables adjacent to a flowsheet object containing user-selected information.

- ✓ Right mouse-click on the Quenched Blowdown stream and select Add Callout from the dropdown list.

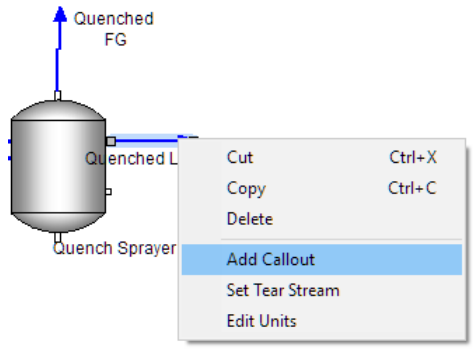


Figure 13-1 - The Add Callout action item

The default setting is for the callout to display the temperature, pressure, and pH. We are interested in pH (to see if any strong acid is present) and also the stream flow. That flow is not present, and so it will be added next.

- ✓ Double-click on the callout table to activate the Select Variable window.
- ✓ Expand the Phase Flows section.
- ✓ Add Volume Liq1 to the Selected field and then press OK to close the window.

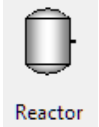
Quench Bowdown	
T (°F)	133.235
P (psia)	14.696
pH	2.83762
Volume Liq1 (gal/min)	135.383

The quench blowdown flow is 135 gpm. This compares to the Prequench Water flow of 482 gpm. The difference is evaporation. Note the outlet temperature is 133 F, representing evaporative cooling of the 330 F inlet flue gas.

Adding the Scrubber Reactor

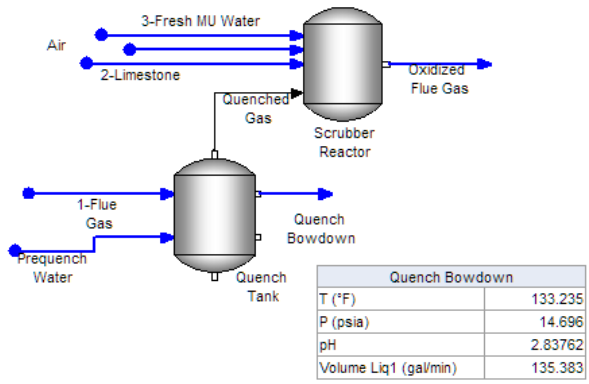
The Scrubber reactor represents the mass-transfer-limited and kinetic-limited oxidation elements of the overall Scrubbing process. Oxidation-Reduction is one of the standard OLI calculations, and these REDOX reactions are assumed to reach equilibrium. SO_2 oxidation, however, does not reach equilibrium. Rather, there are mass-transfer and kinetic limitations. The specific mechanism for both limits are not known here, and so simulating these reactions mechanistically is beyond the scope of this case. You will, therefore, estimate SO_2 to SO_3 oxidation using a conversion fraction. According to plant data, SO_2 removal is about 95%. This will be the conversion value.

- ✓ Click on the Reactor block in the Library.



- ✓ Drag it to the upper right of the Quench tank.
- ✓ Label it Scrubber Reactor.
- ✓ Link the Quenched Gas stream to the inlet of this block.

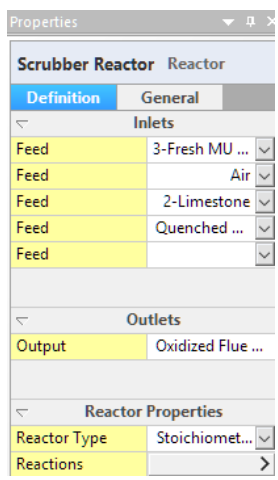
- ✓ Link the three other external streams you created earlier to this block: 3-Fresh MU Water, Air, and 2-Limestone.
- ✓ Click on the Add stream button and add an outlet stream to the Reactor block.
- ✓ Label this stream Oxidized Flue Gas.



- ✓ Click on the Scrubber Reactor block to access the Properties panel.

There is a section called Reactor Properties. It contains two entries, Reactor Type and Reactions. There are three reactor types, Kinetics, Stoichiometric Conversion, and Gibbs. You will use the Stoichiometric Conversion.

- ✓ Change the Reactor Type to Stoichiometric Conversion.
- ✓ The Reactions properties now appear.



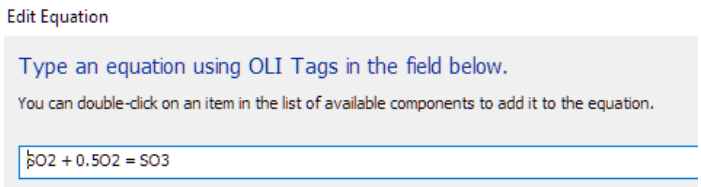
This instructs the software that you will create a chemical reaction and that the extent of the reaction will be fixed by a conversion value. That conversion value will be specific to a reactant, in this case the 95% conversion of SO2.

- ✓ Click on the Reactions button.
- ✓ Click on the Edit link to open the Reaction Editor.
- ✓ Click on the Add button.

The top field is empty. The following reaction will be added to it: SO2 + 0.5O2 = SO3

- ✓ Enter the above reaction in that field. Be careful to use the appropriate syntax and

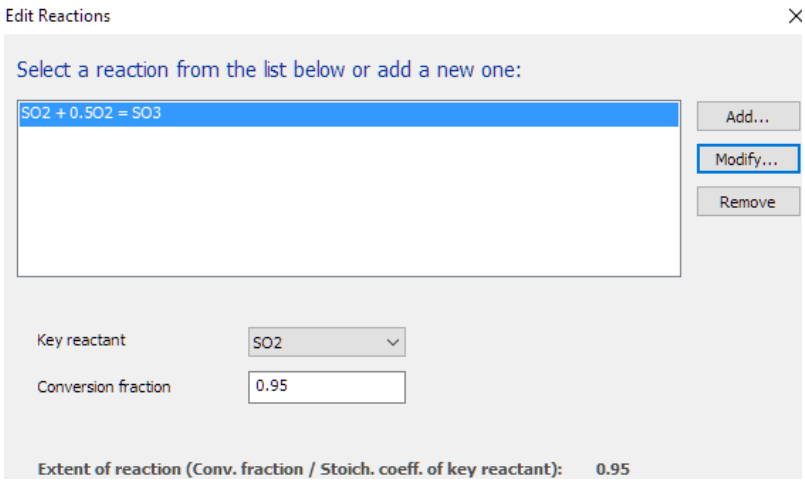
symbols. You can also use the available species in the list provided in the Editor.



- ✓ When completed, press OK to close the window.

The Main Reaction Editor contains two settings in the center of the window, Key Reactant and Conversion fraction.

- ✓ Set the Key reactant to SO2.
- ✓ Set the Conversion fraction to 0.95 and press OK.



The Reactor is complete and the partially-completed case is ready for a test calculation

- ✓ Calculate.

Comparing the SO2 flow upstream and downstream of the Scrubber Reactor

- ✓ Right-mouse-click on the Quench Gas stream and select Add Callout.
- ✓ Double-click on the Callout table to open the Variables window.
- ✓ Expand the "MBG Totals, Combined" category.
- ✓ Add S(+4) to the selected list.
- ✓ Remove the Pressure and pH variable from the Selected list.

Quenched Gas	
T (°F)	133.235
S(+4) (lb/min)	49.5437

Repeat these steps for the Oxidized Flue Gas stream.

- ✓ Right-mouse-click on the Oxidized Flue Gas stream and add the Callout.
- ✓ Double-click on the callout to open the Variables window.
- ✓ Open the "MBG Totals, Combined" group and add S(+4).

- ✓ Remove the Pressure variable and close the Variables window.

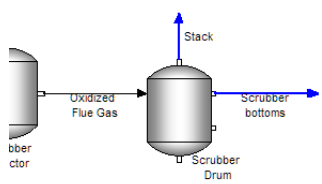
Oxidized Flue Gas	
T (°F)	132.467
pH	6.3236
S(+4) (lb/min)	2.47718

The S(+4) amount in the Quenched Gas Oxidized is twenty times greater than the Oxidized flue gas, and consistent with the ratio expected. This is the scale expected from the conversion reaction settings.

Adding the Scrubber drum

The next step is to add the main scrubber vessel. This vessel will separate the vapor, liquid and solid phases.

- ✓ Click on the Separator object in the Library and drag it to the right of the Scrubber Reactor.
- ✓ Label the object Scrubber Drum.
- ✓ Connect the Oxidized Flue Gas stream to the feed of the drum.
- ✓ Add two new streams to the Vapor and Liquid outlets.
- ✓ Label the vapor stream Stack.
- ✓ Label the liquid stream Scrubber bottoms.

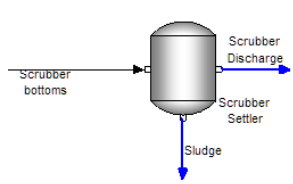


The reactions were completed in the previous block and so this block is added to separate the resulting phases.

Add the solids Settler

The last object in this base case is to add the settler unit.

- ✓ Click on the Settler object in the Library panel and drag it to the right of the Scrubber drum.
- ✓ Label it Scrubber Settler.
- ✓ Link the Scrubber Bottoms stream to the settler feed.
- ✓ Add two new streams to the two settler outlets.
- ✓ Label the bottom outlet stream Sludge and the right outlet stream Scrubber Discharge.

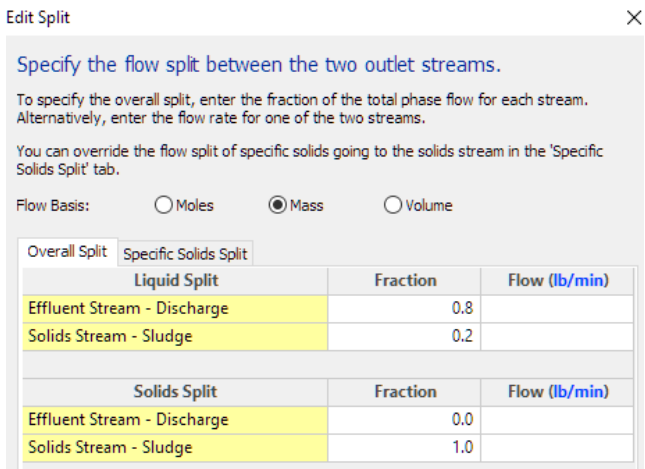


- ✓ Click on the Settler to access the Properties window.

- ✓ In Parameters, click on the Edit window.
- ✓ Change the Flow Basis to Mass.
- ✓ Enter in the Liquid Split section, enter 0.8 for the Effluent Stream – Scrubber Discharge split and press Enter.

When you press Enter, a value of 0.2 will be added automatically to the the Solids Stream – Sludge.

- ✓ In the Solids Split section, enter 0 for the Effluent Stream – Scrubber Discharge and press Enter.



- ✓ Close the window.
- ✓ Calculate.

Reviewing results using the Callouts tables

- ✓ Add a callout table to the Scrubber Discharge stream.
- ✓ Add the variable "Volume-Liquid 1" to the Scrubber Discharge table (in the Phase Flows category).
- ✓ Add a callout table to the Sludge stream.
- ✓ Add the following variables to the Sludge stream table:

Phase Flow Category	Solids Category
Mass Liquid-1	CaCO3 (calcite)
Mass Solid	CaSO4 (anhydrite)
Volume Liquid-1	CaSO4.2H2O (gypsum)
Volume Solid	

Discharge	
T (°F)	132.467
P (psia)	14.696
pH	6.3236
Volume Liq1 (gal/min)	131.087

Sludge	
T (°F)	132.467
P (psia)	14.696
pH	6.3236
Mass Liq1 (lb/min)	270.906
Mass Solid (lb/min)	326.661
Volume Liq1 (gal/min)	32.7719
Volume Solid (gal/min)	13.6936
CaCO3 (Calcite) Solid (mass %)	39.3184
CaSO4 (Anhydrite) Solid (mass %)	60.6816
CaSO4.2H2O (Gypsum) (mass %)	0.0

The Scrubber Discharge liquid rate is 131 gpm, and 33 gpm liquid exits in the Sludge. The liquid flow fraction was set to 80%, and this 4:1 liquid ratio is observed in the Callout tables. The sludge solids mass rate is 327 lb/min and the liquid rate is 270 lb/min. This is a 45% water retention. The sludge will be dewatered in a later chapter.

Lastly, view the solids formed. Of the 327 lb/min solids formed, 128 lb/min is unreacted calcite. You will compare this value to the initial amount of limestone added.

- ✓ Add a Callout table to the 2-Limestone stream.
- ✓ Add the Mass Solid variable to the Callout table.

2-Limestone	
T (°F)	68.0
P (psia)	14.696
pH	10.0507
Mass Solid (lb/min)	279.291

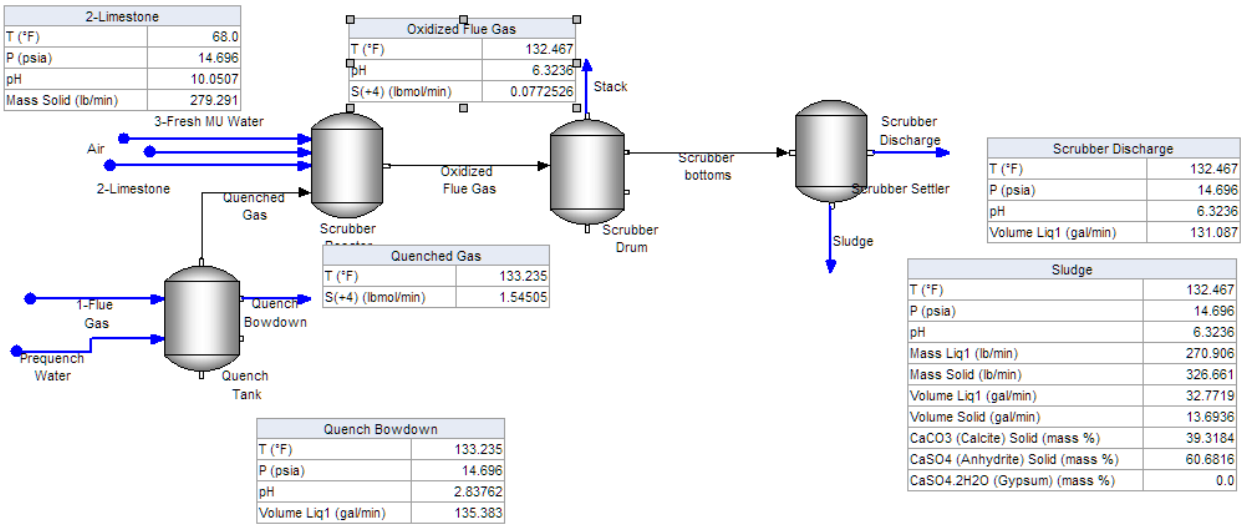
There is 279 lb/min limestone (calcite) added to the scrubber. Therefore, about 50% of what is added did not react. It is possible to optimize the limestone addition and reduce the amount of sludge formed. This will also be done in a later chapter.

Below is what your flowsheet should look like at this point. Save your file and we can move to the next chapter.

Summary

This chapter introduces the basic scrubber process. Flue gas is quenched and sent to a scrubber. The scrubber is split into two sections, a reactor and separator. A Reactor block simulates the rate/mass transfer-limited SO2 oxidation step. A separator block then removes the vapor phase. The extent of oxidation can be modified within the Reactor block. The downstream settler block then separates the calcium sulfate from the discharge water. The fraction of water that is entrained in the solids vs discharged is set here.

In the next chapter, you will modify the process to include a dewatering system and a water softening reactor.

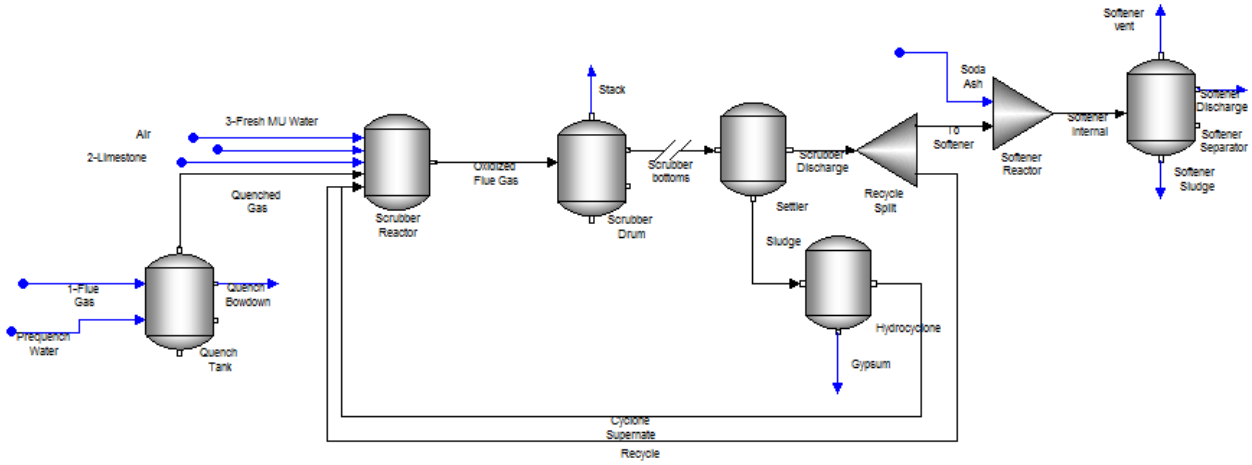

2-Limestone
T (°F) 68.0
P (psia) 14.696
pH 10.0507
Mass Solid (lb/min) 279.291
Oxidized Flue Gas
T (°F) 132.467
pH 6.3236
S(+4) (lbmol/min) 0.0772526
Stack
3-Fresh MU Water
Air
2-Limestone
Quenched Gas
Oxidized Flue Gas
Scrubber Reactor
Scrubber Drum
Scrubber bottoms
Scrubber Discharge
Scrubber Settler
Sludge
Quenched Gas
T (°F) 133.235
S(+4) (lbmol/min) 1.54505
1-Flue Gas
Prequench Water
Quench Bowdown
Quench Tank
Scrubber Discharge
T (°F) 132.467
P (psia) 14.696
pH 6.3236
Volume Liq1 (gal/min) 131.087
Sludge
T (°F) 132.467
P (psia) 14.696
pH 6.3236
Mass Liq1 (lb/min) 270.906
Mass Solid (lb/min) 326.661
Volume Liq1 (gal/min) 32.7719
Volume Solid (gal/min) 13.6936
CaCO3 (Calcite) Solid (mass %) 39.3184
CaSO4 (Anhydrite) Solid (mass %) 60.6816
CaSO4.2H2O (Gypsum) (mass %) 0.0
Quench Bowdown
T (°F) 133.235
P (psia) 14.696
pH 2.83762
Volume Liq1 (gal/min) 135.383

Chapter 14 Coal Boiler Flue Gas Scrubber II

The Application

The following case study is a continuation of the base case scenario created previous chapter. The base case scenario contained four process objects; the quench tank, scrubber reactor, scrubber drum and the settler.

In this chapter, you will add two additional units, a soda ash softener and a hydrocyclone/filter press. You will also recycle some of the discharge water back to the scrubber in order to reduce the amount of makeup water used. When complete, the process should look like the following:



Creating the Chemistry Model

Opening the existing case

- ✓ Open the case saved in the previous chapter. If you have not already created it, contact AQSim for the work file.

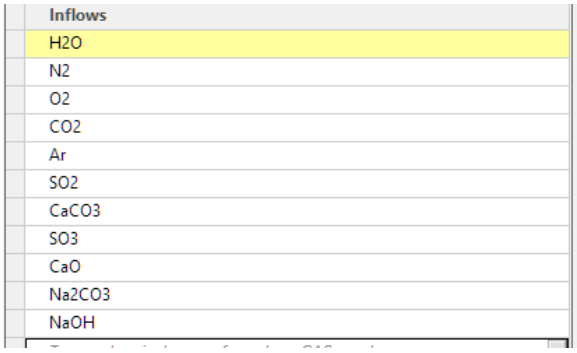
Modifying the Chemistry Model

This scenario includes a softening unit. This generally means inputs of lime, soda ash and caustic,

depending on the inlet stream composition. You will add all three components to the model, but will only use soda ash in the simulation.

- ✓ Click on the Chemistry tab.
- ✓ Click on the Inflows sub tab.
- ✓ Enter the following three components.

CaO
Na2CO3
NaOH

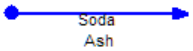


Building the process

Adding the new Units

Create the Soda Ash stream

- ✓ Click on the Flowsheet tab.
- ✓ Click on the Add Stream button in the Toolbar -
- ✓ Add a new stream above and to the right of the Settler object – do not attach it to anything.
- ✓ Name the stream Soda Ash.



Entering the stream compositions

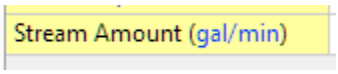
The table below contains the inflow composition for Soda Ash.

Property	Soda Ash
Temperature (°F)	77
Pressure (psia)	14.696
Stream Amount	10 lb/min
Inflows	mass%
H2O	
CaO	0
Na2CO3	100

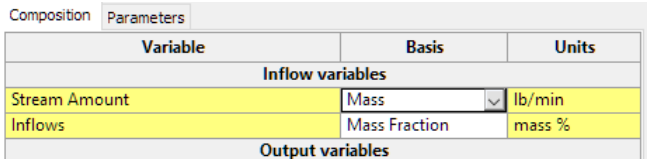
NaOH	0
Set Phase	Solid Only

Notice that the units for flow and composition are different. You will therefore edit the stream's unit set before entering the data.

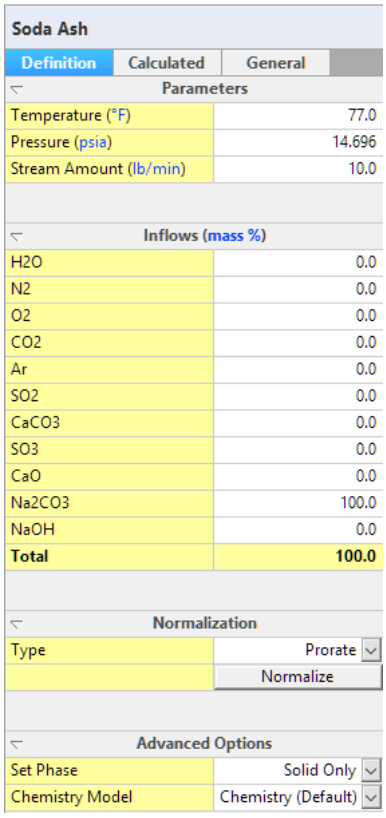
- ✓ Click on the Soda Ash stream to access the Properties panel.
- ✓ Click on the Stream Amount units link to open the Units Editor.



- ✓ Change the Stream Amount from Volume to Mass.

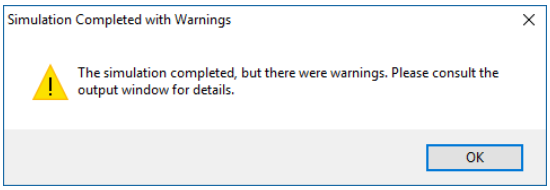


- ✓ Close the Unit Edit window and enter the data from the above table.



Eliminating the warnings cause by the compositions not summing to 100%

You created two streams whose composition did not sum to 100%. Consequently, each time the case is run, a pop-up window appears warning of this inconsistency.



The same message is also reported in the Error tab at the bottom of the screen.

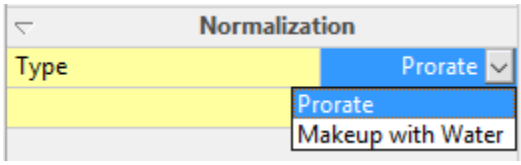
Description	Object
The sum of all inflows must equal 100.0. Please adjust the inflows or use the normalization function to correct this error.	1-Flue Gas
The sum of all inflows must equal 100.0. Please adjust the inflows or use the normalization function to correct this error.	Air

Having a stream that does not sum to 100% is not critical, since the software will normalize it automatically. Nonetheless, the software will continue to remind the user that this issue is present. To eliminate this warning, you will need to adjust the composition, which is quite simple.

- ✓ Click on the 1-Flue Gas stream to access the Properties Panel.

Inflows (mole %)	
H2O	10.53
N2	72.9
O2	8.6
CO2	7.0
Ar	0.9
SO2	0.0697
CaCO3	0.0
SO3	0.0
CaO	0.0
Na2CO3	0.0
NaOH	0.0
Total	99.9997
Normalization	
Type	Prorate
	Normalize

- ✓ Click on the down arrow adjacent to the name Prorate in the Normalization section.



There are two normalization options, Prorate and Makeup with Water. The Prorate will adjust all inflows by 100/99.997. The Makeup with Water will increase the water by 0.0003%. Each approach has its advantages and disadvantages.

- ✓ Select Makeup with Water.

You will take the same action on the Air stream.

- ✓ Click on the Air stream.
- ✓ Set the Normalization Type to Makeup with Water.

1-Flue Gas	
Definition / Calculated / General	
Parameters	
Temperature (°F)	330.0
Pressure (psia)	14.696
Stream Amount (Mft3/min)	1280.0
Inflows (mole %)	
H2O	10.5303
N2	72.9
O2	8.6
CO2	7.0
Ar	0.9
SO2	0.0697
CaCO3	0.0
SO3	0.0
CaO	0.0
Na2CO3	0.0
NaOH	0.0
Total	**100.0**
Normalization	
Type	Makeup wit...

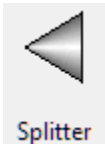
Air	
Definition / Calculated / General	
Parameters	
Temperature (°F)	70.0
Pressure (psia)	14.696
Stream Amount (ft3/min)	34110.0
Inflows (mole %)	
H2O	2.06
N2	76.4
O2	20.6
CO2	0.04
Ar	0.9
SO2	0.0
CaCO3	0.0
SO3	0.0
CaO	0.0
Na2CO3	0.0
NaOH	0.0
Total	**100.0**
Normalization	
Type	Makeup wit...

Adding the Softener unit

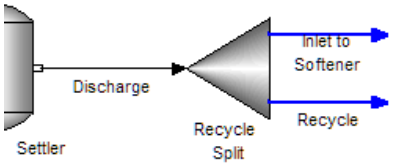
Adding a Flow Splitter to create the recycle stream

The Scrubber Discharge will be split into two streams, a recycle stream and an inlet stream to the Softener unit. The split fraction will be set to 50% as a starting point, since it will eventually need to be optimized using a total dissolve solids (TDS) controller.

- ✓ Click on the Splitter block in the Library and drag it to the right of the Settler.

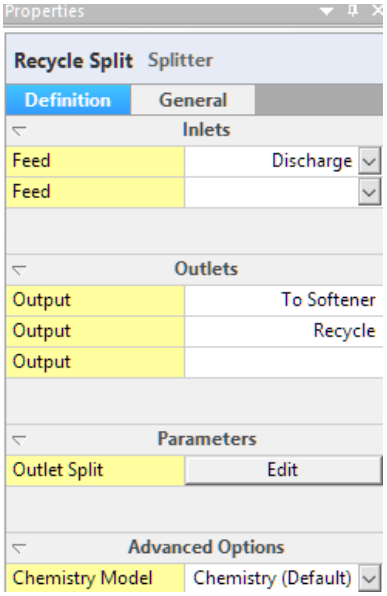


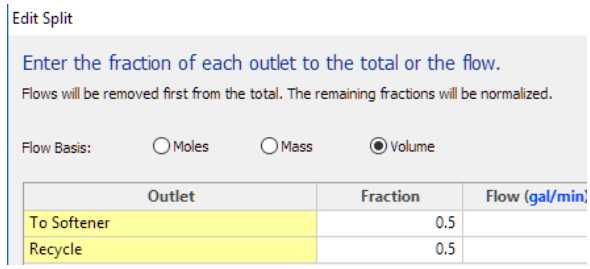
- ✓ Label it Recycle Split.
- ✓ Link the Scrubber Discharge stream to its inlet.
- ✓ Add two streams to the outlet.
- ✓ Label the upper stream Inlet to Softener.
- ✓ Label the lower stream Recycle.



- ✓ Click on the Recycle Split object to access the Properties panel.

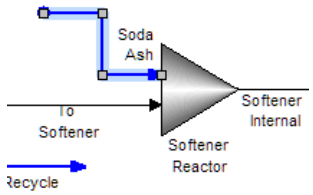
- ✓ Click on the Edit button in the Parameters section.
- ✓ Change the Flow basis to Volume.
- ✓ Enter Fractions of 0.5 for both outlets.





Add the Softener Reactor section

- ✓ Click on the Mixer object in the Library and drag it to the right of the Recycle Split.
- ✓ Label it Softener Reactor.
- ✓ Link the Inlet To Softener stream to the inlet.
- ✓ Link the Soda Ash stream to the inlet.
- ✓ Add an Outlet stream to the Softener Reactor and label it Softener Internal.

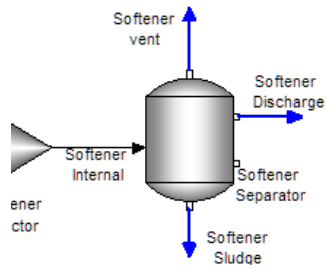


Add the Softener Separator section

- ✓ Click on the Separator object in the Library.

- ✓ Drag it to the right of the Softener Reactor.
- ✓ Label it Softener Separator.
- ✓ Link the Softener Internal stream to the Inlet of the Softener Separator.
- ✓ Add three new streams to the block; to the vapor, liquid-1 and solids outlets.

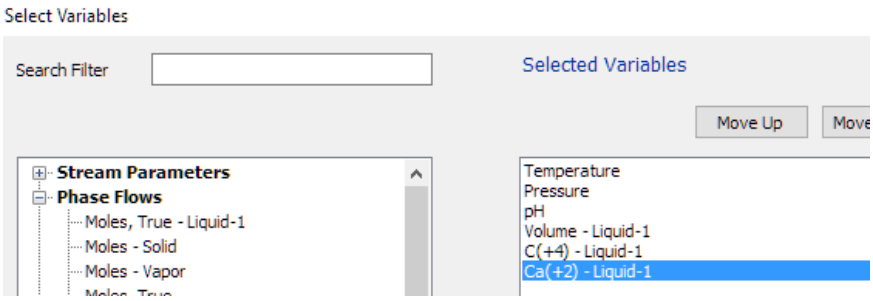
- ✓ Label them Softener vent, Softener Discharge and Softener Sludge, respectively.



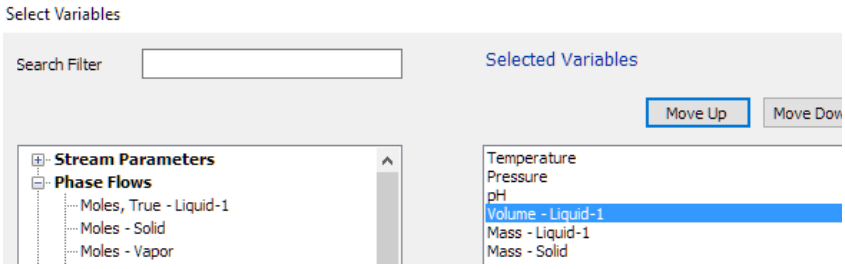
- ✓ Click on the Softener Separator object to access its Properties panel.
- ✓ Click on the Entrainment button.
- ✓ Set the Liquid in Solid (g/g) value to 0.4.
- ✓ Calculate.

Add Callouts for the Inlet to Softener, Softener Discharge and Softener Sludge streams

- ✓ Right-mouse-click on the Inlet to Softener stream and add a Callout table.
- ✓ Double-click on the Callout to open the Variables table.
- ✓ Expand Phase Flows and add Volume – Liquid-1.
- ✓ Expand the MBG Totals, Liquid-1 and add C(+4) and Ca(+2).



- ✓ Close the window.
- ✓ Repeat the above steps for the Softener Discharge stream.
- ✓ Create a Callout for the Softener sludge stream.
- ✓ Open the Variables table.
- ✓ Expand Phase flow and add Volume Liquid-1, Mass Liquid-1, and Mass Solid.



- ✓ Close the window.

Review the total dissolved calcium, Ca(+2) in the Inlet to Softener stream. The soda ash reduced the dissolved calcium by forming CaCO3 solids that exits with the sludge. Note the liquid content in the solids to be sure that it meets the expected fraction. This amount of water exiting with the solids should be small relative to the total liquid discharge flow.

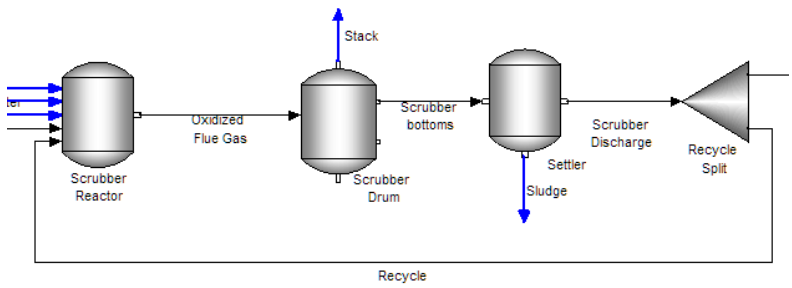
Inlet to Softener	
T (°F)	132.475
P (psia)	14.696
pH	6.3236
Volume Liq1 (gal/min)	65.5482
C(+4) Liq1 (mass %)	3.36965e-3
Ca(+2) Liq1 (mass %)	0.15171

Softener Discharge	
T (°F)	134.58
P (psia)	14.696
pH	9.83414
Volume Liq1 (gal/min)	65.473
C(+4) Liq1 (mass %)	0.164649
Ca(+2) Liq1 (mass %)	5.84618e-5

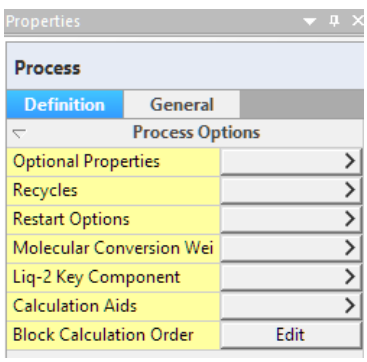
Softener Sludge	
T (°F)	134.58
P (psia)	14.696
pH	9.83414
Volume Liq1 (gal/min)	0.0978958
Mass Liq1 (lb/min)	0.820835
Mass Solid (lb/min)	2.05209

Linking the Recycle stream to the front of the process

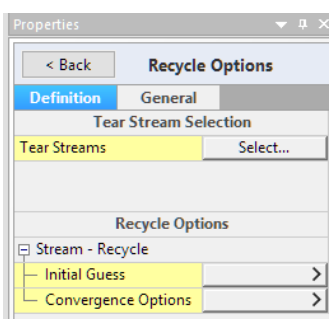
- ✓ Click on the Recycle stream and link it to the Scrubber Reactor.



- ✓ Click anywhere on the white section of the Flowsheet so that no object is selected. This exposes the Properties Panel of the Process.

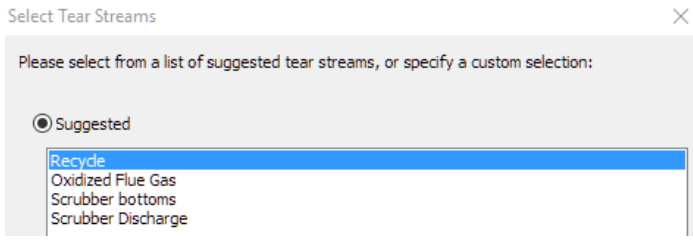


- ✓ Click the Recycles button and select the Tear Streams button.



- ✓ Click the Select button to open a window that contains a list of available tear streams.

- ✓ Highlight Recycle and close the window.



- ✓ Click on the Initial Guess button.
- ✓ View the composition in this panel.

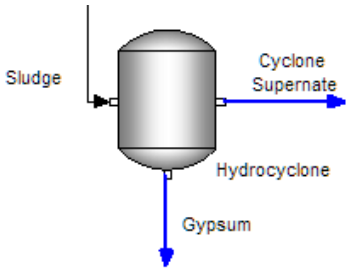
This composition is the initial guess for the simulation. It will change as the simulation is converged. Keep this panel open so that you can see how it changes with each iteration.

- ✓ Calculate.

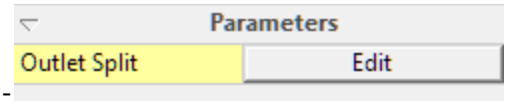
Adding the Hydrocyclone to dewater the Scrubber sludge

- ✓ Click on the Filter block in the Library and drag it below the Settler block.

- ✓ Label it Hydrocyclone.
- ✓ Link the Sludge to the inlet.
- ✓ Add two streams to the outlets.
- ✓ Label the liquid stream Cyclone Supernate and the solid stream Gypsum.



- ✓ Click on the Hydrocyclone block to access the Properties panel.
- ✓ Click on the Outlet Split Edit button -



- ✓ Set the Liquid Split to 0.8 and 0.2 (see image below); this is 80% liquids recovery.
- ✓ Set the Solids Split to 0 and 1; all solids exit in the Gypsum stream.

Edit Split

Specify the flow split between the two outlet streams.

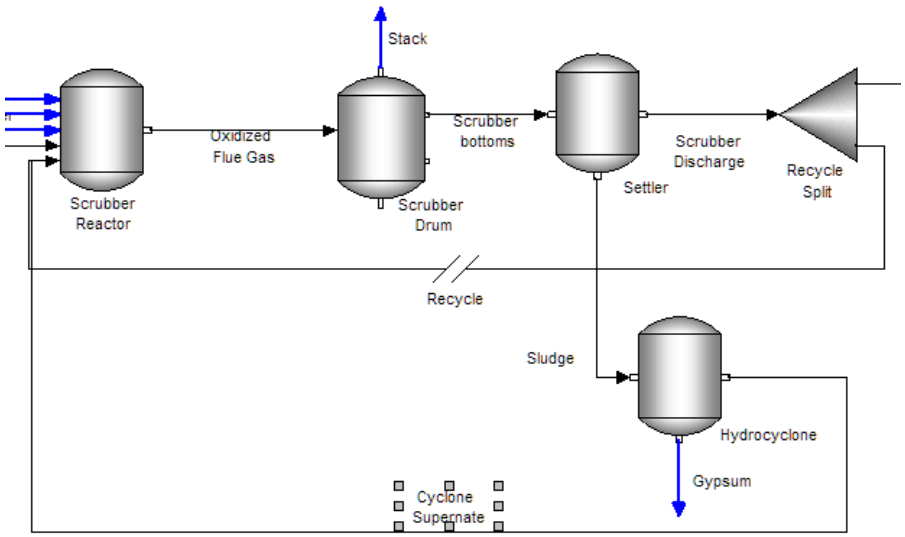
Enter the fraction of the total phase flow for each stream. Alternatively, enter the flow rate for one of the two streams.

Flow Basis: (•) Moles ( ) Mass ( ) Volume

Liquid Split	Fraction	Flow (lbmol/min)
Filtrate Stream - Cyclone Supernate	0.8	
Solids Stream - Gypsum	0.2	

Solids Split	Fraction	Flow (lbmol/min)
Filtrate Stream - Cyclone Supernate	0.0	
Solids Stream - Gypsum	1.0	

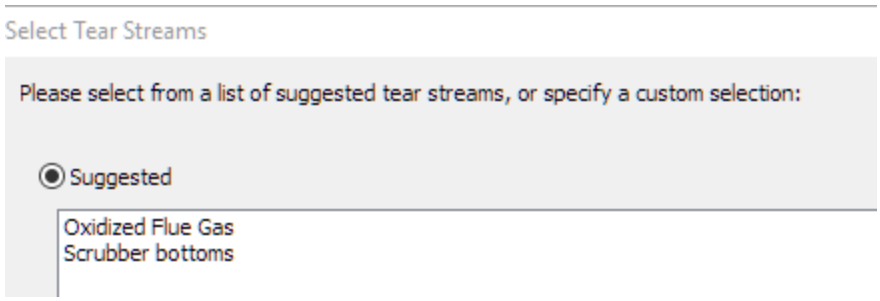
- ✓ Click on the Cyclone Supernate stream and link it to the front of the Scrubber Reactor



You have now created two recycle streams, Recycle and Cyclone Supernate. Both return to the scrubber reactor, and both need to be known in order for the reactor to be computed. Therefore, they both need to be tear streams.

Alternatively, a single Tear stream inside the recycle loop can replace both. For instance, if the Oxidized Flue gas is selected as a Tear, then the Scrubber drum is computed first. The other option is the Scrubber Bottoms stream. You will change the Tear stream to the Scrubber Bottoms.

- ✓ Click anywhere on the flowsheet to access the Process Properties Panel.
- ✓ Select the Recycles button in the Panel.
- ✓ Click on the Tear Stream Select button.
- ✓ Click on the Suggested radio button and highlight Scrubber Bottoms from the list.



✓ Close the window and calculate.

Summary

A more advanced version of the Flue gas scrubber is simulated. It contains a softener unit and hydrocyclone. In addition, some of the supernate is sent back to the scrubber unit. This is done with the intention of reducing the makeup water requirements.

There are several additional tasks required to complete this work. There is excess limestone added. Only about 60% added is used, with the remaining limestone settling with the sludge volume. A controller can be used to minimize limestone needs using the discharge pH as the controller setting. The Makeup water is added with no specified target flow or output. In addition, discharge water is recycled. Therefore, a controller can be added to minimize makeup water requirements by controlling the TDS or salinity of the discharge water exiting to the softener. Lastly, a Soda Ash controller will maximize its inflow based on total dissolved calcium targets in the Softener discharge. These will be done in the next chapter.

Appendix – Stream inflow composition

The table below contains a list of three inflow streams associated with lime softening. In this examples soda ash is used. If you want to test other additives on the softener, then use the following table to add the lime and 50% caustic.

Property	Soda Ash	Lime	50% Caustic
Temperature (°F)	70	70	70
Pressure (psia)	14.696	14.696	14.696
Stream Amount	10 lb/min	10 lb/min	10 lb/min
Inflows	mass%	mass%	mass%
H2O			50
CaO	0	100	0
Na2CO3	100	0	0
NaOH	0	0	50
Set Phase	Solids Only	Solids Only	No Special Cond.

Properties

Lime

Definition | Calculated | General

Parameters	
Temperature (°F)	70.0
Pressure (psia)	14.696
Stream Amount (lb/min)	10.0

Inflows (mass %)	
H2O	0.0
N2	0.0
O2	0.0
CO2	0.0
Ar	0.0
SO2	0.0
CaCO3	0.0
SO3	0.0
CaO	100.0
Na2CO3	0.0
NaOH	0.0
Total	**100.0**

Normalization	
Type	Prorate
	Normalize

Advanced Options	
Set Phase	Solid Only

Properties

50% Caustic

Definition | Calculated | General

Parameters	
Temperature (°F)	70.0
Pressure (psia)	14.696
Stream Amount (lb/min)	10.0

Inflows (mass %)	
H2O	50.0
N2	0.0
O2	0.0
CO2	0.0
Ar	0.0
SO2	0.0
CaCO3	0.0
SO3	0.0
CaO	0.0
Na2CO3	0.0
NaOH	50.0
Total	**100.0**

Normalization	
Type	Prorate
	Normalize

Advanced Options	
Set Phase	No Special ...

Chapter 15 Seawater Evaporation – Effect 3

The Application

This process will evaporate seawater using a three-effect system and a crystallizer. The process will include two external steam feeds, one feeding the three effects and the other to the crystallizer. The seawater will flow at 10 mT/hr and the effective evaporation will be 95%. At 95%, NaCl salts should begin to form.

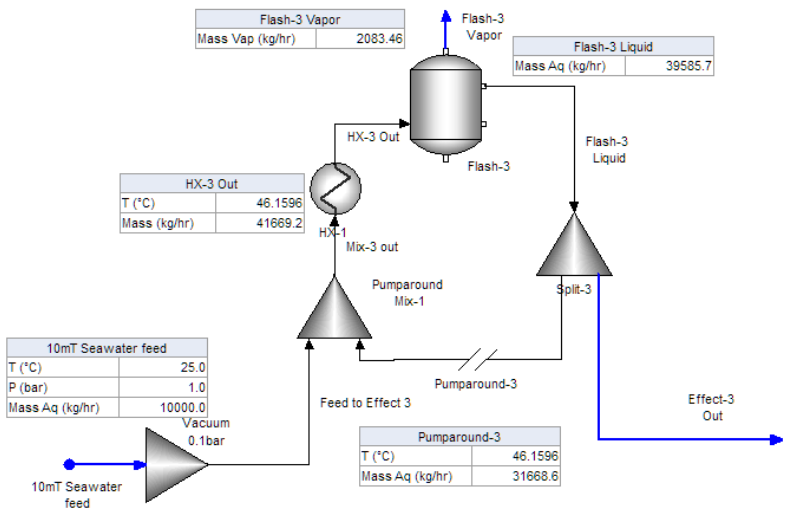


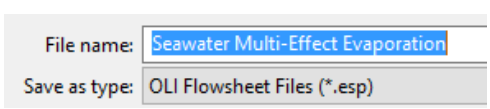
Figure 15-1- Effect 3 of the overall seawater evaporation process

Creating the Chemistry Model

Creating the Case file

This is a new case, so create a new file.

✓ Save the new file with the name Seawater Multi-Effect Evaporation.



Adding Chemistry to the Model

You will start with a simple salt-water composition. The Seawater chemistry contains multiple inflows, including Ca, Mg, SO4, HCO3, Br, and other components. However, the goal here is to keep the chemistry simple until the simulation is converged. Then the remaining components can be added. NaCl is by far the most significant salt in seawater, and so most of the mass required is obtained with H2O and NaCl.

- ✓ Click on the Chemistry tab and then the Inflows subtab.
- ✓ Enter NaCl to the list.

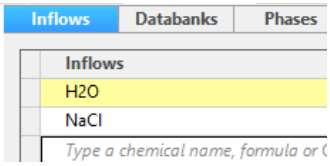


Figure 15-2 – Adding NaCl to the Chemistry Inflows List

- ✓ Return to the flowsheet view.

Building the Process

Building the Third Effect

The Inflow seawater rate is 10,000 kg/hr. The third effect will evaporate 20% of this seawater and the pumparound recycle will have a 4:1 ratio. Those are the basic settings. Also, as explained above, the seawater contains NaCl only until the complete process is converged. Then the remaining components will be added.

Specifications	Value
Seawater Feed rate	10,000 kg/hr
Steam Rate	20% (+/- 1%)
Recycle Ratio	80% (4:1)

Figure 15-3 - Third Effect Specifications

Setting the Units

Setting the units for the flowsheet before adding any streams or blocks eliminate a significant amount of editing time once the simulation work begins. Setting the units before starting work is good practice for all work in Flowsheet ESP.

- ✓ Open the Units Manager window using the Units button on the Toolbar
- ✓ Change the process units to Metric-Flowing-Mass.

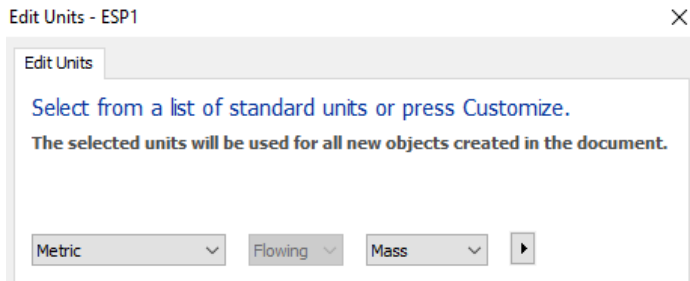
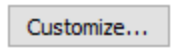


Figure 15-4 - The Units Manager window

- ✓ Click on the Customize button - 

to open the Units Editor.
- ✓ Make the following changes:

Variable	Basis or units
Aqueous Composition	Concentration
Solid Composition	Concentration
Mass	kg/hr
Volume	m3/hr
Pressure	bar
Energy	kJ/hr

Table 15-1 - Changes to the global flowsheet units

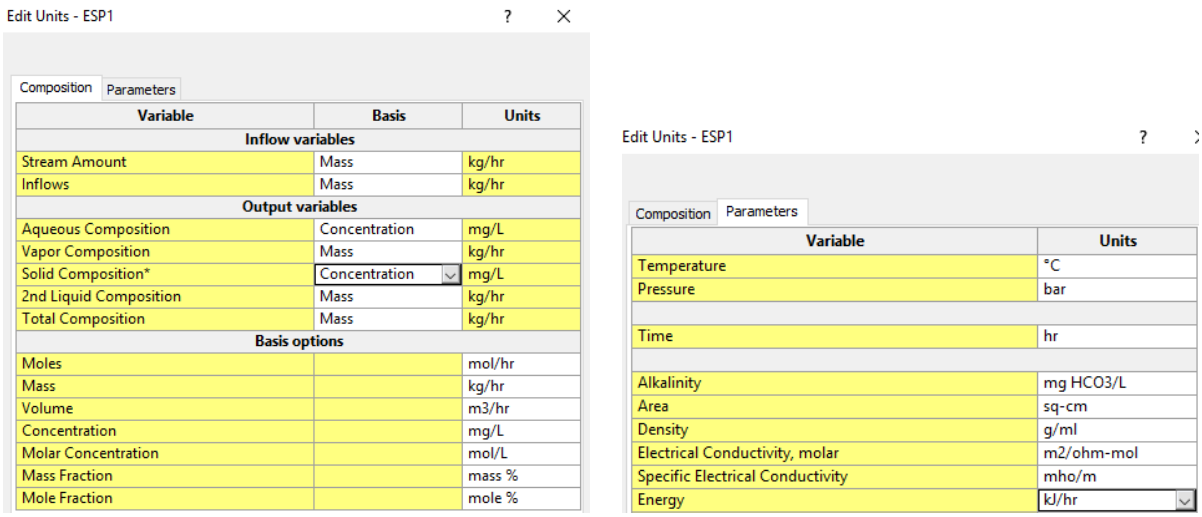


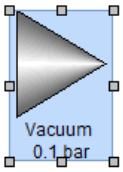
Figure 15-5 - Updated Units Editor windows

- ✓ Close the windows when done.

Building the process

Create the feed stream and the Vacuum unit

- ✓ Click on the Mixer object in the library, and drag it to the bottom-left of the screen.
- ✓ Label it Vacuum – 0.1 bar.



- ✓ Change the Pressure setting to Absolute Pressure and enter a value of 0.1 bar.

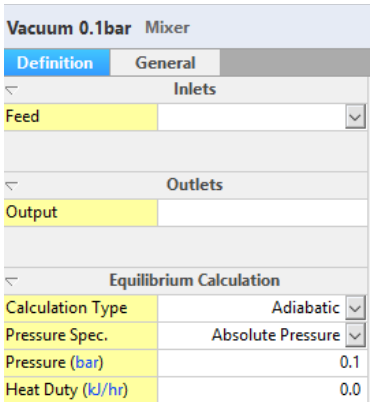
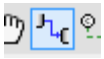
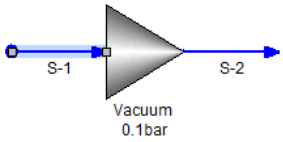
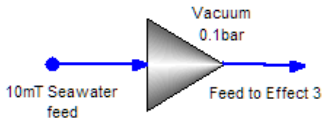


Figure 15-6 - Updated parameters to the Vacuum 0.1 bar block

- ✓ Click on the Add Stream button - 
- ✓ Create one stream to the inlet and one stream to the outlet.
- ✓ Press Esc to deactivate the Add Stream action.



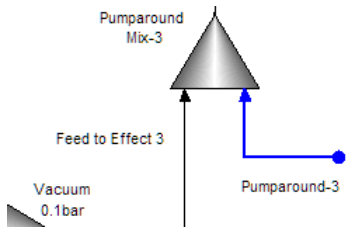
- ✓ Label the inlet stream 10mT Seawater feed.
- ✓ Label the outlet stream Feed to Effect-3.



Create the Pumparound Mix-3 and the Pumparound-3 stream

- ✓ Click on the Mixer block from the Library and drag it to the upper right of the Vacuum block.
- ✓ Label it Pumparound Mix-3.
- ✓ Rotate the block counter-clockwise
- ✓ Link the Feed to Effect-3 stream to the Mixer.
- ✓ Add a new stream to the inlet and outlet of the Pumparound Mix-3.

✓ Label the inlet stream Pumparound-3 and the outlet stream Mix-3 out.



✓ Enter the following composition for the Seawater feed and Pumparound-3 streams:

Component	Seawater Feed	Pumparound-3
Temperature, C	25	25
Pressure, bar	1	0.1
Stream Amount, kg/hr	10,000	32,000
H2O	96.629	96.629
NaCl	2.626	2.626

Table 15-2 - Composition of the Seawater feed and the Pumparound stream

10mT Seawater feed

Definition | Calculated | General

Parameters	
Temperature (°C)	25.0
Pressure (bar)	1.0
Stream Amount (kg/hr)	10000.0
Inflows (kg/hr)	
H2O	96.629
NaCl	2.626
Total	**99.255**

Initial Guess - Pumparound-3

Definition | Calculated | General

Parameters	
Temperature (°C)	25.0
Pressure (bar)	0.1
Total Flow (kg/hr)	32000.0
Inflows (kg/hr)	
H2O	96.629
NaCl	2.626
Total	**99.255**

Figure 15-7 - updated Parameters table for the Seawater and Pumparound-3 streams

✓ Calculate.

✓ Review the Mix-3 Out results.

Calculated | General

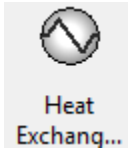
Stream Parameters	
Temperature (°C)	25.0054
Pressure (bar)	0.1
pH	6.99186
Moles, True (mol/hr)	2.30769e6
Moles, Apparent (mol/hr)	2.28868e6
Mass (kg/hr)	42000.0
Volume (m3/hr)	41.3587

Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	0.0
Total, Apparent (Molecular) (kg/hr)	
H2O	40888.8
NaCl	1111.2

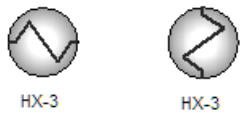
Figure 15-8 - Updated Parameters table for the Mix-3 Out block

Adding the Heat Exchanger and Flash Drum

✓ Click on the Heat Exchanger object in the library and drag it above the Mix-3 Out stream.



- ✓ Label it HX-3.
- ✓ Rotate the HX-3 block counterclockwise -



- ✓ Change the HX-3 Spec type to Vapor Fraction and enter a value of 5 mass%.

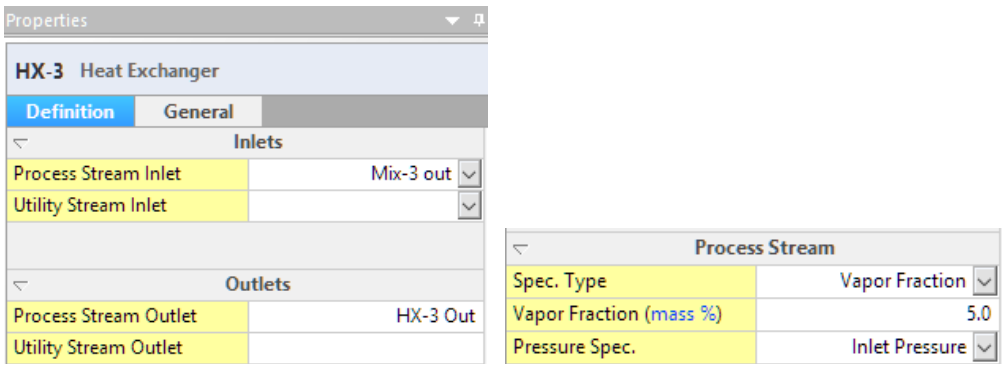
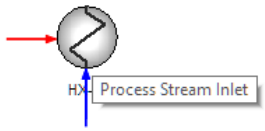
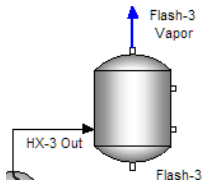


Figure 15-9 - Updated Parameters for the HX-3 block

- ✓ Link the Mix-3 Out stream to the inlet of the HX-3.



- ✓ Add an outlet stream from the HX-3. Name it HX-3 Out.
- ✓ Click on the Separator block in the Library and drag it to the upper right of the HX-3.
- ✓ Label it Flash-3.
- ✓ Link the HX-3 stream to the inlet.
- ✓ Add two new streams, one to the Vent and one to the Liquid-3 outlet.
- ✓ Label these streams, Flash-3 Vapor and Flash-3 Liquid.



- ✓ Calculate.

Adding Callouts to review the results

- ✓ Right-mouse-click on the Seawater feed stream and select Add Callout.
- ✓ Double-click on the Callout table and add Mass – Aqueous from the Phase Flows section.

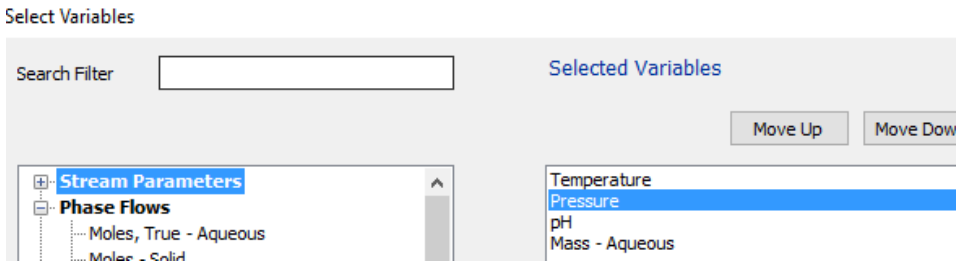
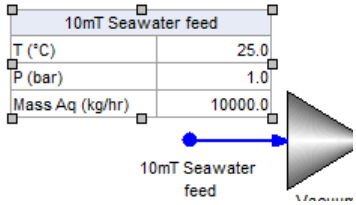


Figure 15-10 - The Select Variables window showing the variable list and the selected variables fields



- ✓ Add Callout tables for the Pumparound, HX-3 Out, Flash-3 Vent, and Flash-3 Liquid streams. Use the following variables (delete all others).

Table 15-3 - The Variables to be in each Callout table

10mT Seawater Feed	Pumparound-3	HX-3 Out	Flash-3 Vapor	Flash-3 Liquid
Temperature Pressure Mass-Aqueous	Temperature Mass Aqueous	Temperature Mass	Mass-Vapor	Mass-Aqueous

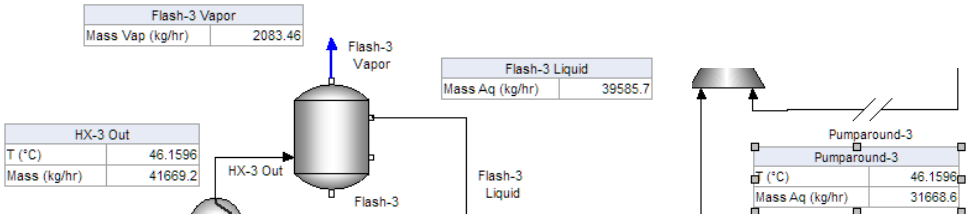
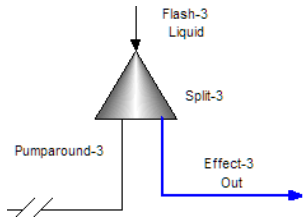


Figure 15-11- The Flowsheet diagram with the Callout tables added

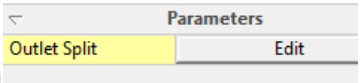
Adding the Flow Splitter and linking the Recycle stream

- ✓ Click on the Splitter block in the Library and drag it to the lower right of the Separator.
- ✓ Name it Split-3.
- ✓ Rotate the block clockwise -
- ✓ Link the Flash-3 Liquid stream to the inlet of the Split-3 block.
- ✓ Link the Pumparound-3 stream to the outlet of the Split block.
- ✓ Add a new stream to the Outlet of the Split block – label this Effect-3 Out.



✓ Click on the Split-3 block to access the Properties panel.

✓ Click on the Edit button in the Parameters section



✓ Enter the following specifications:

Flow Basis	Mass
Pumparound-3	0.8 fraction
Effect-3 out	0.2 fraction

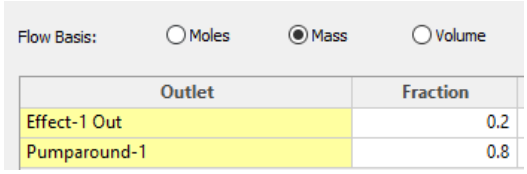


Figure 15-12 - The updated flow fractions for the Split-3 block

✓ Right-mouse-click on the Pumparound-3 stream, and select Set Tear Stream.

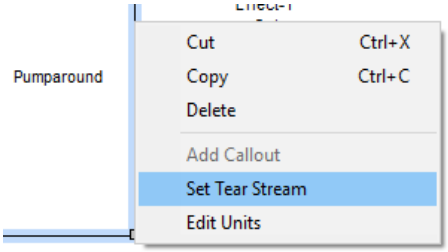


Figure 15-13 - Setting the Tear (recycle) stream using the right-mouse-click dropdown window

✓ Calculate

The simulation should converge quickly, because the Pumparound-3 guess with which we started is close to the converged state.

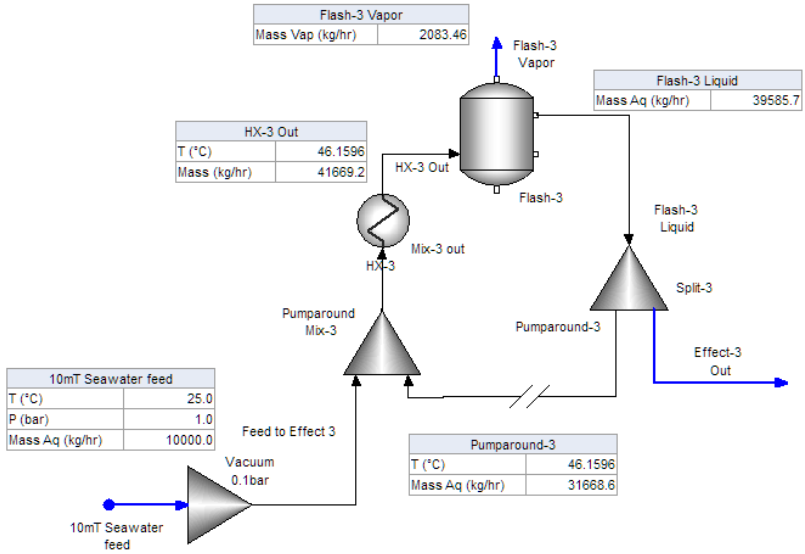


Figure 15-14 - The converged process using the initial settings

The Flash-3 Vapor mass is 83 kg/hr above the 2000 kg/hr target value. This target can be tightened by changing the Vapor Fraction setting in HX-3. It is currently set to 5%. The flow exiting the heat exchanger is 41,669 kg/hr, and so to achieve 2000kg/hr the vapor fraction is 4.8%.

✓ Change the Vapor Fraction (mass %) value to 4.8.

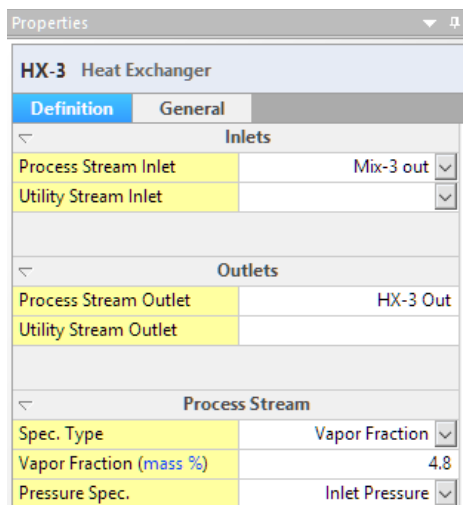


Figure 15-15 - updating the HX-3 vapor fraction to 4.8%

✓ Calculate.

The updated vapor rate is now 2013 kg/hr. This is slightly high than desired, and is because the recycle rate increased by about 300 kg/hr. This is well within the 1% tolerance set in the specification at the beginning of the chapter.

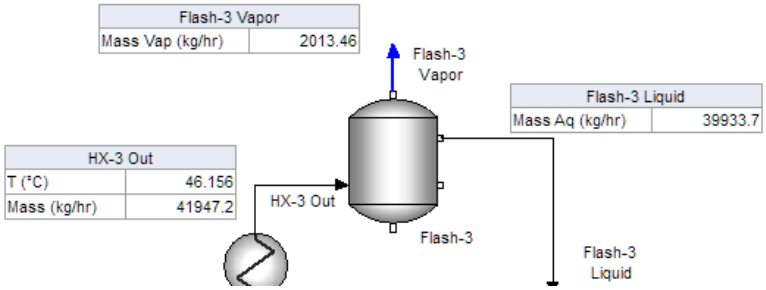
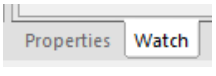


Figure 15-16 - Updated vapor flow after setting the HX-3 vapor fraction to 4.8%

- ✓ Save the file.

Review the HX-3 energy balance

- ✓ Click on the HX-3 block to access the Properties panel.
- ✓ Click on the Watch tab at the bottom of the panel - 

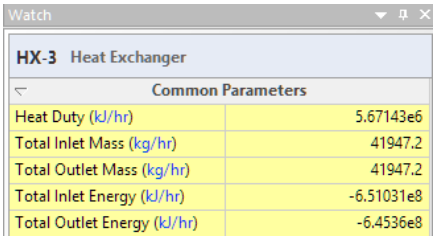


Figure 15-17 - The Heat Balance surrounding the HX-3 block

The required heat duty is $5.67e^{6}$ KJ/hr ($5.67e^{9}$ J/hr). At this point in the simulation procedure, this energy is simulated. There is no utility steam to provide the energy. Once the remaining effects are created, the counter-current steam will be linked.

Summary

This chapter presents the basic approach to set up an evaporator effect. It converged easily because a good initial guess was used in the Pumparound-3 stream. A good guess was possible because the flow and recycle specification are known. Lastly, this process does not include the counter-current steam streams to supply the heat to the HX-3 block. This will be done in later chapters once the system is completed.

Chapter 16 Seawater Evaporation – Effects 2 and 1

The Application

This process is a continuation of the previous chapter. It is evaporating seawater in a three-effect system plus a crystallizer. The first effect is already completed, and it will be used to create the two effects shown in this chapter. The objective in this effect is to evaporate 30% of the inlet flow.

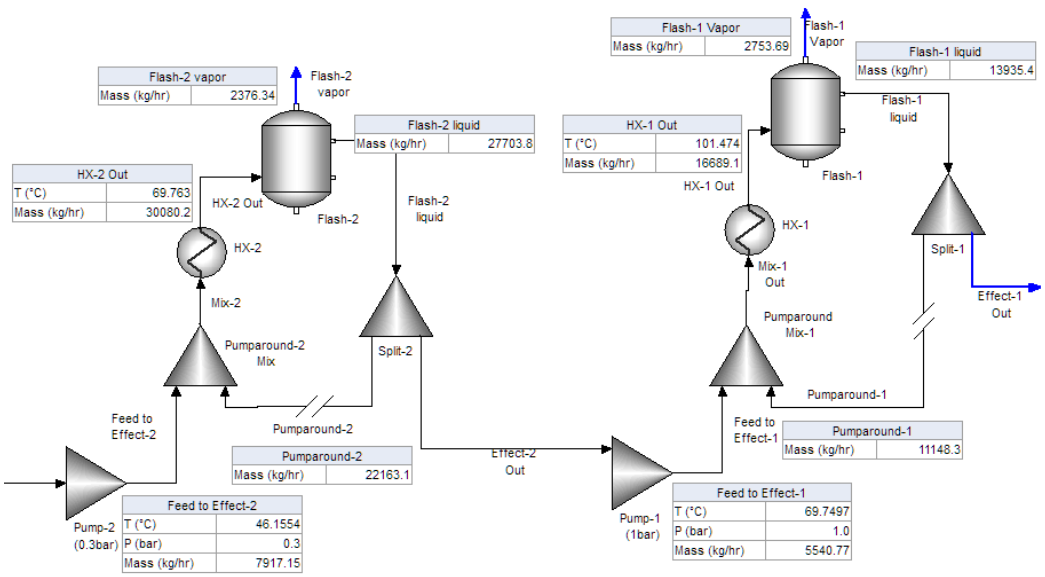
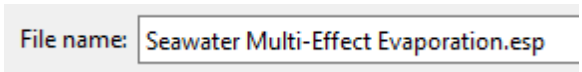


Figure 16-1- Effects 2 and 3 of the overall seawater evaporation system

Creating the Chemistry Model

Open the existing Case file

✓ Open the existing file created in the last chapter, Seawater Multi-Effect Evaporation.



There is no change to the chemistry model in this chapter.

Building the Process

Building the Second Effect

The second effect is nearly identical to the first effect, with the differences being the settings. Therefore, the simplest way to create it is by following the procedure in the previous chapter. The Main instructions will be included here.

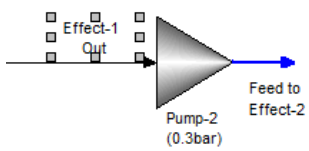
Adding the five blocks in the second effect

The following table contains the specifications for the five new blocks. Three of the blocks contain Parameter specifications: Pump-2, HX-2, and Split-2.

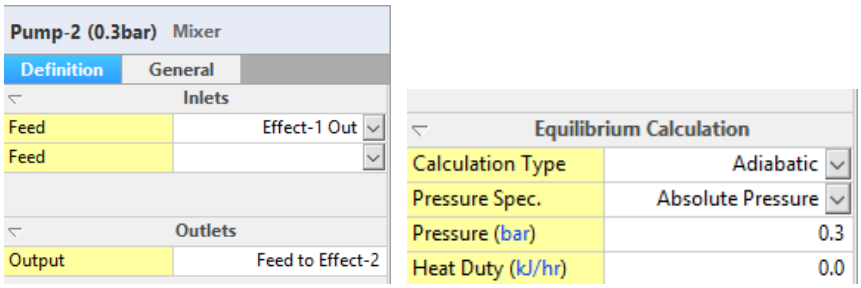
Block name	**Pump-2**	**Pumparound Mix-2**	**HX-2**	**Flash-2**	**Split-2**
Block type	Mixer	Mixer	Heat Exchanger	Separator	Flow Splitter
Inlet Streams	Effect-1 Out	Feed to Effect 2 Pumparound-2	Mix-2 Out	HX-2	Flash-2 liquid
Outlet Stream	Feed to Effect 2	Mix-2 Out	HX-2 out	Flash-2 Vapor Flash-2 Liquid	Pumparound-2 Effect-2 Out
Parameter Specification	Absolute pressure		Vapor Fraction		Flow basis = mass
Parameter Value	0.3 bar outlet pressure		7.5 mass% in vapor		Pumparound-2=0.8 Effect-2 out=0.2

Pump-2 (0.3 bar)

- ✓ Add a Mixer block to the lower right of the Split-1 stream and label it Pump 2 (0.3 bar).
- ✓ Link the Effect-1 out stream to it.
- ✓ Add a new outlet stream and label it Feed to Effect-2.



- ✓ Change the Pressure specifications to Absolute pressure and enter a value of 0.3bar.



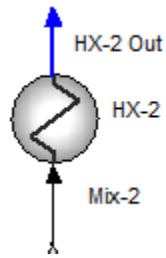
Pumparound Mix-2

- ✓ Add another Mixer block to the upper right of Pump-2 and label it Pumparound Mix-2.
- ✓ Rotate the block counterclockwise.

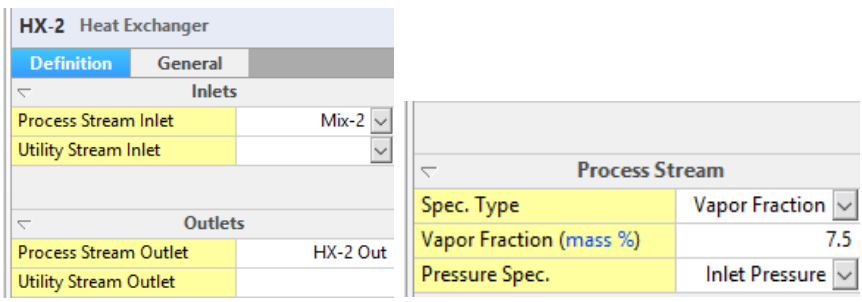
- ✓ Link the Feed to Effect-2 stream to the inlet.
- ✓ Create a new inlet stream and label it Pumparound-2.
- ✓ Create a new outlet stream and label it Mix-2 Out.

HX-2, heat exchanger

- ✓ Add a Heat exchanger above the Mix-2 block and label it HX-2.
- ✓ Rotate the block counterclockwise.
- ✓ Link the Mix-2 Out stream to it.
- ✓ Add a new stream and label it HX-2 out.

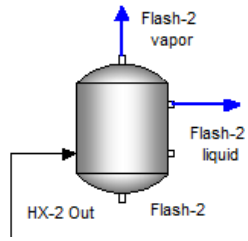


- ✓ Change the Process Stream Spec. type to Vapor Fraction.
- ✓ Enter 7.5%.



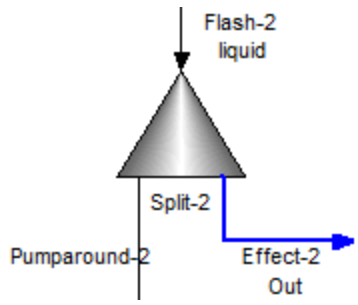
Flash-2 flash drum

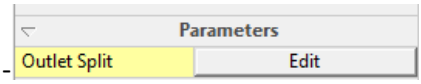
- ✓ Add a separator to the upper right of HX-2 and label it Flash-2.
- ✓ Link the HX-2 Out stream to it.
- ✓ Create new Vapor and Liquid outlet streams and label them Flash-2 vapor and Flash-2 liquid.



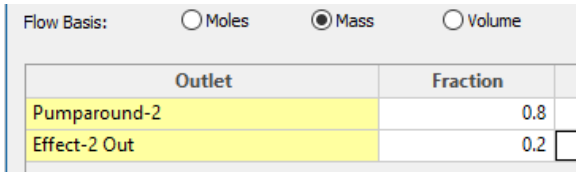
Split-2 (flow splitter)

- ✓ Add a Flow splitter to the lower-right of the flash-2 block and label it Split-2.
- ✓ Rotate it clockwise.
- ✓ Link the Flash-2 Liquid to the inlet.
- ✓ Link the Pumparound-2 stream to its outlet.
- ✓ Create a new outlet stream and label it Effect-2 Out.



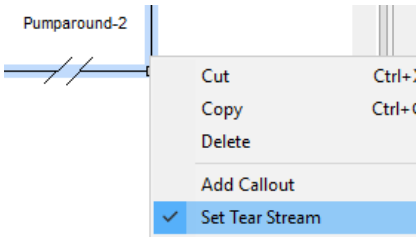
- ✓ Open the Split-2, Outlet Split Edit window - 

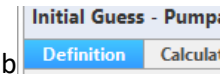
- ✓ Change the Flow basis to Mass and the fraction as shown in the image below.



Setting the Pumparound-2 as the Tear stream

- ✓ Right-mouse-click on the Pumparound-2 stream and select Set Tear Stream.



- ✓ Click on the Pumparound-2 stream again and select the Definition tab 

in the Properties panel.
- ✓ Enter the following values:

Composition	Value
Temperature	80 C
Pressure	0.3 bar
Stream Amount	25000 kg/hr
H2O	95 kg
NaCl	5 kg

Table 16-1 – Pumparound-2 composition guess

If you cannot access the Definition tab, click off the Pumparound-2 stream and then click back on. The panel may need to be refreshed, because you just signaled to the software that this stream is a tear stream.

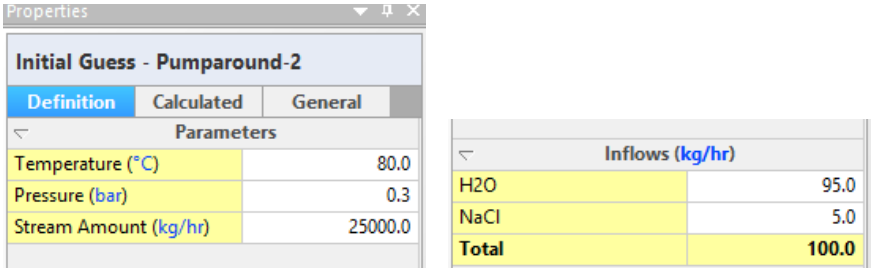


Figure 16-2 - Initial guess to the Pumparound-2stream that will be used to converge the recycle

- ✓ Calculate.

The calculation should converge quickly because a good initial guess was provided, and because the process is straightforward. If it does not converge quickly, check your work to see if something was missed.

Add the Callouts

- ✓ Add callout tables to the Feed to Effect-2, HX-2 out, Flash-2 vapor, Flash-2 liquid, Pumparound, and Effect-2 out.
- ✓ Use the following variables for each callout:

Feed to Effect-2	HX-2 Out	Flash-2 Vapor	Flash-2 Liquid	Pumparound-2
Temperature Pressure Mass	Temperature Mass	Mass	Mass	Mass

Table 16-2 - The Variables to be in each Callout table

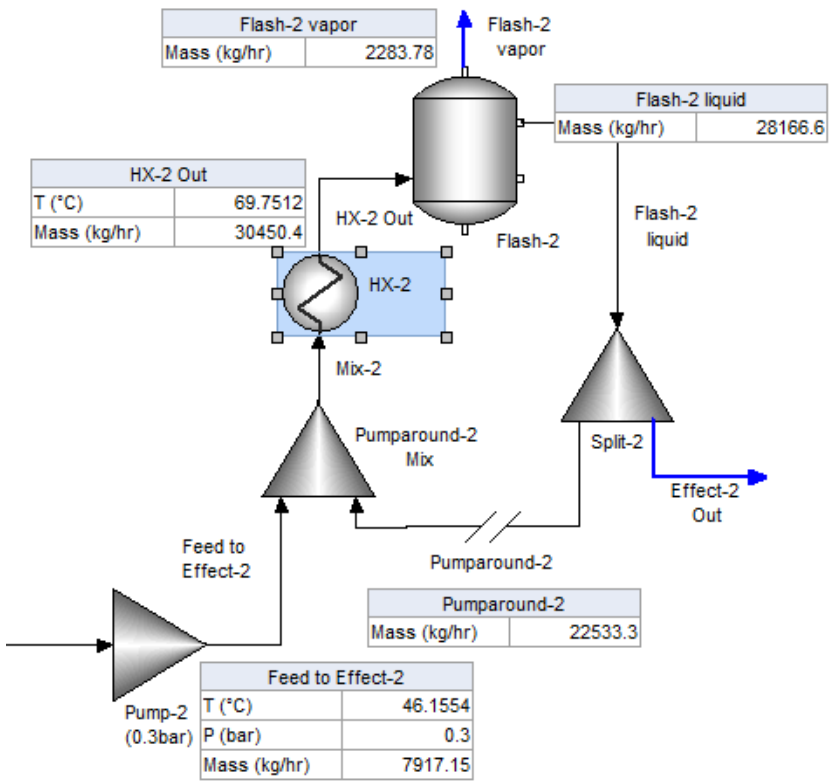


Figure 16-3- The converged flowsheet with the Callout tables added to the second effect streams

The Vapor mass is 2283 kg/hr which is 28.8% of the feed to Effect-2 (7917 kg/hr). The target is 30% evaporation of the inlet feed. So you will increase the HX-2 vapor fraction value to 7.9%.

- ✓ Click on the HX-2 block to activate the Properties panel.
- ✓ Change the Vapor Fraction (mass %) value to 7.9.

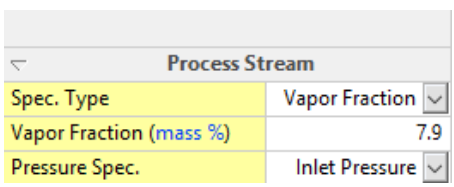


Figure 16-4 - updating the HX-1 vapor fraction to 7.9%

- ✓ Calculate.

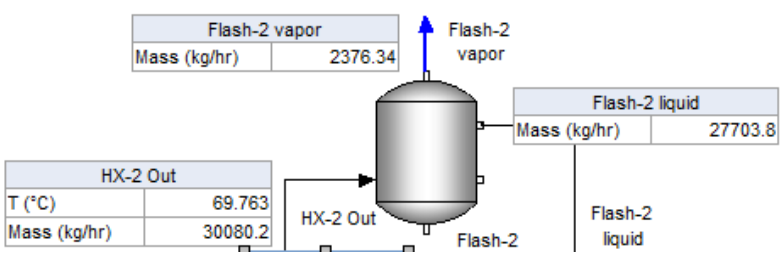
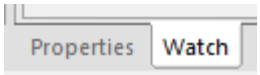


Figure 16-5 - Updated vapor flow after setting the HX-2 vapor fraction to 7.9%

The updated vapor rate is now 2376 kg/hr. This is 30% of the inlet rate and so the target specifications are met.

- ✓ Save the file.

Review the HX-1 energy balance

- ✓ Click on the HX-2 block to access the Properties panel.
- ✓ Click on the Watch tab at the bottom of the panel - 

HX-2 Heat Exchanger	
Common Parameters	
Heat Duty (kJ/hr)	6.30749e6
Total Inlet Mass (kg/hr)	30080.2
Total Outlet Mass (kg/hr)	30080.2
Total Inlet Energy (kJ/hr)	-4.60877e8
Total Outlet Energy (kJ/hr)	-4.5457e8

Figure 16-6 - The Heat Balance surrounding the HX-2 block

The required heat duty is $6.31e^6$ KJ/hr. This energy will be sourced from the vapor phase produced by the third effect. It will be set up in the next chapter.

Building the First Effect

The third effect is again nearly identical to the first and second effect. The difference is the settings. The third effect will evaporate 50% of the inlet feed. You will use the same procedure as above to create this section.

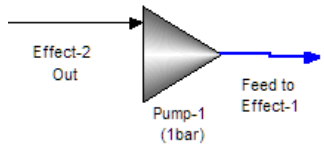
Adding the five blocks in the first effect

The following table contains the specifications for the five new blocks. Three of the blocks contains Parameter specifications, Pump-1, HX-1, and Split-1.

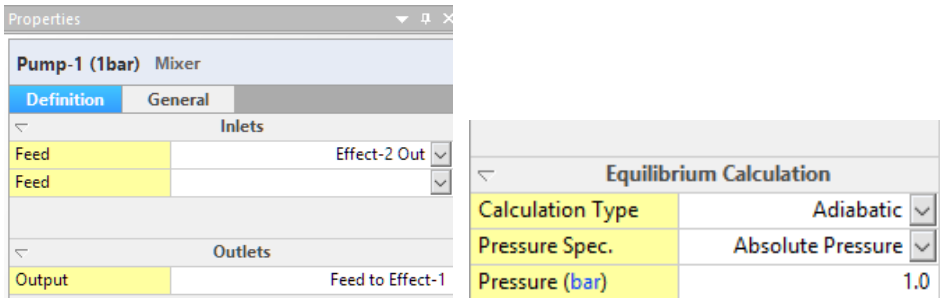
Block name	**Pump-1**	**Pumparound Mix-1**	**HX-1**	**Flash-1**	**Split-1**
Block type	Mixer	Mixer	Heat Exchanger	Separator	Flow Splitter
Inlet Streams	Effect-2 Out	Feed to Effect-1 Pumparound-1	Mix-1 Out	HX-1	Flash-1 liquid
Outlet Stream	Feed to Effect-1	Mix-1 Out	HX-1 out	Flash-1 Vapor Flash-1 Liquid	Pumparound-1 Effect-1 Out
Parameter Specification	Absolute pressure		Vapor Fraction		Flow basis = mass
Parameter Value	1 bar outlet pressure		12 mass% in vapor		Pumparound-1=0.8 Effect-1 out=0.2

Pump-1 (1 bar)

- ✓ Add a Mixer block to the lower right of the Split-2 stream and label it Pump 3 (1 bar).
- ✓ Link the Effect-2 Out stream to it.
- ✓ Add a new outlet stream and label it Feed to Effect-1.

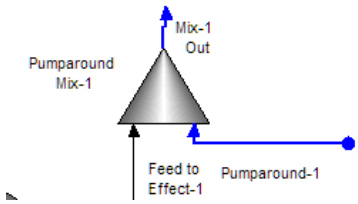


- ✓ Change the Pressure specifications to Absolute pressure and enter a value of 1 bar.



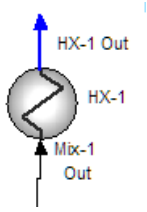
Pumparound Mix-1

- ✓ Add another Mixer block to the upper right of Pump-1 and label it Pumparound Mix-1.
- ✓ Rotate the block counterclockwise.
- ✓ Link the Feed to Effect-1 stream.
- ✓ Create a new inlet stream and label it Pumparound-1.
- ✓ Create a new outlet stream and label it Mix-1 out.



HX-1, heat exchanger

- ✓ Add a Heat exchanger above the Mix-1 block and label it HX-1.
- ✓ Rotate the block counterclockwise.
- ✓ Link the Mix-1 Out stream to it.
- ✓ Add a new stream and label it HX-1 out.

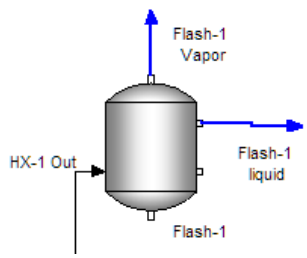


- ✓ Change the Process Stream Spec. Type to Vapor Fraction.
- ✓ Enter 12%.

Process Stream	
Spec. Type	Vapor Fraction
Vapor Fraction (mass %)	12.0
Pressure Spec.	Inlet Pressure

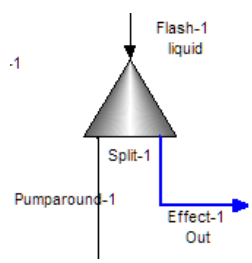
Flash-1 flash drum

- ✓ Add a separator to the upper right of HX-1 and label it Flash-1.
- ✓ Link the HX-1 Out stream to it.
- ✓ Create new Vapor and Liquid outlet streams and label them Flash-1 vapor and Flash-1 liquid.



Split-1 (flow splitter)

- ✓ Add a Flow splitter to the lower-right of the Flash-1 block and label it Split-1.
- ✓ Rotate it clockwise.
- ✓ Link the Flash-1 Liquid to the inlet.
- ✓ Link the Pumparound-1 stream to its outlet.
- ✓ Create a new outlet stream and label it Effect-1 Out.



- ✓ Open the Split-1, Outlet Split Edit window -

Parameters	
Outlet Split	Edit

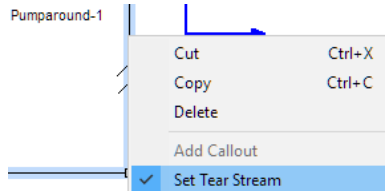
- ✓ Change the Flow basis to Mass and the fraction as shown in the image below:

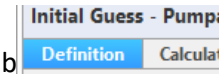
Flow Basis: ○ Moles ◉ Mass ○ Volume

Outlet	Fraction
Pumparound-2	0.8
Effect-2 Out	0.2

Setting the Pumparound-2 as the Tear stream

- ✓ Right-mouse-click on the Pumparound-1 stream and select Set Tear Stream.



- ✓ Click on the Pumparound-1 stream again and select the Definition tab 

in the Properties panel.

- ✓ Enter the following values:

Composition	Value
Temperature	100 C
Pressure	1 bar
Stream Amount	15000 kg/hr
H2O	90 kg
NaCl	10 kg

Table 16-3 - Pumparound-1 composition guess

If you cannot access the Definition tab, click off the Pumparound-1 stream and then click back on. The panel may need to be refreshed, because you just signaled to the software that this stream is a tear stream.

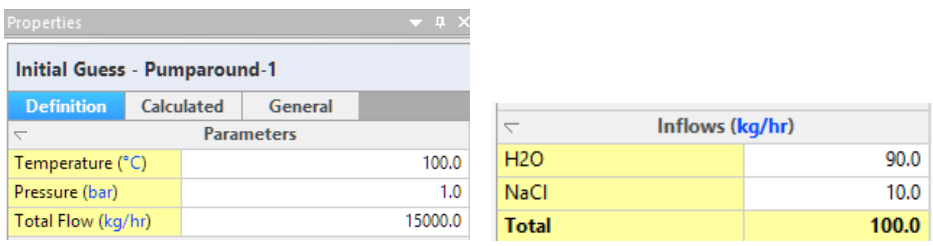


Figure 16-7 - Initial guess to the Pumparound-1 stream that will be used to converge the recycle

- ✓ Calculate.

The calculation should converge quickly, because a good initial guess was provided, and because the process is straightforward. If it does not converge quickly, check your work to see if something was missed.

Add the Callouts

- ✓ Add callout tables to the Feed to Effect-1, HX-1 out, Flash-1 vapor, Flash-1 liquid, Pumparound, and Effect-1 out.

- ✓ Use the following variables for each callout:

Feed to Effect-1	HX-1 Out	Flash-1 Vapor	Flash-1 Liquid	Pumparound-1
Temperature Pressure Mass	Temperature Mass	Mass	Mass	Mass

Table 16-4 - The Variables to be in each Callout table

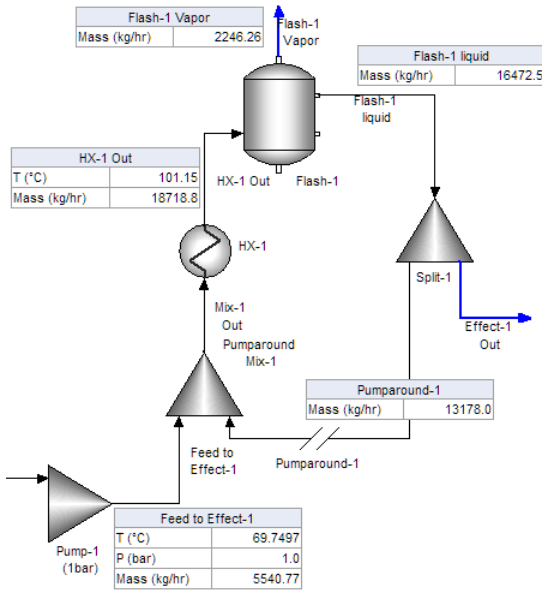


Figure 16-8- The converged flowsheet with the Callout tables added to the third effect streams

The Vapor mass is 2246 kg/hr which is 40.5% of the Feed to Effect-1 flow (5541 kg/hr). The target is 30% evaporation of the inlet feed. So you will increase the HX-2 vapor fraction by 25% value to 15%.

- ✓ Click on the HX-1 block to activate the Properties panel.
- ✓ Change the Vapor Fraction (mass %) value to 15.

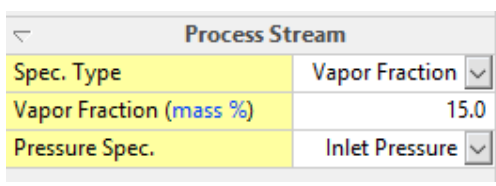


Figure 16-9 - updating the HX-1 vapor fraction to 15%

- ✓ Calculate.

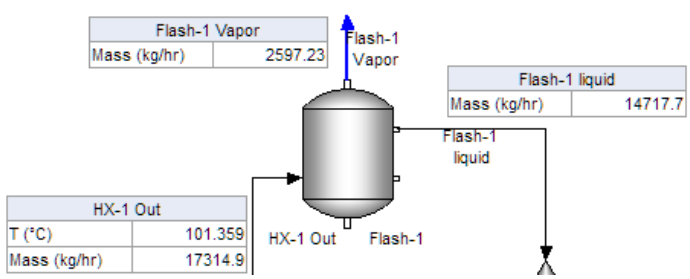


Figure 16-10 - Updated vapor flow after setting the HX-2 vapor fraction to 15%

The updated vapor rate is now 2597 kg/hr. This is 47% of the inlet rate and still not within the target value. You will change the value once again, 10% higher or 16.5%.

- ✓ Click on the HX-1 block to activate the Properties panel.
- ✓ Change the Vapor Fraction (mass %) value to 16.5.

Process Stream	
Spec. Type	Vapor Fraction
Vapor Fraction (mass %)	16.5
Pressure Spec.	Inlet Pressure

Figure 16-11 - updating the HX-1 vapor fraction to 16.5%

✓ Calculate.

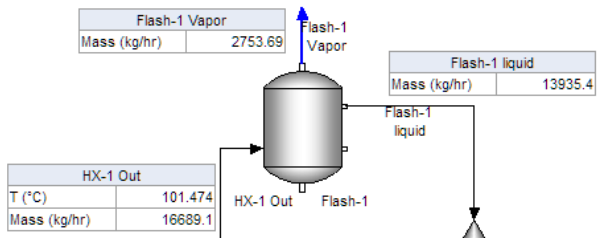


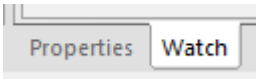
Figure 16-12 - Updated vapor flow after setting the HX-2 vapor fraction to 16.5%

The updated vapor rate is now 2754 kg/hr. This is 49.7% of the inlet rate and is within the target range.

✓ Save the file.

Review the HX-1 energy balance

✓ Click on the HX-1 block to access the Properties panel.

✓ Click on the Watch tab at the bottom of the panel - 

Watch

HX-1 Heat Exchanger	
Common Parameters	
Heat Duty (kJ/hr)	6.92956e6
Total Inlet Mass (kg/hr)	16689.1
Total Outlet Mass (kg/hr)	16689.1
Total Inlet Energy (kJ/hr)	-2.48833e8
Total Outlet Energy (kJ/hr)	-2.41904e8

Figure 16-13 - The Heat Balance surrounding the HX-1 block

The required heat duty is $6.93e^{6}$ KJ/hr. This energy will be sourced from an inlet Steam that will be added in the next chapter.

Summary

This chapter includes instructions to add the second and third effect. All three effects are easy to converge because good initial guesses were used and because the three recycle streams are not interdependent. This will change in the next chapters where the counter-current steam and flash vapor is used in the HX-1 and HX-2.

Chapter 17 Seawater Evaporation – Adding the Steam

The Application

This process is a continuation of the previous chapters. It a seawater evaporation system using three-evaporators and a crystallizer. All three effects are completed. Yet to be competed are the counter-current steam and vapor streams that supply the energy source to the three heat exchangers. The objective in this chapter is to add the steam and to converge the three-effect system.

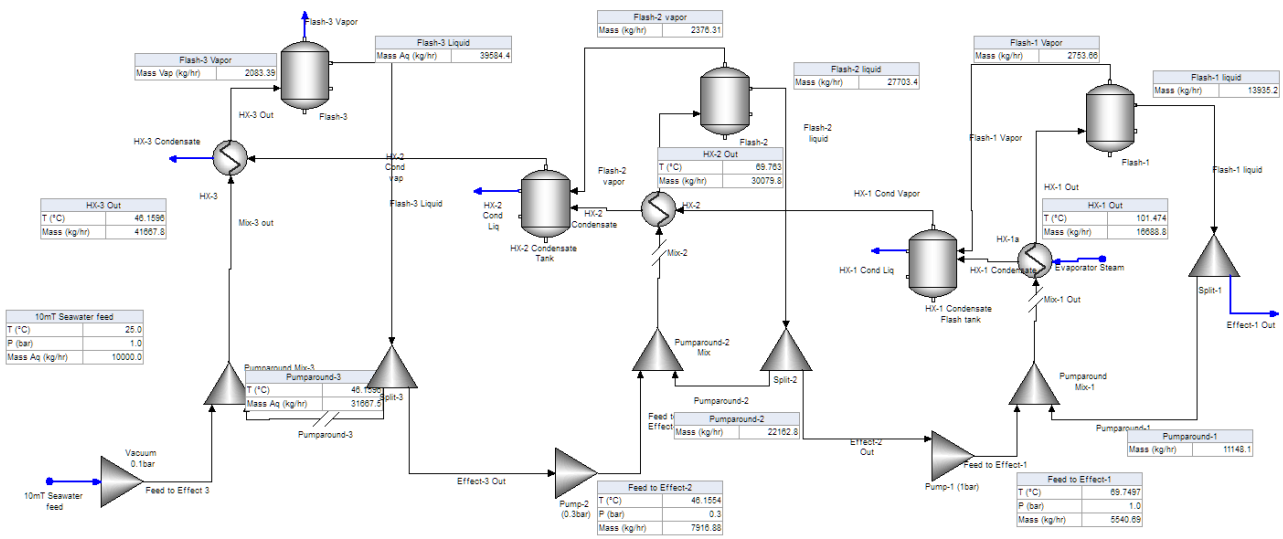


Figure 17-1- Three-effect evaporation system containing the counter-current steam flow

Creating the Chemistry Model

Open the existing Case file

✓ Open the existing file created in the last chapter, Seawater Multi-Effect Evaporation

File name: Seawater Multi-Effect Evaporation.esp

There is no change to the chemistry model in this chapter.

Building the Process

Adding the Steam

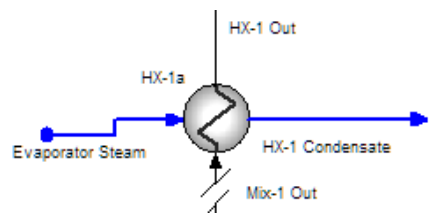
The process build procedure in this chapter is straightforward. Steam is added to HX-1. Its condensate is flashed to create additional steam. This flashed steam is combined with the HX-1 vapor exiting the Flash-1 and sent to the HX-2 block. This condensate will be flashed again at a lower pressure and mixed with Vapor from HX-2 and sent to HX-3 to provide its energy requirements.

Setting up HX-1 with a steam utility stream

What may be new to the reader is using the Utility configuration of the heat exchanger. In this case, the exchanger is modeled with a utility stream, and the heat transfer will be based on a temperature approach. The process stream inlet temperature is known, and the outlet temperature was set in the previous chapters. The differential temperature setting option sets the temperature difference between the process stream outlet and the utility inlet at 5C. Thus, the unknown is only the utility stream exit temperature.

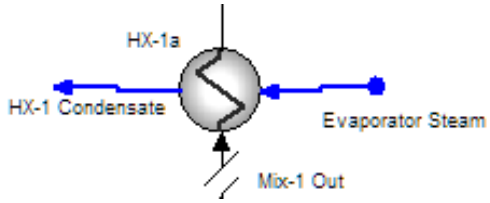
HX-1 block with a utility stream

- ✓ Add a new stream to the Utility inlet of the HX-1 block.
- ✓ Label the stream Evaporator Steam.
- ✓ Add a new stream to the Utility outlet of the HX-1 block.
- ✓ Label it HX-3 Condensate.



Notice that the flow direction is from left to right. This is opposite of the process, and so you will change the HX-3 orientation.

- ✓ Rotate the HX-3 block horizontally (if necessary). You may have to rearrange your streams to keep the flowsheet clean.



- ✓ Click on the Evaporator Steam stream and enter the following composition:

Table 1 - Evaporator steam composition

Composition	Value
Temperature	165 C
Pressure	6.909 bar
Stream Amount	4000 kg/hr
H2O	100 kg

Evaporator Steam

Definition | Calculated | General

Parameters	
Temperature (°C)	165.0
Pressure (bar)	6.909
Stream Amount (kg/hr)	4000.0

Inflows (kg/hr)	
H2O	100.0
NaCl	0.0
Total	**100.0**

Figure 17-2 – Evaporator Steam composition

✓ Click on the HX-1 block to access the Properties panel.

HX-1 Heat Exchanger

Definition | General

Inlets	
Process Stream Inlet	Mix-1 Out
Utility Stream Inlet	Evaporator Ste...

Outlets	
Process Stream Outlet	HX-1 Out
Utility Stream Outlet	HX-1 Condensate

Process Stream	
Spec. Type	Vapor Fraction
Vapor Fraction (mass %)	16.5
Pressure Spec.	Inlet Pressure

Utility Stream	
Spec. Type	Flow
Pressure Spec.	Inlet Press...

Heat Exchanger	
Flow Geometry	Counter-c...
Min. Temp. Approach (°C)	5.0

Advanced Options	
Chemistry Model	Chemistry ...

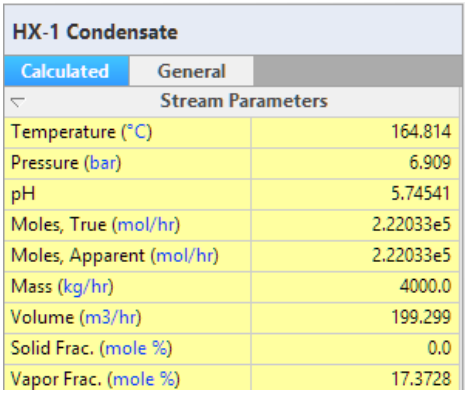
Figure 17-3 - Initial settings of the HX-1 block after the utility streams are added but before any adjustments are made

The panel should look like the image above. There is now a utility stream inlet and outlet. The Utility Stream Specifications (at the bottom of the panel) are set to Flow and Inlet Pressure (no pressure drop across the exchanger). The Heat Exchanger specifications are set to Counter-current flow with a 5C temperature approach.

✓ Calculate.

The simulation should converge quickly (within seconds). Our interest is to see how much available energy is left for the remaining exchanger. So, you will review the HX-1 condensate stream.

✓ Click on the HX-1 Condensate stream and review the Properties panel.



HX-1 Condensate

Calculated | General

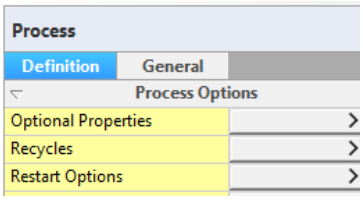
Stream Parameters	
Temperature (°C)	164.814
Pressure (bar)	6.909
pH	5.74541
Moles, True (mol/hr)	2.22033e5
Moles, Apparent (mol/hr)	2.22033e5
Mass (kg/hr)	4000.0
Volume (m3/hr)	199.299
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	17.3728

Figure 17-4 - The properties for HX-1 Condensate. There is 17% steam remaining.

Updating the process with the converged recycle streams

Each time the simulation is converged the three recycle streams are converged to new flows and compositions. To this point, however these new compositions have not been updated into the streams. Thus, each time the process is calculated it starts with the initial guess. The next step will update the three recycle guesses with the converged values.

- ✓ Click anywhere on the white section of the sheet to access the Flowsheet Properties panel.



Process

Definition | General

Process Options	
Optional Properties	>
Recycles	>
Restart Options	>

Figure 17-5 - The Process Properties panel focusing on the Recycle and Restart sections

- ✓ Select the Restart Options button and then press the Update All button on the next page.

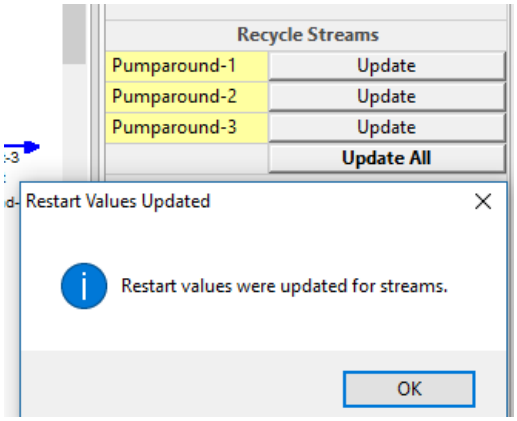
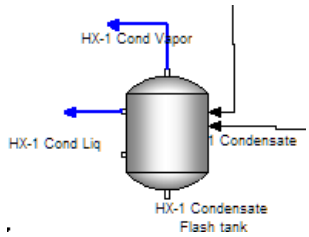


Figure 17-6 - The recycles have been updated with the most recent converged results

The software will report back that the three recycle streams have been updated with the converged values. You are doing this now because as the simulation becomes more complex, starting from a better initial guess is important.

Adding the HX-1 Condensate Flash tank to create steam for HX-2

- ✓ Double click on the Separator object in the Library to add it to the flowsheet.
- ✓ Label the block HX-1 Condensate Flash tank.
- ✓ Rotate the block horizontally -
- ✓ Link the HX-1 Condensate and the Flash-3 Vapor stream to the inlet.
- ✓ Add a new stream to the Vapor and to the liquid outlets. Label them HX-1 Cond Vapor and HX-1 Cond Liq.



- ✓ Click on the HX-1 Condensate Flash tank to access the Properties panel.
- ✓ Set the Pressure Spec. to Absolute Pressure with a value of 1 bar.

HX-1 Condensate Flash tank Separator

Definition | General

Inlets	
Feed	Flash-1 Vapor
Feed	HX-1 Condensate
Feed	

Outlets	
Liquid	HX-1 Cond Liq
Solids	
Vapor	HX-1 Cond Vapor
Organic	

Equilibrium Calculation	
Calculation Type	Adiabatic
Pressure Spec.	Absolute Pressure
Pressure (bar)	1.0
Heat Duty (kJ/hr)	0.0
Entrainment	

Figure 17-7 - The HX-1 Condensate Flash tank specifications

- ✓ Calculate.
- ✓ Review the HX-1 Cond Vapor stream properties.

HX-1 Cond Vapor	
Common Parameters	
T (°C)	99.7019
P (bar)	1.0
pH	
Moles, True (mol/hr)	2.1583e5
Moles, Apparent (mol/hr)	2.1583e5
Mass (kg/hr)	3888.26
Volume (m3/hr)	6635.57
Solid Frac (mole %)	0.0
Vap Frac (mole %)	100.0
Liq2 Frac, Apparent (mole %)	0.0

	Total, Apparent (Molecular) (kg/hr)
H2O	3888.26
HCl	4.10049e-14

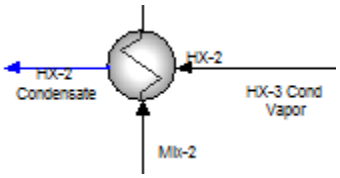
Figure 17-8 - The Stream parameters for the HX-1 condensate vapor

There is nearly 4000 kg/hr of 1-bar steam. Notice also that there is an insignificant amount of HCl in the steam. This HCl came from the HX-1 vapor stream.

Linking the HX-1 Cond Vap stream to the HX-2 Utility

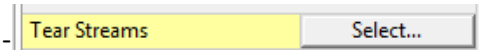
The next step is straightforward, but it will create complications with the recycle streams. Once this stream is linked, a new recycle loop is created. You will be required to make adjustments to the recycle settings.

- ✓ Click on the HX-2 block and rotate it horizontally
- ✓ Link the HX-1 Cond Vapor stream to the inlet of the HX-2 utility inlet.
- ✓ Add a new stream to the HX-2 utility outlet and label it HX-2 Condensate.

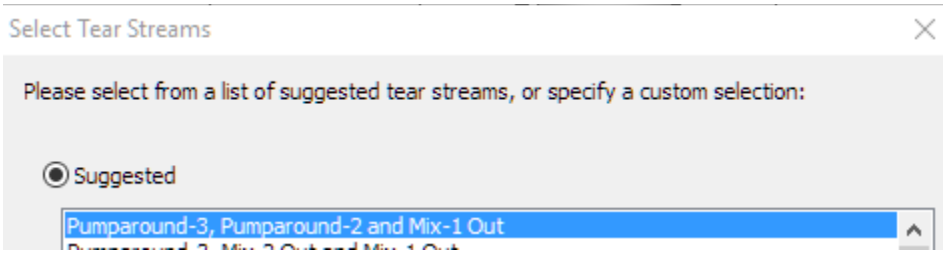


Adjusting the Recycles

- ✓ Click on white section of the Flowsheet to access the Properties panel.
- ✓ Click on the Recycles button -

- ✓ Click on the Select button for the Tear Streams- 

- ✓ Click on the Suggested radio button and then select the top choice:



New tear stream selection
Pumparound-3
Pumparound-2

Mix-1 Out

- ✓ Press OK to close the Tear Stream window.
- ✓ Click on the Initial Guess button for the Mix-1 out stream to see if there is an initial guess present.

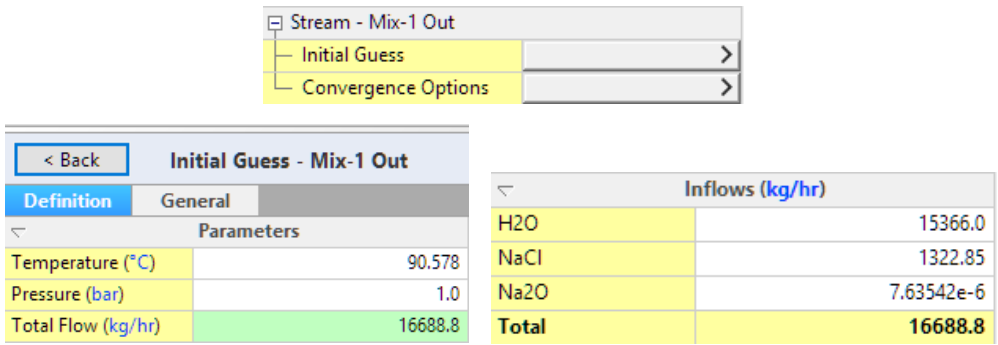


Figure 17-9 - The Initial guess for the Mix-1 Out stream. It is present because the previously converged results were entered.

An initial guess is available, which again, will improve the convergence process.

- ✓ Calculate.

The process should once-again converge within seconds.

- ✓ Click on the HX-2 Condensate stream to review its properties.

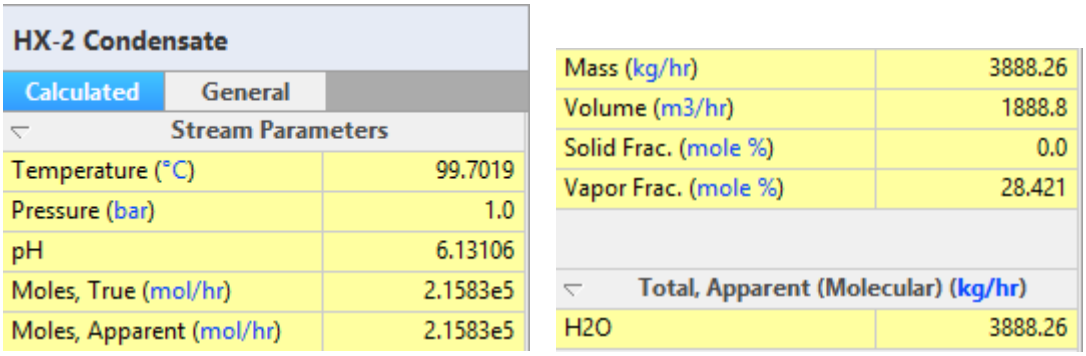
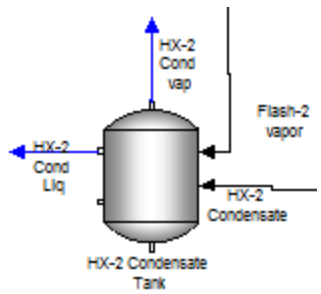


Figure 17-10 - The HX-2 Condensate stream parameters showing the existing water and vapor phases

The HX-2 condensate contains 28% vapor. This is a largely mathematical result because the boiling point range of this nearly-100% H2O stream is exceedingly small.

Adding the HX-2 Condensate Flash tank to create steam for HX-3

- ✓ Double click on the Separator object in the Library to add it to the flowsheet.
- ✓ Label the block HX-2 Condensate Flash tank.
- ✓ Rotate the block horizontally -
- ✓ Link the HX-2 Condensate and the Flash-2 Vapor stream to the inlet.
- ✓ Add a new stream to the Vapor and to the liquid outlets. Label them HX-2 Cond Vap and HX-2 Cond Liq, respectively.



- ✓ Click on the HX-2 Condensate Flash tank to access the Properties panel.
- ✓ Set the Pressure Spec. to Absolute Pressure with a value of 0.3 bar.

HX-2 Condensate Tank Separator

Definition | General

Inlets	
Feed	HX-2 Condensate
Feed	

Outlets	
Liquid	HX-2 Cond Liq
Solids	
Vapor	HX-2 Cond vap

Equilibrium Calculation	
Calculation Type	Adiabatic
Pressure Spec.	Absolute Pressure
Pressure (bar)	0.3
Heat Duty (kJ/hr)	0.0
Entrainment	

Figure 17-11 - The HX-2 Condensate Tank specifications

- ✓ Calculate.
- ✓ Review the HX-2 Cond Vap stream properties.

HX-2 Cond Liq

Calculated | General

Stream Parameters	
Temperature (°C)	69.101
Pressure (bar)	0.3
pH	6.41228
Moles, True (mol/hr)	1.4449e5
Moles, Apparent (mol/hr)	1.4449e5
Mass (kg/hr)	2603.03

Volume (m3/hr)	2.66037
Solid Frac. (mole %)	0.0
Vapor Frac. (mole %)	0.0

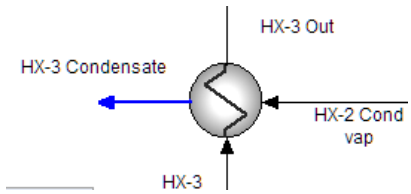
Total, Apparent (Molecular) (kg/hr)	
H2O	2603.04
HCl	1.29951e-7

Figure 17-12 - The HX-2 Condensate Liquid stream parameters

Linking the HX-2 Cond Vapor to HX-3

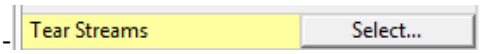
This is the last step of the chapter. You will create the link as before. This will also require that you change the recycle stream selection.

- ✓ Click on the HX-3 block and rotate it horizontally
- ✓ Link the HX-2 Cond Vap stream to the Utility Inlet of the HX-3 block.
- ✓ Add a new stream to the outlet of the HX-3 block and label it HX-3 Condensate.

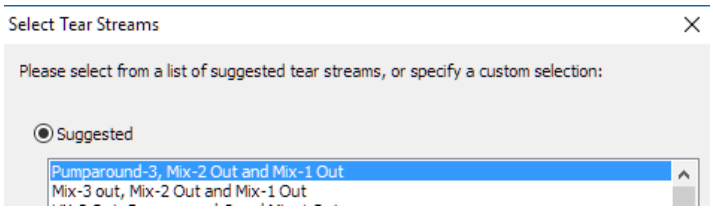


Changing the recycle stream

- ✓ Click anywhere on flowsheet to access the Properties panel for the Process.
- ✓ Click on the Recycles button -

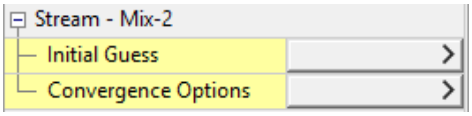
- ✓ Click on the Select button for the Tear Streams- 

- ✓ Click on the Suggested radio button and then select the top choice:



New tear stream selection
Pumparound 1
Mix-2 Out
Mix-1 Out

- ✓ Press OK to close the Tear Stream window.
- ✓ Click on the Initial Guess button for the Mix-2 Out stream to see if there is an initial guess present.



< Back **Initial Guess - Mix-2**

Definition | General

Parameters	
Temperature (°C)	63.4828
Pressure (bar)	0.3
Stream Amount (kg/hr)	30079.8

Inflows (kg/hr)	
H2O	28757.0
NaCl	1322.85
Na2O	4.72745e-7
Total	**30079.8**

Figure 17-13 - The Initial Guess present in the Mix-2 Out stream. It is present because the stream was converged previously

An initial guess is available, which again, will improve the convergence process.

- ✓ Calculate.

Updating the recycles with the most recent results

- ✓ Click anywhere on flowsheet to access the Properties panel for the Process.
- ✓ Click on the Restart Options button -

✓ Click on the Update All button

Recycle Streams	
Pumparound-3	Update
Mix-2 Out	Update
Mix-1 Out	Update
	Update All

The Evaporator portion of the process is complete. The outstanding work in this section is to add the remaining components to the seawater. This is not important now, and so will be done in a later chapter.

Summary

This chapter includes instructions to add the counter-current steam. The procedure was straight forward, and only a few blocks were needed. The more complicated part was to change the recycle streams because the configuration had changed. In the remaining chapters, the crystallizer will be added and the complete water analysis for seawater will be included.