OLI systems, inc.

INTRODUCTION TO

OLI Flowsheet: ESP

V11.5

think simulation

getting the
chemistry right

Introduction to OLI Flowsheet: ESP

Version : OLI Flowsheet: ESP V11.5

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Disclaimer

This manual was produced using the OLI Flowsheet: ESP 11.5 build 5 (11.5.5). At the time this manual was produced, the product was still in beta and some screen images may reflect that fact.

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.

Table of Contents

Chapter I – Getting Started with OLI Flowsheet: ESP

A tour of OLI Flowsheet: ESP – The basics

With version 11.5 the default thermodynamic framework is the Mixed-solvent Electrolyte (MSE) framework. However, for most of the examples in this guide we will use the legacy Aqueous (AQ) thermodynamic framework. When we are using a thermodynamic framework other than AQ we will so indicate it.

This tour of OLI Flowsheet: ESP is based on a sample application - a pH neutralization problem. Suppose we have two waste streams that must be mixed. One of the streams is an acid stream (in that the pH is less than 7.0 at room temperature) and the other stream is a base stream. We know from general chemistry that when acid and base streams mix, generally heat is evolved resulting in gases being produced. In addition, if the pH changes significantly, solids may form.

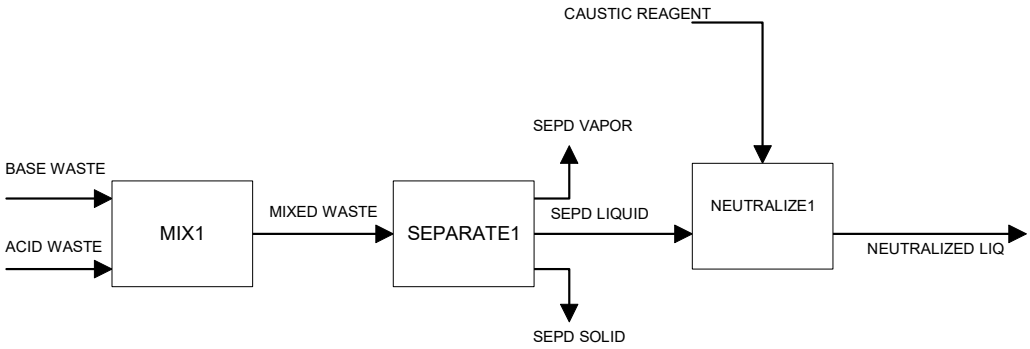
We want to treat any resulting gases from this mixing separately (we may need to recover the gases for another process) and we also want to remove any solids which may form. Finally, we want to make sure that the pH of the resulting liquid has been made basic.

Creating the Process

A diagram which represents this process in OLI Flowsheet: ESP, is shown below.

MIX1 is a mixer which adiabatically mixes the acid stream and the base stream. The resultant stream has a pH, temperature, and composition different from those of the inlet streams.

The next block chosen is a separator called SEPARATE1. This unit allows us to physically separate the multiphase product stream from MIX1 into separate vapor, liquid, and solids streams.



	Base Waste	Acid Waste	Caustic Reagent
Temperature (C)	40	25	30
Pressure (Atm)	1	1	1
Total Flow (mole/hr)	200	150	100
H2O	55.51	55.51	55.51
NH3	1.0	0	0
CO2	0.1	0	0
SO2	0.1	0	0
HCL	0	0.1	0
H2SO4	0	1	0
NaOH	0	0	1

Figure 1 Process Diagram pH Neutralization

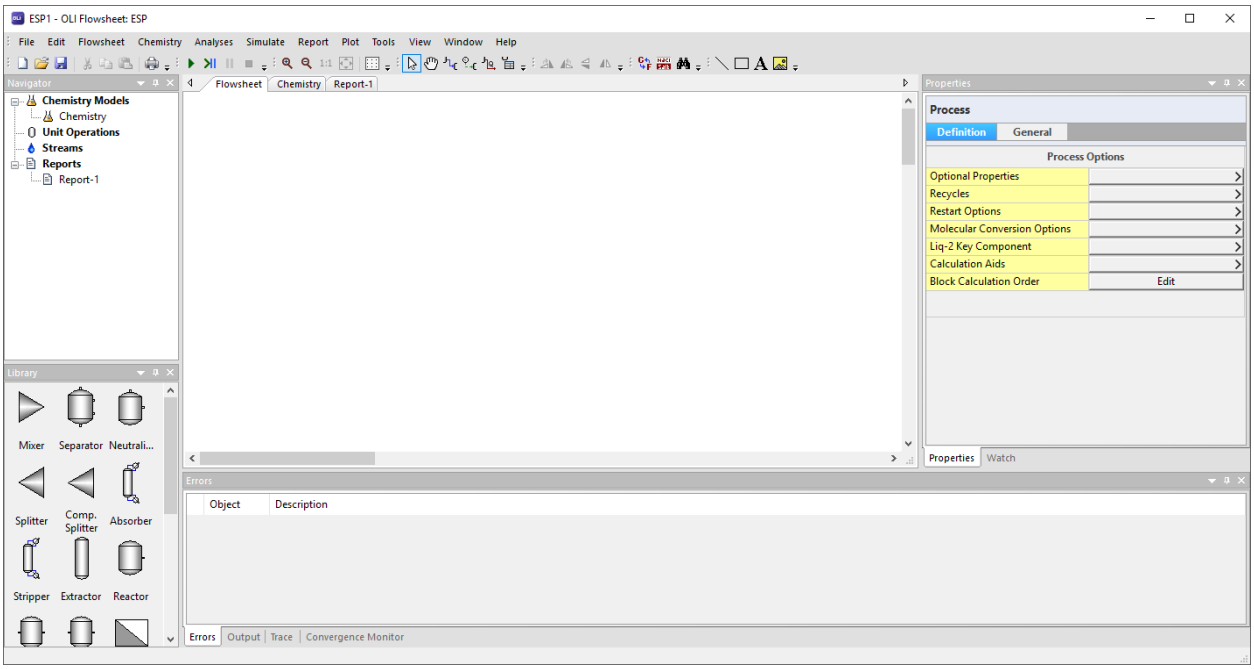
The combination of the mixer and separator represents a surge tank. Generally, a surge tank would be used in a pH neutralization process to dampen flow and composition fluctuations as well as to vent vapor release and to settle solids.

The neutralizer block then adds a reagent to adjust the pH of the liquid from that of the separator effluent liquid to the desired value.

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

Starting the tour

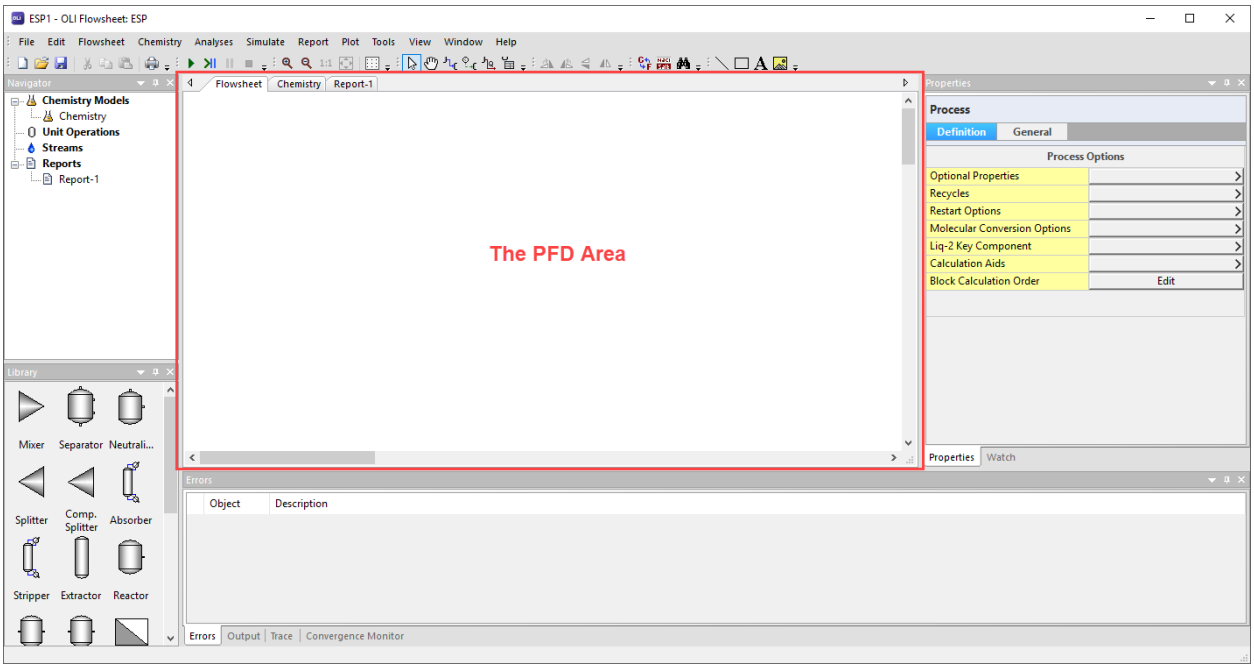
Start OLI Flowsheet: ESP by ether clicking the icon on the desktop or via the start menu options.



The standard layout

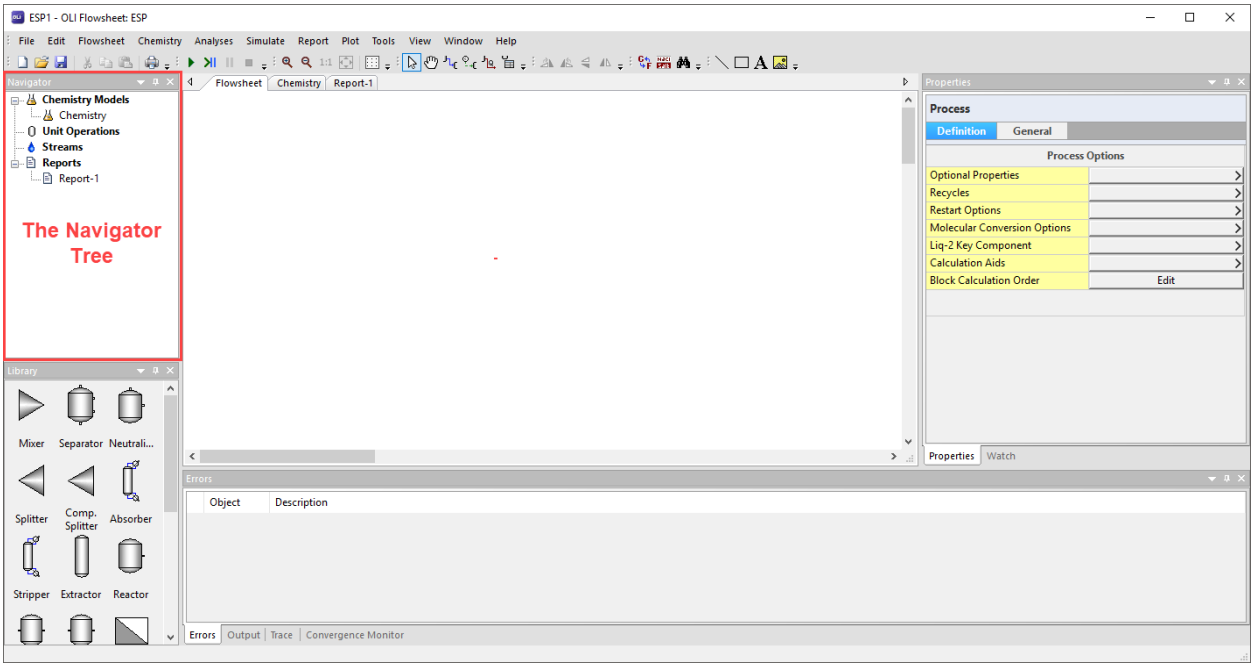
Let's begin by describing the various sections of the program.

The PFD (Process Flow diagram)



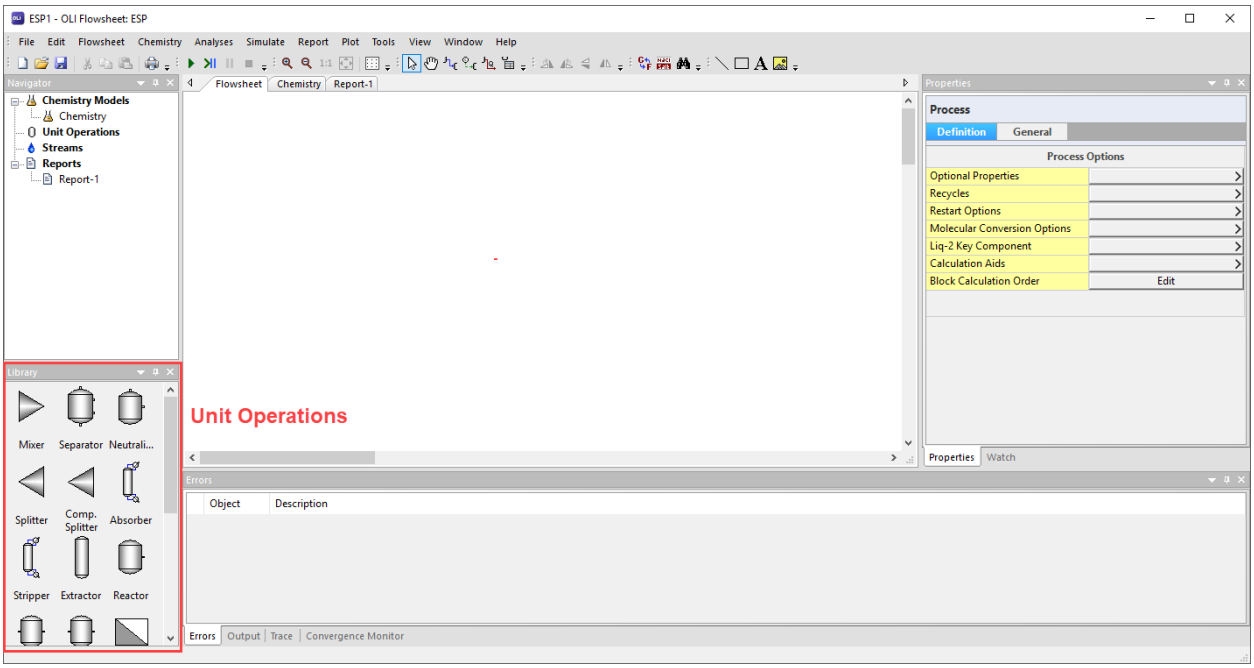
This is the area where we will build the process diagram. The tabs at the top are where we will define the chemistry and create our reports.

The Navigator Tree



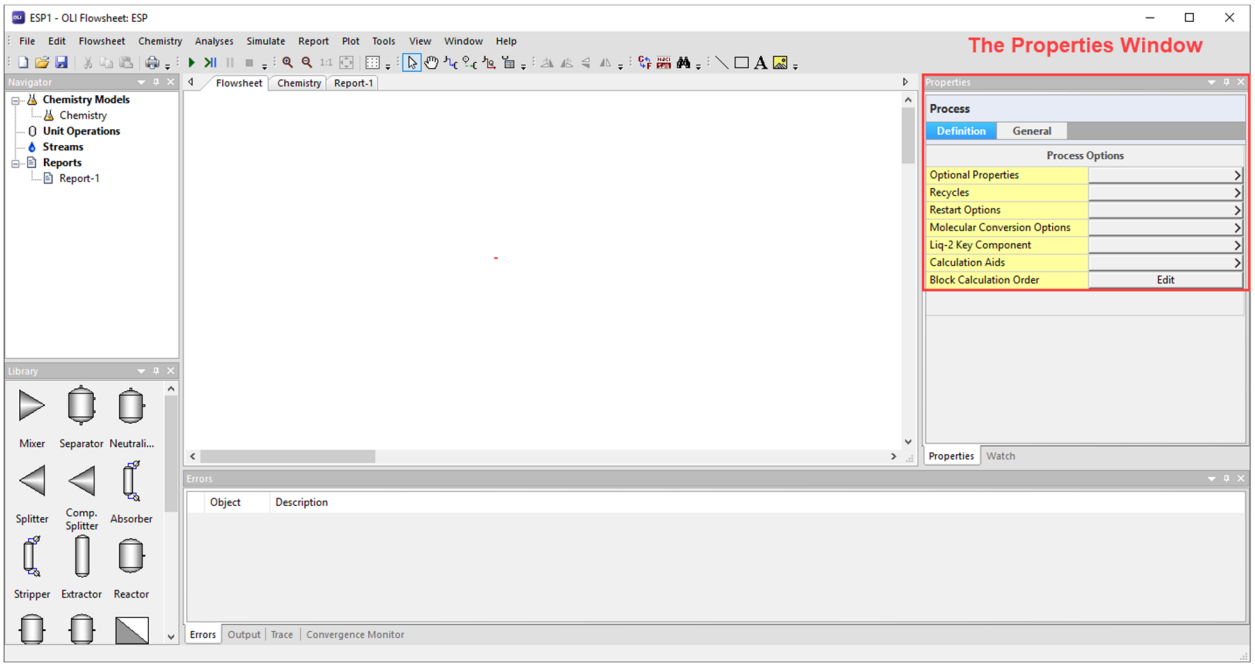
On this tree-view we can see all the objects, reports and chemistry models that exist in this document.

Unit Operations



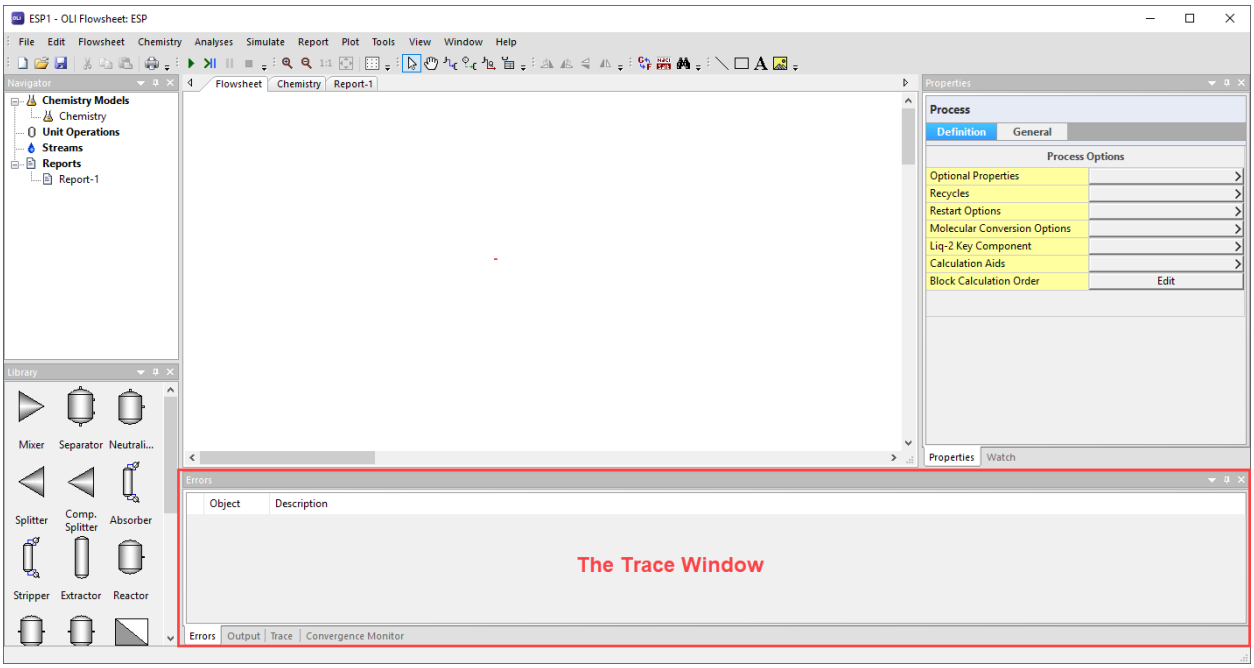
This is the palate of unit operations available in OLI Flowsheet: ESP. These will be described in more detail in the following chapters.

Properties



This window changes depending on the object highlighted. Right now, it is displaying options for the entire flowsheet.

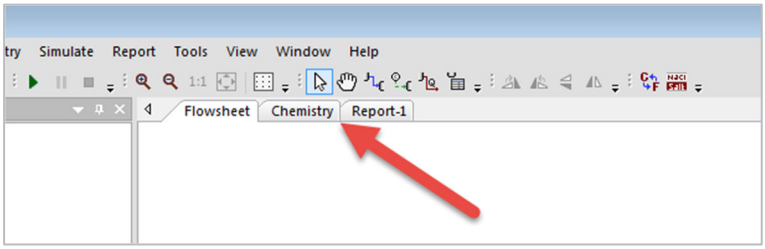
The Trace Window (Optional)



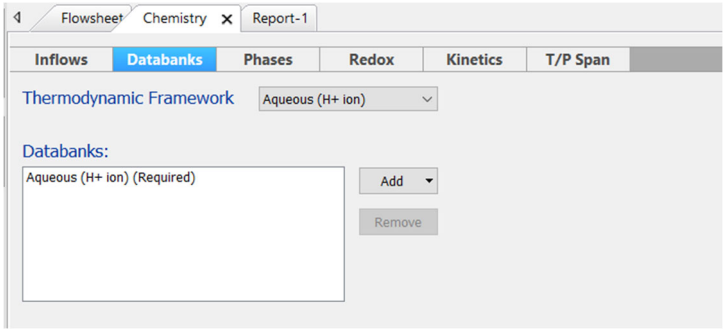
Various output messages about the state of the simulation are displayed here including warnings, errors, and convergence messages.

Defining the chemistry for this application

To begin to define the chemistry for this application we need to click on the **Chemistry Tab** located at the top of the PFD area.



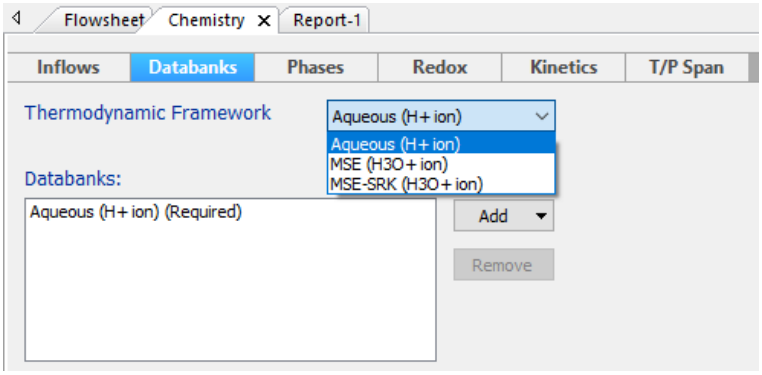
We can have multiple chemistry models in this application but for now we will only use a single model.



If you have used other OLI Software before then many of the objects on this screen will be familiar to you. We will describe them here.

The default view of the chemistry tab is the **Databanks Tab**. Here we have several buttons and fields.

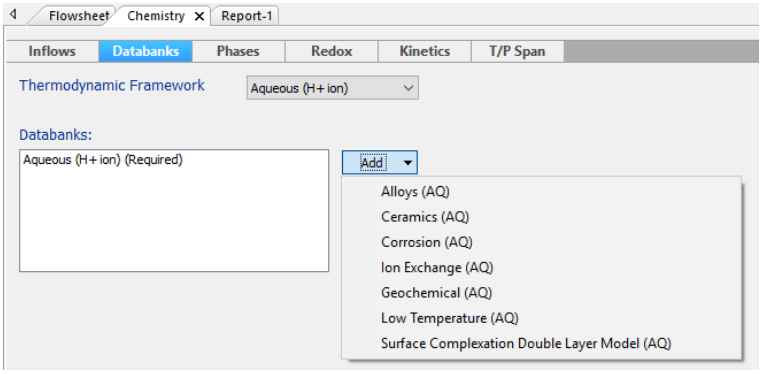
Thermodynamic Framework Button



Here we can choose the thermodynamic framework for the simulation. For this application use the **Aqueous (H+ Ion)** framework.

Adding user/private databanks

The user can add some additional databanks or their own databanks. This is usually required when the default OLI databank is missing some components or OLI has recently made an interim release of new data and components.. The currently selected databanks are displayed (Aqueous (H+ ion)[1] in this example) but additional databanks can be selected via the **Add** button.

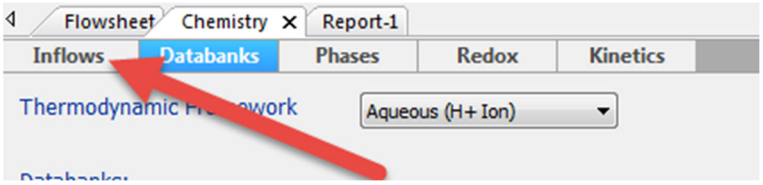


These databanks will be discussed in later chapters. For this application do not select any additional databanks.

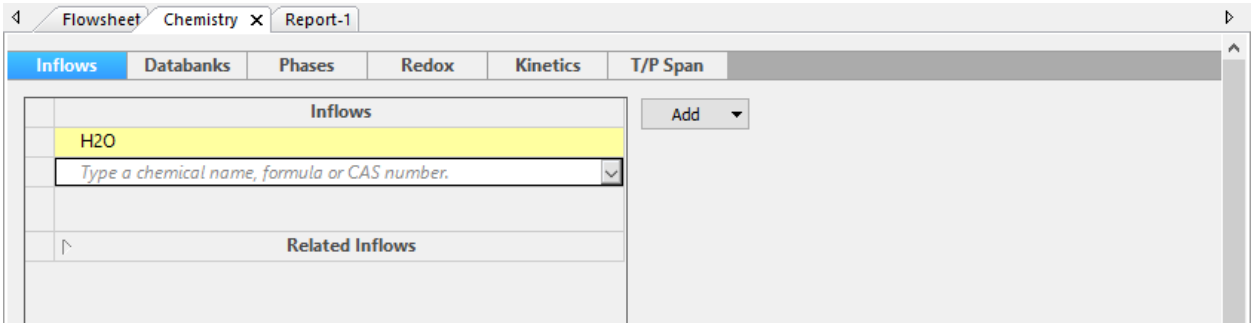
[1] Sometimes OLI will refer to this database as the PUBLIC database. The PUBLIC database is the default database for the AQ thermodynamic framework.

Creating the inflow chemistry

Now click on the **Inflows Tab** to enter the inflow list of components.

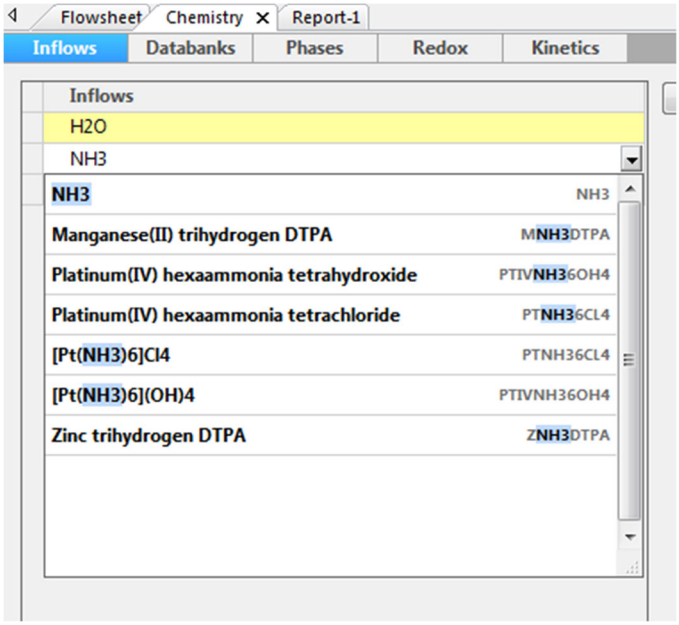


Entering components.

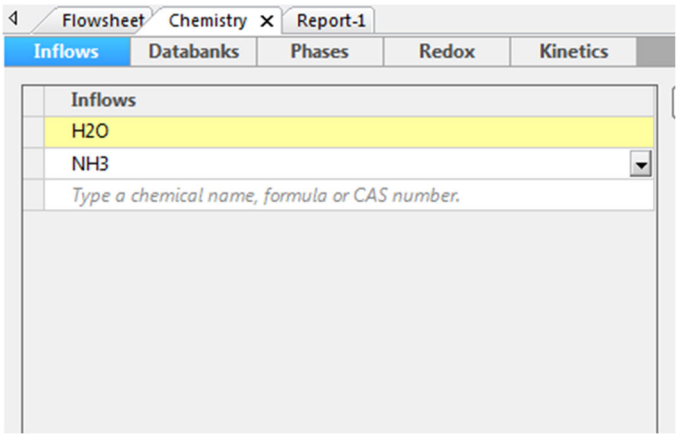


We can start to enter the name of our components. Experienced uses of OLI software know that they can either type in the chemical formula or enter the OLI TAG name. In version 11, common component names can be entered as well. The inflow grid will automatically start to search for your components. We can also add special components such as petroleum assays and pseudo components via the **Add** button. This functionality will be discussed in later chapters.

For now, please enter the species formula for ammonia, **NH3**



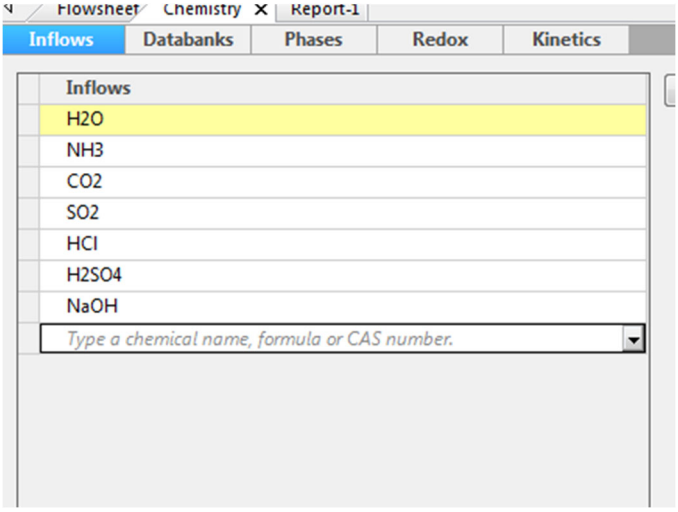
You can see that we automatically begin searching the selected databank for the characters “NH3”. There are several components to select, for this example select the first entry NH3.



Now please enter the remaining components for this application. These components are (enter each on a separate line):

CO2
SO2
HCl
H2SO4
NaOH

The grid should be like the image below when complete.

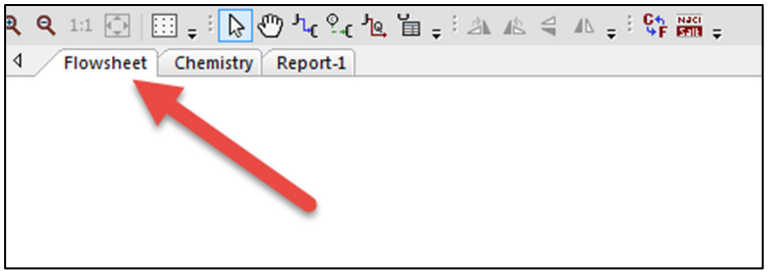


We can also modify the phase phenomena, oxidation and reduction chemistry, and reaction kinetics. We will leave this for later examples.

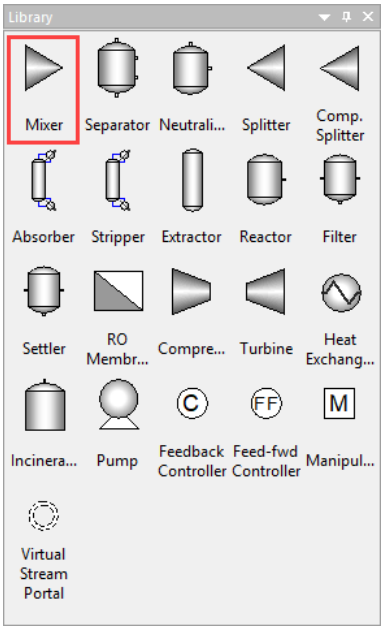
Building the process

We are ready to define the individual unit operations which make up the process shown in Figure 1 Process Diagram pH Neutralization on page 7

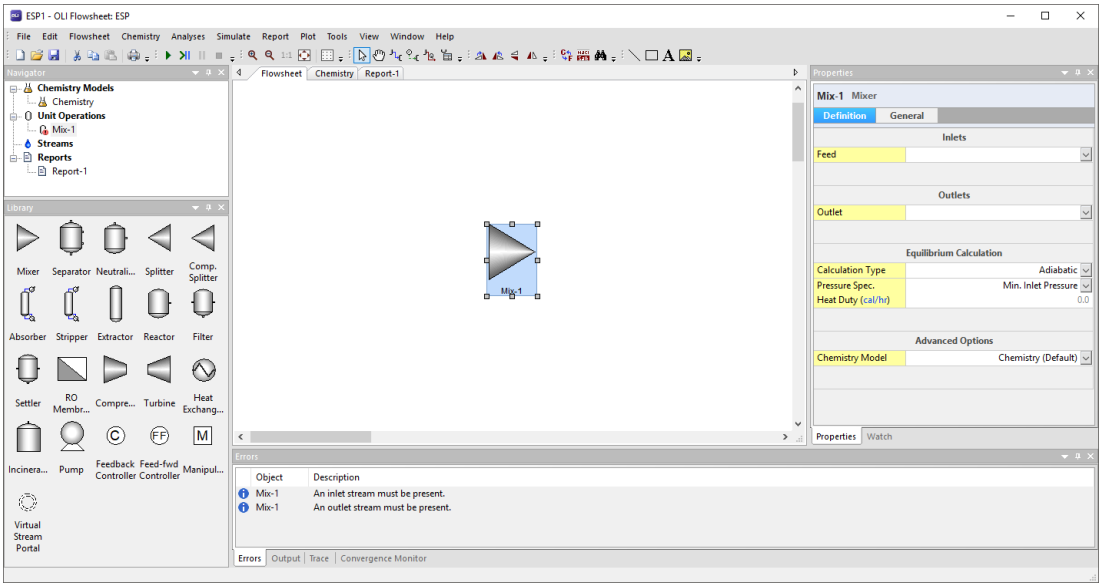
The first thing we should do is to click on the Flowsheet tab in the PFD area.



The **Mixer** is the first unit operation we need. Locate the **Mixer** in the unit operations library.

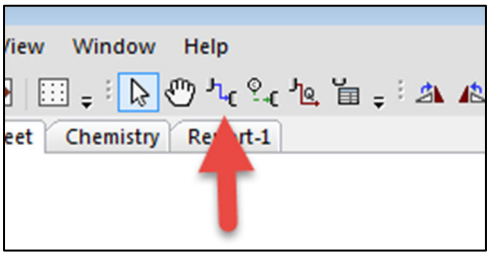


Double-clicking the object will add it to the PFD. Please note that the unit operation can also be dragged and dropped from the palette into the flowsheet area.



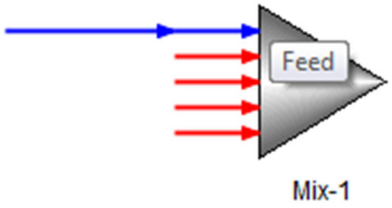
A lot of messages and properties suddenly became visible in the program. The object is centered on the PFD but you can click and drag it where you want. Right now, it is acceptable where it is located. The

Properties window has updated with some information. We will come back to this window. Right now, we need to add some streams. The mixer needs two inlets (although a single inlet is permitted) and a single outlet. To start adding streams we need to **click** the streams icon above the PFD in the tool bar.

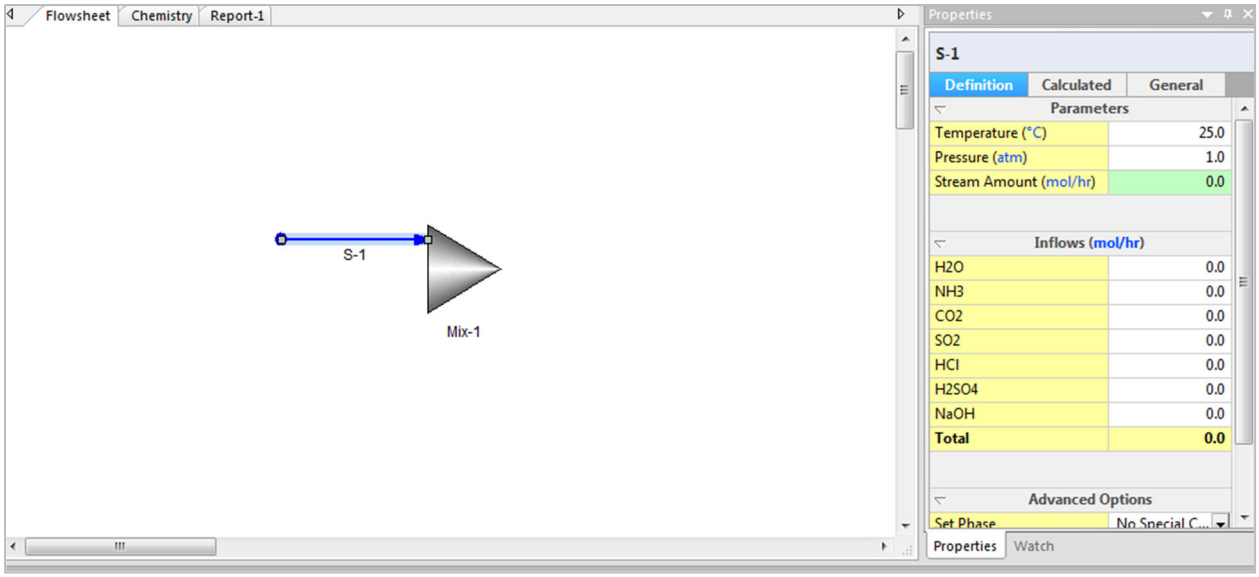


The Streams toolbar button

Now position the mouse pointer near the inlet side of the mixer.



As you click and drag the inlet select streams become visible as red lines. Just drop the end of the stream on the red line. Pressing the ESC key exits the add stream function if you so desire.

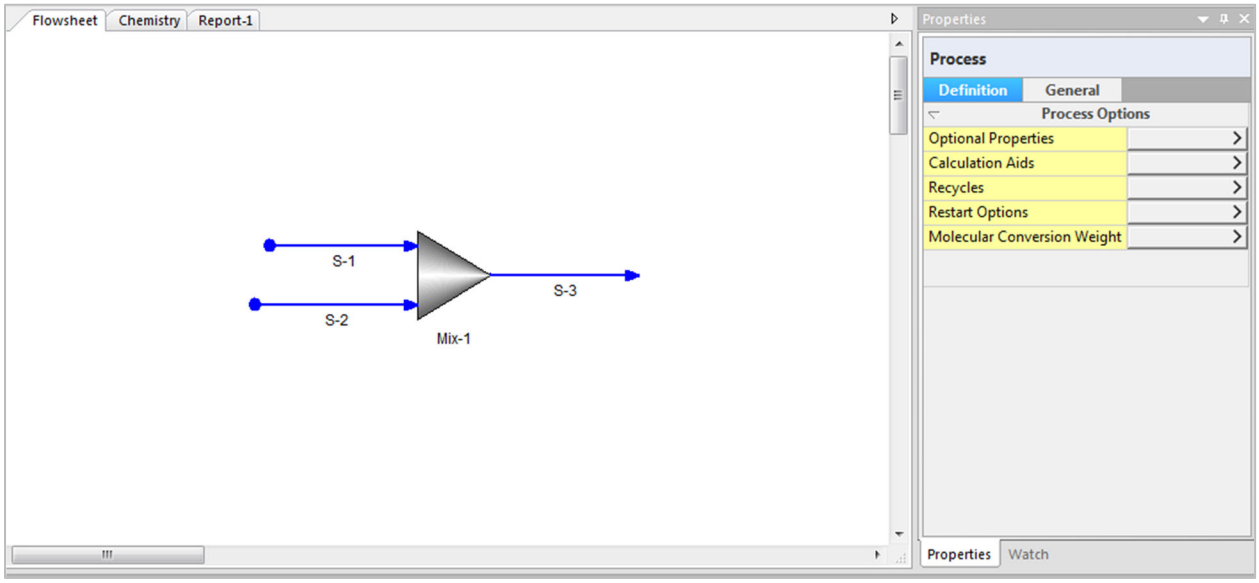


Added stream with the properties window displayed.

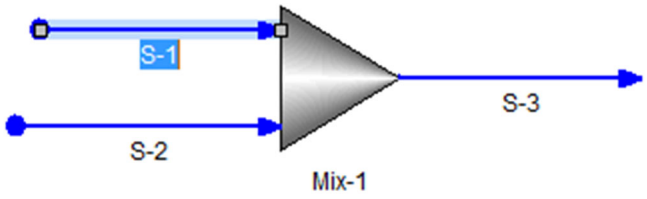
At this point you have some options. The desired stream name is “Base Waste” and you can change it now or later. Some users prefer to change the name as they go and others after the blocks are connected.

For this example, we will complete adding the inlet and outlet stream.

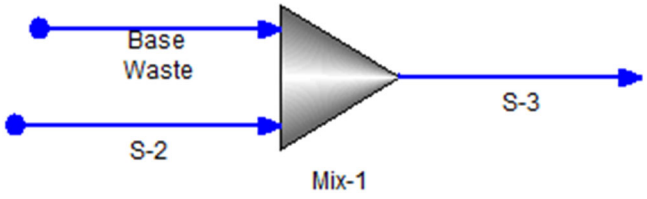
Re-click the **Add Stream** toolbar button and add a second inlet stream, and then an outlet stream. Your diagram should look like the following figure.



Now let's change the stream names to match Figure 1 Process Diagram pH Neutralization on page 7 iLike any good windows-based program there are several methods to accomplish this task. The first is to double-click the stream to put you into edit mode. Double-click the stream S-1 (or whatever name currently exists).

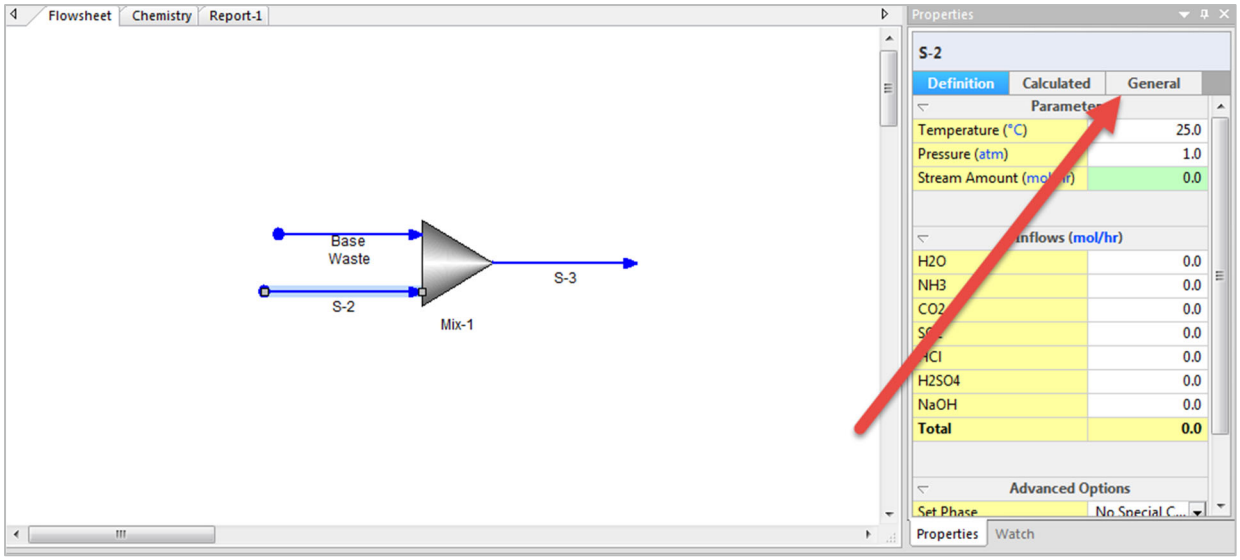


The name of the stream is highlighted. You can now just type the name you desire. In this case, please change the name to "Base Waste".



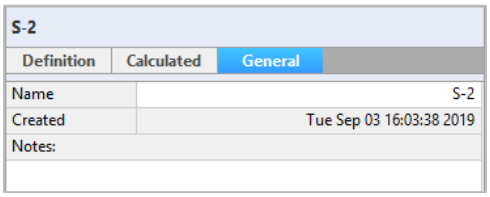
The text can be moved around to make the PFD more readable. We will do that in a later chapter.

The other method to change the name of a stream is to use the property window. In this case just click the stream "S-2"

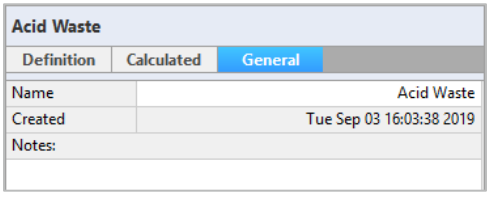


Changing the stream name via the properties window

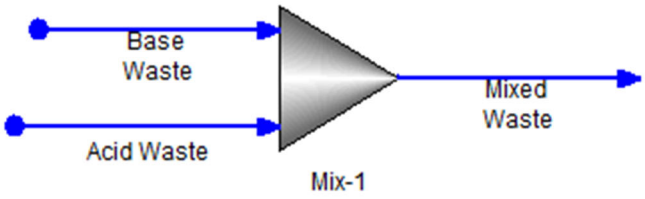
Click the **General** tab in the properties window for this stream.



Here you can rename the stream name “S-2” to “Acid Waste” as you would in any windows program.



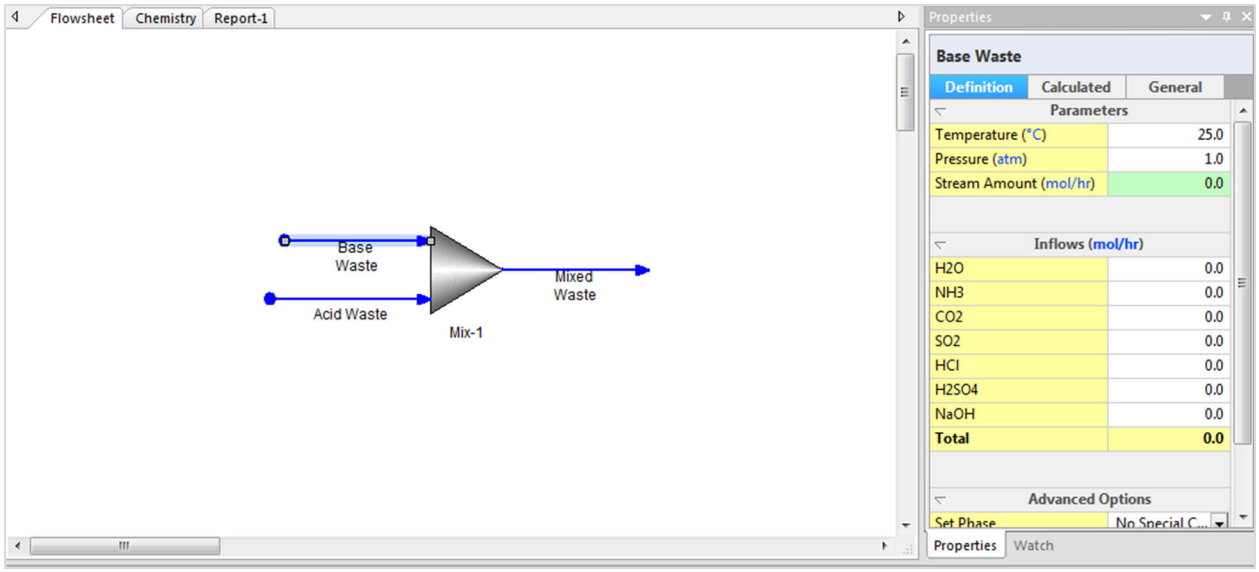
Now for the remaining stream, change the name to “Mixed Waste” using either method.



The fully named block

You can also rename the block itself using the same methods.

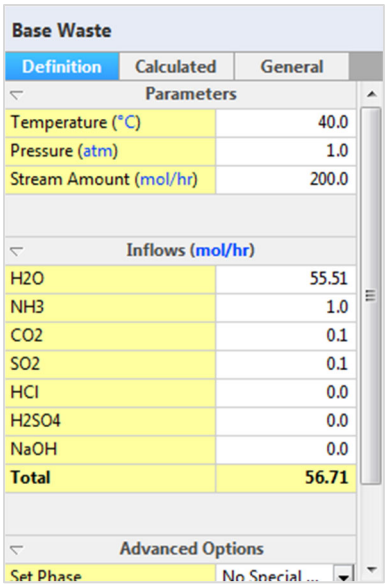
Now we need to define the composition of the streams and the operating conditions of the mixer. Click on the stream “Base Waste” and then click on the **Definition** tab in the properties window.



The composition of Base-Waste is given in the Table below:

Stream Name	Base Waste
Temperature, ºC	40.0
Pressure, Atm	1.0
Stream Amount, mole/hr	200
Inflows, mol/hr	
H2O	55.51
NH3	1.0
CO2	0.1
SO2	0.1

Enter these values in the grid; notice that we have not entered any values for HCl, H2SO4 or NaOH.



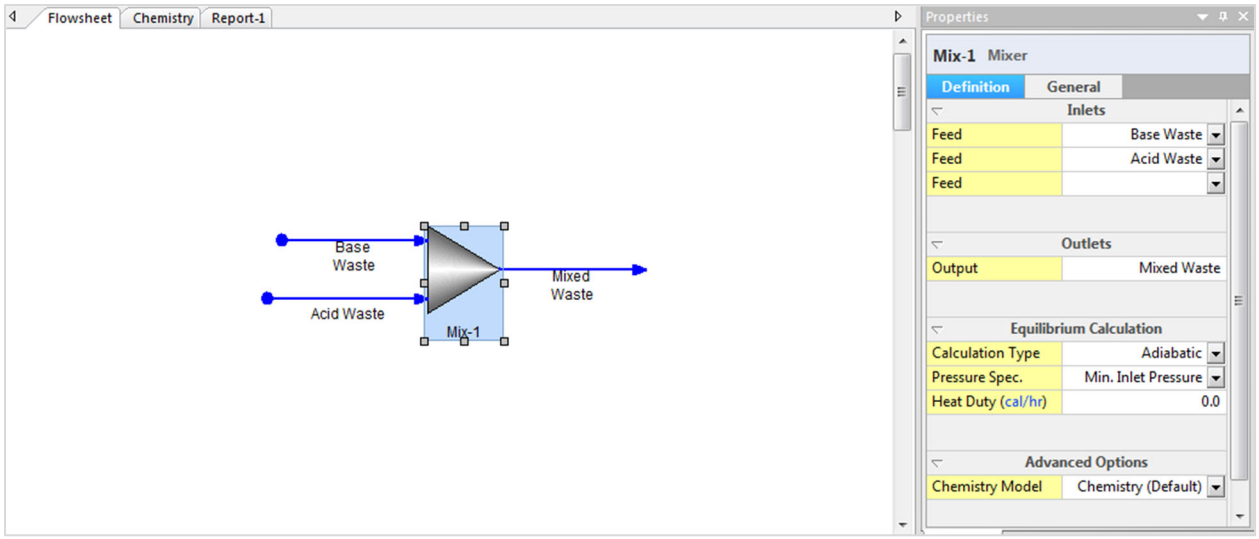
A few comments about this stream; notice that the “Stream Amount” and the “Total” do not match. This is by design. Many times, a user will know the stream amount in a different unit such as kg/hour and the inflows in mass fractions. In that scenario, the two values do not match. What the internal numerical engine will do is to normalize the inflows to match the stream amount.

Please enter the composition for the stream “Acid Waste” in the same manner.

Stream Name	Acid Waste
Temperature, ºC	25.0
Pressure, Atm	1.0
Stream Amount, mole/hr	150
Inflows, mol/hr	
H2O	55.51
HCl	0.1
H2SO4	1.0

Now we are ready to define the unit operation parameters.

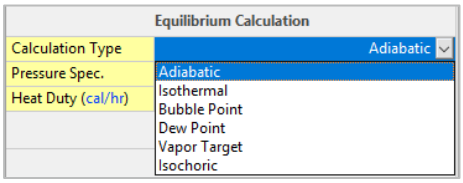
Click on the mixer block.



In the properties window, we have several options. These options differ for each type of unit operation. We can see the names of the inlet streams and outlet streams. We can use the drop-down arrows to select different streams if required.

Please look at the section labeled “Equilibrium Calculation.” Here we can set some basic parameters for a mixer block.

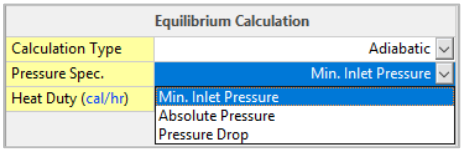
Calculation Type



We can have several types of calculations for a mixer. These will be described in detail in a later chapter. The default mixer type is “Adiabatic” which means the heat out of the block equals the sum of the heat into the block (duty = 0) and the temperature is calculated to meet that condition.

For this example, we will leave the **Calculation Type** at the default value of “Adiabatic”.

Pressure Spec.



Many unit operations have pressure options, and these often depend on the type of calculation being specified. For our example, we will leave the default value of “Min. Inlet Pressure” which means we will survey the inlet streams and use the smallest value. In this example the inlet streams both have a pressure of 1.0 atmosphere so that will be the pressure used.

Heat Duty

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

For adiabatic type calculations (where the temperature is calculated) we can add some type of offset value. This is a rare calculation, so we will use the default value of 0.0.

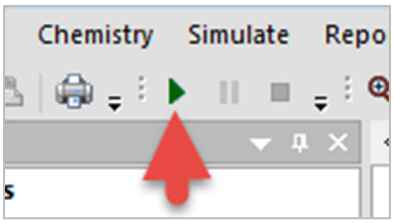
Running the calculation

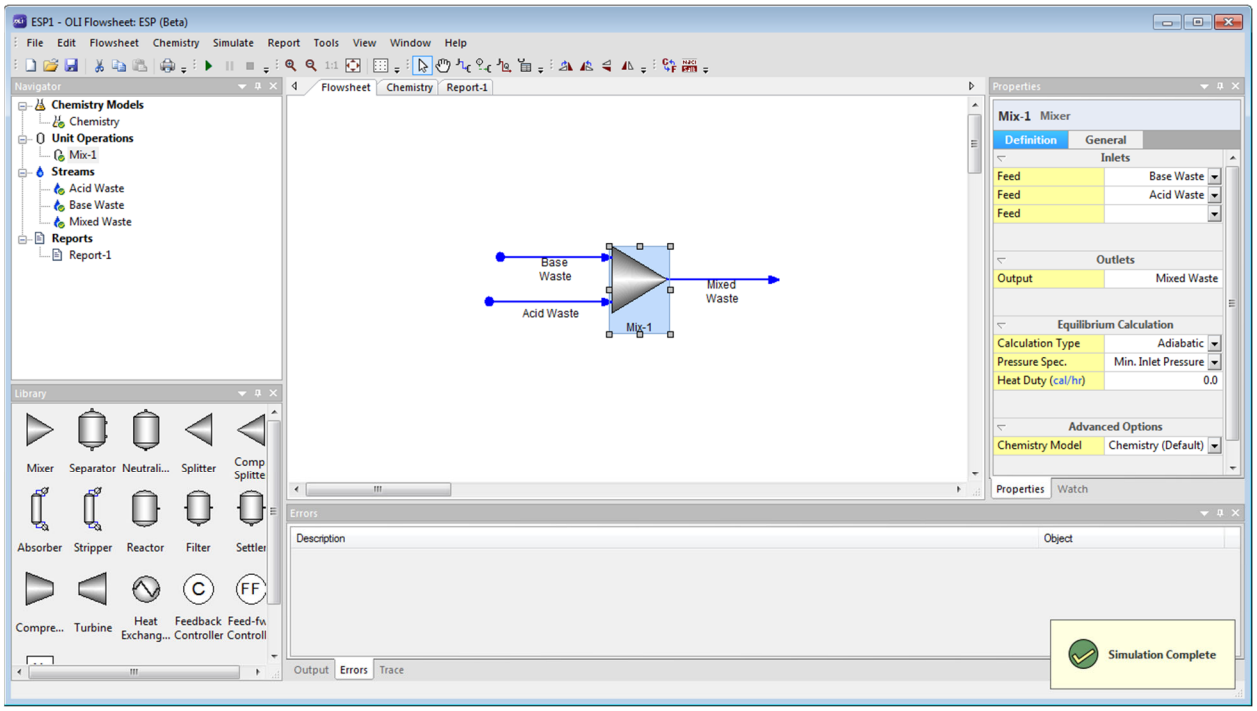
We have partially completed the process. There are several schools of thought on how to build a process. Some want to layout the process first then run the simulation. Others will build the process in parts and run each part. Both have advantages and disadvantages.

For this simulation, we will run the simulation for our partially completed process.

To run this simulation, please look for the “run button” in the toolbar.

Click the run button to run the simulation.



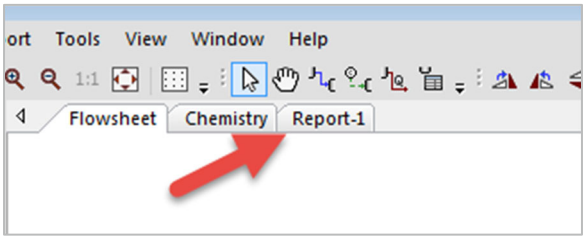


The simulation has been completed successfully.

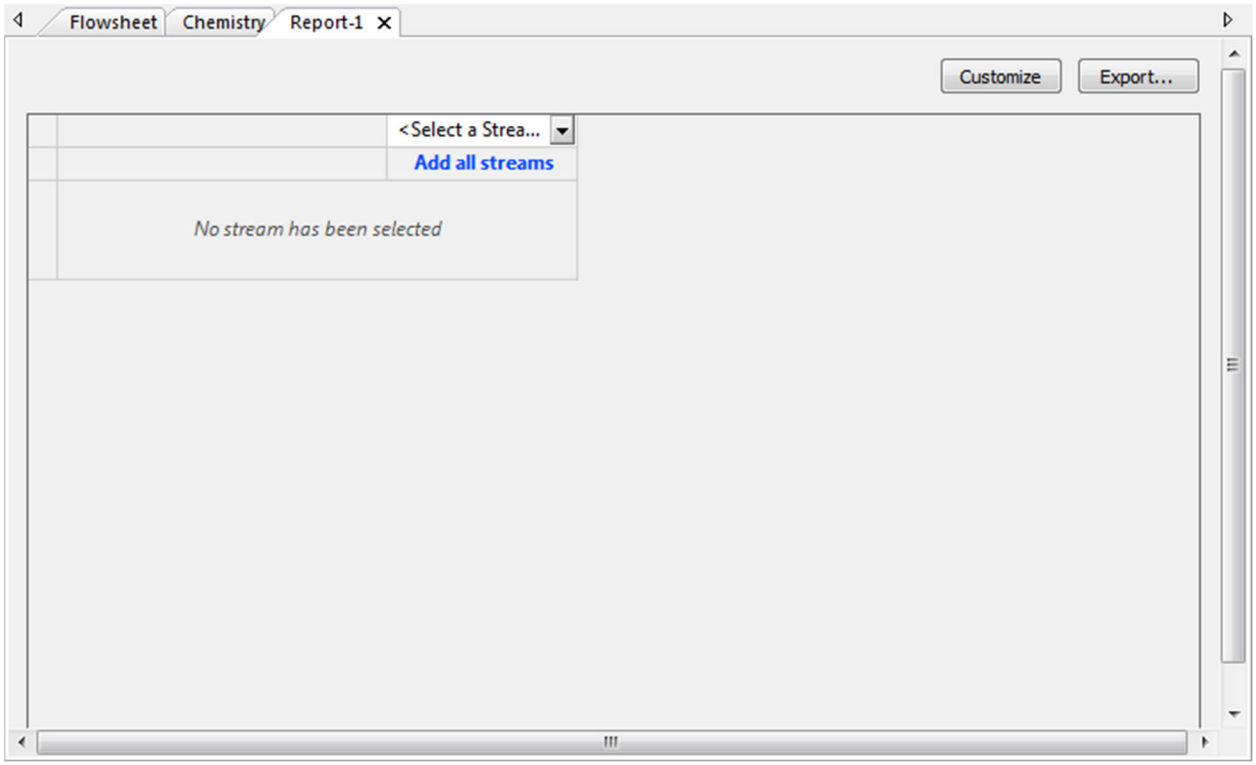
Obtaining preliminary results

Now that we have a converged simulation, we can obtain some results. These may not be (and probably will not be) the final results, but it is a good idea to investigate our preliminary results to see if they are reasonable. For example, we expect our “Acid Waste” stream to have low pH values and similarly the “Base Waste” stream to have high pH values.

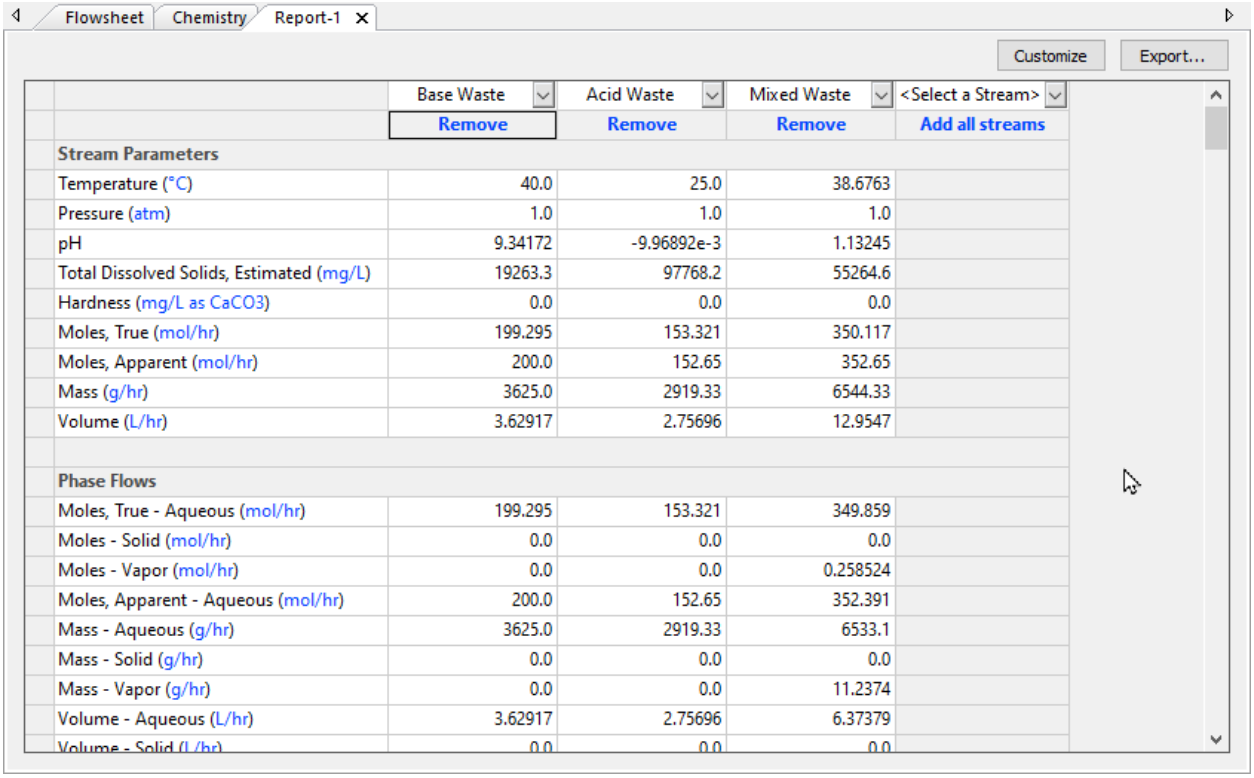
Click on the **Report-1** tab at the top of the PFD area (note: the “-1” means that is the first report for this document, the number may change).



This will display a report where the stream of interest needs to be selected first, before any information is shown.



We have many options here. We can see a single stream,multiple streams, or all the streams. The process, currently, only has three streams. Click the **Add All Streams** hyperlink.

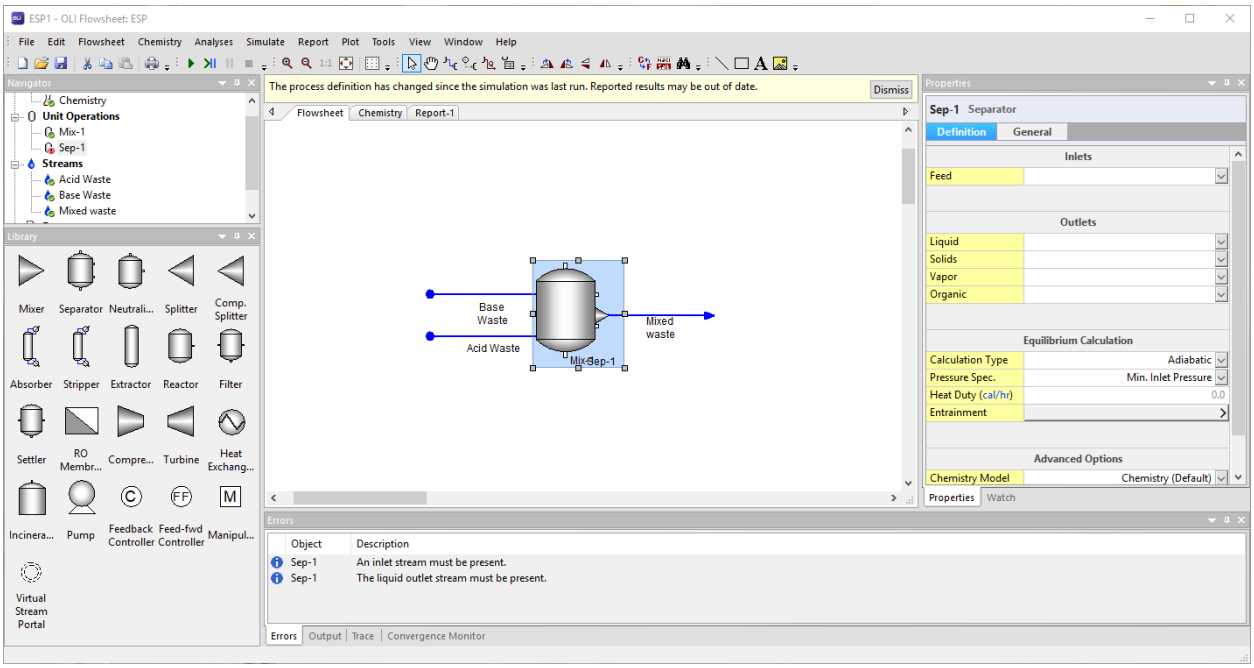


This report is a table. It can be copied and pasted into another program such as Microsoft Word or Excel. You can use the **Export** button to create a CSV file for direct import into Excel. Right now, we will not dwell on too much of the contents since we have more unit operations to add. You can see, however, that our "Base Waste" and "Acid Waste" streams have pH values representative of the type of stream that they are.

Finishing the application

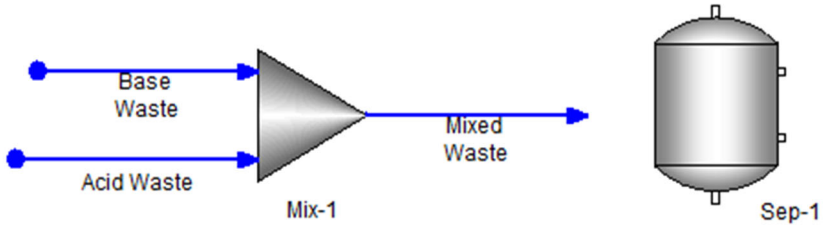
We will now finish the application by adding the remaining Separator and Neutralizer.

Click back on the **Flowsheet** tab above the PFD. From the **Library** please double-click the **Separator** unit operation.



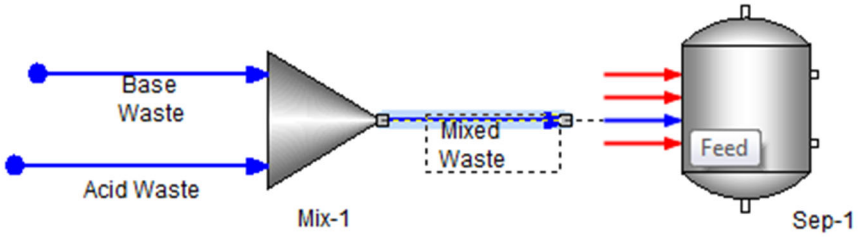
Adding a separator block

You can see that double-clicking the unit operation put it dead-center in the PFD. There is a slightly better method of adding a block which we will show you with the neutralizer. Drag the separator to the right of the mixer. Notice that a warning has appears informing you that the process definition has changed. Click the **Dismiss** button.

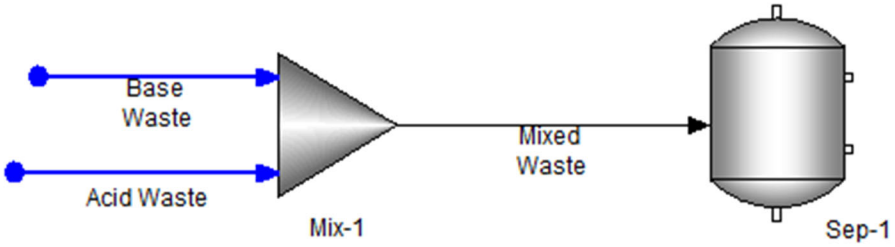


Now this part is tricky, click the arrowhead at the end of the stream “Mixed Waste” and drag it towards the separator “Sep-1.”

As you get close to the separator the inlet stream become live.



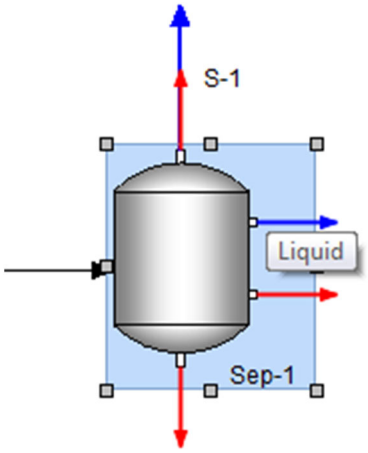
Connect the “Mixed Waste” stream to any inlet stream.



Notice now that the connected stream went from blue (which indicates an inlet or outlet stream) to a thin black line. Thin black lines represent internal streams. Blue lines with a dot on the end are inlet streams and blue line with just an arrowhead our outlet streams.

As we did with the mixer, we now need to add the outlet streams using the stream toolbar. Connect a line at the top, sides, and bottom.

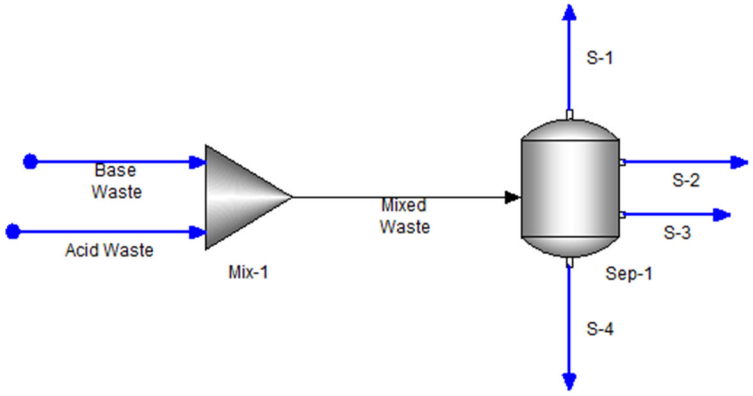
You will notice that as you add streams to a separator block, we display some tags.



Displaying stream tags

These tags tell you what kind of stream is expected for that outlet port. The top stream is expected to be vapor and the bottom is solids. The top-most side stream is a liquid (water rich) and the bottom-most side stream is an organic stream (hydrocarbon-rich). We will discuss separators in more detail in later chapters.

The completed separator unit block now looks like this:



We have started re-using the original stream names. We need to rename these streams according to the process design for pH neutralization shown on page 7.

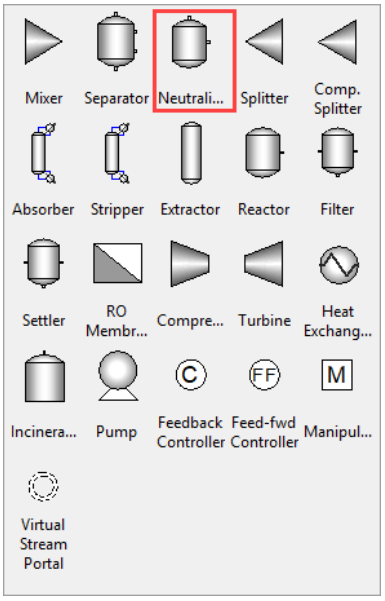
Separator Stream Definitions – Sep-1	
Line	**Name**
Vapor	Sep Vapor
Liquid	Sep Liq
Organic	Sep Org
Solid	Sep Solid

Using the methods outlined for the mixer, change the name as indicated in the above table.

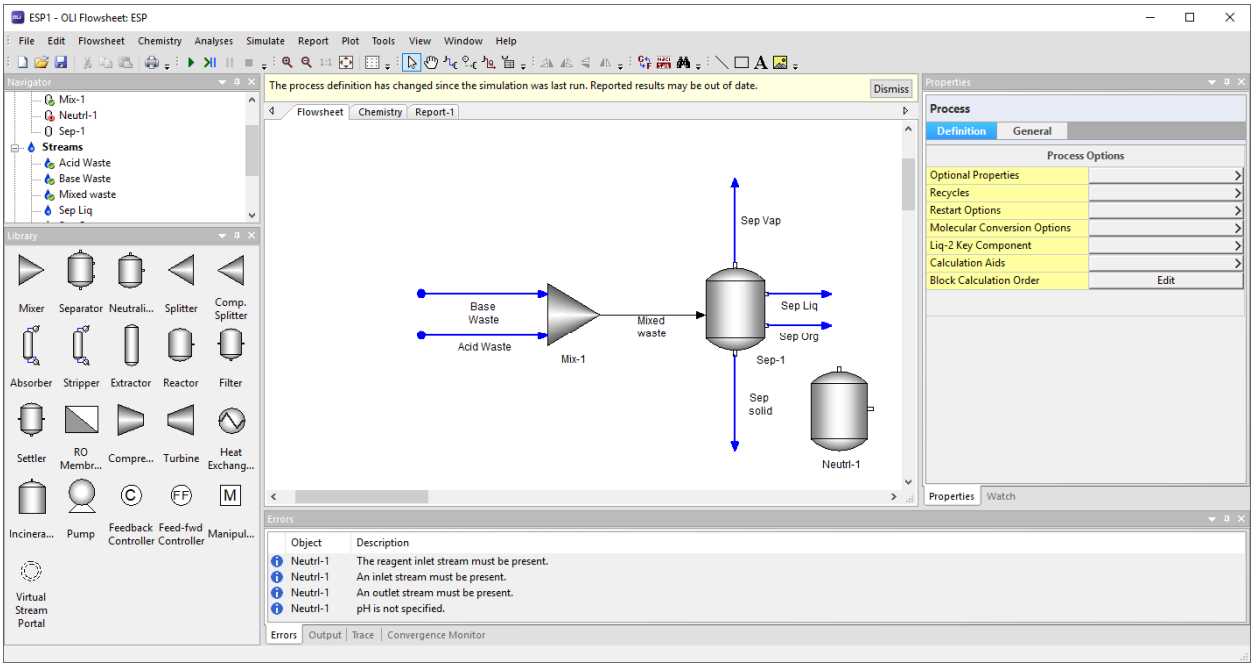
The separator also has its own properties which need to be defined. The separator also supports all the mixer calculations plus some entrainment options. We will not change any of these properties. The block properties are (we will use this table format for future examples).

Block Properties – Sept-1	
Block Type	Separator
Block Name	Sep-1
	Equilibrium Calculation
Calculation Type	Adiabatic (default)
Pressure Spec.	Min. Inlet Pressure (default)
Duty	0.0 (default)
Entrainment (sub-menu)	All values are default

We will now add the final block which is a neutralizer block. Locate the neutralizer block from the **Library** (you may need to scroll down to locate it).



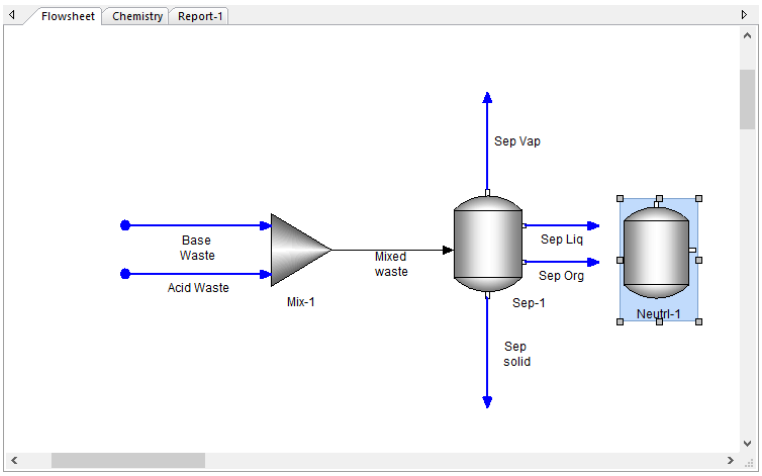
This time do not double-click the block. Click and then drag it to the PFD.



This is not a very convenient place to locate the block. Using the scroll bars move the entire PFD to the left (scrolling right):

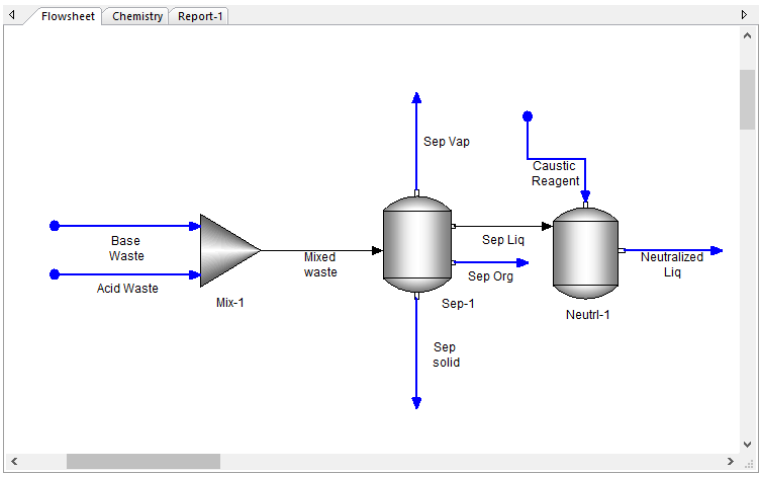
Scrolling right (moving left)

Now drag the neutralizer up a bit to be in line with the other blocks.



As with the separator, drag the stream “Sep Liq” to the neutralizer and connect to an inlet. Then add a new inlet stream to the top of the neutralizer. Rename the new inlet stream to “Caustic Reagent” and create an outlet stream named “Neutralized Liq”.

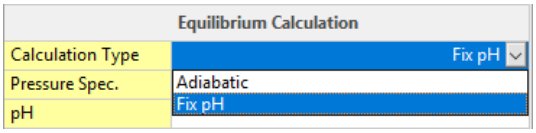
The process should look like the one shown in the figure below:



Now let’s finish adding the component inflows and block properties.

Stream Name	Caustic Reagent
Temperature, ºC	30.0
Pressure, Atm	1.0
Stream Amount, mole/hr	100
Inflows, mol/hr	
H2O	55.51
NaOH	1.0

Now we will enter the block properties for the neutralizer. The **Calculation Type** defaults to “Fix pH” for the neutralizer block. If it is not this option you can change it by using the drop-down menu to find the correct setting:



Block Type	Neutralizer
Block Name	Neutrl-1
Equilibrium Calculation	
Calculation Type	Fix pH
Pressure Spec.	Min. Inlet Pressure (default)
pH	9.0

Running the final simulation design

We are now ready to run the simulation for the final design. However, good computing practices dictate that we should save the simulation before we run it.

Click the **File | Save** menu item or use the Save toolbar button. This function is the same as the standard windows conventions. Save the file in a folder where you remember the location.

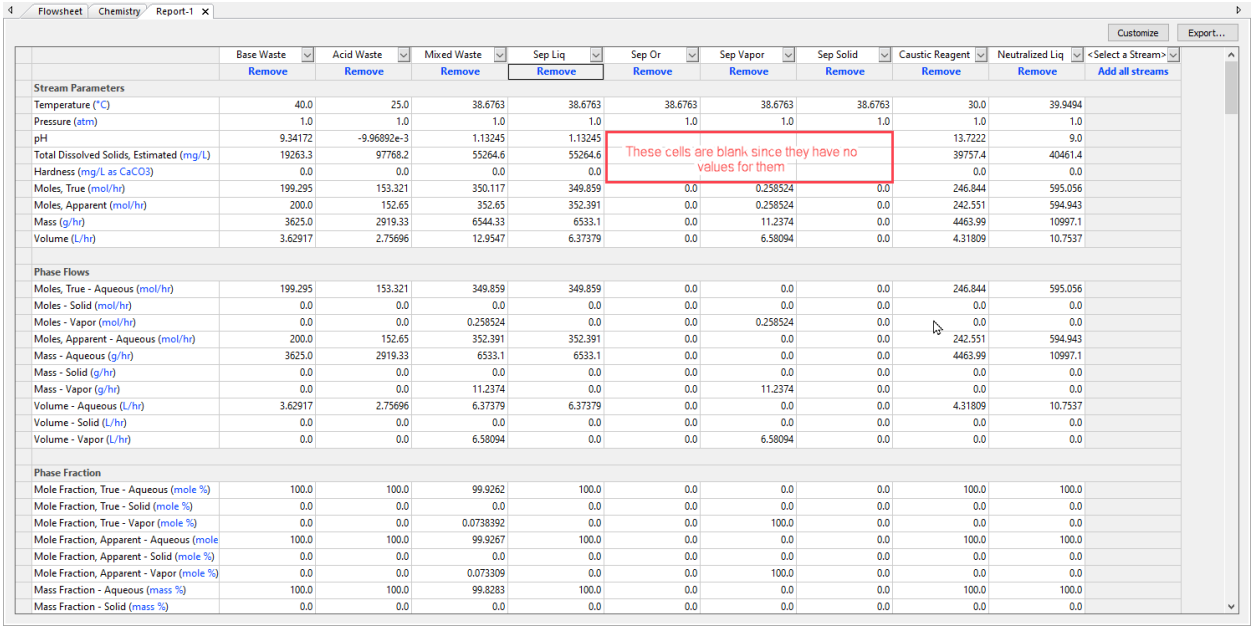
OLI recommends the name "**Neutral1-basic design**" as the file name. The file type is "ESP".

Click the run button.

Once complete, please click on the **Report-1** tab. The original list of streams will still be there and updated with new data if necessary. As we did previously, please click the **Add all streams** hyperlink.

We can modify the current report to display or hide streams and contents. If you are already familiar with OLI Studio, then you know much about the report sections for each stream. We previously looked at the streams "Base Waste" and "Acid Waste". These streams are straightforward to analyze, and we will not look at them here.

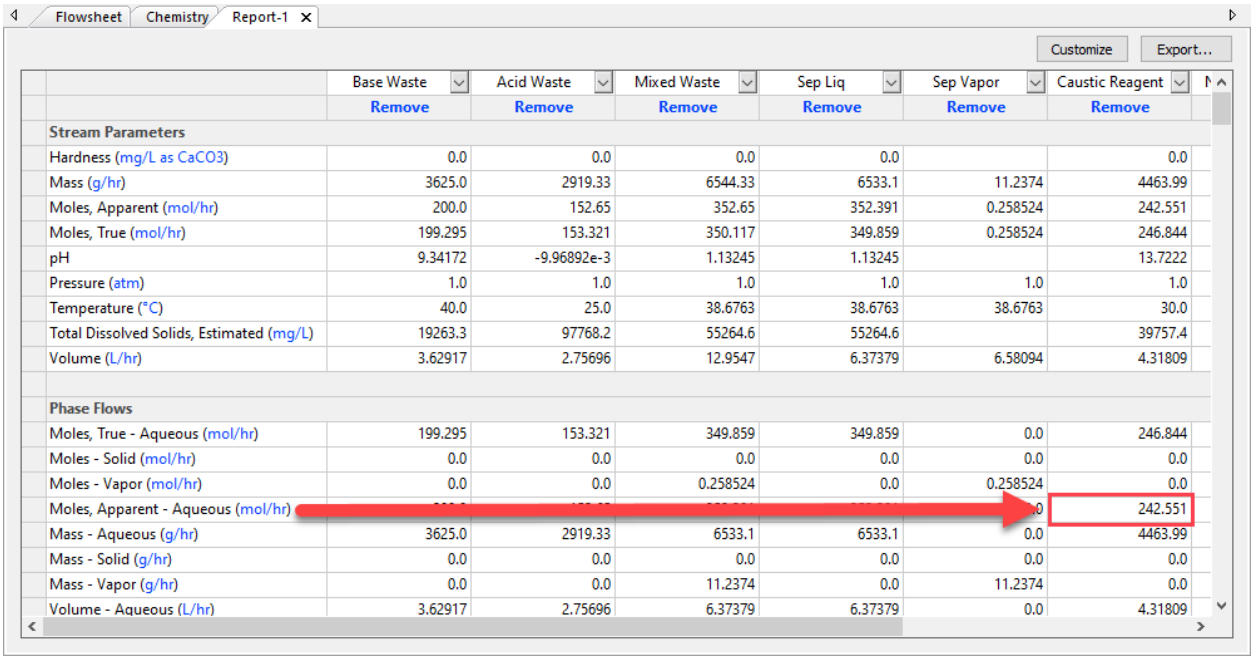
Click the **Remove** hyperlink under those streams to remove them from the report. You should have a screen like the following (you may need to scroll left or right to see all the values depending on your screen resolution).



	Base Waste	Acid Waste	Mixed Waste	Sep Liq	Sep Or	Sep Vapor	Sep Solid	Caustic Reagent	Neutralized Liq	<Select a Stream>
	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Remove	Add all streams
Stream Parameters										
Temperature (°C)	40.0	25.0	38.6763	38.6763	38.6763	38.6763	38.6763	30.0	39.9494	
Pressure (atm)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	
pH	9.34172	-9.96892e-3	1.13245	1.13245				13.7222	9.0	
Total Dissolved Solids, Estimated (mg/L)	19263.3	97768.2	55264.6	55264.6				39757.4	40461.4	
Hardness (mg/L as CaCO3)	0.0	0.0	0.0	0.0				0.0	0.0	
Moles, True (mol/hr)	199.295	153.321	350.117	349.859	0.0	0.258524	0.0	246.844	595.056	
Moles, Apparent (mol/hr)	200.0	152.65	352.65	352.391	0.0	0.258524	0.0	242.551	594.943	
Mass (g/hr)	3625.0	2919.33	6544.33	6533.1	0.0	11.2374	0.0	4463.99	10997.1	
Volume (L/hr)	3.62917	2.75696	12.9547	6.37379	0.0	6.58094	0.0	4.31809	10.7537	
Phase Flows										
Moles, True - Aqueous (mol/hr)	199.295	153.321	349.859	349.859	0.0	0.0	0.0	246.844	595.056	
Moles - Solid (mol/hr)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Moles - Vapor (mol/hr)	0.0	0.0	0.258524	0.0	0.0	0.258524	0.0	0.0	0.0	
Moles, Apparent - Aqueous (mol/hr)	200.0	152.65	352.391	352.391	0.0	0.0	0.0	242.551	594.943	
Mass - Aqueous (g/hr)	3625.0	2919.33	6533.1	6533.1	0.0	0.0	0.0	4463.99	10997.1	
Mass - Solid (g/hr)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Mass - Vapor (g/hr)	0.0	0.0	11.2374	0.0	0.0	11.2374	0.0	0.0	0.0	
Volume - Aqueous (L/hr)	3.62917	2.75696	6.37379	6.37379	0.0	0.0	0.0	4.31809	10.7537	
Volume - Solid (L/hr)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Volume - Vapor (L/hr)	0.0	0.0	6.58094	0.0	0.0	6.58094	0.0	0.0	0.0	
Phase Fraction										
Mole Fraction, True - Aqueous (mole %)	100.0	100.0	99.9262	100.0	0.0	0.0	0.0	100.0	100.0	
Mole Fraction, True - Solid (mole %)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Mole Fraction, True - Vapor (mole %)	0.0	0.0	0.0738392	0.0	0.0	100.0	0.0	0.0	0.0	
Mole Fraction, Apparent - Aqueous (mole	100.0	100.0	99.9267	100.0	0.0	0.0	0.0	100.0	100.0	
Mole Fraction, Apparent - Solid (mole %)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Mole Fraction, Apparent - Vapor (mole %)	0.0	0.0	0.073309	0.0	0.0	100.0	0.0	0.0	0.0	
Mass Fraction - Aqueous (mass %)	100.0	100.0	99.8283	100.0	0.0	0.0	0.0	100.0	100.0	
Mass Fraction - Solid (mass %)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Notice that the “Moles, True (mol/hr)” line for the streams “Sepd Org” and “Sepd Solid” equals zero (0.0). This means that these streams have zero content. For this analysis we can remove these streams from the report by clicking the **Remove** link.

We now have a much more reasonable list. Going back to the flowsheet process presented on page 7 the original flowrate of the “Caustic Reagent” stream was 100 mol/hr. The value now is 242.5 mol/hr.



	Base Waste	Acid Waste	Mixed Waste	Sep Liq	Sep Vapor	Caustic Reagent
	Remove	Remove	Remove	Remove	Remove	Remove
Stream Parameters						
Hardness (mg/L as CaCO3)	0.0	0.0	0.0	0.0		0.0
Mass (g/hr)	3625.0	2919.33	6544.33	6533.1	11.2374	4463.99
Moles, Apparent (mol/hr)	200.0	152.65	352.65	352.391	0.258524	242.551
Moles, True (mol/hr)	199.295	153.321	350.117	349.859	0.258524	246.844
pH	9.34172	-9.96892e-3	1.13245	1.13245		13.7222
Pressure (atm)	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (°C)	40.0	25.0	38.6763	38.6763	38.6763	30.0
Total Dissolved Solids, Estimated (mg/L)	19263.3	97768.2	55264.6	55264.6		39757.4
Volume (L/hr)	3.62917	2.75696	12.9547	6.37379	6.58094	4.31809
Phase Flows						
Moles, True - Aqueous (mol/hr)	199.295	153.321	349.859	349.859	0.0	246.844
Moles - Solid (mol/hr)	0.0	0.0	0.0	0.0	0.0	0.0
Moles - Vapor (mol/hr)	0.0	0.0	0.258524	0.0	0.258524	0.0
Moles, Apparent - Aqueous (mol/hr)					.0	242.551
Mass - Aqueous (g/hr)	3625.0	2919.33	6533.1	6533.1	0.0	4463.99
Mass - Solid (g/hr)	0.0	0.0	0.0	0.0	0.0	0.0
Mass - Vapor (g/hr)	0.0	0.0	11.2374	0.0	11.2374	0.0
Volume - Aqueous (L/hr)	3.62917	2.75696	6.37379	6.37379	0.0	4.31809

Why is it different from the input? The Neutralizer block has a target pH of 9.0. We can see from the streams that the “Sep Liq” stream has a pH of 1.13 so it will take some titrating of the caustic stream to raise it to 9.0.

Why did we look at the **Apparent** value instead of the **True** value? The true value is the sum of all species in the stream; vapor, solids, neutrals and ions. The apparent value has the ions converted back into neutral species and better compares to the neutral inputs we originally used.

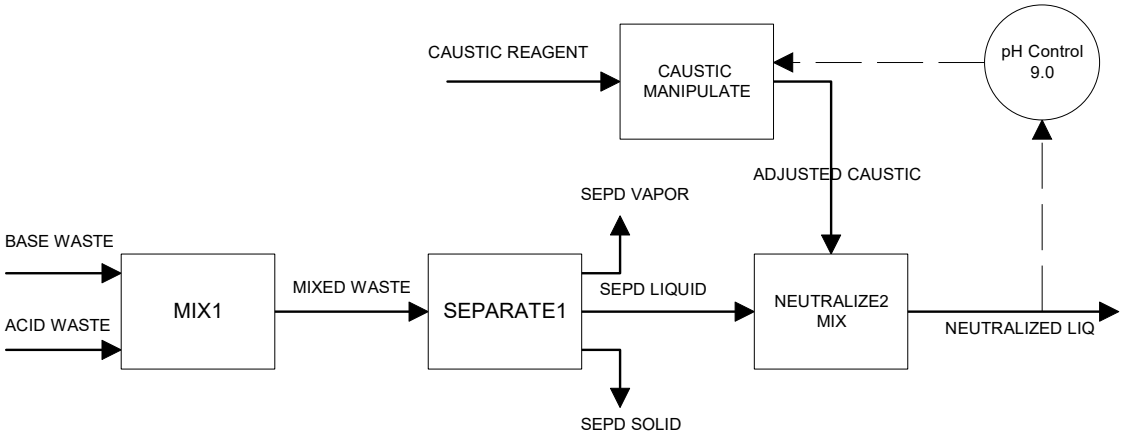
Later chapters will have a more complete discussion.

Once again, time to save your work.

A tour of OLI Flowsheet: ESP – Some Advanced Features

In this application we will continue to use the example process **Neutral1-basic design** but will add a pH control loop rather than the neutralizer block. We frequently use a control loop for pH in cases where the set point of the controller is near the equivalence point of the solution (an area in which mathematical solutions are difficult to obtain).

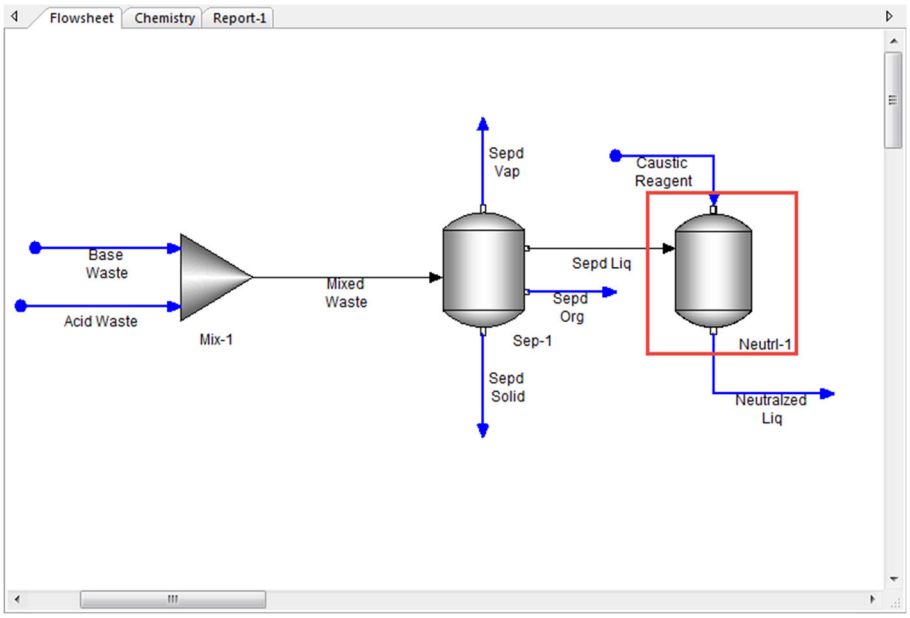
We will be re-using portions of the **NEUTRAL1** process[2] described. The revised process diagram can be seen in the figure below.



Neutralization Process with Manipulate/Mix Block and pH Controller

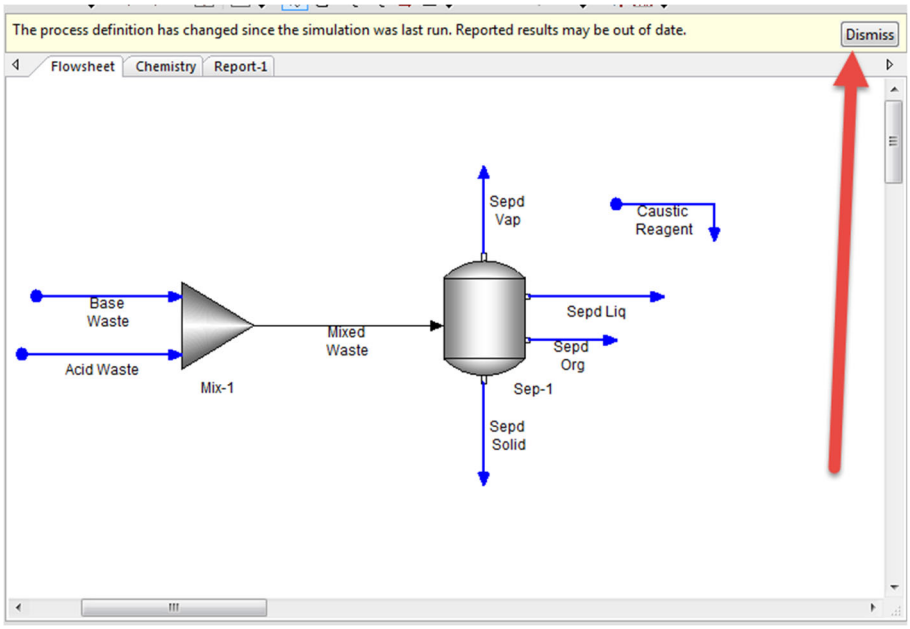
Let's save the file with a new name so we have the older file as a reference. Using the standard windows tools save the file with the name **Neutral 1 – pH controller.**

Locate the **Neutrl-1** block on the existing PFD.



[2]Or use the name you supplied.

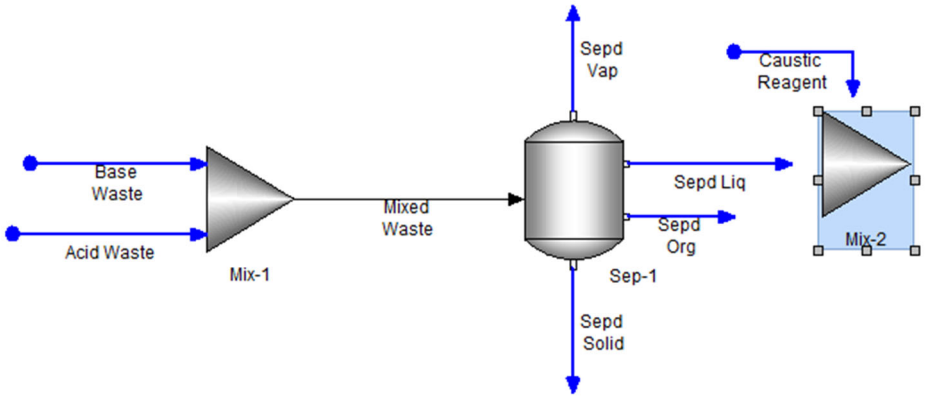
Press the delete key to remove this block.



Two things have happened at this point. First, the old neutralizer has been deleted but the associated inlet stream remains on the PFD. In addition, a warning has appeared to remind you that the process has been modified. To proceed, please click the **Dismiss** button at the top of the PFD.

We have several options now. You can either add the manipulator block as described above or start with a mixer. Either is acceptable. For this tour we will first add the new mixer and call it a neutralizer.

Select a **Mixer** from the library and drag it to approximately the same location as the old neutralizer.



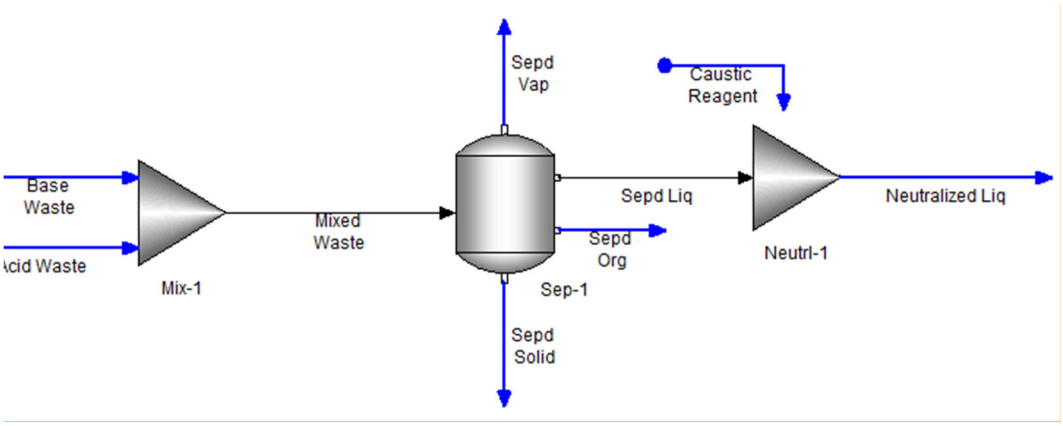
.

Change the parameters for the mixer as described in the following table:

Block Type	Mixer
Block Name	Neutrl-1
Inlet(s)	Sep Liq
Outlet(s)	Neutralized Liq
Equilibrium Calculation	
Calculation Type	Adiabatic

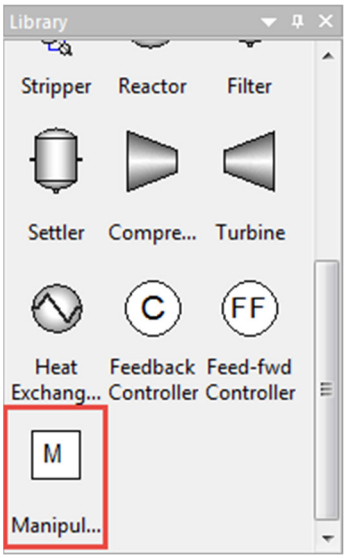
Pressure Spec.	Min. Inlet Pressure
Heat duty	0.0
Advanced Options	
Chemistry Model	Chemistry (Default)

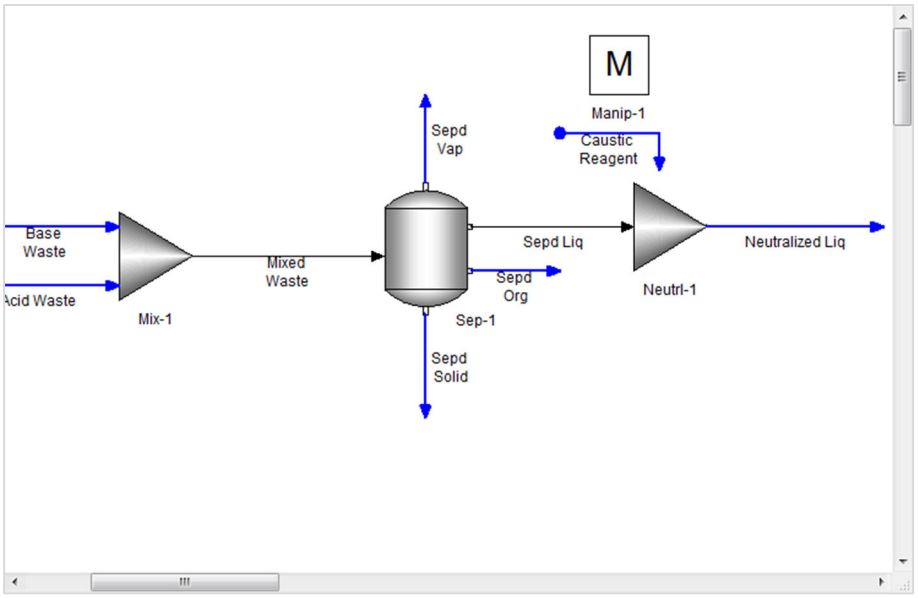
The PFD is now updated like this:



We now need to add a manipulator block. Manipulate blocks are very simple in operation. Either the total flow of the inlet stream is multiplied by some factor or a specific component in the stream is *multiplied* by a factor. This factor can be controlled by a *Controller Block*.

Locate the **Manipulate** block from the library and then drag it to the PFD above the **Neutrl-1** block.

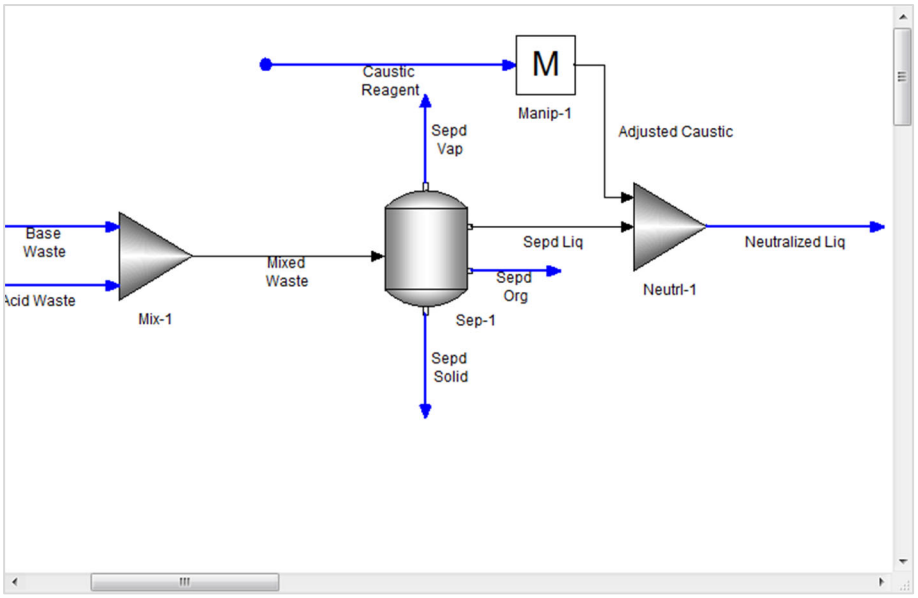




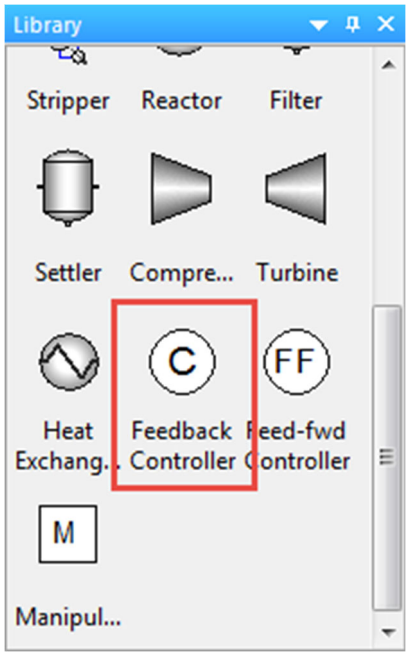
We will now connect the **Caustic Reagent** stream to the manipulate block and add an outlet stream which will be named **Adjusted Caustic.** See Table below for manipulator parameters:

Block Type	Manipulator
Block Name	Manip-1
Inlet(s)	Caustic Reagent
Outlet(s)	Adjusted Caustic
Parameters	
Manipulation Type	Total Flow
Factor, Flow	1.0
Advanced Options	
Chemistry Model	Chemistry (Default)

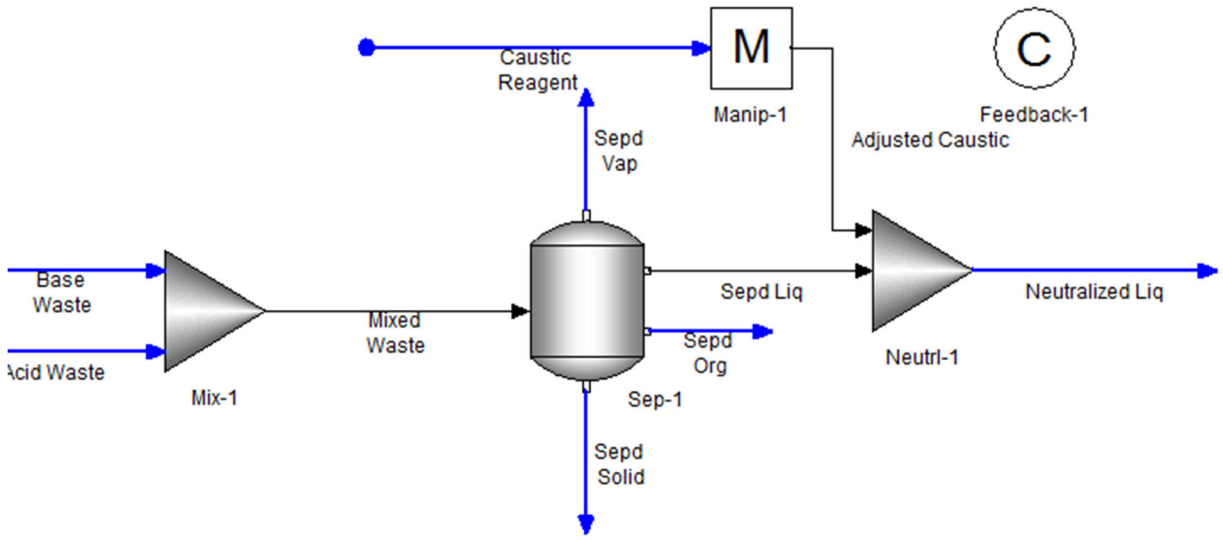
The PFD should be updated as follows:



You may notice that we have moved blocks and streams around to make it easier to read the PFD. We will now add the final block for this process which is a control block. Locate the feedback controller from the library.



Now drag this block to slighlyt above and to the right of the mixer "**Neutrl-1**"

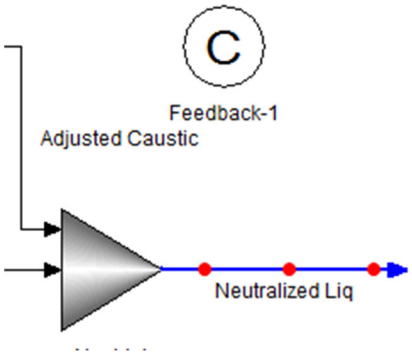


The connections to the controller are different than those of other blocks. The connections only carry information and not mass and energy. These connections are made with a different tool in the toolbar.

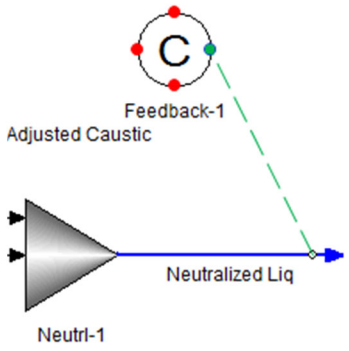
Controller connection tool

When you select this tool, you can drag lines from the measured object (usually a stream) to the controller and from the controller to the object under control (usually a block). Target points will appear when you drag the controller connector to the object.

Click the **Controller Connector** and drag a line from the stream **Neutralized Liq** to the **Feedback-1** controller.

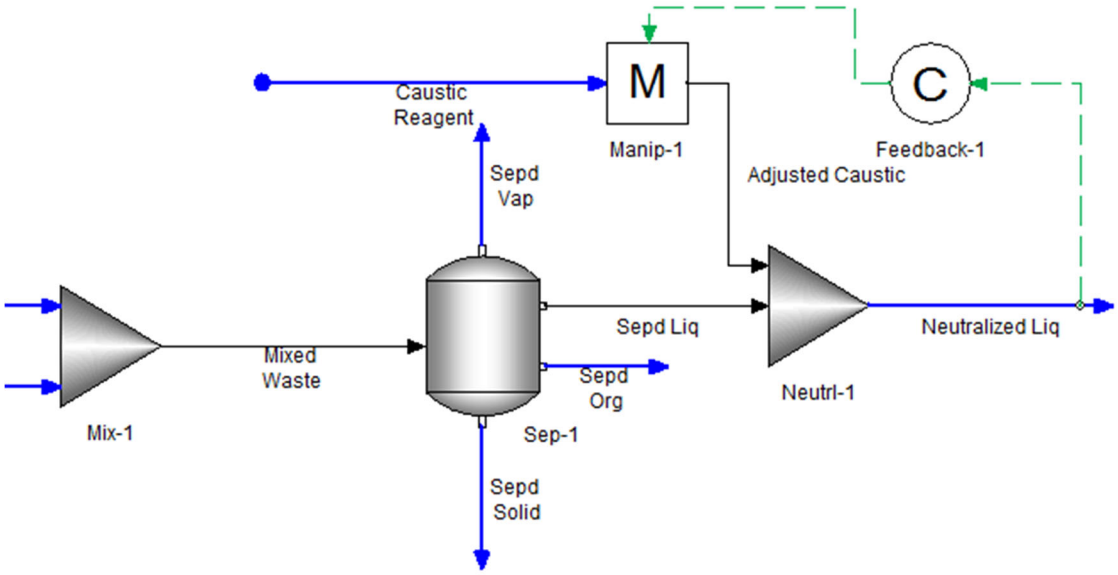


As the controller connection approaches, targets appear. Select any one of them.



As the controller connect approaches the Feedback-1 block new targets appear

Complete the connections by dragging a line from the **Feedback-1** controller to the **Manip-1** block.



The connected feedback controller

We now need to define the parameters for the feedback controller.

Block Type	Feedback Controller
Block Name	Feedback-1
Target Specification	
Target Stream	Neutralized Liq
Spec. Type	pH
Target Value	9.0
Control Parameters	
Controlling Block	Manip-1
Block Parameter	Factor, Flow
Options	
Calculate After	<Automatic>
Convergence Options	Fly Out Menu (all default)

We are now ready to run the process. Like all good process simulators (that's you!) please save the process first.

Now run the process.

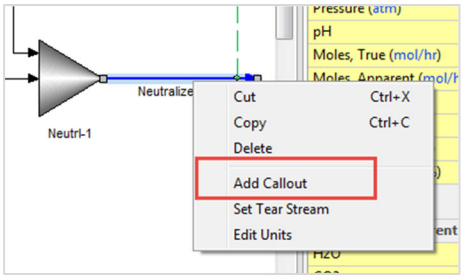
You may not see much going on. What we need to review is the following:

- pH of the **Neutralized Liq** stream
- The flowrate of the **Adjusted Caustic** stream.

We can do this via the report feature we looked at previously, but we can get quick information directly on the PFD instead. We use a tool called "Callouts".

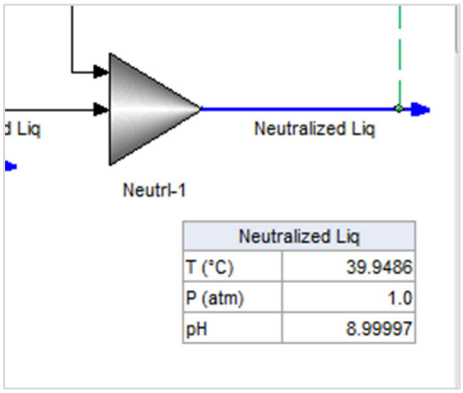
Right-click the stream **Neutralized Liq**.

Select **Add Callout**.



Right-click to add Callout

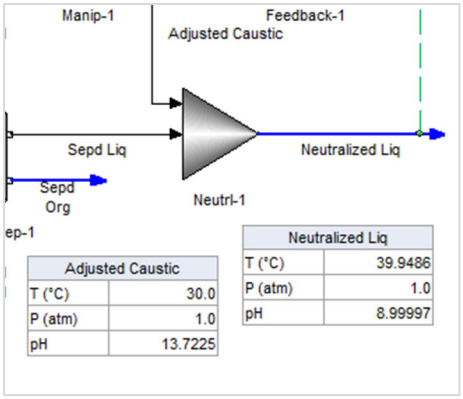
A callout is displayed on the PFD (if it seems to have moved partially off screen you can grab it and drag it to where you can see it)



Callout for the stream "Neutralized Liq"

You can see that the pH is nearly 9.0. The reason it is not exactly 9.0 is because there is a tolerance in the controller algorithm. This will be explained in later chapters.

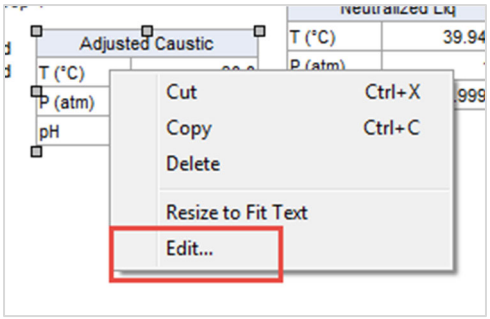
Right-click on the **Adjusted Caustic** stream and add the callout.



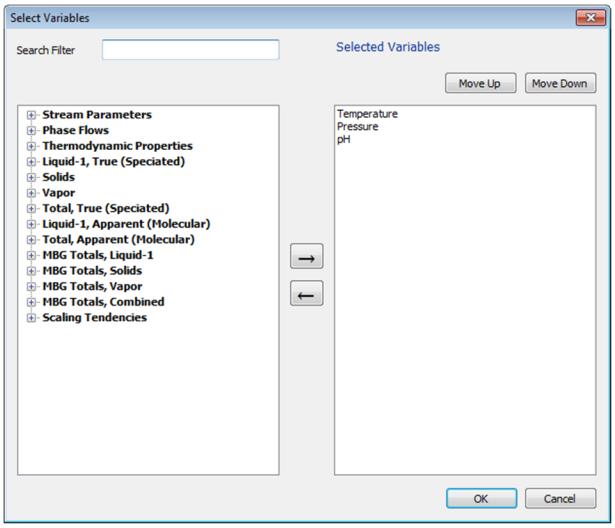
Adding the "Adjusted Caustic" callout

We have dragged the **Adjusted Caustic** callout to where we can view it. Unfortunately, it does not contain the flowrate information we require.

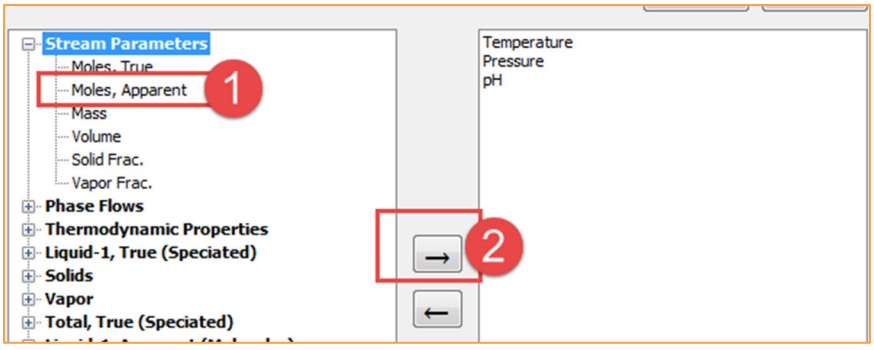
Fortunately, we can edit the callout to add the information. Right-click the **Adjusted Caustic** callout box.



This will display the **Select Variables** dialog. Users of the OLI Studio program will be familiar with this dialog.

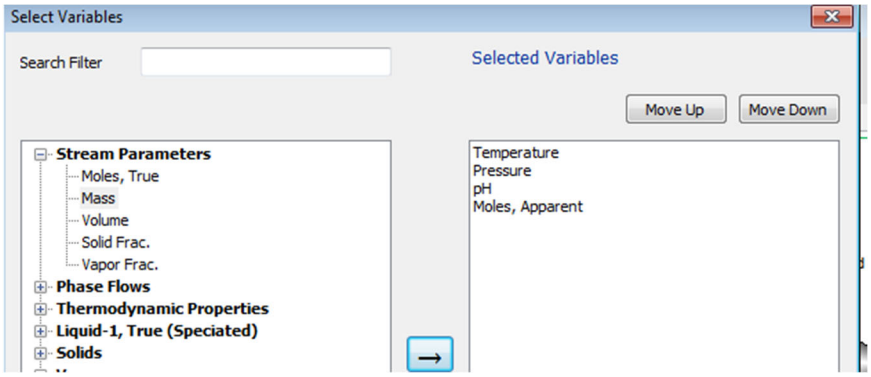


Expand the tree under **Stream Parameters**



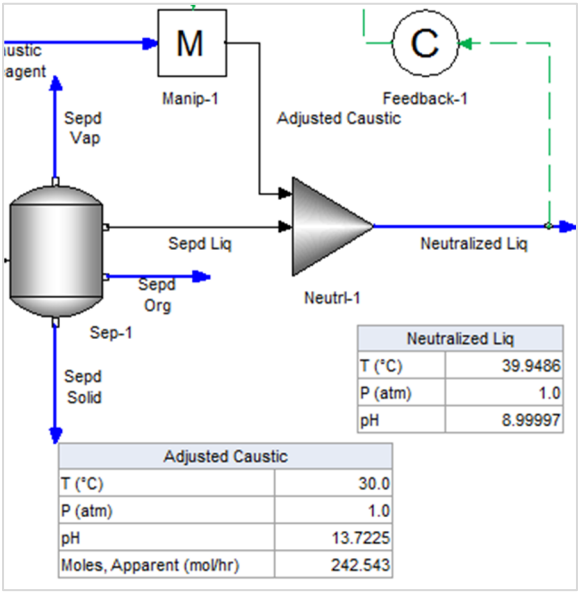
First select **Moles, Apparent** and then Second, click the right-arrow to select it (or just double-click the first option).

This updates the selected variables.



Click **OK** to close the dialog.

The callout on the PFD is updated with the newly selected variables.



You can see that the flowrate is 242.5 mol/hr for the adjusted caustic reagent stream. Compare this to the value previously found in page 32.

Please save your file.

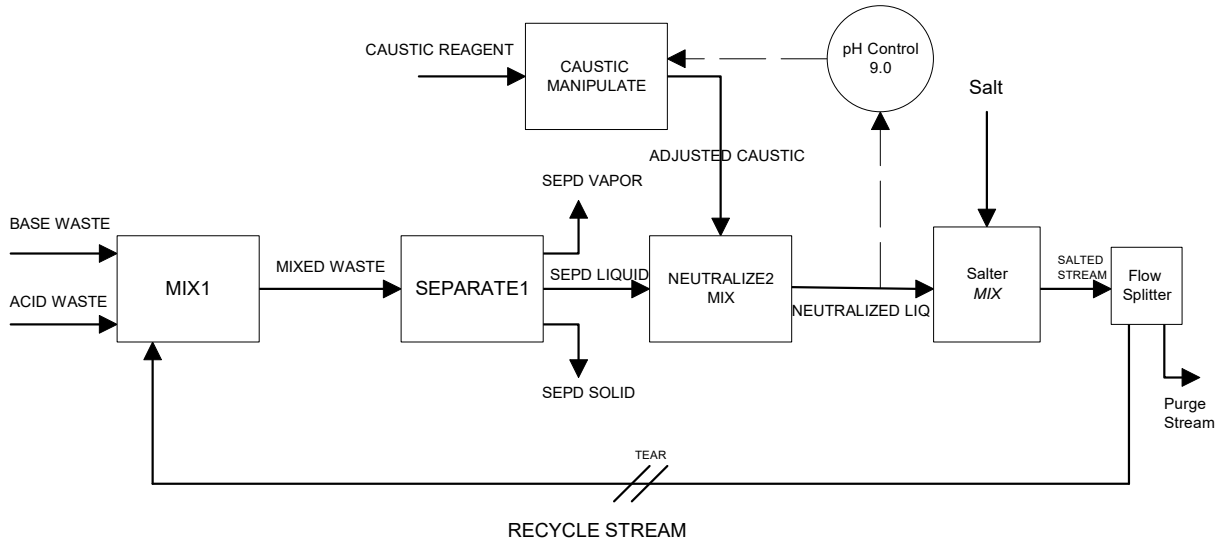
A tour of OLI Flowsheet: ESP – More Advanced Options

We have just seen that a control block, combined with mix blocks and manipulate blocks, can be used to control the pH of a stream. Frequently a process recycles part or all of certain streams back to upstream units. There are many reasons for this including minimization of waste, increase of residence time, and purification of product.

This application extends the previous application by adding a new mix block, a split block and a recycle stream. We will be adding sodium chloride (salt) to the process to remove some solids from the solution. We will then recycle some of those solids back to an upstream unit to see the effect, if any, on the amount of caustic required to adjust the pH.

We will be reusing the previous process **Neutral 1 – pH controller** [3]. Please load this file (if not already loaded) and then let's save the file with a new name. OLI recommends **Neutral 1 – recycle.**

The figure below shows the layout of the new process.

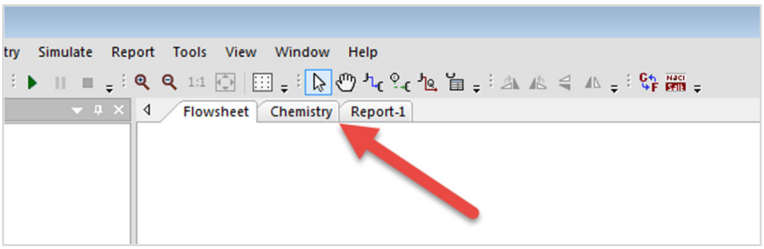


Neutralization Process with Manipulate/Mix Block, pH Controller, and Recycle Loop.

[3] Or the name you supplied.

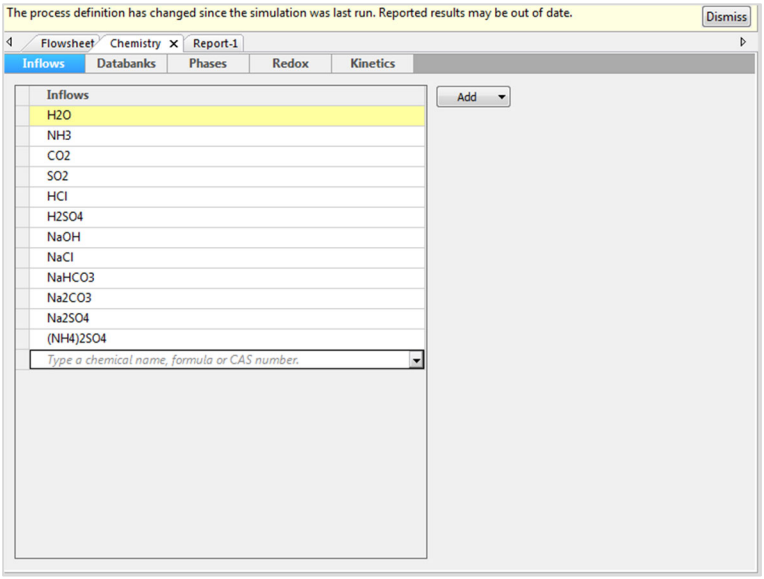
Modifying the chemistry

For this example, we need to add some components to the chemistry model. Click the **Chemistry** tab at the top of the PFD.



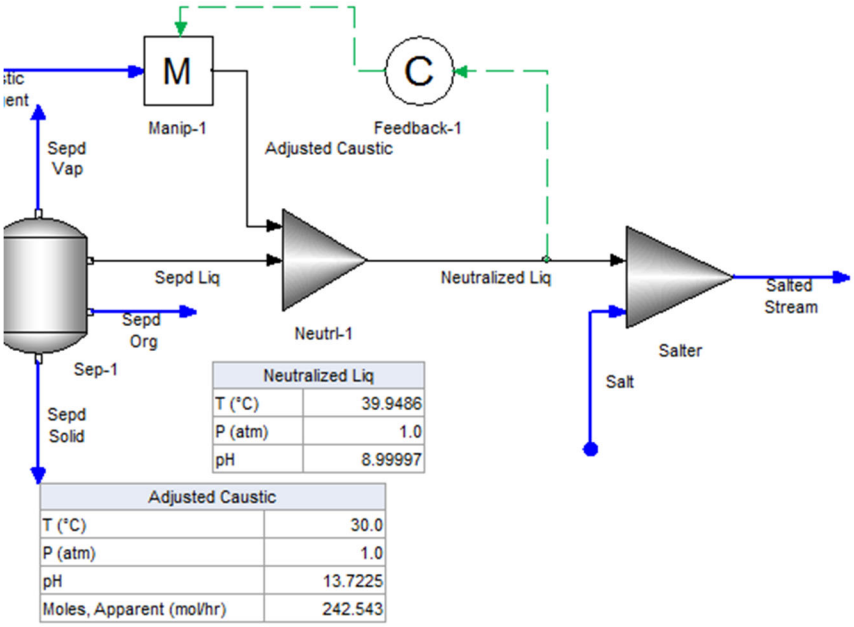
Add the following components to the **Inflows** list:

NaCl
NaHCO3
Na2CO3
Na2SO4
(NH4)2SO4



Click **Dismiss** to clear the warning message and then click on the **Flowsheet** tab.

We are going to add a new mixer block and a new stream to the mixer. Please add these two objects to the PFD and connect them as indicated. The PFD should look like this (the details of the objects will follow):



Stream Name	Salt
Temperature, ºC	25.0
Pressure, Atm	1.0
Stream Amount, mole/hr	75.0
Inflows, mol/hr	
NaCl	75.0
Advanced Options	
Set Phase	Solids Only
Chemistry Model	Chemistry(Default)

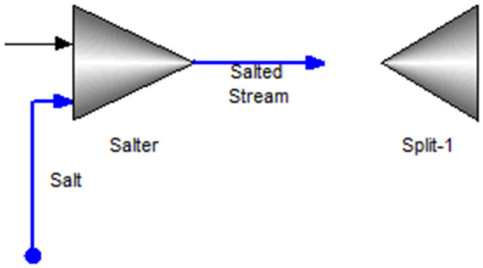
There is no water associated with this stream. Under most conditions, we require water as a component. In those cases, where we specifically do not want water in a stream, we must use the option **Set Phase: Solids Only**.

In the table below, you will find the “Salter” Mixer parameters.

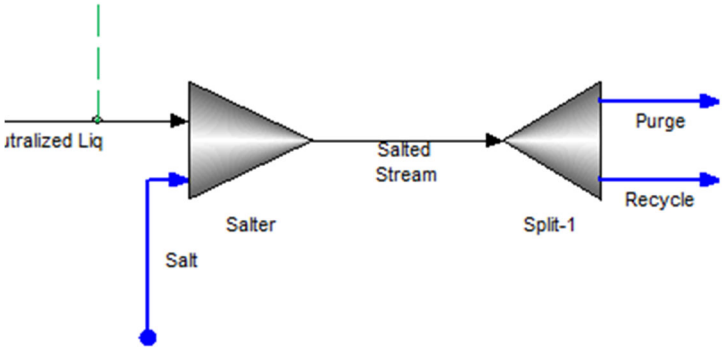
Block Type	Mixer
Block Name	Salter
Inlet(s)	Neutralized Liq
	Salt
Outlet(s)	Salted Stream
Equilibrium Calculation	
Calculation Type	Isothermal
Pressure Spec.	Min. Inlet Pressure
Temperature (ºC)	40.0
Advanced Options	
Chemistry Model	Chemistry (Default)

We will now split the **Salted Stream** to discharge some of the material and recycle some of the material. We now need to add a flow splitter to the PFD. A flow splitter is named “Splitter” in the library. By now you should be able to find unit operations in the library, so we will not show you an image for this.

Drag the **Splitter** and place it to the right of the **Salted Stream** on the PFD.



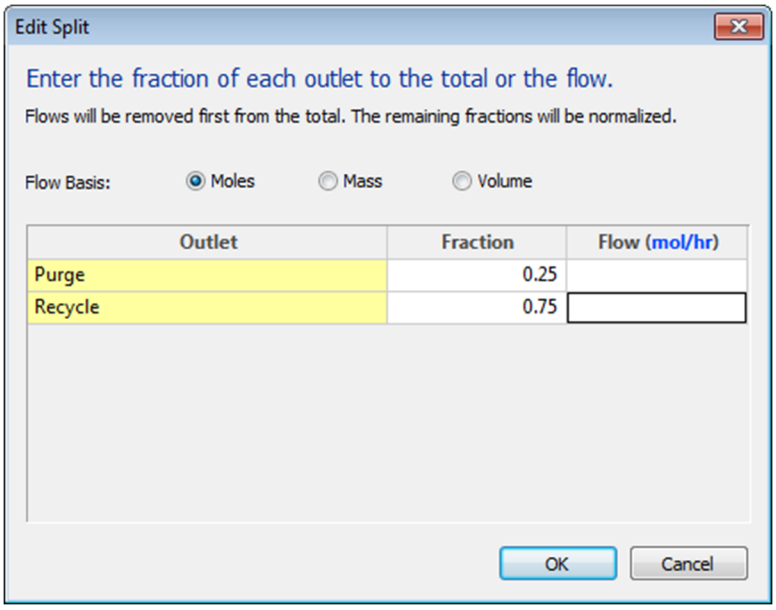
As with other objects we need to connect the streams. The **Salted Stream** will be connected to the inlet of the **Split-1** block and two outlets will be defined, **Purge** and **Recycle**.



The parameters for the **Split-1** block are found in the table below:

Block	Splitter (flow)
Block Name	Split-1
Inlets(s)	Salted Stream
Outlet(s)	Purge
	Recycle
Parameters	
Outlet Split	Flyout (edit) This launches a new dialog.
Advanced Options	
Chemistry Model	Chemistry (Default)

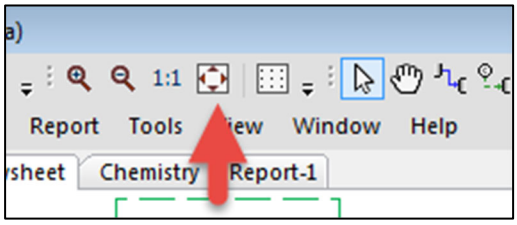
Enter the fractions that you want to purge and recycle:



Click **OK** to close the dialog.

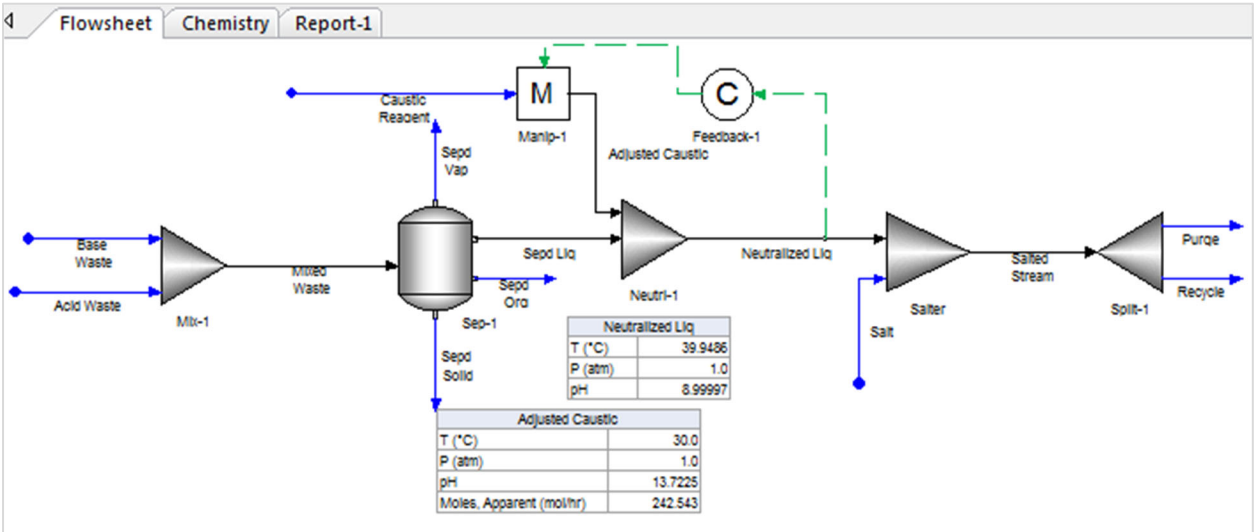
Right now, the PFD may look skewed or shifted to the right. We can zoom and center the diagram with a tool in the toolbar.

Click the **Zoom to Fit** tool button.

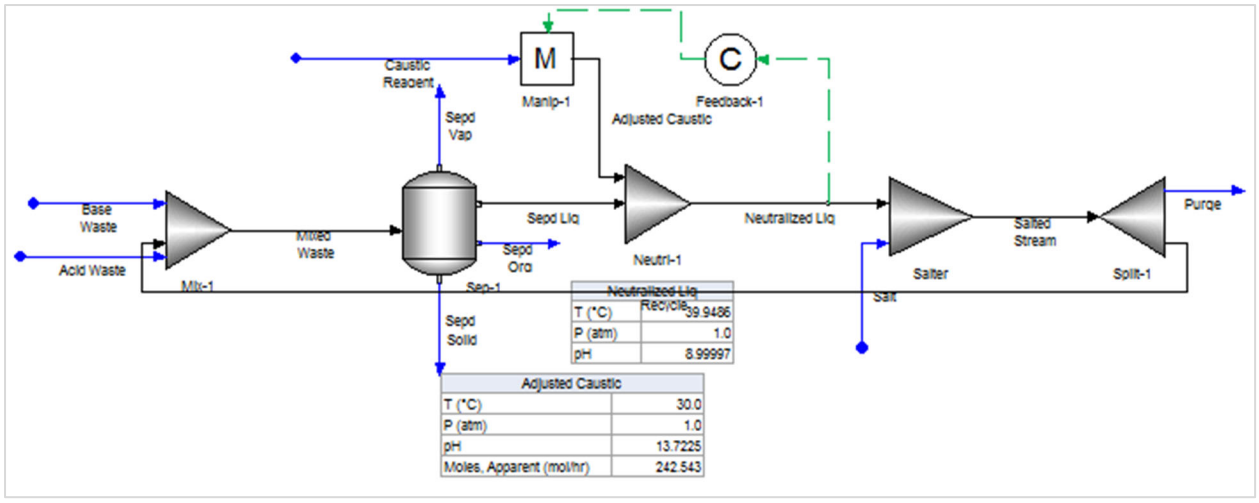


Zoom to Fit tool

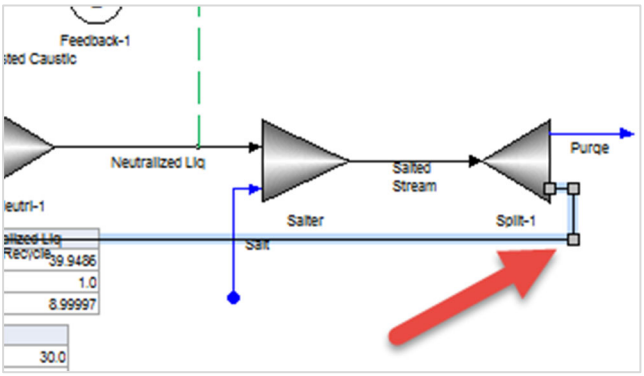
We now need to connect the **Recycle** stream back to the upstream block **Mix-1**.



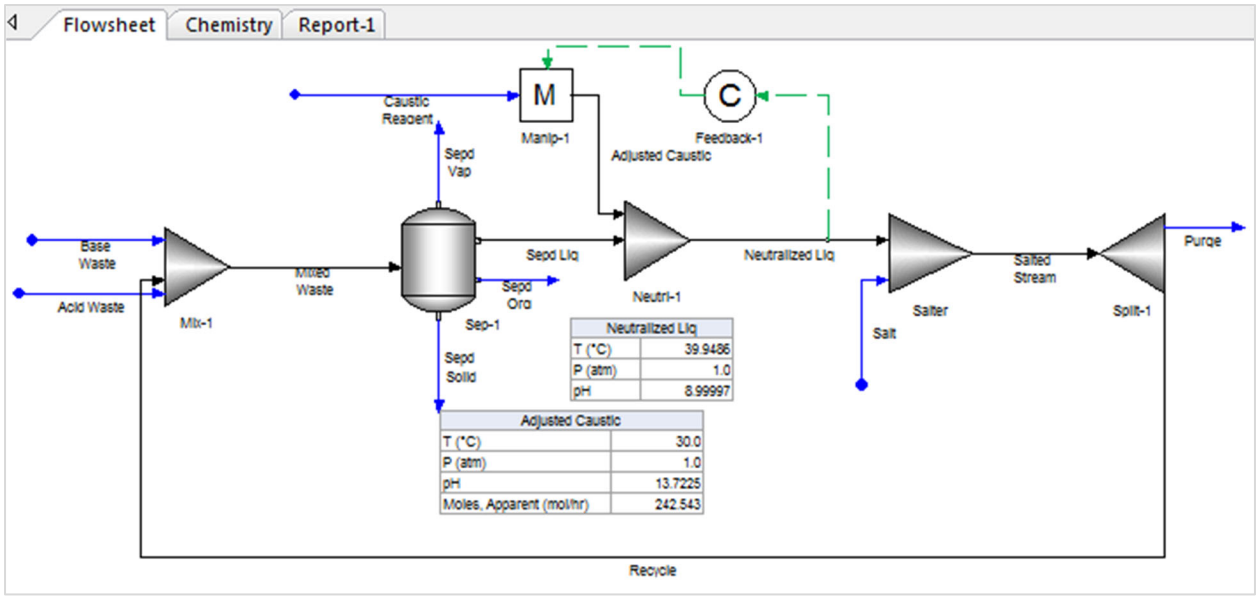
The PFD should look that the image below:



This is a bit messy to read. We can drag our **Recycle** stream down to the PFD is easier to read. Click the stream and find one of the "Anchors" and drag the stream down.



Finding the "Anchor"

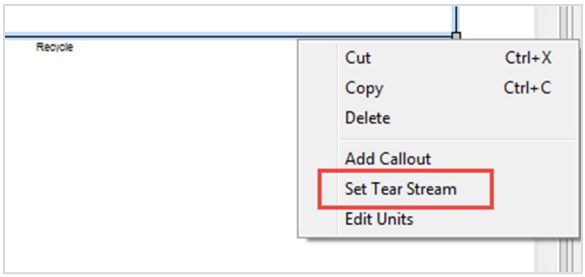


This PFD is certainly easier to read than the previous image.

Processes with recycle streams require some additional information to be provided prior to running the simulation. In processes without a recycle stream, the order of block calculation is easy to determine. Generally, the first block defined is the first block that is calculated.

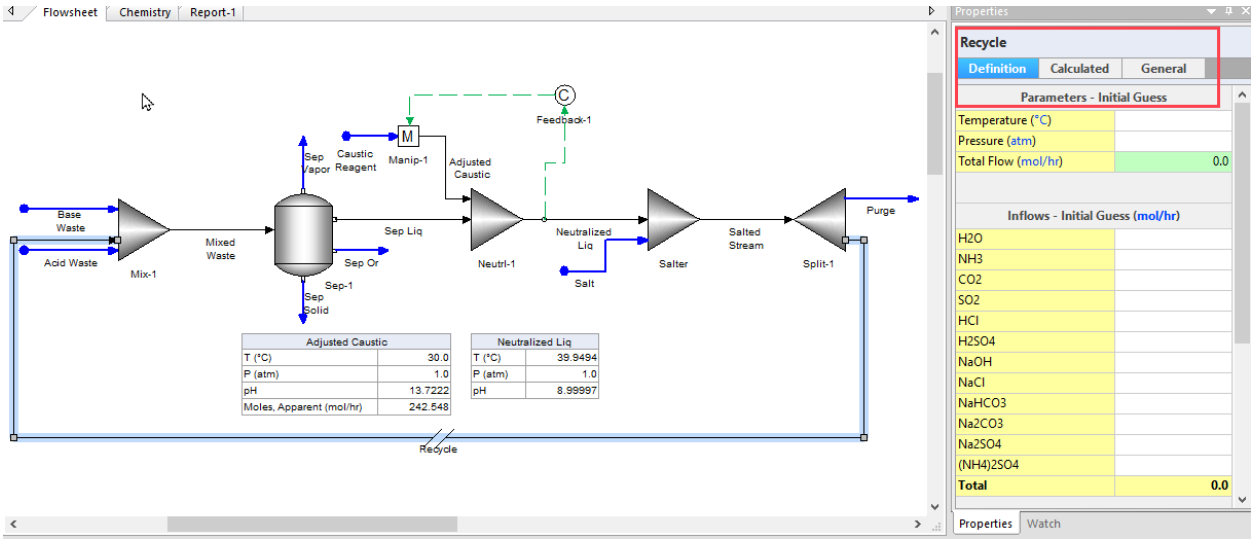
In recycle processes, we must tell the program where to begin calculating. We do this by defining a process stream as a *Tear* stream. Tear streams are treated as normal process entry streams and require an initial composition. These compositions should be representative of the process and some care should be taken in specifying the stream.

In this example, the stream **Recycle** is a likely candidate for a ***TEAR*** stream. Right-click the stream **Recycle**.



Setting a TEAR stream

When you select a ***TEAR*** stream you get the opportunity to specify an initial guess. The OLI Flowsheet: ESP program updates with a new stream definition when the ***TEAR*** stream is highlighted.



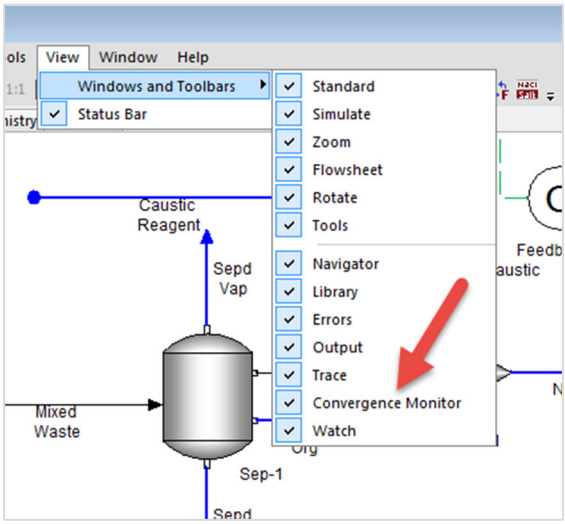
Entering the initial guess for the TEAR stream

Notice that the ***TEAR*** stream is indicated with a double-hash mark ("//")

Enter the following initial values for the ***TEAR*** stream (note that some values were skipped in the input):

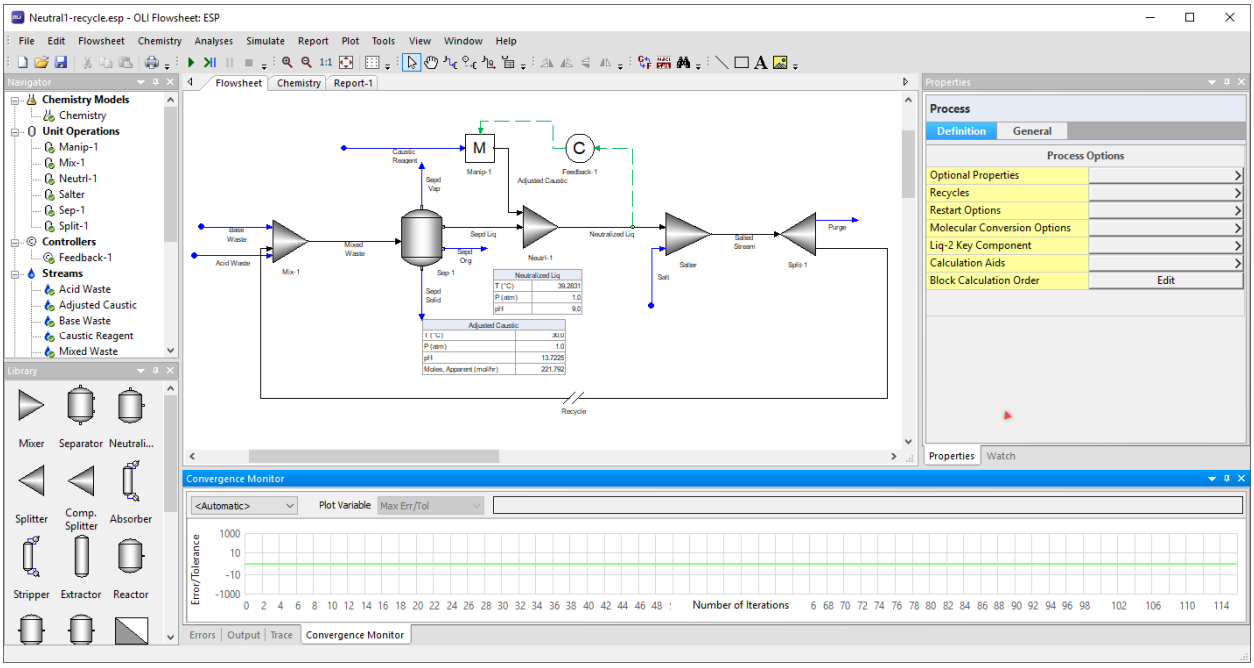
TEAR Stream Initial Guess	Recycle
Temperature, °C	40.0
Pressure, atm	1.0
Stream Amount, mole/hr	213.19
Inflows, mol/hr	
H2O	186.74
NH3	0.331
CO2	0.002
HCl	0.0006
NaCl	25.1
NaHCO3	0.005
Na2CO3	0.023
Na2SO4	0.46
(NH4)2SO4	0.42

Process simulations with ***TEAR*** streams may take a long time to converge. We can monitor the approach to convergence with a tool called the **Convergence Monitor**. You enable the **Convergence Monitor** via the **Menu > View >Windows and Toolbars > Convergence Monitor**.



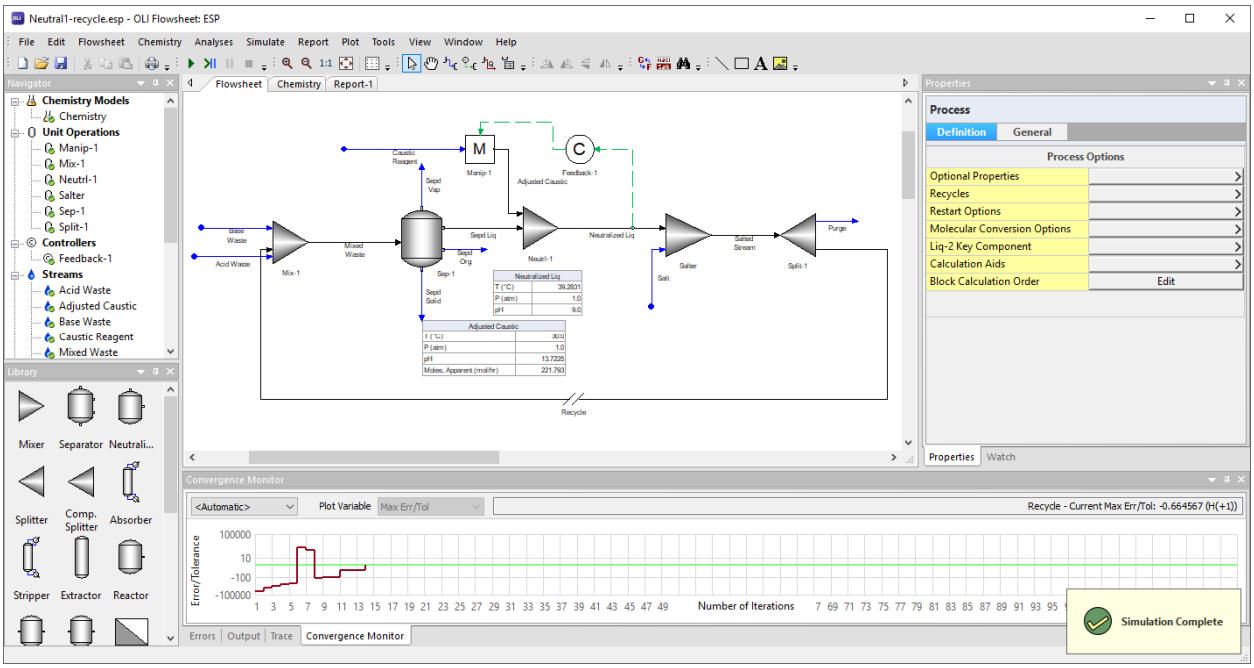
Enabling the convergence monitor

This creates a new panel in the program. The new panel appears below the PFD.



Save the file and then run the process.

Unlike the previous tours, this tour will recalculate many of blocks as the program attempts to converge the recycle stream, in other words, to make the values in the recycle loop consistent between successive iterations. This may take several iterations to complete.



The case has converged. The convergence monitor has shown the state of the convergence of the ***TEAR*** stream over approximately 14 iterations. We will explain this convergence in later chapters.

What has happened in this process? We left the callouts from the previous tour in place. You can see that the pH of the neutralized stream is 9.0 which is what we required. The amount of the **Adjusted Caustic** stream is approximately 222 mol/hr which is less than the 242 moles we found in the example without the recycle stream. This means some of the unreacted caustic stream was used to neutralize the solution.

You can explore many other options and reports and we encourage you to do so. These worked examples will be on the OLI Wiki page in the following link:

Getting Started Examples for OLI Flowsheet: ESP

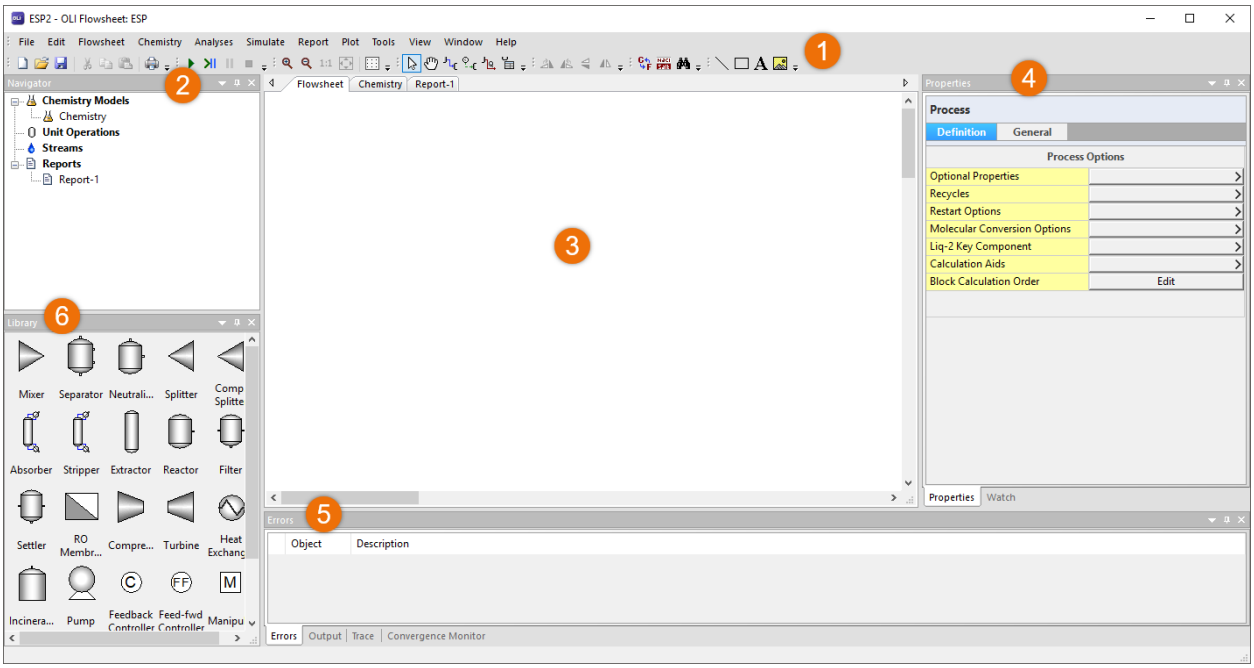
Please save your file.

Chapter II – Process Options

Overview

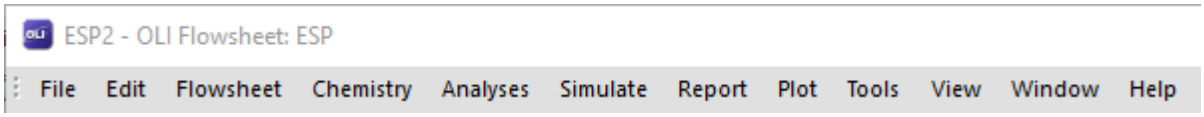
The OLI Flowsheet: ESP screen is roughly divided into 6 sections.

The top section is Menu Items and Toolbar
Left most section is the Navigator Panel. The navigator panel will have the tree of all the objects in the current flowsheet.
The middle section is Flowsheet window. This view can be switched by the tabs at the top to Chemistry view or Report view
The Properties Pane has two tabs, properties variables and watch variables.
The bottom section has four tabs, Errors, Trace, Convergence Monitor and Output
Left bottom corner is the Library, it has all the unit operations



Menu Items

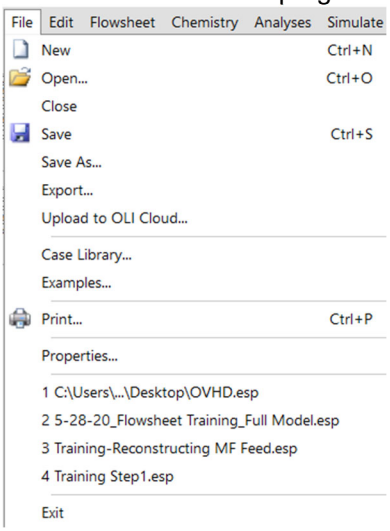
Following image shows the menu items:



File

The options under File are as follows:

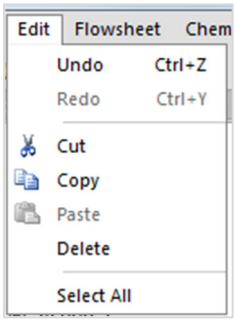
- *Ctrl+N* short cut or the New file icon will open a new file.
- *Ctrl+O* shortcut of the Open file icon will open an existing file.
- *Close* will close the file.
- *Ctrl+S* shortcut or Save icon will save the file.
- *Export* options exports the .bin file and associated file types from a OLI Flowsheet: ESP type file. .bin file is compatible with ESP Original program
- *Upload to OLI Cloud…* will upload the current file to the OLI App Builder account associated with the user
- *Case Library* allows access to OLI's repository of sample simulation files from multiple industries
- *Examples* option has sample files created for the OLI Flowsheet: ESP program.
- *Ctrl+P* shortcut of Print option will print the Flowsheet section
- Below print, recently opened files are automatically pinned
- *Exit* will exit the F-ESP program.



Edit

The options under Edit are as follows:

Ctrl+Z shortcut or Undo will undo the latest action in the Flowsheet, Chemistry or Report section
Ctrl+Y shortcut or Redo will redo the latest action in any of the above three sections
Cut will cut an object
Copy will copy the object
Paste will paste the object
Delete will delete the object
Select All will select all the objects

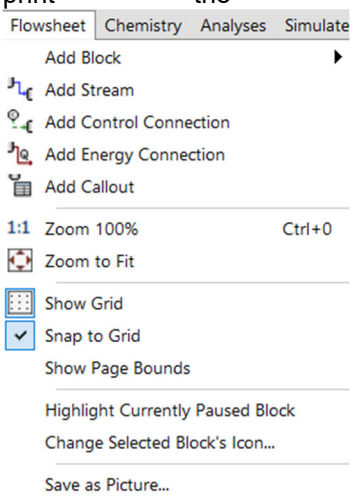


Flowsheet

The options under Flowsheet are as follows:

Add Block: Will add a Block
Add Stream: Will add a Stream

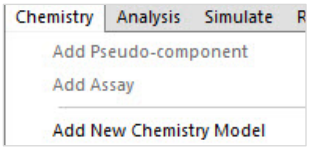
Add Control Connection: Will add a Control Connection
Add Energy Connection: Will add an Energy Connection
Add Callout: Will add a call out with information about the stream
Zoom 100%: Ctrl+O is a shortcut for a 100% zoom
Zoom to Fit: This option will fit the flowsheet to the screen
Show Grid: You can change the display options on the flowsheet screen and use a grid as a background
Snap to Grid: Snaps the objects back to the grid
Show Page Bounds: You can see the limits of the page
Highlight Currently Paused Block: Shows in the simulation the last converged block when using the step through calculation run button
Changed Selected Block's Icon: Once selected, a block may have different icons available for the user to choose from and more closely resemble their process
Save as Picture: This tool is useful to print the flowsheet



Chemistry

The options under Chemistry are as follows:

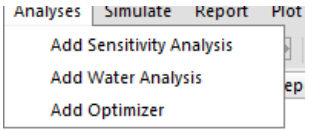
Add Pseudo-Component
Add Assay
Add New Chemistry Model



Analysis

The options under Analysis are as follows:

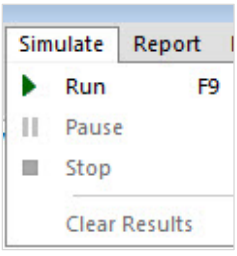
Sensitivity Analysis
Water Analysis
Optimizer



Simulate

The options under Simulate are as follows:

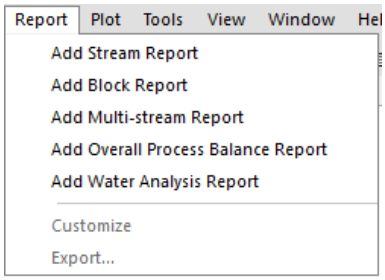
Run (F9)
Pause
Stop
Clear Results



Report

The options under Report are as follows:

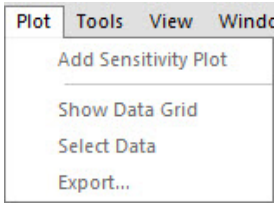
Add Stream Report
Add Block Report
Add Multi-stream Report
Add Overall Process Balance Report
Add Water Analysis Report
Customize
Export



Plot

The options under Plot are as follows:

Add Sensitivity Plot
Show Data Grid
Select Data
Export

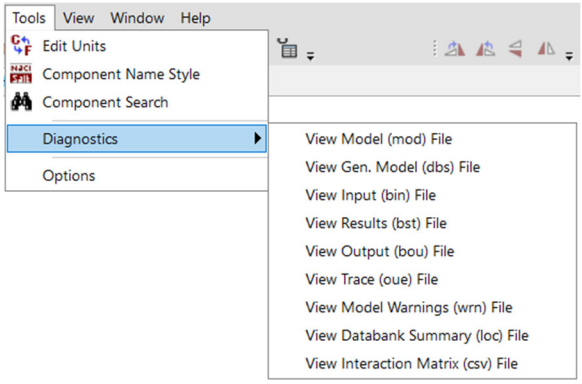


Tools

The options under Tools are as follows:

- Edit Unit
- Component Name Style
- Component Search
- Diagnostics
- Options

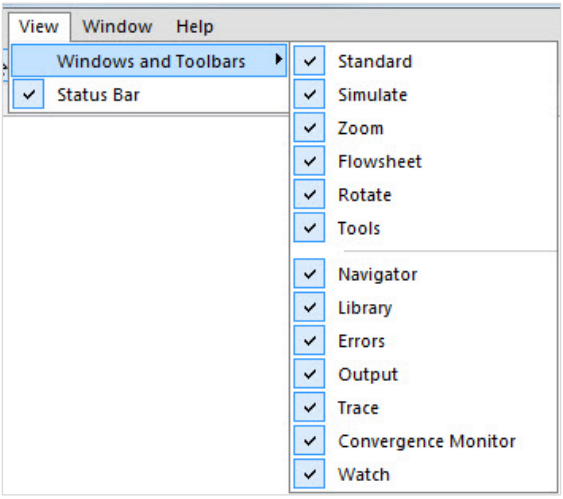
The sub-options under Diagnostics are as follows:



View

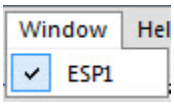
The options under View are as follows:

Windows and Toolbars
Status Bar



Window

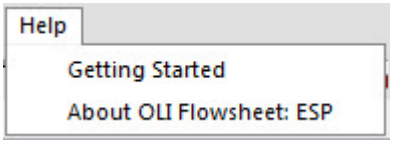
The options under Window are the last file name that had been opened.



Help

The options under Help are as follows:

Getting Started
About OLI Flowsheet: ESP



Toolbar

The top toolbar for OLI Flowsheet: ESP:

Toolbar is divided into six sections.

1. File Management

This section has file options:

New
Open
Save
Cut
Copy
Paste
Print

2. Simulation or execution options

This section has execution options:

- Run
- Step
- Pause
- Stop

3. View options

This section controls the Grid and View options.

- Zoom in
- Zoom out
- Resize
- Pan
- Center
- Grid

4. Design Control Options

- Mouse Pointer
- Pan
- Add a Stream
- Add a Control Connection
- Add a Utility stream
- Add a Call out

5. Rotation Controls

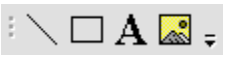
- Rotate 90° to the right
- Rotate 90° to the left
- Flip Vertical
- Flip Horizontal

6. Managers

- Unit Manager
- Names Manager
- Component Search

7. Drawing Tools

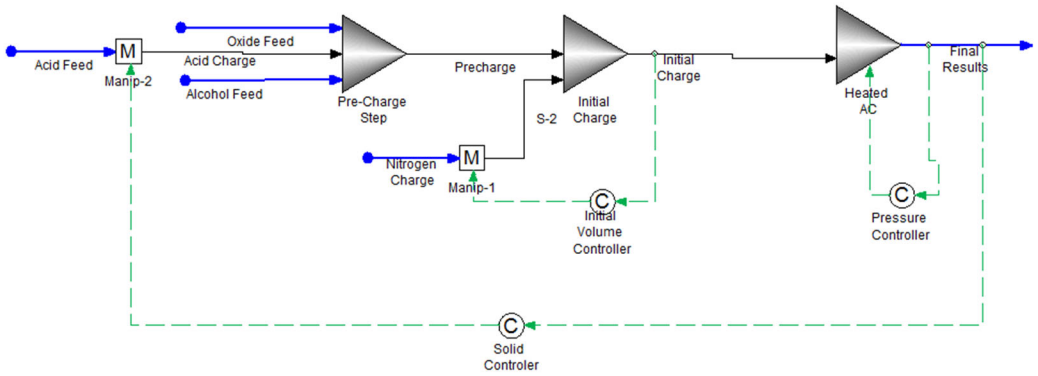
- Insert a line
- Insert a rectangle
- Insert text
- Insert image



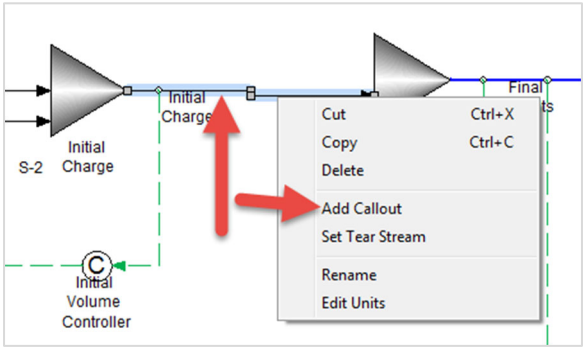
Adding callouts

Callouts are extremely useful in describing what your process is doing right on the PFD. You can always get detailed information using the reports but sometimes a quick glance is all you need.

There are two methods to place a callout on the PFD. The easiest is to right-click on the stream of interest and select **Add Callout**. In this example, we have a process to which we wish to add a callout:

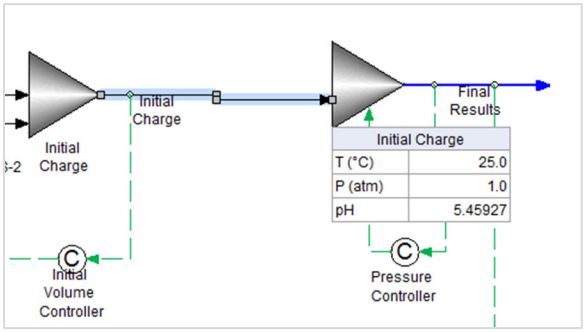


This actual process is a simulation of an autoclave. Frequently we need to know the volumetric flow of a stream. In this example, we will right-click the stream **Initial Charge** and then select **Add Callout.**

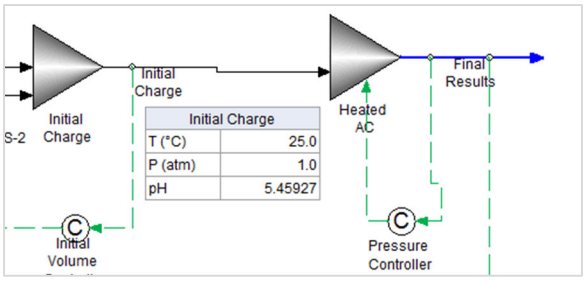


Adding a callout

Sometimes OLI Flowsheet: ESP doesn't put objects in convenient places, as is shown below:

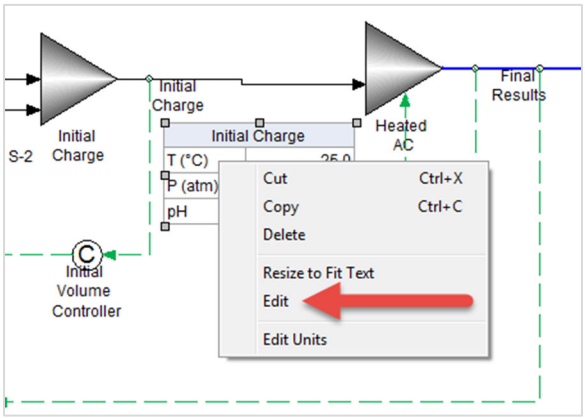


If you click the callout out, you can move it to a more readable location:



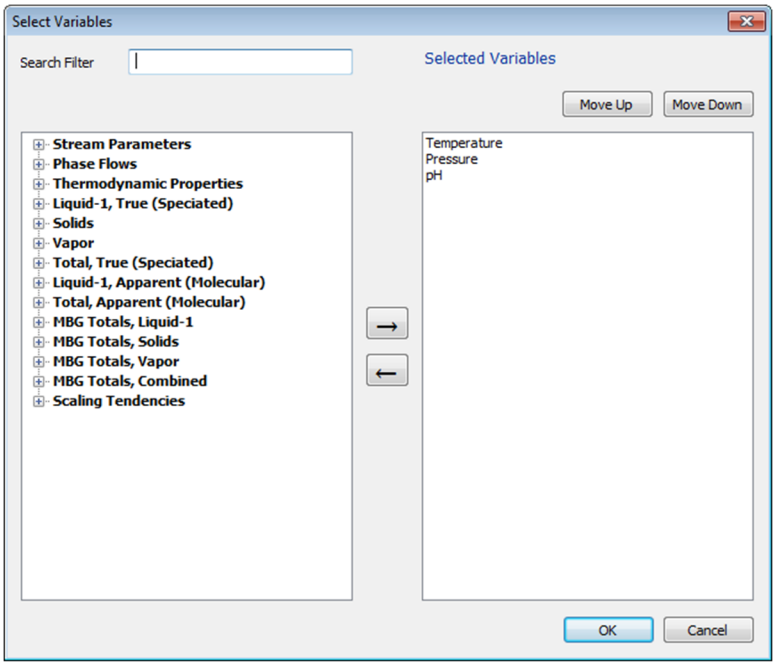
Editing a callout

The default values for any callout are Temperature, Pressure and pH. We are interested in these but what we really need to know is the total volumetric flow. Right click the callout and select **Edit**.

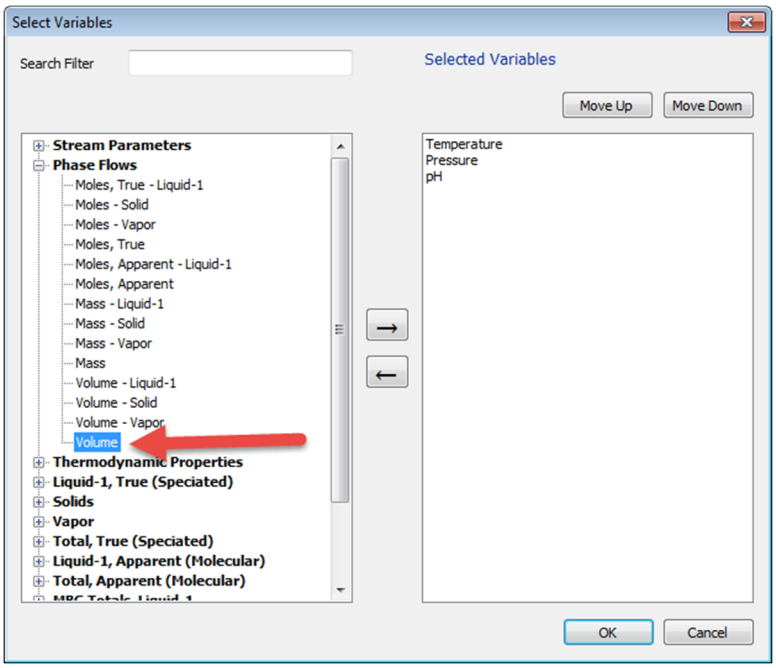


Editing a callout

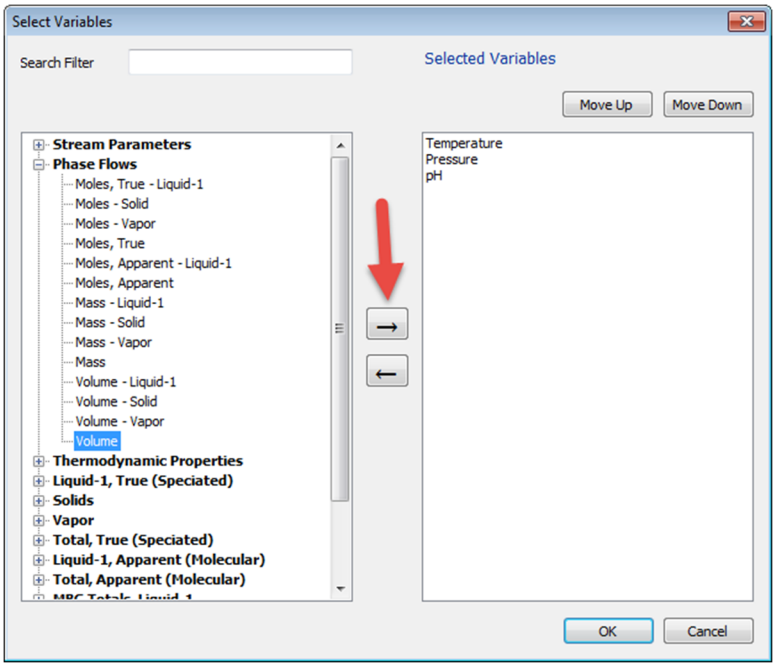
This will display a select variables dialog that is very much like the select variables dialog in OLI Studio



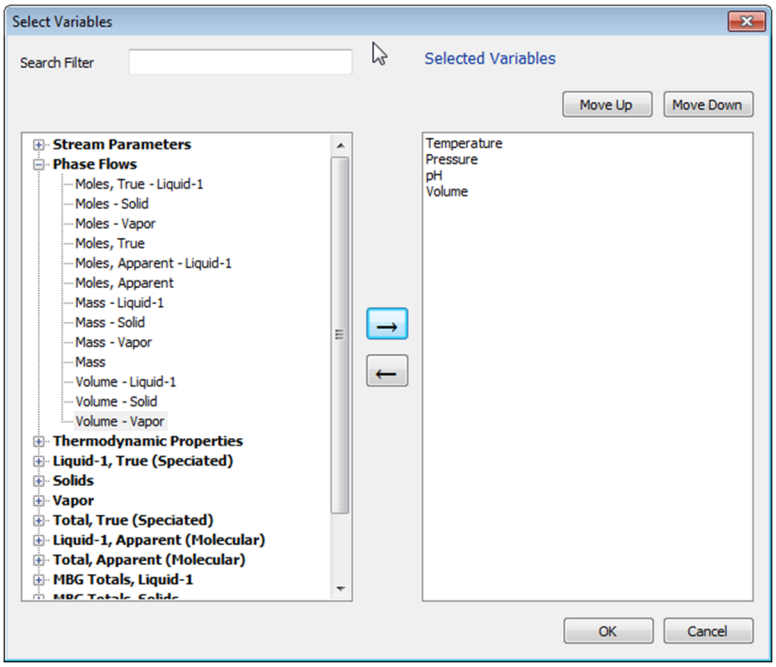
Expand the **Phase Flows** category and locate the variable **Volume**:



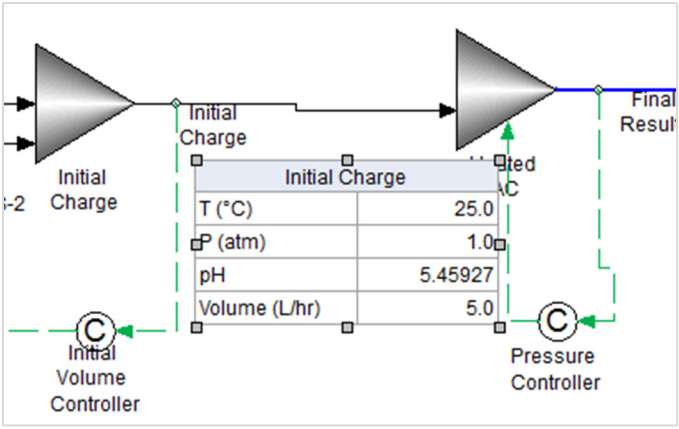
This variable is the sum of the volumes for all phases. Click the right-arrow key to select it.



Using the right arrow key (you could also double-click the variable to select it)



Click the **OK** button to continue.



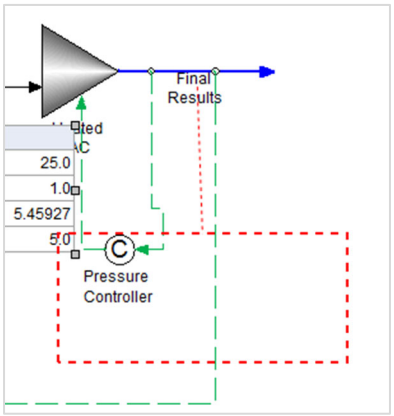
The alternative method to add a callout is to use the menu bar. For this example, we are going to select the stream **Final Results.**

Locate the Callout toolbar button:

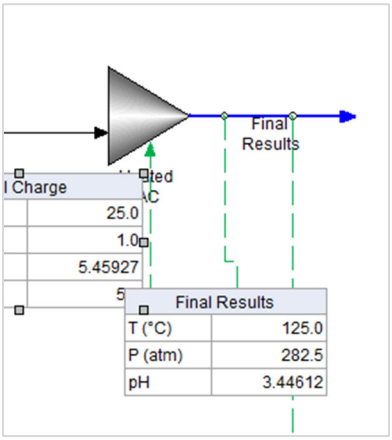
The callout toolbar button

When you click this button the cursor changes shape to a small hand like object and a red dotted lined box appears when you are hovering over an acceptable object such as a stream or block.

Click to place the box.



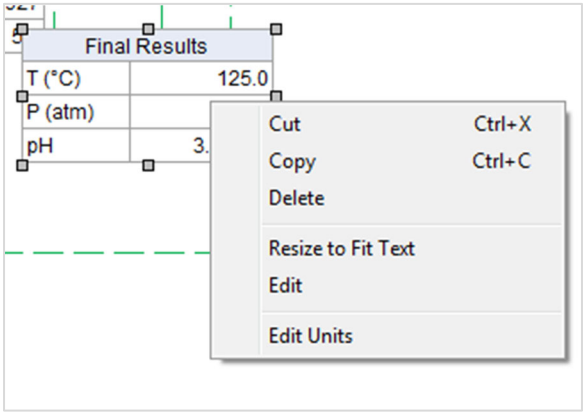
A dotted box appears



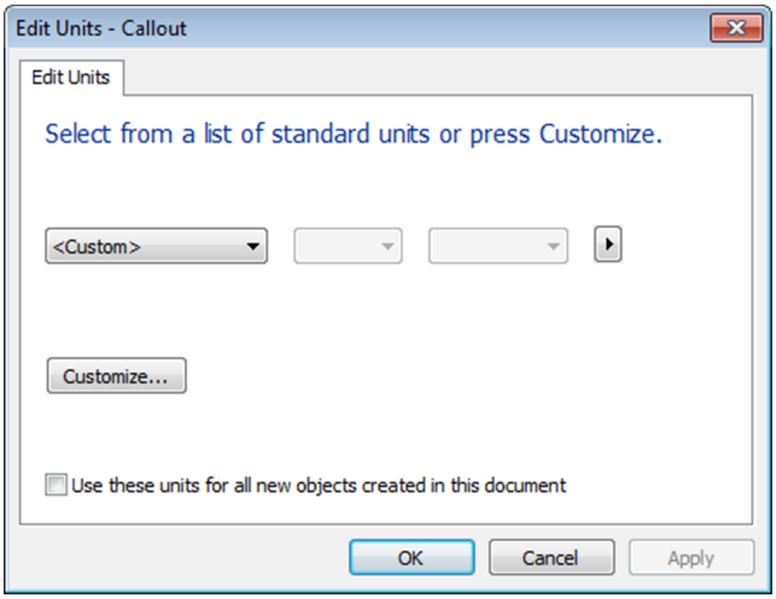
The dotted box has turned into a callout box

Editing the units for a callout

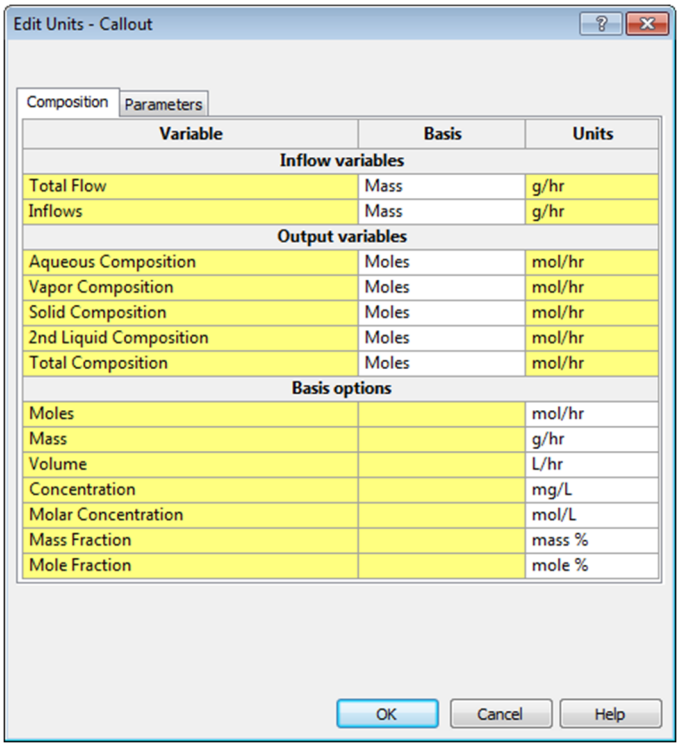
The units manager is similar to the units manager in OLI Studio and elsewhere in OLI Flowsheet: ESP. Once the callout has been placed you can right-click and select **Edit Units**.



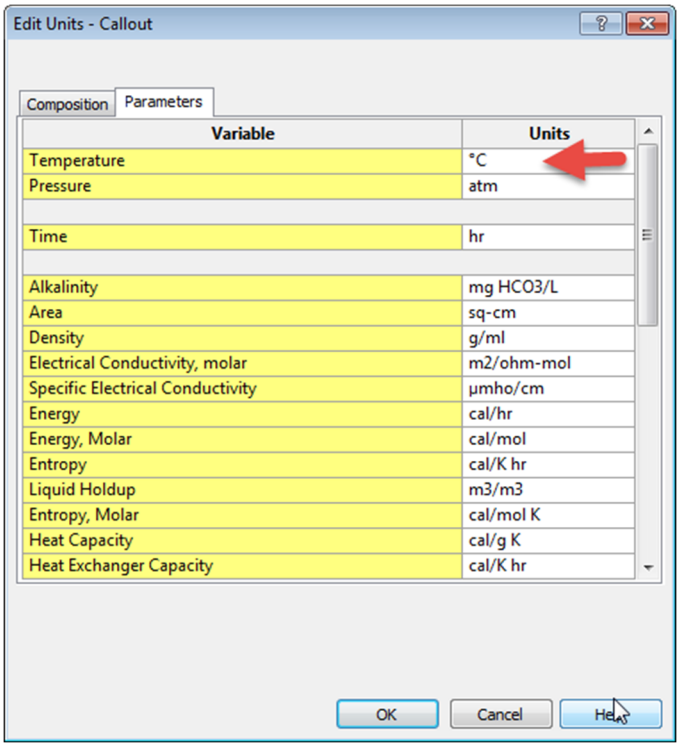
This will bring up the initial edit units dialog:



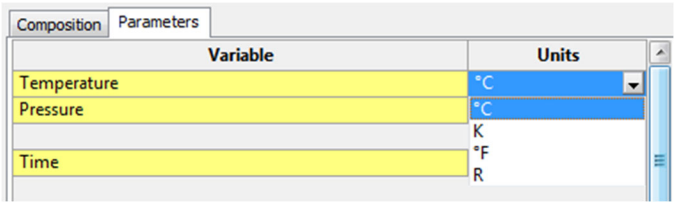
Normally for a callout we do not need to make global changes. For this example, we are going to change the temperature units from degrees centigrade to Fahrenheit. Click the **Customize** button.



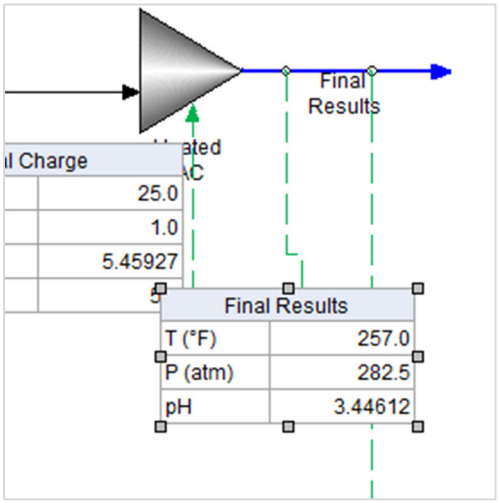
Click the **Parameters** minitab.



If you click in the box where you wish to change the unit, a dropdown menu will appear:



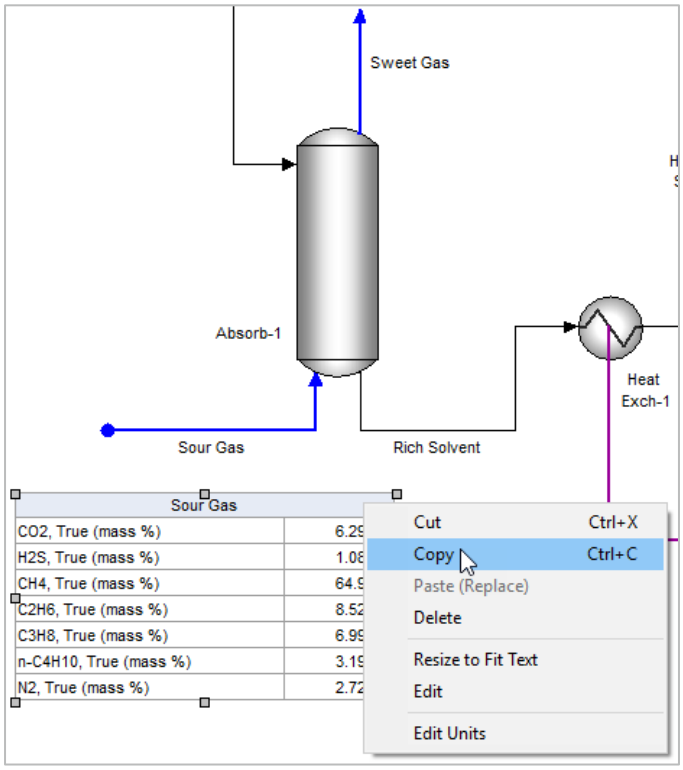
You can select the desired unit. You will need to click the **OK** button several times to return to the PFD.



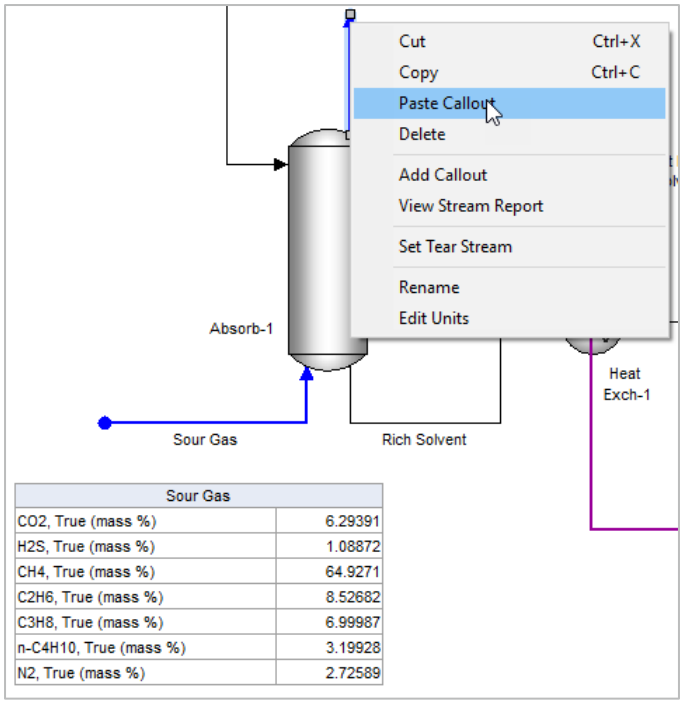
Copy and paste a callout

Once you are satisfied with the parameters and units that you want to show in your callout, you can easily copy and paste on a different stream where you want to see the same variables. This reduces the time to make the customized callouts for different streams.

To do this select the callout that you want to replicate, right click, and select copy.

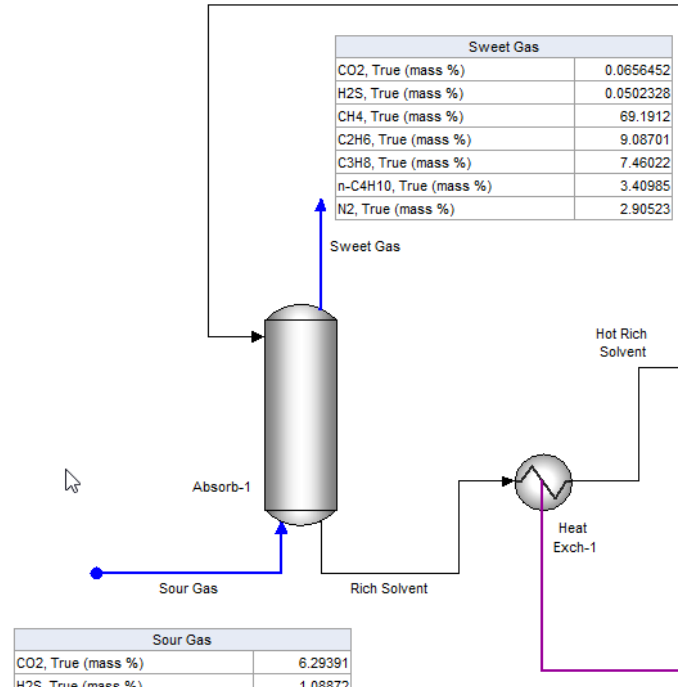


Then, select the stream where you want to place the callout, and select Paste Callout.



Sour Gas	
CO2, True (mass %)	6.29391
H2S, True (mass %)	1.08872
CH4, True (mass %)	64.9271
C2H6, True (mass %)	8.52682
C3H8, True (mass %)	6.99987
n-C4H10, True (mass %)	3.19928
N2, True (mass %)	2.72589

The same information and units have been transferred to a different stream.

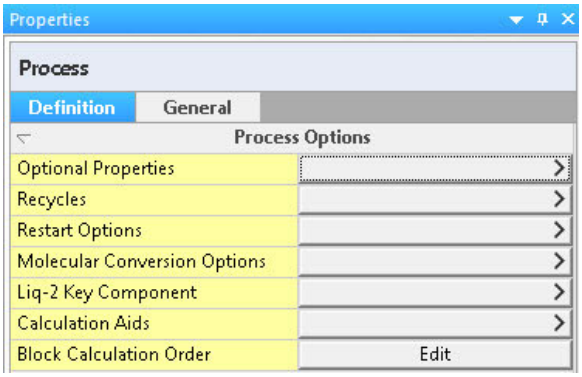


Sweet Gas	
CO2, True (mass %)	0.0656452
H2S, True (mass %)	0.0502328
CH4, True (mass %)	69.1912
C2H6, True (mass %)	9.08701
C3H8, True (mass %)	7.46022
n-C4H10, True (mass %)	3.40985
N2, True (mass %)	2.90523

Sour Gas	
CO2, True (mass %)	6.29391
H2S, True (mass %)	1.08872
CH4, True (mass %)	64.9271
C2H6, True (mass %)	8.52682
C3H8, True (mass %)	6.99987
n-C4H10, True (mass %)	3.19928
N2, True (mass %)	2.72589

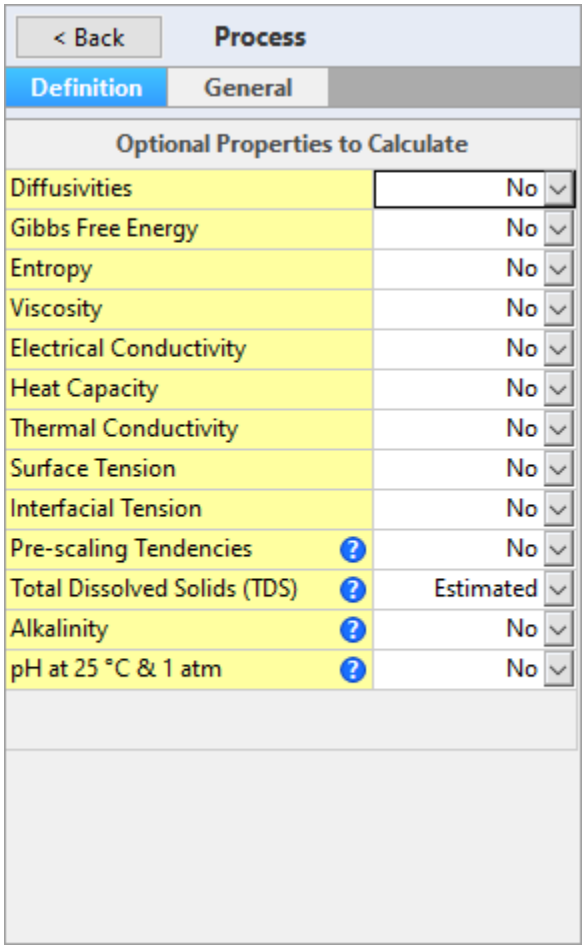
Process Options

The Properties Panel has two tabs. The Definition Tab has seven process options. The general tab contains the information specified by the user about the name of the application being built.



Optional Properties

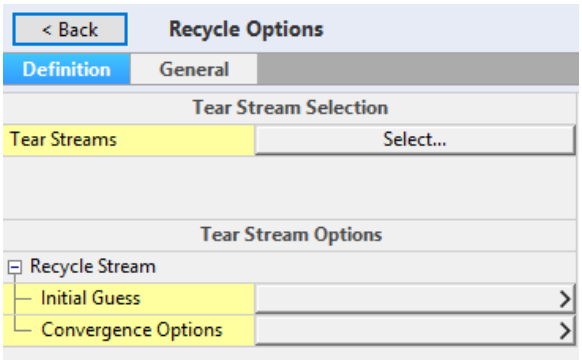
This section has the optional properties that can be calculated while running the simulation. The screen lets users choose from an option of a dropdown if they want to enable or disable the calculation of that property. Following is the list of available properties.



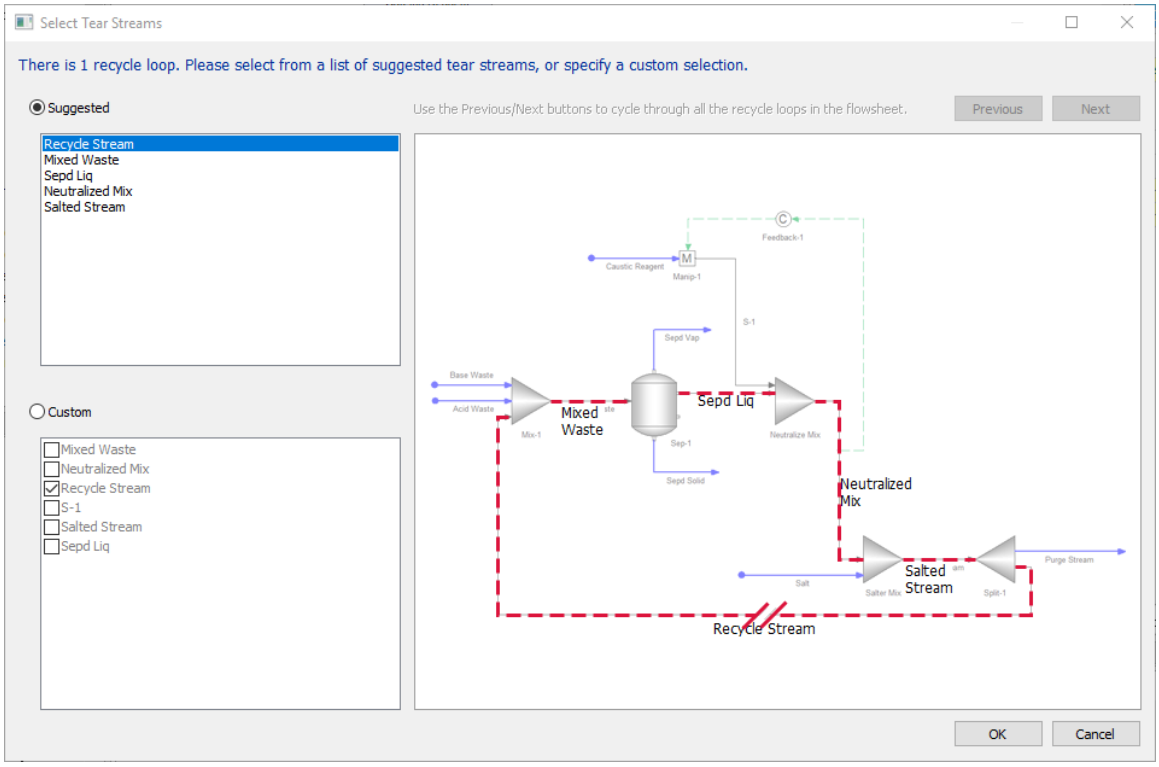
To enable the calculation of any of the properties, click on the drop-down arrow and select **Yes.**

Recycles

When this facility is selected, an analysis for process recycle streams is done automatically and, if recycle exists, the user can choose from several options to define the tear stream and recycle convergence.

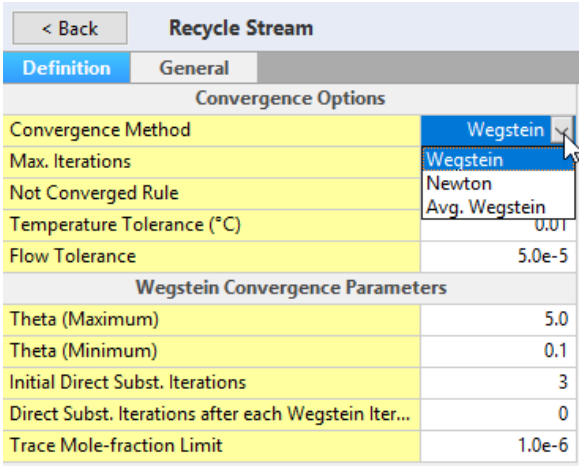


Tear Stream: When clicking ***Select***, in Tear Streams in the recycle options, a new window will open.



In the previous window a suggested tear stream is given, however the user can specify a custom tear stream.

Convergence options can be specified after selecting a tear stream are as follows:



Convergence Method: Three different convergence method are available:

Wegstein
Newton
Avg. Wegstein

A brief explanation of how these methods work is given below:

Wegstein's method: The traditional method of converging a recycle loop. In this method the update guess for the tear stream is given by:

$$X_{n+1} = (1 - \theta)F(X_n) + \theta\, X_n$$

Where

$$\theta = \frac{s}{s - 1}$$

and

$$s = \frac{F(X_n) - F(X_{n-1})}{X_n - X_{n-1}}$$

The value of θ can give an indication of the quality of convergence

θ (theta) = 1	Direct substitution
θ (theta) < 1	Slow, stable convergence
θ (theta) > 1	Can speed convergence but introduce instability

Direct substitution:

In this method the previous computed stream values becomes the input for the next iteration. This method is often slow to converge.

$$X_{n+1} = F(X_n)$$

Newton's Method: This method perturbs each material balance group, temperature, pressure, and flow to obtain a matrix of derivatives. This allows for a slope-like technique to converge a recycle stream. This is very useful when the Wegstein's method seems to be unstable.

Newton's method requires the derivative information for obtaining the guess for the next iteration.

$$X_{n+1} = X_n - \frac{F'(X_n)}{F(X_n)}$$

Where $F'(X_n)$) is the analytical/Numerical derivative.

Average Wegstein's Method This method uses the previous 3 Wegstein theta values and averages them. This becomes the new theta value. The method then uses a rolling average based on the last three theta values to set the new theta value.

Max Iterations: Change the default number of iterations that will be performed before a non-convergent case will be terminated.

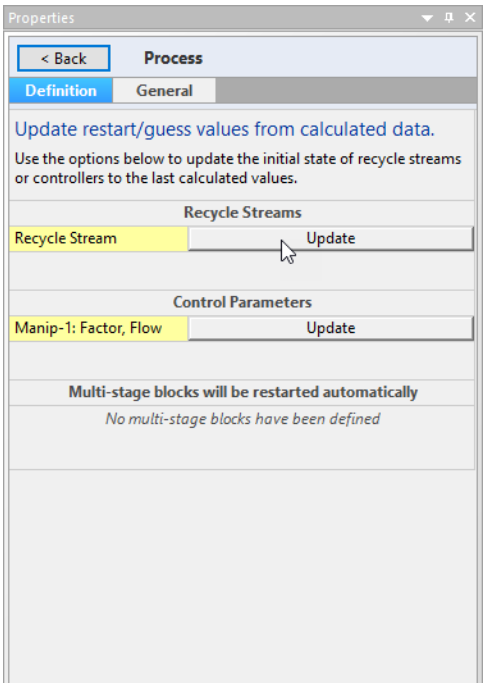
Not Converged Rule: The choice to continue or stop when a loop does not converge.

Temperature Tolerance (ºC): Temperature tolerance that determines when the case converges.

Flow Tolerance: Flow tolerance that determined when the case converges.

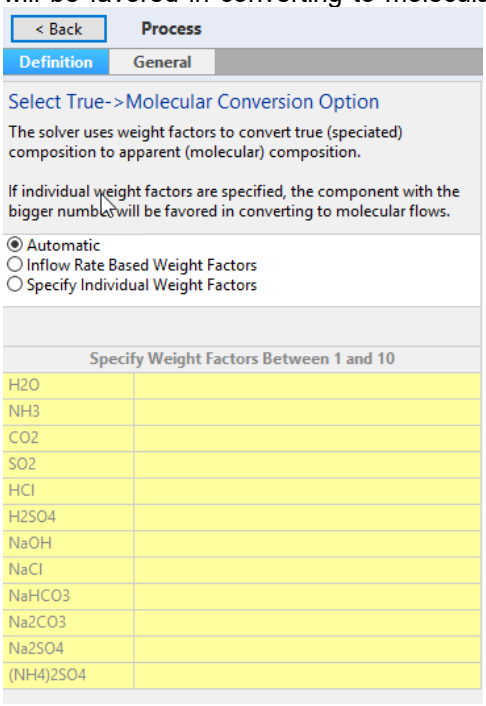
Restart Options

This facility gives the user the option of initializing a recycle stream or a Multi-stage process block with the results from the previous case run.



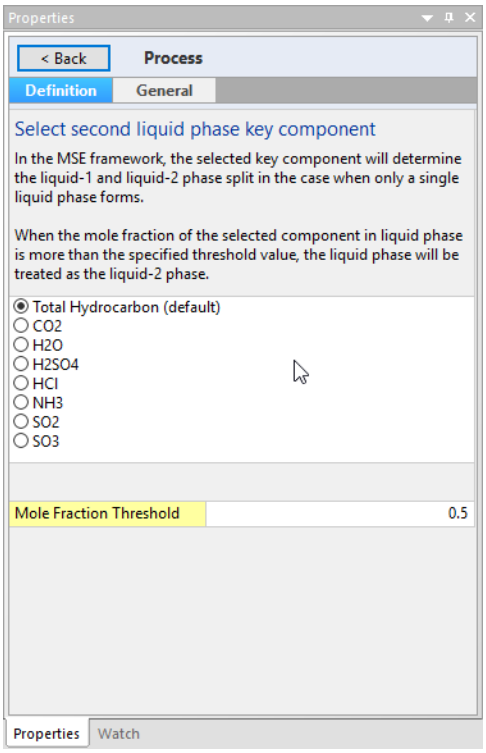
Molecular Conversion Weights

The solver uses weight factors to convert true (speciated) composition to apparent (molecular) composition. If individual weight factors are specified, the component with the bigger number will be favored in converting to molecular flows.



Liq-2 Key Component

In the MSE framework, the selected key component will determine the liquid-1 and liquid-2 phase split in the case when only a single liquid phase forms. When the mole fraction of the selected component in liquid phase is more than the specified threshold value, the liquid phase will be treated as the liquid-2 phase. The Liq-2 key component options lets a user choose their own key component from a chemistry model.



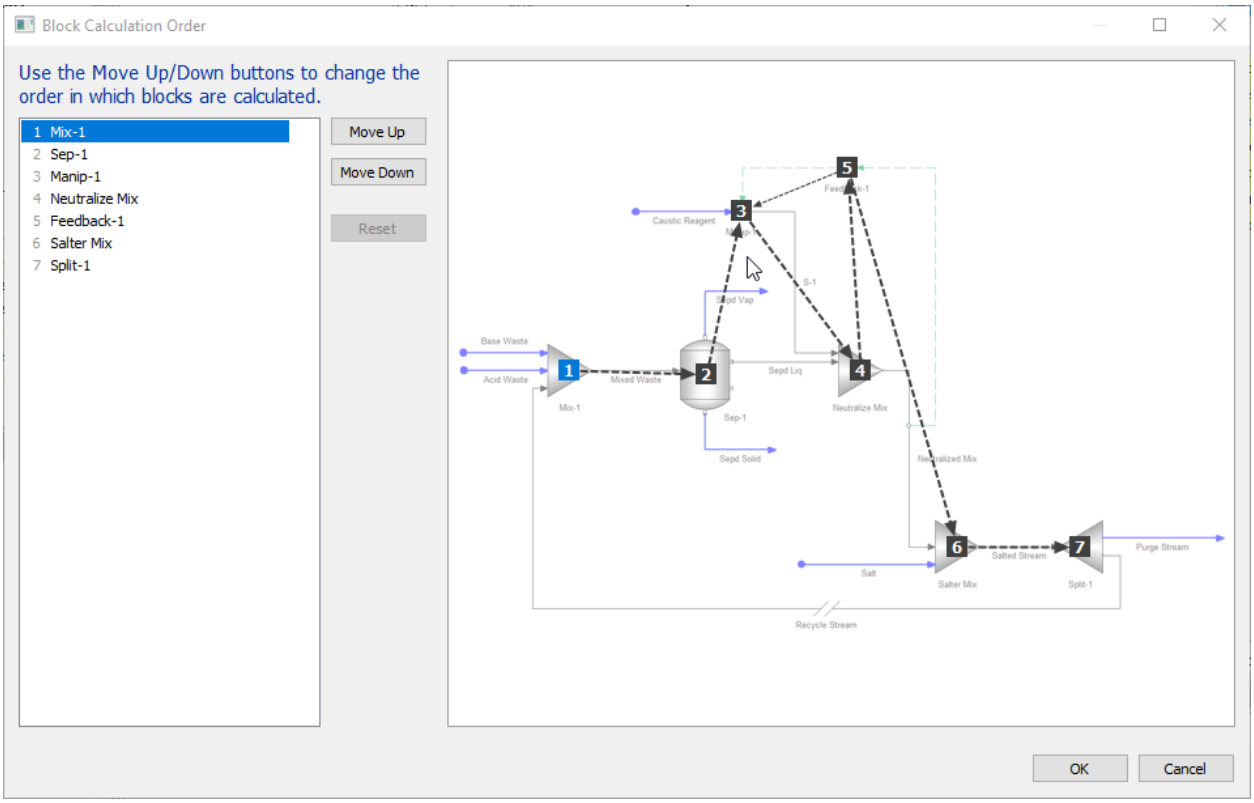
Calculation Aids

One of the current calculation aids are to enable trace, This option will create a file with the extension .oue and will contain a detailed convergence history for all Process Blocks. This is useful in determining probable causes for the nonconvergence of Process Block calculations.

Block Calculation Order

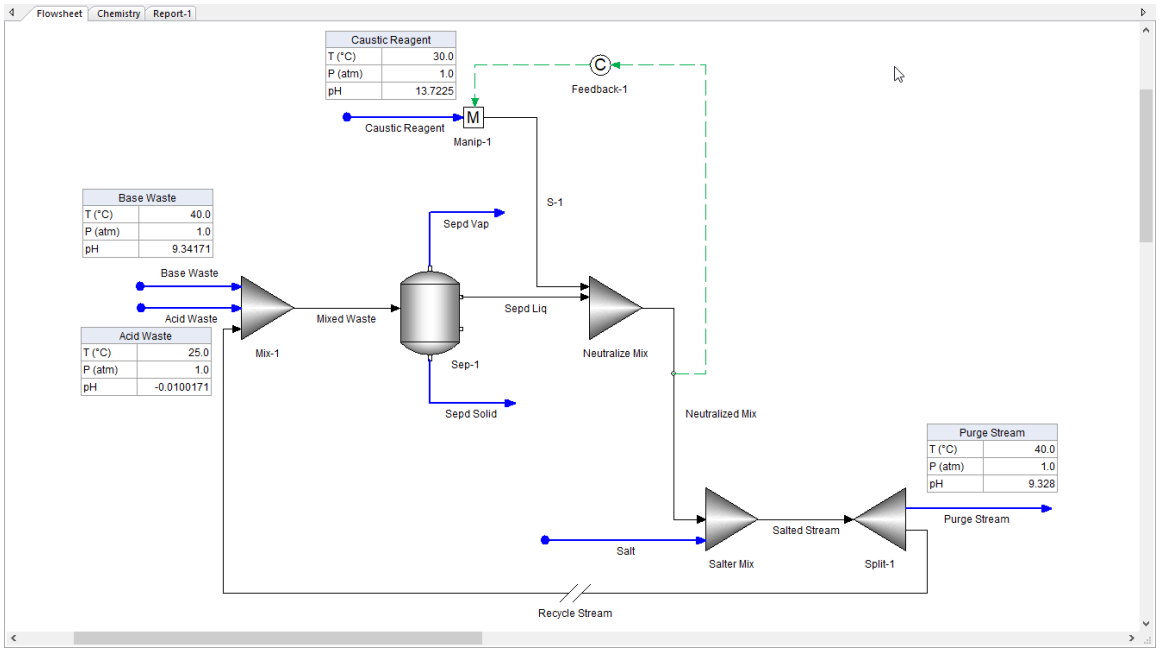
This option will allow the user to specify the order of the blocks to be calculated. It will also allow the choice of executing only part of the process.

The user can change the order of the process by using the Move Up or Move Down Buttons.



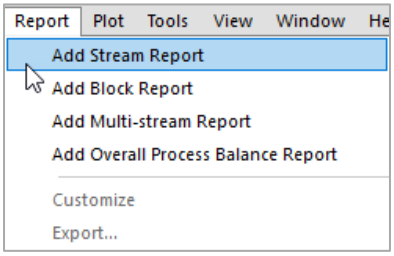
Chapter III – Reports

Let us consider the pH Neutralization with Feedback control and recycle:



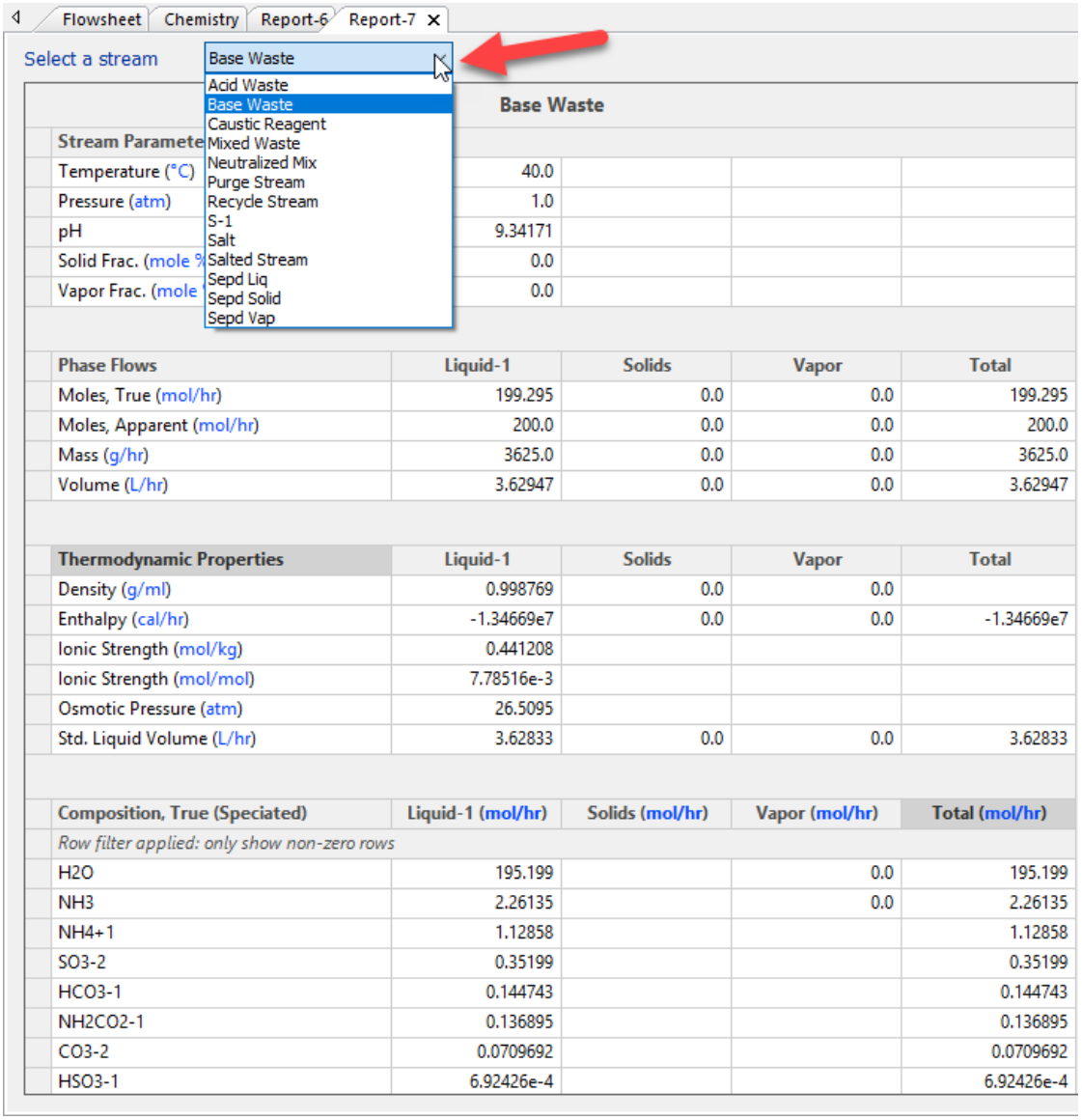
In the Report Tab, we have the following options:

Add a Stream Report
Add a Block Report
Add Multi-Stream Report
Add Overall Process Balance Report
Customize
Export



Stream Report

When using the Stream Report, the user can select a stream for analyzing its properties. Just use the drop-down arrow to select the desired stream:



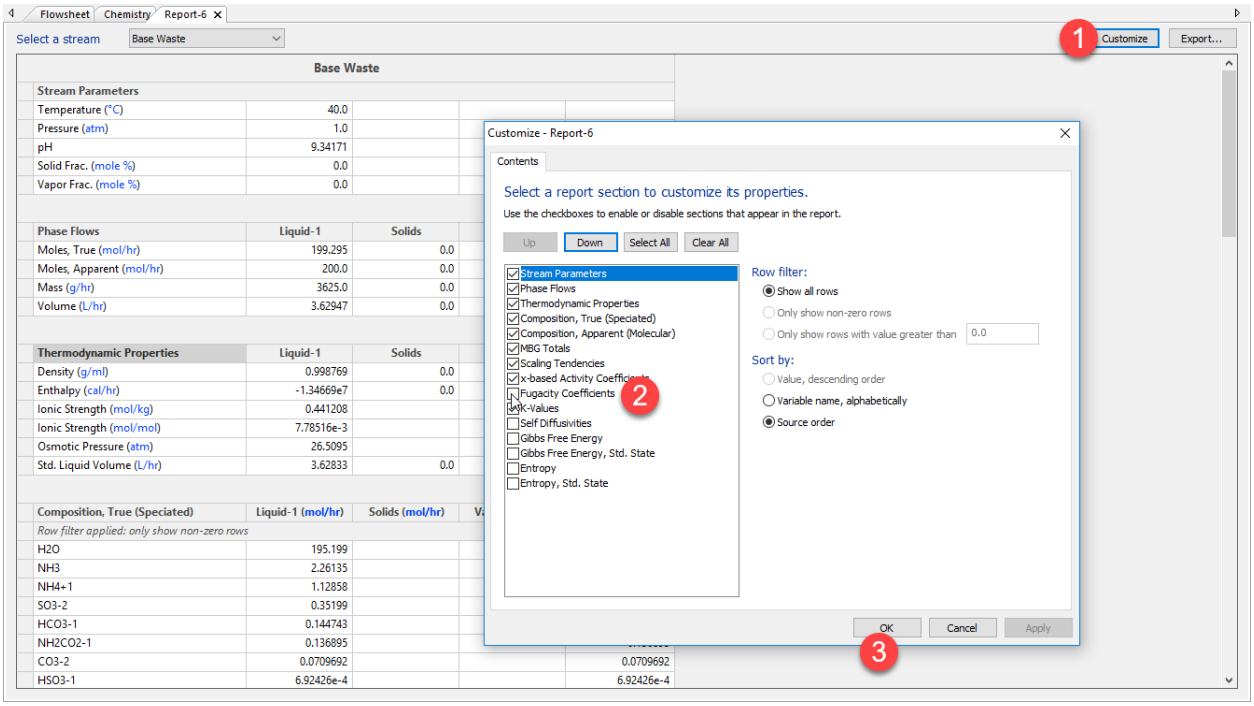
Stream Parameter	Base Waste			
Temperature (°C)	40.0			
Pressure (atm)	1.0			
pH	9.34171			
Solid Frac. (mole %	0.0			
Vapor Frac. (mole	0.0			

Phase Flows	Liquid-1	Solids	Vapor	Total
Moles, True (mol/hr)	199.295	0.0	0.0	199.295
Moles, Apparent (mol/hr)	200.0	0.0	0.0	200.0
Mass (g/hr)	3625.0	0.0	0.0	3625.0
Volume (L/hr)	3.62947	0.0	0.0	3.62947

Thermodynamic Properties	Liquid-1	Solids	Vapor	Total
Density (g/ml)	0.998769	0.0	0.0	
Enthalpy (cal/hr)	-1.34669e7	0.0	0.0	-1.34669e7
Ionic Strength (mol/kg)	0.441208			
Ionic Strength (mol/mol)	7.78516e-3			
Osmotic Pressure (atm)	26.5095			
Std. Liquid Volume (L/hr)	3.62833	0.0	0.0	3.62833

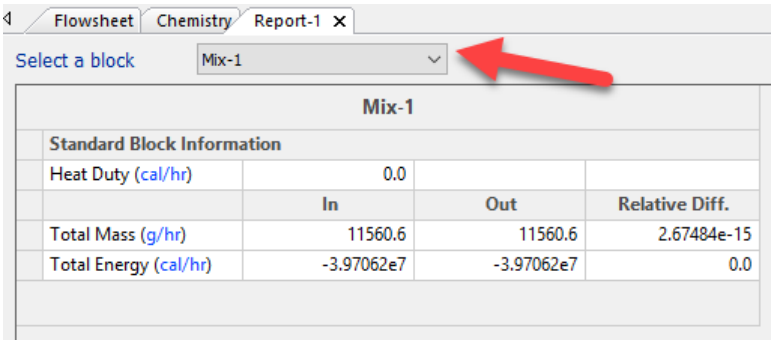
Composition, True (Speciated)	Liquid-1 (mol/hr)	Solids (mol/hr)	Vapor (mol/hr)	Total (mol/hr)
Row filter applied: only show non-zero rows				
H2O	195.199		0.0	195.199
NH3	2.26135		0.0	2.26135
NH4+1	1.12858			1.12858
SO3-2	0.35199			0.35199
HCO3-1	0.144743			0.144743
NH2CO2-1	0.136895			0.136895
CO3-2	0.0709692			0.0709692
HSO3-1	6.92426e-4			6.92426e-4

The Stream Report can be customized with additional properties:



Block Report

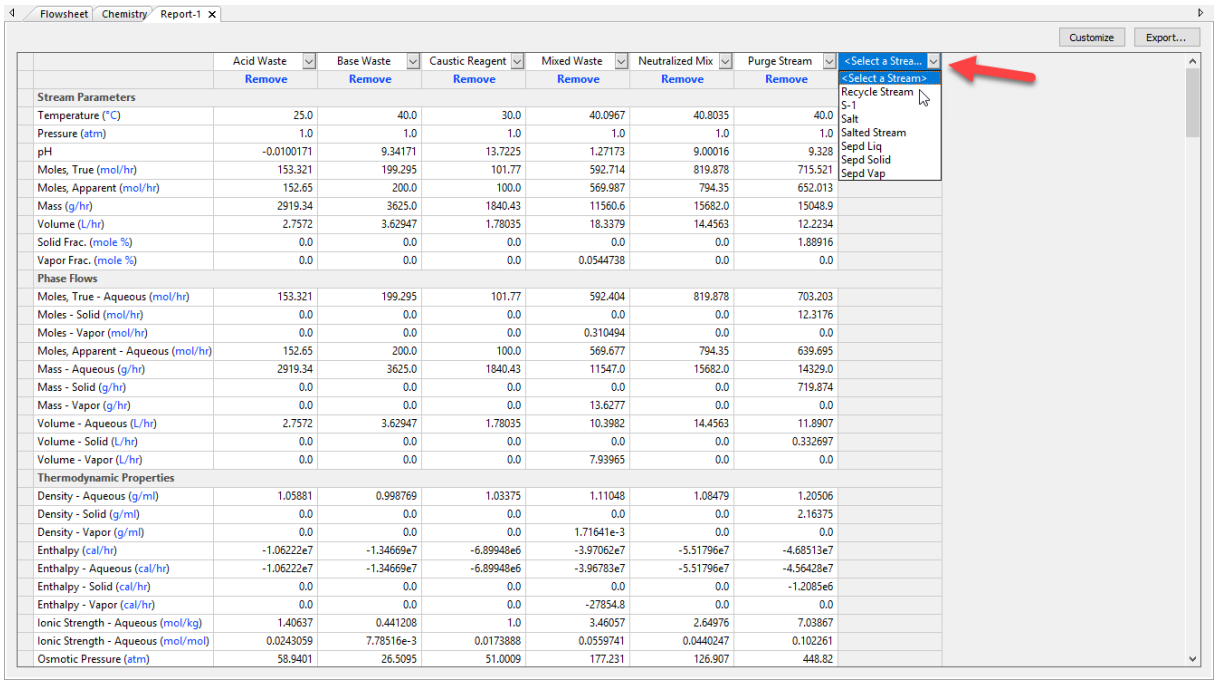
The block report allows the user to view the general information for a specific block. Additionally, the information shown in this table can also be customized.



Multi-stream Report

The Multi-Stream Report gives us the advantage of showing information of different streams for comparison purposes. You can add either all streams of the streams of interest or just specific streams.

To add an additional stream, you need to click in the drop-down arrow, and select the stream of interest, as is shown in the image below:

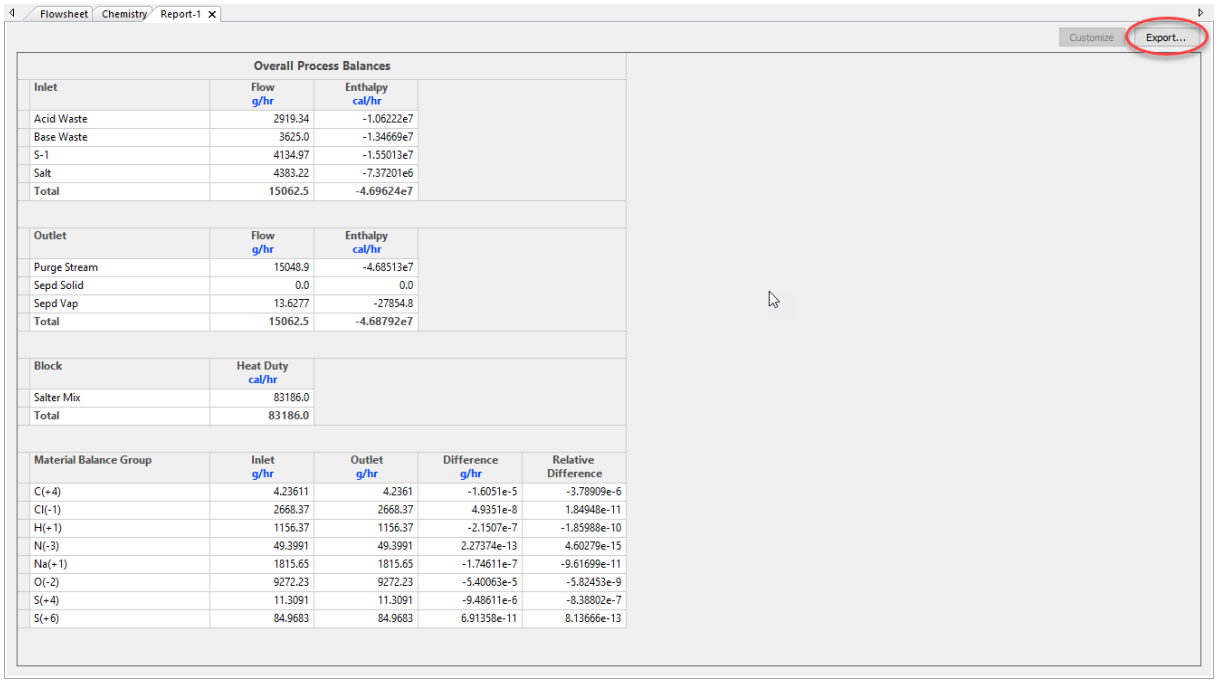


Overall Process Balance Report

The overall process balance report shows the information of all inlets and outlets of the process, and information calculated for different blocks.

A material balance group table is also displayed.

The information of the this, report (and all the reports previously explained), can be exported in a .csv file, for posterior analysis in Excel.



Chapter IV – Chemistry Models

Overview

In most cases, the user defines a chemistry model by simply entering the names of the chemicals to be covered by the model and the software does the rest. However, this chapter describes all the advanced facilities available to the user.

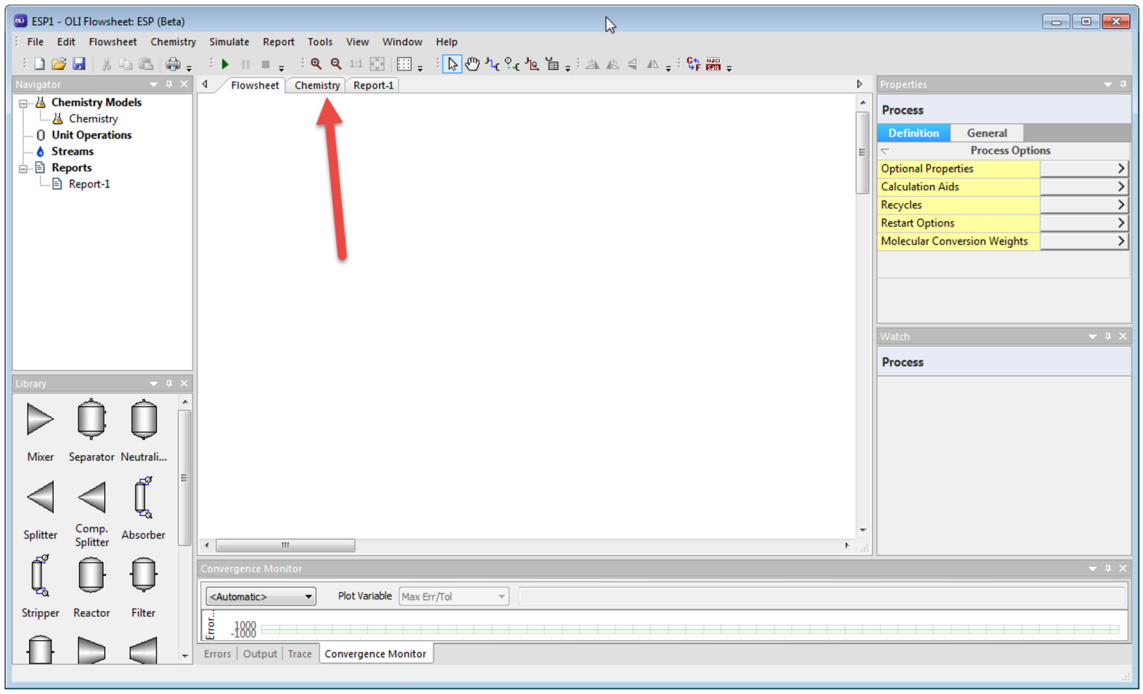
This section describes in detail the requirements to build a Chemistry Model. The Chemistry Model is important as it describes the specific chemical species and chemical equilibria involved in the application being considered.

The building of a basic Chemistry Model is a quick and simple operation. It is also an essential requirement for the modeling of an electrolyte system. Generally, from a user statement of molecular chemical species, a model is automatically created by the software. This file contains a list of the chemical species in each phase (i.e., vapor, aqueous molecules and ions, and anhydrous and hydrated solids) and the corresponding thermodynamic phase and aqueous speciation equilibrium relationships for the system.

For many OLI applications, this created model is all that is needed to describe the chemistry of the system. However, if required, the model can be augmented by the user to include chemical reaction kinetics, and surface phenomena.

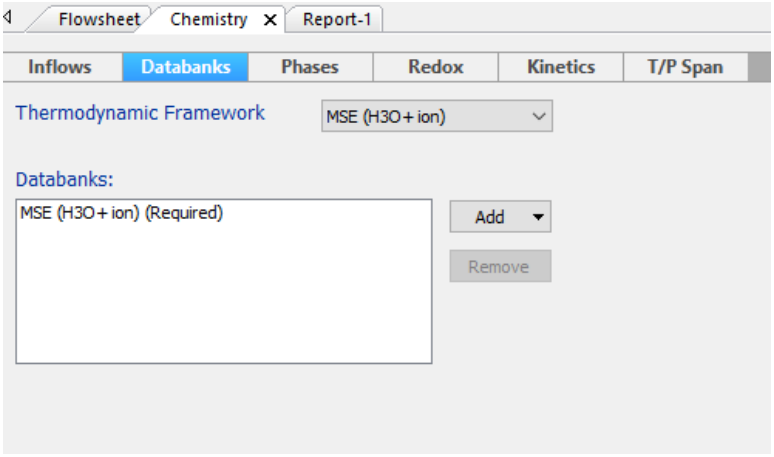
Chemistry Tab

The OLI Flowsheet: ESP chemistry model is accessible via the **Chemistry** tab on the PFD. It is recommended that the user start with some basic chemistry before building the process.



Locating the Chemistry Model

Clicking on the **Chemistry** tab will display the options for the chemistry model.

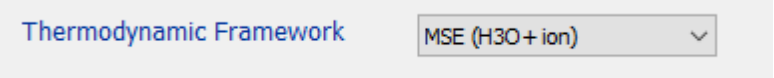


We start on the default tab **Databanks**. Here we will modify the data-sets used for this process if required.

Thermodynamic Framework

The user can choose between the default **MSE (H3O+ Ion)** framework, the MSE-SRK (H3O+ Ion) framework, or the **Aqueous (H+ Ion)** framework.

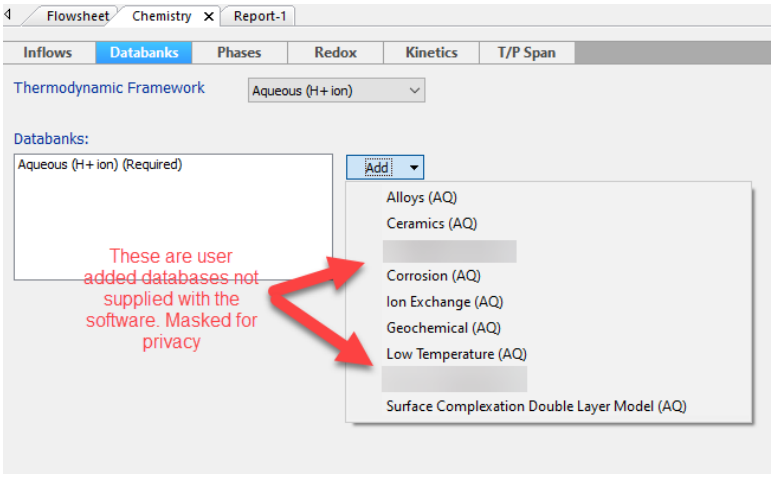
The default version of the thermodynamic framework is the MSE (H30+ Ion) framework



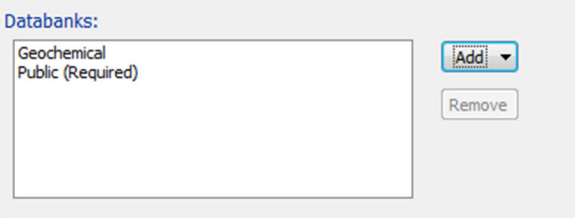
Databanks

The default databank for each thermodynamic framework is shown. The user cannot make any modifications to the default databank. For the AQ thermodynamic framework, the default databank is **Aqueous (H+ ion)**. For the MSE thermodynamic framework the default databank is **MSE (H3O+ ion)**.

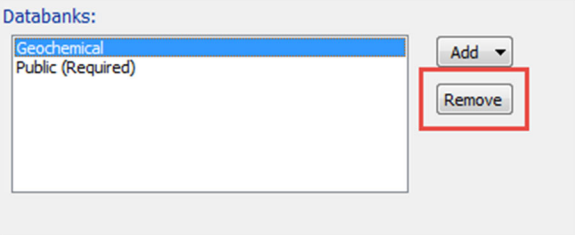
The add button allows the user to add additional databanks to the process. Here we are showing the installed additional databases for the AQ thermodynamic framework.



The user just selects the desired databank, and it is added to the current list. For this example, we are selecting a commonly used databank **Geochemical**.



To remove a databank, simply highlight the databank and then click the **Remove** button. The default databank cannot be removed.



What are the OLI Supplied Databanks?

Below is a list of the databanks supplied with the OLI Flowsheet: ESP program:

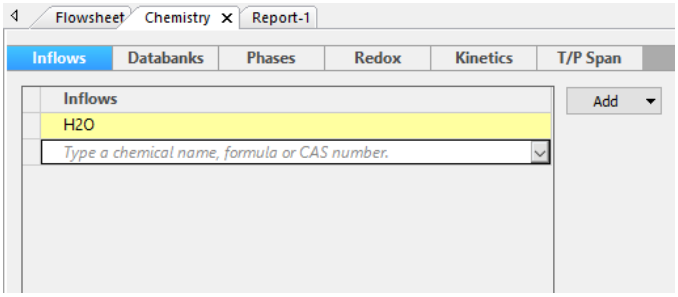
AQ Databank Name	MSE Databank Name	Description
Alloys	<none>	This contains special solids that are like alloys. Such an example is CuNi alloys. This is an AQ thermodynamic framework only databank. There is no corresponding MSE databank
Ceramics	<none>	This contains special solids that are like ceramics. This was to support work done for the ceramics lab at the Rutgers University. This is an AQ thermodynamic framework only databank. There is no corresponding MSE databank
Corrosion	MSE Corrosion	This contains special elements to generate Pourbaix diagrams. Some of the species have had their Gibb's Free Energy of Formation values adjusted to match traditional Pourbaix Diagrams. It is not recommended for use with OLI Flowsheet: ESP

Exchange	<none>	This contains ion-exchanging resins. This is an AQ thermodynamic framework only databank. There is no corresponding MSE databank
Geochemical	MSE Geochemical	This contains minerals that are primarily found in geothermal applications. These minerals typically do not reform under traditional chemical process conditions.
Low Temperature	<none>	This databank contains minerals that form below 0°C (273.15 K). This is an AQ thermodynamic framework only databank. There is no corresponding MSE databank
Surface Complexation Capacitance Model	<none>	This databank contains surface species following Dzombak's model for capacitance. This is an AQ thermodynamic framework only databank. There is no corresponding MSE databank
Surface Complexation Double Layer Model	Surface Complexation Double Layer Model (MSE)	This databank contains surface species following Dzombak's model for Double-layers capacitance.
Surface Complexation Non-Electrostatic Model	<none>	This databank contains surface species following Dzombak's model for non-electrostatic interactions. This is an AQ thermodynamic framework only databank. There is no corresponding MSE databank
Surface Complexation Triple Layer Model	<none>	This databank contains surface species following Dzombak's model for Triple-layers. This is an AQ thermodynamic framework only databank. There is no corresponding MSE databank
<none>	MSE Urea	This databank contains surface species that support high temperature formation of urea. It is not recommended unless urea is known to form from NH_3 and CO_2. Generally, such formations are kinetically limited. This is an MSE thermodynamic framework only databank. There is no corresponding AQ databank

Inflows Tab

The inflows tab is where the components you desire are entered. Unlike OLI Studio, this grid automatically searched for a component in the selected databanks. You enter the name, chemical formula, CAS number or OLI TAG name. The displayed name is based on the Names Manager tool.

Water (H_2O) is a required inflow component even in systems where water is not present. This is a requirement of the software. Component flowrates for water may be zero in the simulation if required.



Entering a chemical name

When entering a chemical name, the grid will expand to show likely components. Here we are entering *diethylamine.*

As we started to enter text, the grid begins to start a search. At this point in Figure 2 we have only entered the text “diethyla” and all the species that contain that text are displayed. Just click the one you require.

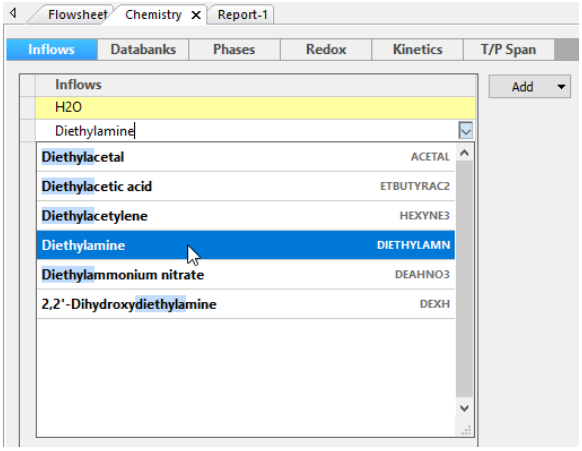
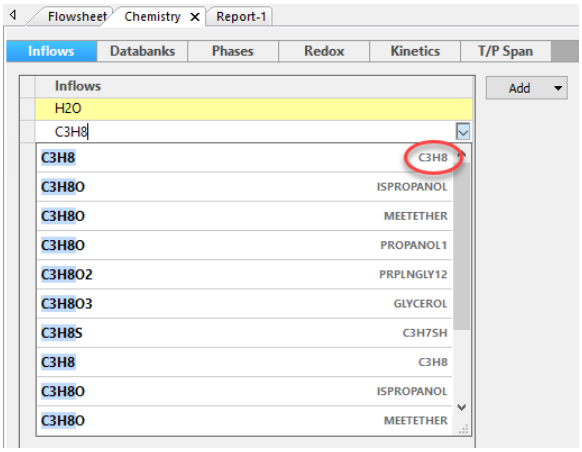


Figure 2 entering species names

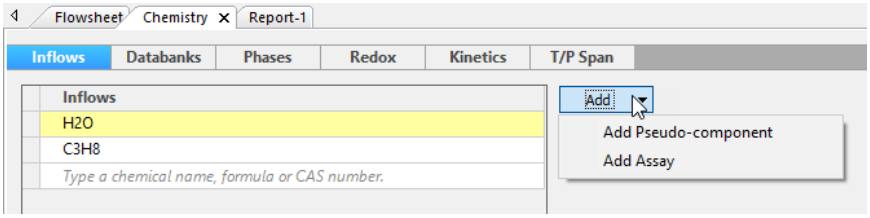
You can also enter by formula such as C3H8 (n-propane).

The input grid also displays alternative names (OLI TAG) for the species to the right. Users of ESP Original and some alliance partners will be familiar with these names.



Add Button

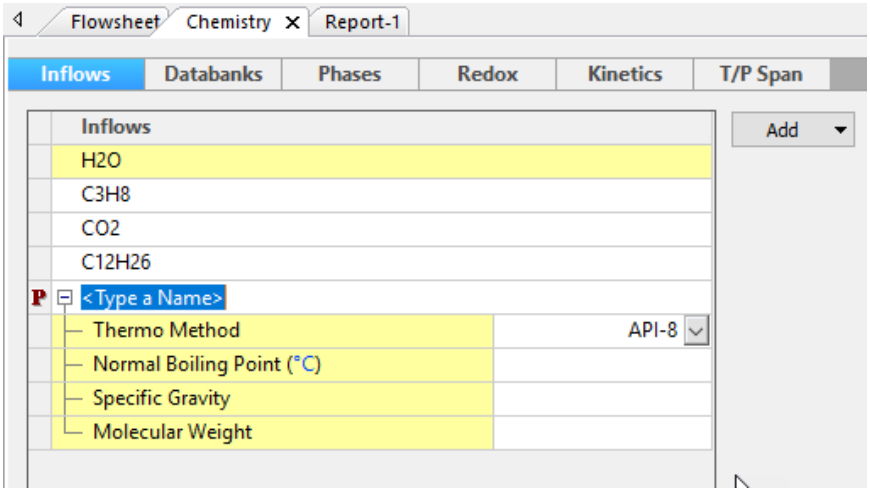
The **Add Button** allows the user to add different types of chemistry. The user can add a Pseudo-Component or a Petroleum Assay.



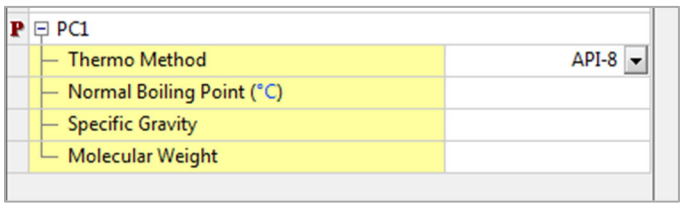
Adding a Pseudo-Component

Pseudo-components are user created species which simulate portions of petroleum products. Typically, a user will have some analysis of an oil sample such as assay data (boiling point data and the like) which will be broken down into individual pseudo-components. This task will be discussed in the next section. Alternatively, the user may have the data for each pseudo-component derived from other sources. This type of data can be entered via this menu item.

Select **Add Pseudo-component**



We have several items to enter for each individual pseudo-component. The first item is a name. Enter a name in the **<Type a Name>** box. This name must be unique to the model and cannot be the name of a component already in the OLI software (the program will warn you accordingly). Typically, the pseudo-component name uses the letters “PC” and some number. Here we will use the name **PC1**.



Thermo Method

We now need to define a thermodynamic method to convert the entered data to a thermodynamic entity. The default method is API-8 (American Petroleum Institute Method 8).

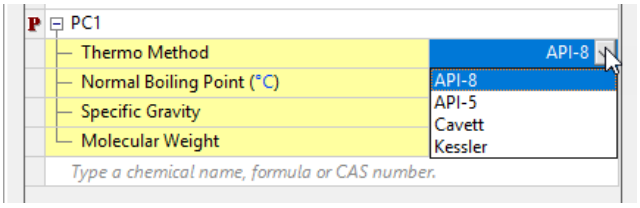


Figure 3 Available pseudo thermodynamic models

OLI Flowsheet: ESP supports the following methods:

API-8 (default)
API-5
Cavett
Kessler

A more detailed explanation of each method is given below:

API 8 and 5 Uses the specific gravity to estimate the critical parameters. The specific gravity, if not entered, can be estimated from the API gravity or the Watson K. The boiling points are taken from the assay data.

Cavett This method uses the API gravity method to determine the critical properties. The API gravity, if not entered can be estimated from the actual specific gravity or the Watson K. The boiling points for the pseudo-components are taken from the assay.

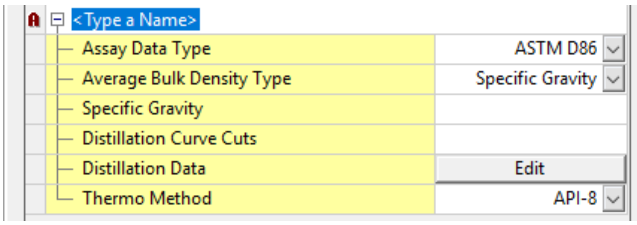
Lee-Kesler This method uses the Watson K and the specific gravity (which can be estimated via the Watson K) to determine the critical parameters.

The user may enter any two of the three parameters listed in**Normal Boiling Point, Specific Gravity, And Molecular Weight.** The parameter not entered will be calculated using the selected thermo method. If all three parameters are entered, then only the parameters **Normal Boiling Point** and **Specific Gravity** will be used.

Adding an Assay

Assays are characteristics of oil samples. Typically, some sort of distillation data has been collected and will be entered into the software. This distillation data will be “Cut” into individual pseudo-components.

Click the **Add Assay** menu item.



As with pseudo-components a name is required that must be unique for this document. The name may not be the same as any component currently in the OLI software (the software will check for this). Typically, a name such as “AS” is used with a number appended (such as AS1). The name is limited to 5 characters and the program will enforce this rule.

The **Assay Data Types** are described in Table 1 Assay Data Types

Table 1 Assay Data Types

Assay Data Type	Description
ASTM D86	Used for light and medium petroleum products and is carried out at atmospheric pressure. The results are converted internally in the OLI model generator to a TBP (True Boiling Point Curve). This curve is then fit to a spline to smooth the curve. The cuts are taken from the spline. Examples are: Naphtha, kerosene/jet fuel, diesel and atmospheric gas oils.
ASTM D1160	Used for heavier petroleum products and is often carried out under vacuum. Sometimes as low as 1 mm Hg. The results are converted internally in the OLI model generator to a TBP (True Boiling Point Curve). This curve is then fit to a spline to smooth the curve. The cuts are taken from the spline. Examples are atmospheric bottoms/resid or vacuum bottoms/resid.
ASTM D2887	Uses gas chromatography to produce the distillation curve and is applicable to a wide range of petroleum products. The results are always reported on a volume percent basis. The results are converted internally in the OLI model generator to a TBP (True Boiling Point Curve). This curve is then fit to a spline to smooth the curve. The cuts are taken from the spline
TBP (True Boiling Point)	This is the true boiling point curve. These curves, in practice, are difficult to obtain. The other methods are usually used instead.

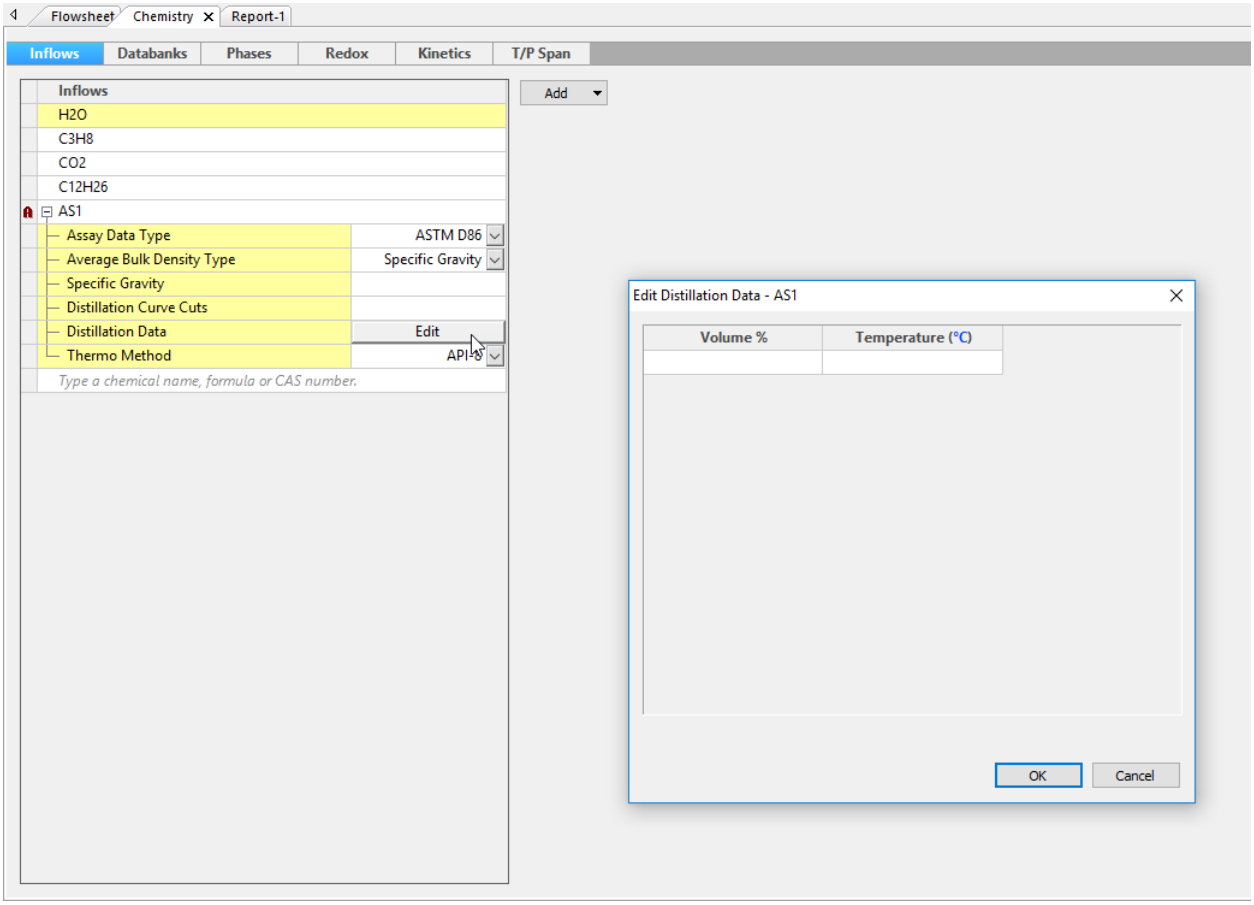
The **Average Bulk Density Type** is described below:

Average Bulk Density Type	Description
Specific Gravity	Relative to the density of water. No units
API Gravity	Reported in Degrees API (^{O}API). Calculated via the following formula: $$°API(60°\text{F}) = \left(\frac{141.5}{SG(60°\text{F})}\right) - 131.5$$ Where, SG is the specific gravity at 60 °F.
Watson K	The Watson K has no units but is calculated via: $$K = \left(\frac{NBP^{\frac{1}{3}}}{SG}\right)$$ Where NBP is the normal Boiling point and SG is the specific gravity.

Distillation Data

The **Distillation Curve Cuts** are the number of pseudo-components that will be created from the distillation data.

The **Distillation Data** is the actual assay data. The type of the data entered depends on the user selection for the **Assay Data Type**. As an example, for the method **ASTM D2887** the distillation data may look like this:

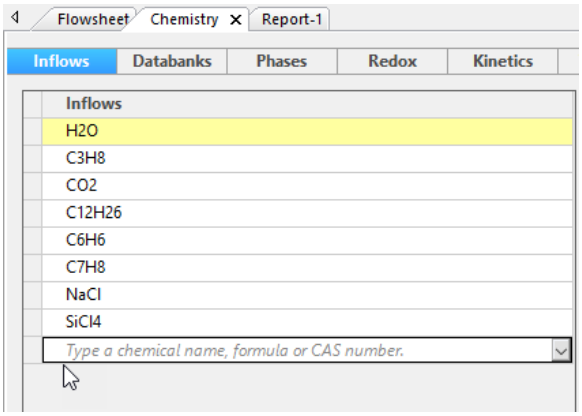


The **Thermo Method** is the same selection for Pseudo-components above.

Once the data has been entered, the program will create the pseudo-components and display a report.

Phases Tab

The **Phases Tab** allows the user to modify the default phase behavior. In this example we have created the follow chemistry using the **Inflows Tab**.

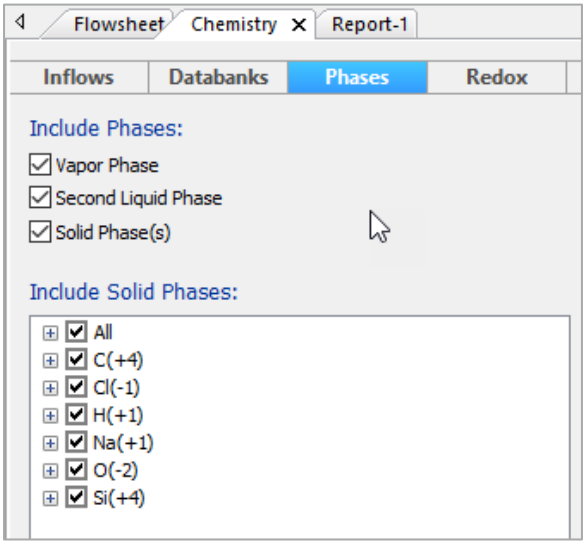


Click on the **Phases** tab.

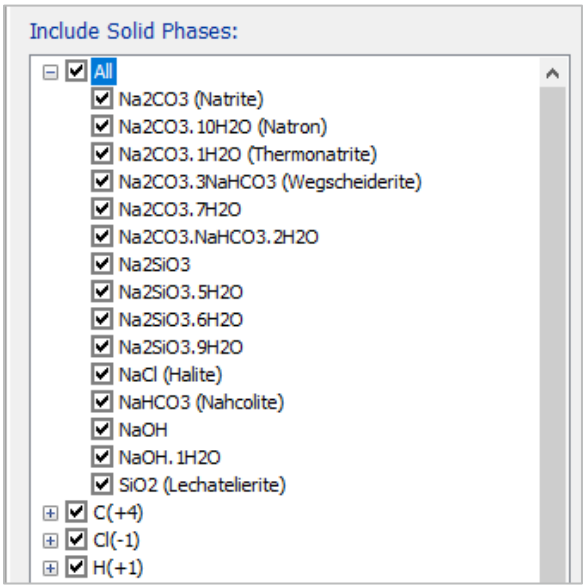
OLI considers the possibility of a vapor phase, second liquid phase (also referred to as an organic phase) and multiple solid phases. OLI always considers a water-rich phase referred to as Liquid 1.

The user can enable or disable phases by unchecking the phase box. In the figure above, all phases have been enabled.

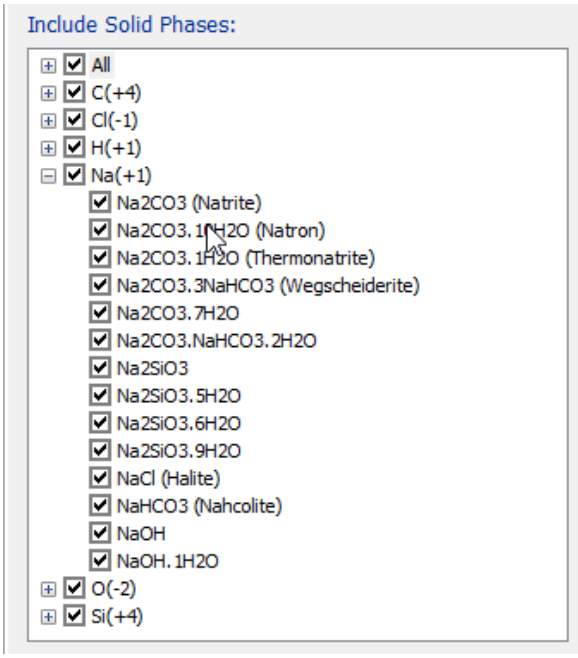
The user may also disable individual solid phases if they are known not to form under the conditions specified in the flowsheet. The solids are grouped by material codes and can be expanded by section.



The **All** group has all the solid displayed.

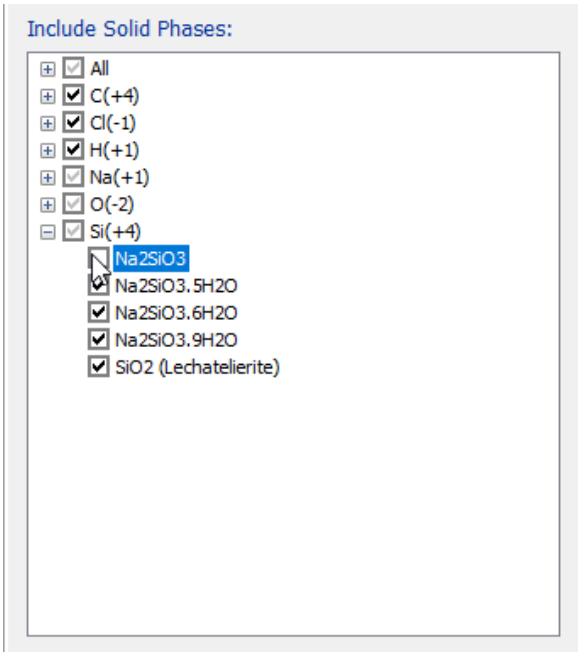


The **Na(+1)** only has species with the sodium ion (+1) material groups displayed.



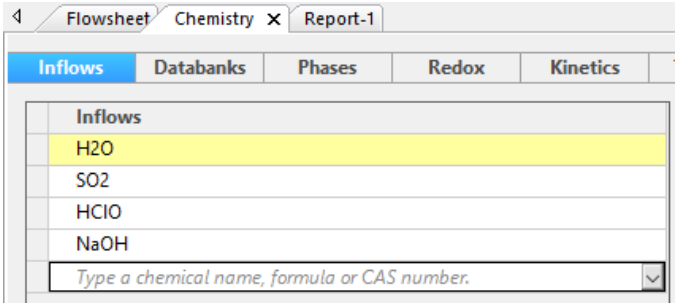
If the solid Na2SiO3 is unwanted it can be unchecked.

You will notice that some other check boxes have turned gray. Since the species Na2SiO3 also contains the materials Na(+1), Si(+4) and O(-2) the corresponding check boxes in those groups have also been removed.



Redox Tab

OLI Flowsheet: ESP allows for changes in oxidation state otherwise known as REDOX. To illustrate this feature, we have created a simple chemistry model:

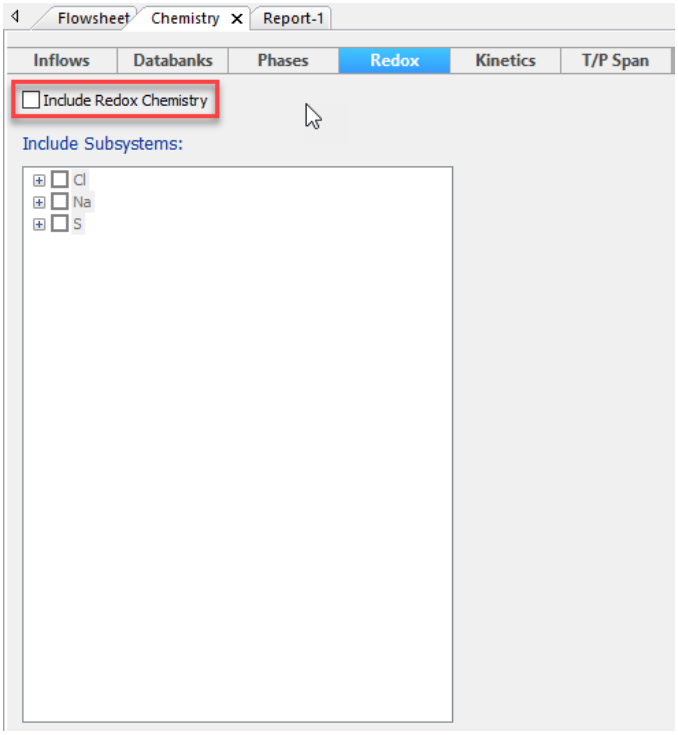


We are going to oxidize the sulfur in Sulfur dioxide - an S (+4) oxidation state- to an S (+6) state commonly found in sulfuric acid. At the same time, we will reduce the chlorine in the hypochlorous acid - a Cl (+1) oxidation state - to chloride in the (-1) oxidation state.

Click on the **Redox** tab.

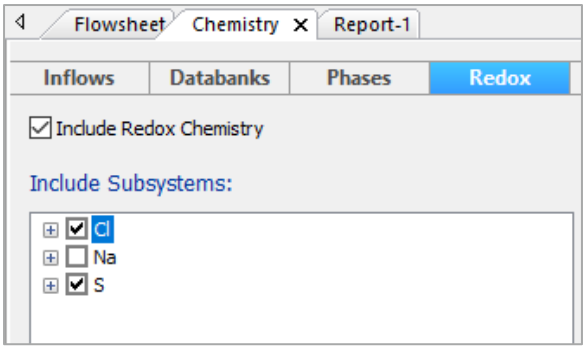
By default, we do not enable Redox chemistry. Enabling redox will add a significant amount of species.

Check the **Include Redox Chemistry** box.



We now can select which subsystems to include. We can check the boxes to enable them. As a best practice, we should not check any elemental metals such as sodium. It is unlikely that we will form metallic sodium in our process unless we add electricity to reduce the metal. OLI Flowsheet: ESP currently does not support such processes. however, if you are starting with a stream that contains metallic sodium then enabling this box would be appropriate.

Check the elements you require.



The current chemistry model now includes these species. We started with Chlorine in the (+1) oxidation state and Sulfur in the (+2) oxidation state. Let's see what we currently have in the chemistry model.

$$Cl^{1-} + 1.25O_{2_{AQ}} + H^+ = ClO_{2_{AQ}} + 0.5H_2O$$

$$SO_3^{2-} + 1.6H^+ = 0.2S_5^{2-} + 0.8H_2O + 1.1O_{2_{AQ}}$$

$$SO_4^{2-} + 1.6H^+ = 0.2S_5^{2-} + 0.8H_2O + 1.6O_{2_{AQ}}$$

$$S^{2-} + 0.4O_{2_{AQ}} + 1.6H^+ = 0.2S_5^{2-} + 0.8H_2O$$

$$S_5O_6^{2-} = S_5^{2-} + 3O_{2_{AQ}}$$

$$HSO_5^{1-} + 0.6H^+ = 0.2S_5^{2-} + 0.8H_2O + 2.1O_{2_{AQ}}$$

$$ClO^- + 0.75O_{2_{AQ}} + H^+ = ClO_{2_{AQ}} + 0.5H_2O$$

$$ClO_4^- + H^+ = ClO_{2_{AQ}} + 0.5H_2O + 0.75O_{2_{AQ}}$$

$$ClO_3^- + H^+ = ClO_{2_{AQ}} + 0.5H_2O + 0.25O_{2_{AQ}}$$

$$S_2O_4^{2-} + 1.2H^+ = 0.4S_5^{2-} + 0.6H_2O + 1.7O_{2_{AQ}}$$

$$S_2O_6^{2-} + 1.2H^+ = 0.4S_5^{2-} + 0.6H_2O + 2.7O_{2_{AQ}}$$

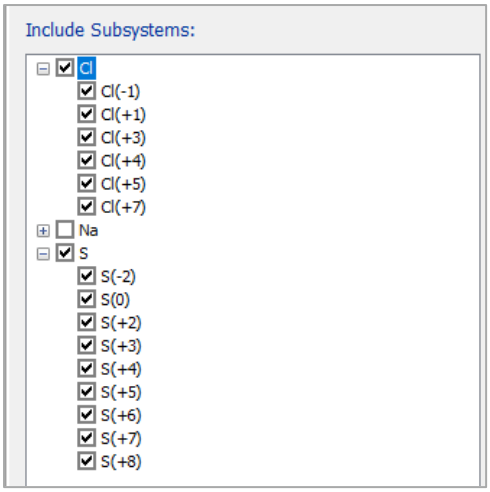
$$S_2O_8^{2-} + 1.2H^+ = 0.4S_5^{2-} + 0.6H_2O + 3.7O_{2_{AQ}}$$

$$ClO_2^- + 0.25O_{2_{AQ}} + H^+ = ClO_{2_{AQ}} + 0.5H2O$$

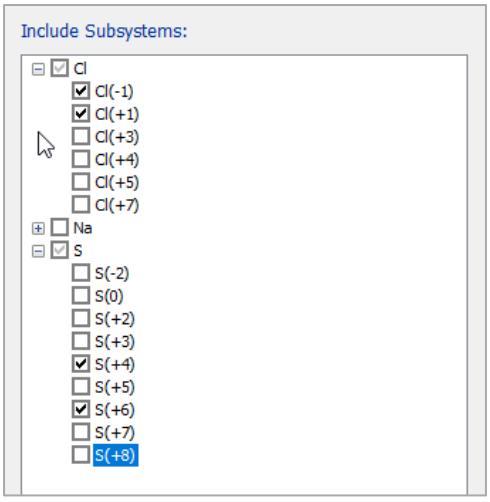
$$0.2H_{2_{AQ}} + 0.1O_{2_{AQ}} = 0.2H_2O$$

As you can see there are a quite a few species with multiple oxidation states for both chlorine and sulfur. If the user knew that only chlorides in the (-1) and (+1) oxidation states are involved as well as sulfur in the (+4) and (+6) oxidation states, then the model can be "adjusted" for just those oxidation states.

In the figure above, expand the "+" symbol to see more oxidation states.



Uncheck the undesired oxidation states. In this example we are only retaining Cl(-1), Cl(+1), S(+4) and S(+6).



The resultant chemistry is drastically altered.

$$Cl^- + 0.5O_{2_{AQ}} = ClO^-$$

$$SO_3^{2-} + 0.5O_{2_{AQ}} = SO_4^{2-}$$

$$0.2H_{2_{AQ}} + 0.1O_{2_{AQ}} = 0.2H_2O$$

Kinetics Tab

Reaction Kinetics Overview

The OLI thermodynamic framework supports reaction kinetics. Reaction kinetics can be defined in standard Arrhenius terms or in terms defined by the user. There are only two different unit operations that support reaction kinetics: REACTOR unit and Multistage COLUMNS such as STRIPPERS and ABSORBERS.

Reaction Types

There are two general types of reaction kinetics:

Type 1: Change in material balance codes across the reaction

As an example, consider the following reaction:

$$CH_4 + 2O_2 = CO_2 + 2H_2O$$

The material balance codes across the reaction are:

Species	Material Balance Codes	=	Species	Material Balance Codes
CH4	1001		CO2	25, 1
O2	57		H2O	1, 21

Due to the material balance code changes across this reaction there will be no equilibrium reaction or any combination of equilibrium reaction to produce this reaction. This assumes that no oxidation/reduction reactions are present in the equilibrium reactions.

In fact, this is a requirement of our kinetic models that kinetics and oxidation/reduction reactions cannot be mixed. You must use all kinetic or all oxidation/reduction, not a mixture of both.

Type 2: No change in material balance codes across the reaction

Consider this reaction:

$$CACO3PPT = CAION + CO3ION$$

The material balance codes across the reaction are:

Species	Material Balance Codes	=	Species	Material Balance Codes
CACO3PPT	6, 25, 21		CAION	6
			CO3ION	25, 21

The material codes on both sides of the equation are the same. Therefore, the equilibrium model will contain this reaction either directly or as a combination of equilibrium reactions. To include this kinetic reaction, the equilibrium model must be changed to remove the equilibrium between these species. The software will re-write the equilibrium reactions by removing the CACO3PPT from the equilibrium reaction

set. Thus, the only way to make or consume $CaCO_{3ppt}$ is by the kinetic reaction. If the user wants to feed $CaCO_{3ppt}$ to the reactor, an additional input has been provided in the interface routine to specify the amount of $CaCO_{3ppt}$ feed. An additional key word has been added to the kinetics section of the model file where the use can specify which species will be removed from the equilibrium calculation.

Kinetics Types

There are two types of kinetics available in OLI Flowsheet: ESP. The first is Arrhenius type (also known as Standard type) and the other is User type (also known as SPEC type).

Standard Rate Expressions

In this mode, the rate of reaction is calculated using a standard rate expression. This expression considers both the forward and reverse reaction rates, the individual species reaction orders, and the forward and reverse reaction constants (determined using the Arrhenius Equation).

The standard rate expression is best illustrated by means of an example. Consider the general equation:

$$aA + bB + \cdots = cC + dD + \cdots$$

where: $a, b, \ldots\ c, d$ are stoichiometric coefficients.

and: $A, B, \ldots$ are reactant species

$C, D, \ldots$ are product species

The standard rate expression is of the form:

$$Rate = \left(k_f a_A^{r1} a_B^{r2} \ldots - k_r a_C^{p1} a_D^{p2}\right) \times Vol$$

where:

$Rate$	=	Reaction rate $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$
k_f	=	Forward reaction rate constant $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$
k_r	=	Reverse reaction rate constant $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$
$a_A, a_B, \ldots$	=	Activities of reactant species (unitless)
$r_1, r_2 \ldots$	=	Reaction order of individual reactant species (normally from experimental data. Default is stoichiometric coefficients; a, b, ...)
$a_C, a_D, \ldots$	=	Activities of product species
$p_1, p_2, \ldots$	=	Reaction order of individual product species (normally from experimental data. Default is stoichiometric coefficients; a, b, ...)
Vol	=	Liquid product volume (m^3)

The forward and reverse reaction rate constants are determined using the general Arrhenius Equation:

$$K = A \exp\left(-\frac{E}{RT}\right)$$

where: K= Reaction rate constant $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$

A = Arrhenius frequency factor for the forward or reverse reaction and is in $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$

E = Forward or reverse activation energy $\left(\frac{joule}{gmole}\right)$

R = Universal gas constant $\left(8.314 \frac{joule}{gmole\ K}\right)$

T = Temperature (K)

When specifying a standard rate expression, the user must define the Arrhenius frequency factor, reaction activation energies divided by the universal gas constant or, alternatively, the reaction rate directly. In addition, the user can specify the individual species order coefficients for the forward and reverse reactions if these differ from the stoichiometric coefficients (which are the default).

Keyword	**Description**
KF	Forward reaction rate constant $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$
KR	Reverse reaction rate constant $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$
AF	Forward reaction Arrhenius factor $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$
AR	Reverse reaction Arrhenius factor $\frac{\left(\frac{mole}{m^3 hr}\right)}{hr}$
BF	Forward reaction activation energy divided by the universal gas constant (K)
BR	Reverse reaction activation energy divided by the universal gas constant (K)
ER_i	Reaction order of reactant species i
EP_i	Reaction order of product species i

It should be emphasized that when the keywords KF and KR, the forward and reverse reaction rate constants are used for a reaction, this would preclude using the other keywords for that reaction. However, these keywords are not normally specified by the user, as these variables are usually calculated by the software from user defined Arrhenius factors and activation energies.

When defining the reaction order for a species, the order in which the species appears in the reaction equation must be defined (i.e., subscript *i*) with a sequential number, for either the reactant or product species. Hence, the first reactant is identified with the number 1, the second, 2 and so on. Similarly, the product species are identified with the integers 1, 2, 3 ... etc.

If any of the keywords are not defined, the software assumes a default value for that variable. These default values are assumed to be zero for the reaction rate constants, Arrhenius factors, and activation energies (divided by the universal gas constant). For the species reaction order coefficients, the reaction stoichiometric values are assumed.

To complete the standard rate expression definition, the reaction temperature and initial reactant molality are included in the process stream composition definition.

You can review a full example for the Standard Reaction Kinetics on page 201 using a reactor block.

Non-Standard (User Defined) Reaction Kinetics

The user can define his/her own reaction kinetics.

You can review a full example for Non-standard Reaction Kinetics on page 208.

T/P Span

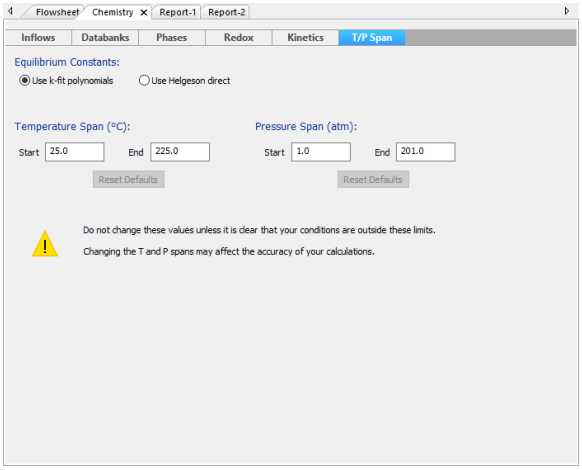
The T/P Span is for the temperature and pressure limits on the equation of state for the model. This only applies to the AQ thermodynamic framework. It is generally recommended that these values not be altered. These values are ignored for both the MSE and MSE-SRK thermodynamic frameworks.

History Lesson

Before 1990, OLI used a mixture of different thermodynamic frameworks to represent the standard state (equilibrium constants). Starting in 1990, OLI migrated to the Helgeson Equation of State[4]. This equation of state provided a consistent representation of the standard state for species in water up to 374 ºC and 5000 atmospheres.

The problem in the 1990's is that computers were slow and the direct method of calculating the equation of state was computationally intensive. Marshall Rafal (OLI – retired) observed that since the equation of state was only a function of temperature and pressure that the equilibrium constants could be pre-fit before calculation time. A matrix of temperatures (T span) and pressures (P span) were generated and then fit to a polynomial equation.

Evaluation of this polynomial is very fast, even in the 1990's, so it is used for the AQ thermodynamic framework. This was too inaccurate for the MSE thermodynamic framework and all values in the T/P are ignored.



This dialog is quite easy to understand. The user has the option to use the K-fit polynomials (Default for AQ thermodynamic framework use) or use the equation of state directly. If the K-fit polynomials are used, then the ranges (spans) can be altered.

The user would only normally alter these ranges if they knew beforehand that the simulation was outside the ranges.

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[4] Helgeson, Harold C., Kirkham, David H and Flowers, George, C. "Theoretical Prediction of the Thermodynamic Behavior of Aqueous Electrolytes at High Pressures and Temperatures – Parts I Though IV." American Journal of Science (1982)

Chapter V – Process Modeling Unit Operations/Blocks

Overview

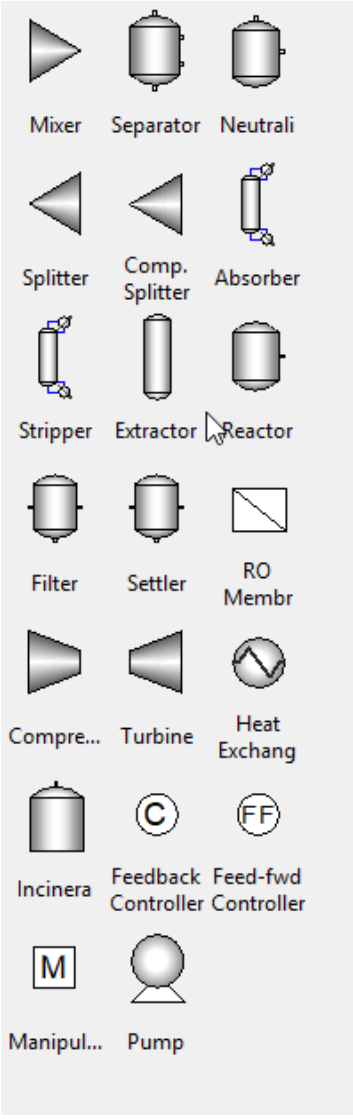
This section is a detailed guide to the use of unit operations, called Process Blocks, and for the use of the steady-state flowsheet simulation facilities provided via OLI Flowsheet: ESP. This chapter contains a brief overview and detailed specifications of the OLI Flowsheet: ESP Process Blocks. Limitations and guidelines for individual units are included.

By selecting pertinent unit operations, a complete process can be modeled by combining individual process blocks into a process flowsheet to describe the process.

Unit Operations/Blocks and Controllers

The current blocks available in OLI Flowsheet: ESP are:

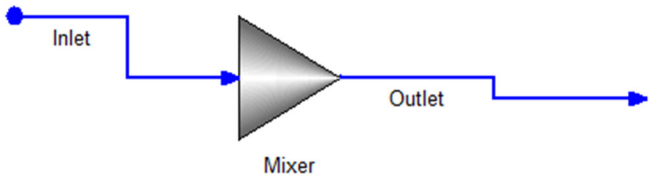
Mixer
Separator
Neutralizer
Splitter
Component Splitter
Absorber
Stripper
Extractor
Reactor
Filter
Settler
RO Membranes
Compressor
Turbine
Heat Exchanger
Incinerator
Feedback controller
Feedforward controller
Manipulator
Pump



Unit Operations/Blocks and Controllers Summary Descriptions

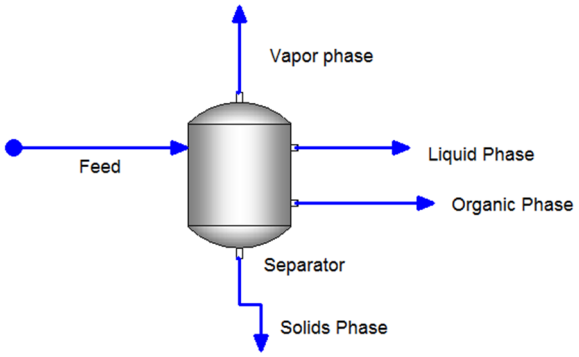
Mixer

A conventional Process Block which allows mixing of several (2-7) inlet streams adiabatically. The resulting phase separation and speciation within each phase is also evaluated.



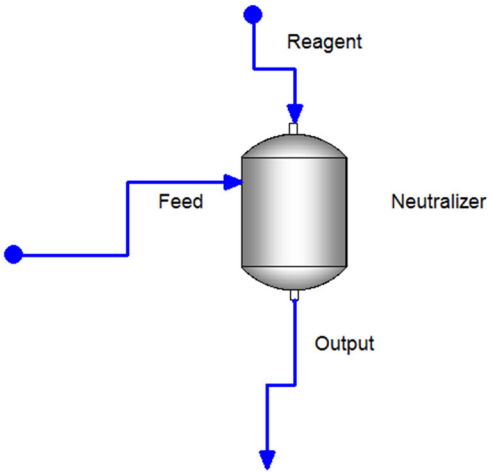
Separator

A conventional Process Block which allows up to 7 inlets to be separated into distinct physical phases. Suspended solids, entrained liquid, dissolved vapor and dissolved liquid can be specified. An equilibrium will be performed adiabatically.



Neutralizer

An Environmental Process Block which allows a specified stream to be neutralized, either by adiabatically mixing the inlet streams, or by varying one of the inlet streams to meet a specified pH point.

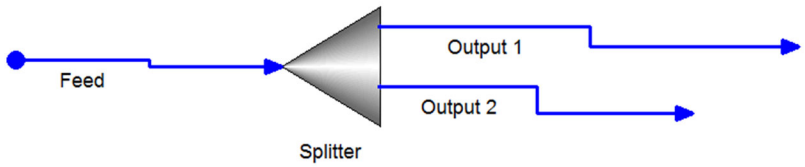


Splitter

A Conventional Process Block which allows a stream to be split into required outlet flow fractions or specified flowrate for one of the streams. There are two types of splits currently supported.

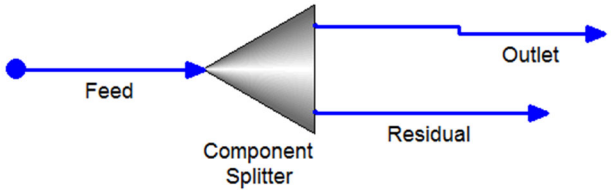
Flow Split – This split allows a single inlet stream to be divided into (2-7) outlet streams, all with the same temperature, pressure and relative species content.

Component splitter – Which is described in the next section.



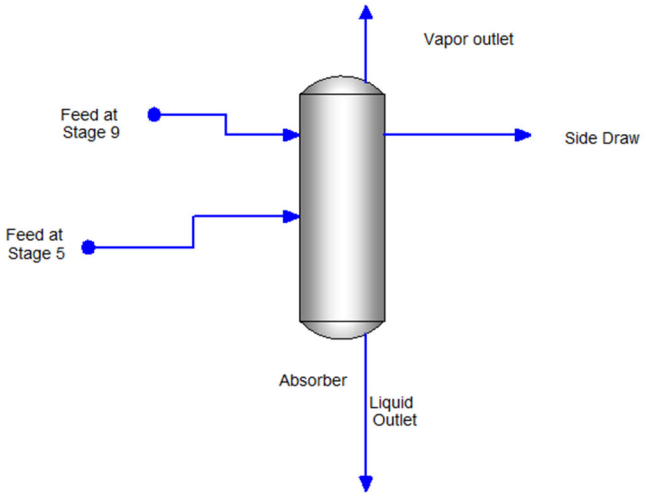
Component Splitter

This type of split allows between 1-7 inlet stream to be divided into 2 outlet streams, one of which contains the required species component fractions.



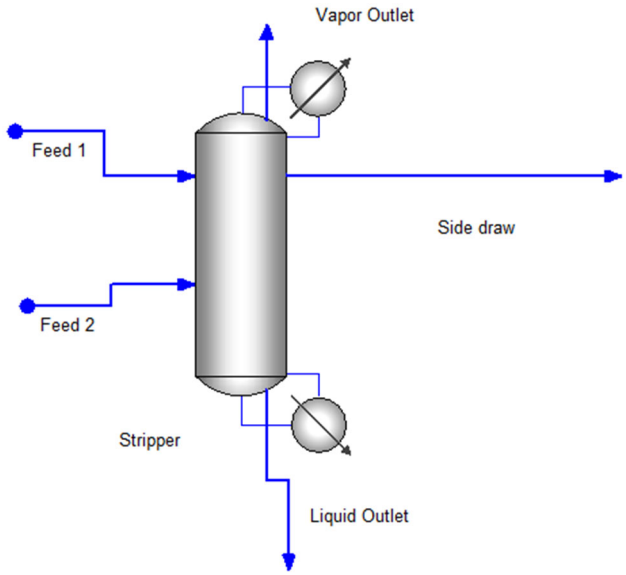
Absorber

A Multi-stage or Environmental Process Block which allows species in a vapor feed to be absorbed by a countercurrent liquid stream. Conventional column capabilities are included, such as: multiple feeds, condenser, reboiler, side streams, pump-arounds, specification/control and stage efficiencies.



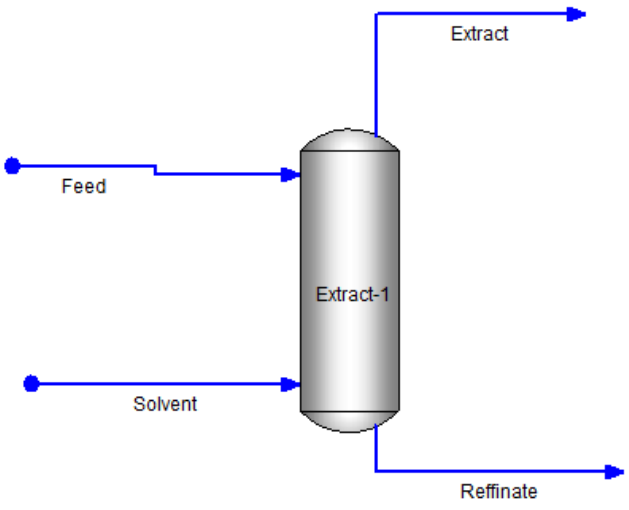
Stripper/Distillation Column

A Multi-Stage Conventional Process Block, allowing species in a liquid feed to be removed by a countercurrent vapor stream. Conventional column capabilities are included, such as: multiple feeds, condenser, reboiler, side streams, pump-arounds, specification/control, and tray efficiencies.



Extractor Unit

This is a multi-stage conventional process unit which allows countercurrent liquid-liquid extraction to be simulated. The unit can hold a maximum of 50 stages, 10 feed and 10 exit streams. Conventional extractor unit capabilities are included, such as: multiple feeds, specification/control, and tray efficiencies.

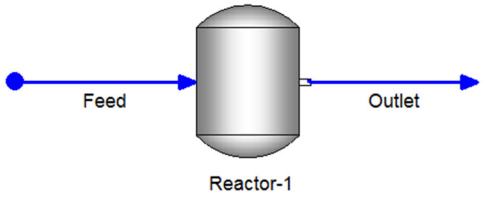


Reactor

An Process Block which determines the phase separation and intraphase speciation for a Chemistry Model including both equilibrium and user-defined rate-limited reactions (i.e., kinetics, redox reactions). Between 1-7 inlet streams are mixed and considered as a single feed. There are two types of reactors currently supported. They are:

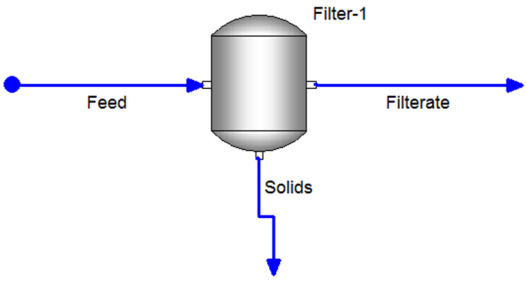
Aqueous – This reactor is used to simulate electrolyte chemical reaction systems.

Non-aqueous – This reactor is used to simulate non-electrolyte chemical reaction systems.



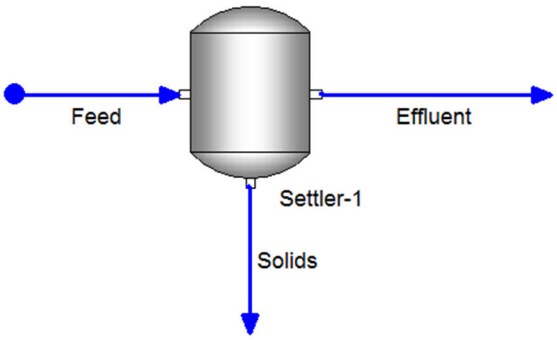
Filter

A crystallization process unit which models the separation of the liquid portion of the feed stream from the solid portion of the feed stream. The liquid and solid are divided between the filtrate and solids outlet streams based upon specified fractions or flows.



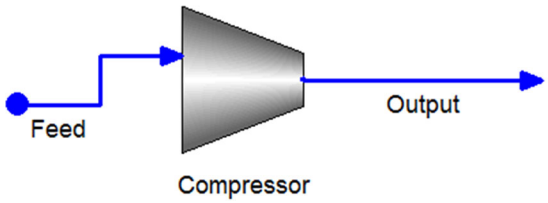
Settler

A crystallization process unit which models the separation of the liquid portion of the feed stream from the solid portion of the feed stream. The liquid and solid are divided between the filtrate and solids outlet streams based upon specified fractions or flows. The solid may be split as a total solid or, differentially, split by individual solid species.



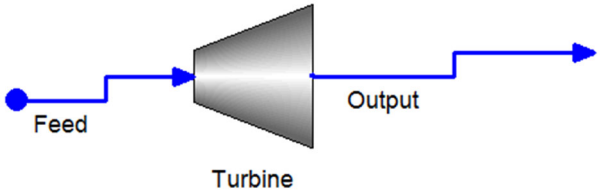
Compressor

A Conventional Process Block for carrying out an isentropic or polytropic pressure change on a product stream comprised of one or more feed streams.



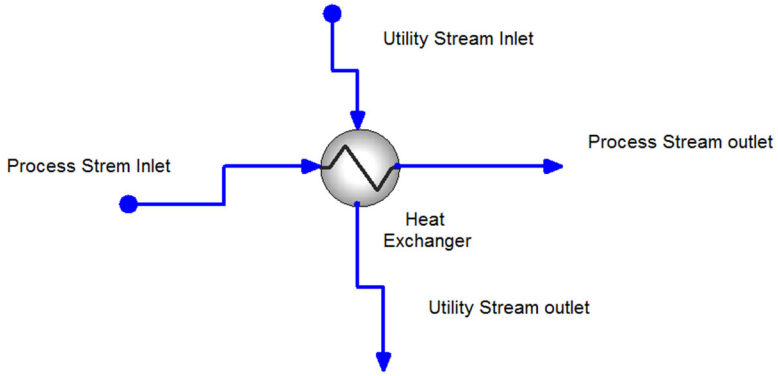
Turbine

A conventional Process Block for carrying out an isentropic or polytropic pressure change on a product stream comprised of one or more feed streams.



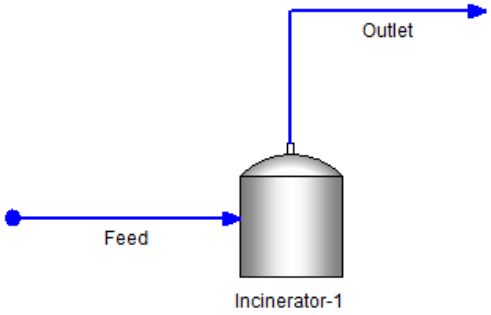
Heat Exchanger

A conventional Process Block which allows energy to be transferred between a process and a utility stream, or allows energy to be added to, or removed from, a single stream. A utility stream may also be a stream from another process block.



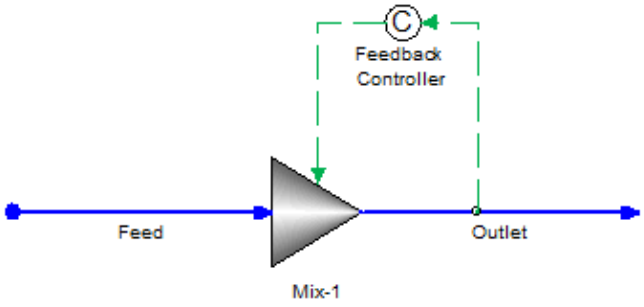
Incinerator

An environmental process block which allows non-electrolyte species to be incinerated either adiabatically or isothermally. A maximum of 7 inlet streams are allowed to the block.



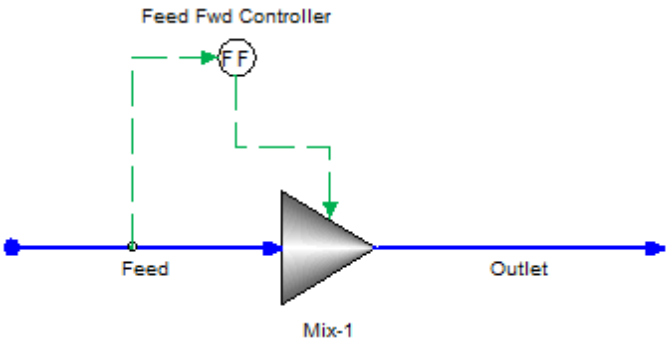
Feedback Controller

An ESP Control Block which sets a stream specification or a block parameter by transferring a block parameter from a downstream unit. The transferred value can be adjusted by addition, subtraction, multiplication, or division.



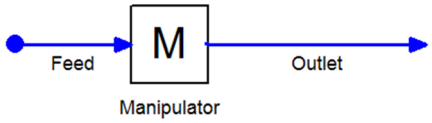
Feed-forward Controller

An ESP Control Block which sets a stream specification or a block parameter by transferring a block parameter from an upstream unit. The transferred value can be adjusted by addition, subtraction, multiplication, or division.



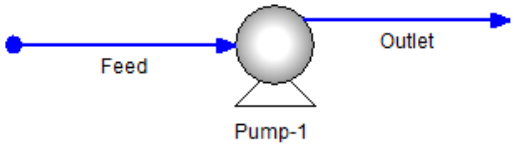
Manipulator

An ESP Control Block which allows a multiplicative factor to be applied to the total flow of a stream, or to the components of a stream.



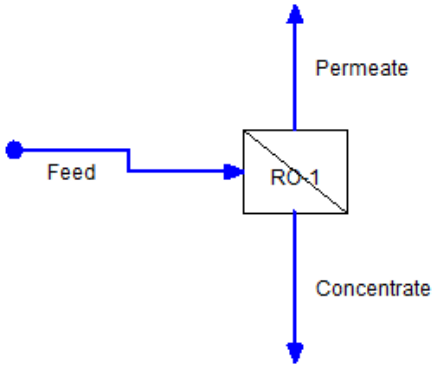
Pump

A Conventional Process Block for increasing fluid pressure to a unit.



RO Membranes (Reverse Osmosis)

A process Block which predicts the distribution (separation) of salts from a single feed and, optional permeate feed, when a membrane is applied with the result that both a permeate (dilute) and concentrated product streams are created.



Virtual Stream Portal

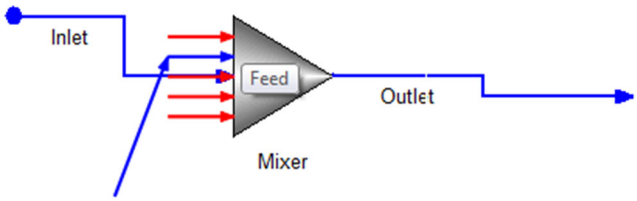
This block allows a stream to be copied exactly to another place in the process. For example, the process may have a stream that needs some side calculations to see how close it is to scaling. We don't want to disturb the main process, so we copy the stream out and perform our scaling calculations separately.

Details of Unit Operations/Blocks

This section describes in detail specific application for the blocks available in OLI Flowsheet: ESP. The procedure for defining each block is described.

1. Mixer Unit

This is a conventional process block which allows the mixing of up to 10 feed streams by one of several types of equilibrium calculations. The resulting phase separation and speciation within each phase is computed.

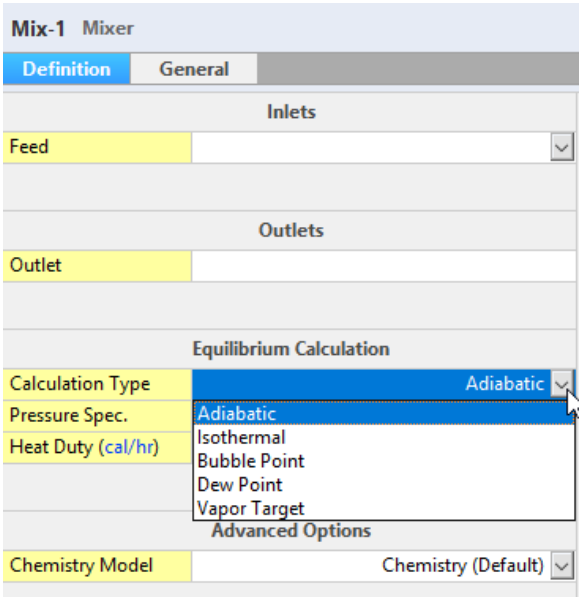


Data Requirement

The unit's stream inflows and exit flow must all be given distinct names. This enables streams and units to be recognized and linked together when building a complex process. A minimum of one feed streams and the respective temperature, pressure, flow and composition must be defined by the user or as a product stream from another Process Block.

Unit Parameters

Calculation Type	Specification Choices
Adiabatic	P, and heat duty
Isothermal	P, T
Bubble Point	P or T
Dew Point	P or T
Vapor Target	P or T, Vapor Amount or V/F



All specifications of pressure can be made by specifying either a pressure loss across the Mix unit or by specifying the exit stream pressure.

If the Parameter facility is not used, a zero pressure drop across the unit is assumed, and the streams will be mixed adiabatically.

Unit Configuration

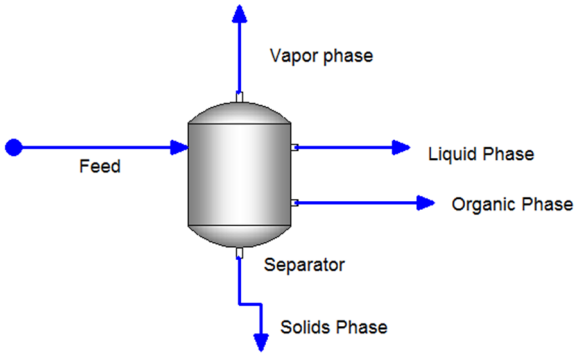
This facility allows the user to add or delete extra feed streams to the unit and is accessed via the Properties pane. An additional nine inlet streams may be defined if required.

Guidelines

When additional streams are to be added to the unit, the user must first ensure the minimum data requirements for the unit are specified prior to adding the streams.

2. Separator Unit

This is a process unit which allows up to 10 inlet streams to be separated into distinct physical phases. Outlet conditions including suspended solids, entrained liquid, dissolved vapor, and dissolved liquid concentrations can be calculated.



Data Requirements

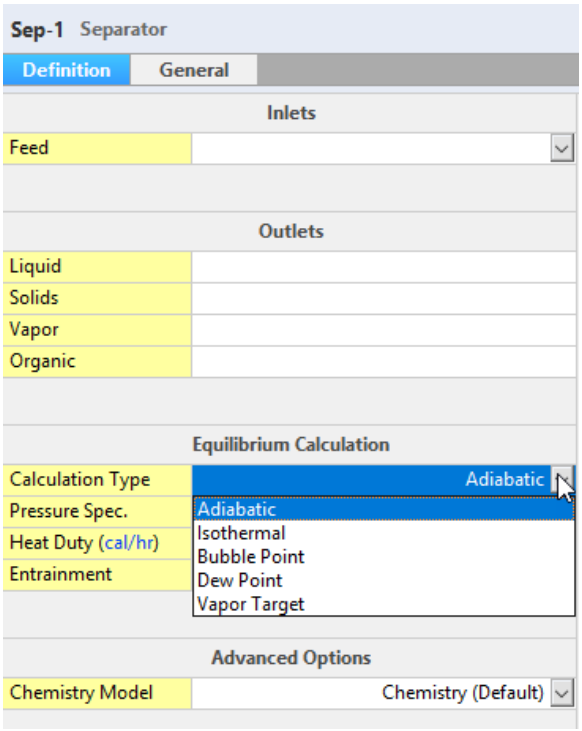
A minimum of one feed and an aqueous exit stream must be defined. The feed stream must be defined by the user or be a product stream from another Process Block. Both streams must be named, and the inlet temperature, pressure, flow, and composition must be specified.

Units Parameters

Different Equilibrium Calculations are available:

- Adiabatic
- Isothermal
- Bubble point
- Dew Point
- Vapor target

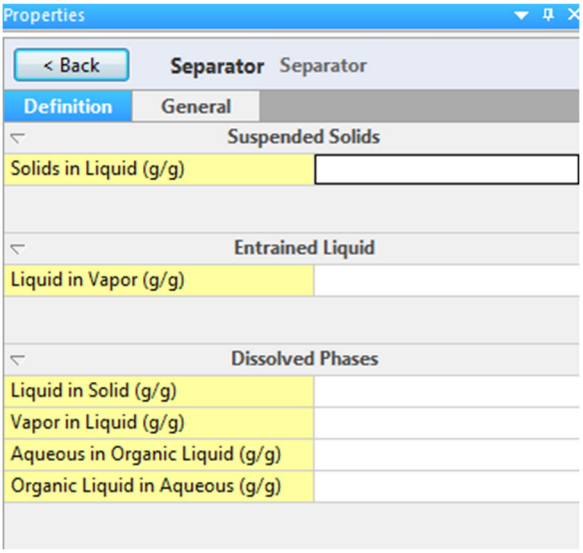
Concentration limits can be defined for phase distribution among the outlet streams and is achieved via the Entrainment option under Equilibrium Calculation section.



These phase distributions include:

Distribution	Stream
Suspended solids	Liquid* outlet stream
Entrained liquid concentration	Vapor outlet stream
Dissolved liquid	Solid outlet stream
Dissolved vapor	Liquid* outlet stream
Dissolved aqueous phase	Organic outlet stream
Dissolved organic phase	Aqueous outlet stream

** The liquid outlet is the combined aqueous and organic outlet streams.*



When the specified limits are exceeded for a particular phase distribution, the surplus quantity remains in its respective phase outlet stream.

Conversely, when one specified phase distribution requires all of the phase, the specification is satisfied, and that phase is eliminated. For example, if the amount specified for the dissolved vapor in the liquid is greater than the amount of vapor present, then all the vapor is put in the liquid outlet, and the vapor outlet is set to zero.

If two specified phase distributions cannot be met, the error condition is raised.

Unit Configuration

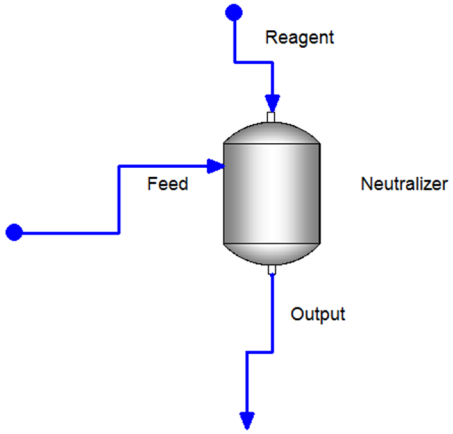
This facility allows the user to add or delete extra inlet streams to the unit and is accessed via the Properties Pane. An additional nine feeds may be defined if required.

Guidelines

When additional streams are to be added to the unit the user must first ensure the minimum data requirements for the unit are specified prior to adding new inlet streams.

3. Neutralizer Unit

This is an environmental process block which allows up to 10 feed streams to be neutralized by the addition of a suitable reagent. The neutralization can be modeled adiabatically by mixing the inlet streams, by varying the neutralizing reagent flow to meet a fixed pH set point.



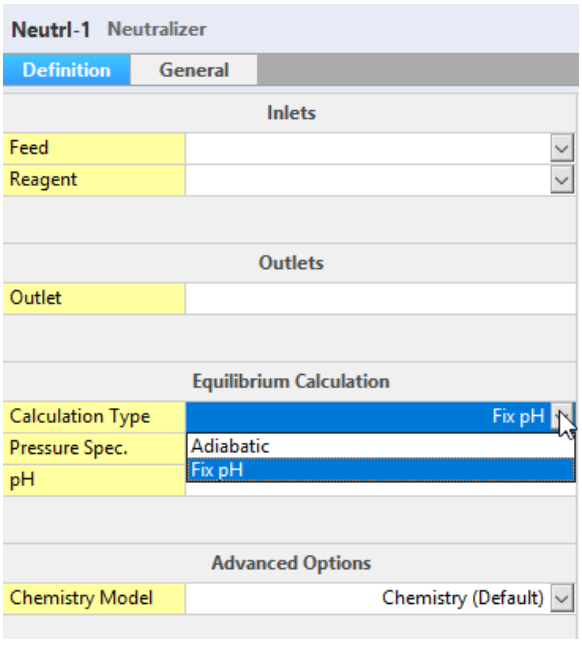
Data Requirements

A minimum of one feed stream and one neutralizing reagent stream must be named. In addition, temperature, pressure, total flow rate and composition data of the feed stream(s) must be specified by the user or be a product stream from another process block. The user must supply the same information for the dosing stream. The dosing stream must be specified as the top entry stream to the process unit. The process block outlet stream must be named. Additionally, the process operating conditions must also be defined by the user.

Unit Parameters

The process mode of operation is defined by using the Properties Pane and selecting the Parameters facility. Two calculation options are currently available to allow the process to be modeled:

- Adiabatic mixing of the feed streams
- Setting pH of the outlet stream



If adiabatic mixing is chosen, the simulator determines the outlet stream properties, based upon the user specified inflows. However, if a fixed exit pH is required for the effluent, the simulator varies the reagent stream flow rate accordingly, until the effluent pH requirement is obtained.

Specifications of pressure can also be made by specifying either a pressure loss across the Mix unit or by specifying the exit stream pressure.

Unit Configuration

This facility is accessed using the Properties Pane. An additional nine feeds may be defined if required.

Guidelines

When additional streams are to be added, the user must first ensure the minimum data requirements for the unit are specified prior to adding new feed streams

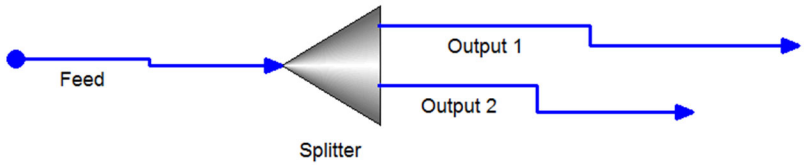
The reagent stream must be a process entry stream. That is, the reagent stream cannot be a product from another process block or be a recycle stream.
A guess for the flow rate of the reagent stream is required.

Systems with difficult chemistry (i.e., multiple phases, multiple solids) may have problems in converging this process block. If the block does not converge, a Crystallizer can be alternately simulated by using a Mix, Manipulate, and Controller block.

Splitter Unit

4.1. Flow Split Unit

This is a conventional process unit which allows a single inlet to be divided into a maximum of 7 outlet streams, all with the same temperature, pressure and relative species content.

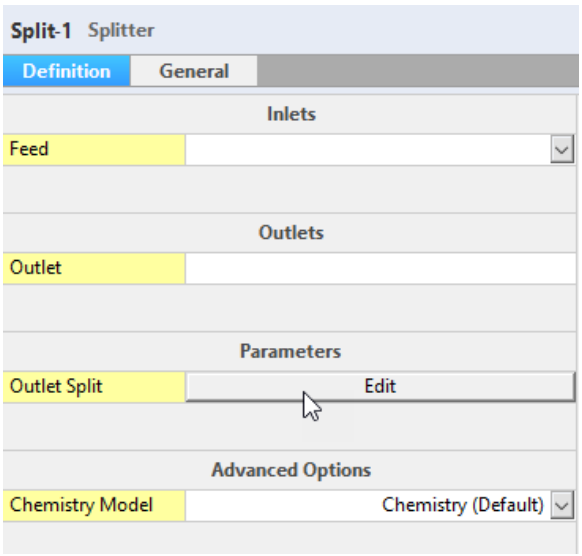


Data Requirement

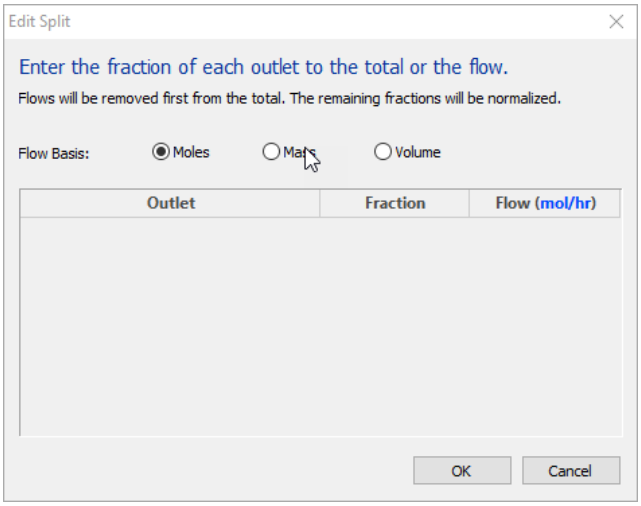
The unit's stream inflow and exit flows must all be given distinct names, so that they can be linked to other process units, if required.

One feed stream, and a minimum of two exit streams must be defined by the user. The inlet stream temperature, pressure, flow and composition data must be defined or be a product stream from another Process Block. Additionally, the split outlet stream fractions or flows must be defined.

Unit Parameters



The stream outlet fractions are defined using the Action Key and then by selecting the Parameters facility. The outlet fractions may be defined on one of a variety of bases, (e.g., mole fractions, flow, etc.) which are then automatically normalized by the software such that the sum of the outlet fractions is equal to 1.



Unit Configuration

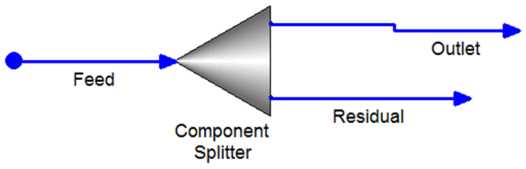
This facility allows the user to add or delete extra outlet streams from the unit and is accessed via Properties Pane. An additional ten exit streams may be defined if required.

Guidelines

When additional streams are to be added, the user must first ensure the minimum data requirements for the unit are specified prior to adding streams.

4.2. Component Split Unit

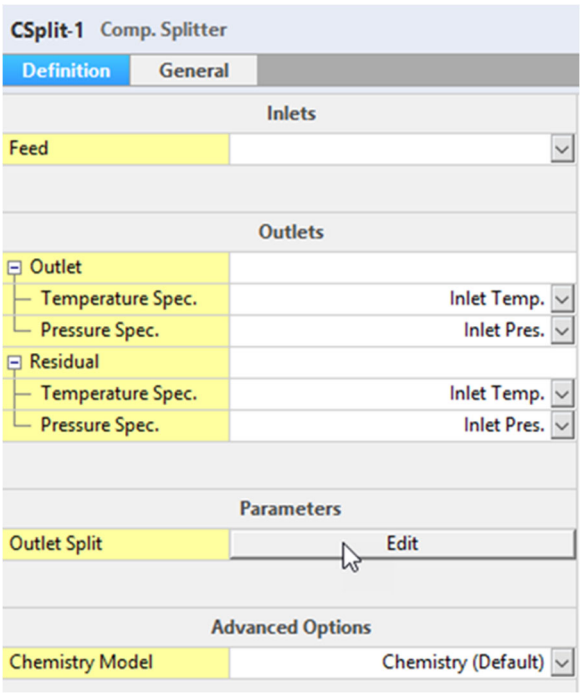
This is a conventional process unit which allows up to a maximum of 10 inlet streams to be divided into two exit streams, one of which contains user defined species component fractions.



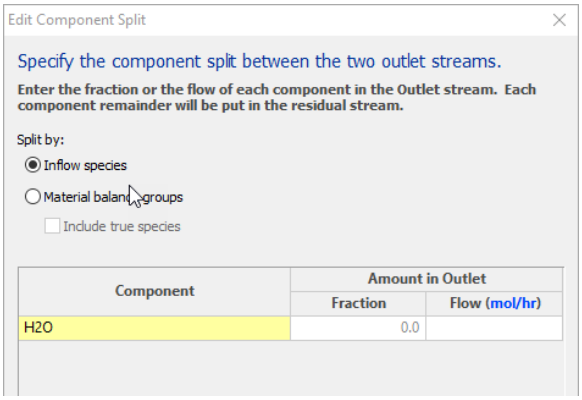
4.2.1. Data Requirement

A minimum of one feed stream and two exit streams must be defined. The inlet stream temperature, pressure, flow and composition data must be defined by the user or as a product stream from another Process Block. The top exit stream from the unit is the stream for which the required species component fractions are specified.

4.2.2. Unit Parameters



The stream outlet fractions are defined using the Action Key and then by selecting the Parameters facility. The species fractions may be specified on either a mole fraction or flow basis, (e.g., mole fractions, flow, etc.) which are then automatically normalized such that the sum of the exit species mole fractions is equal to 1.



4.2.3. Unit Configuration

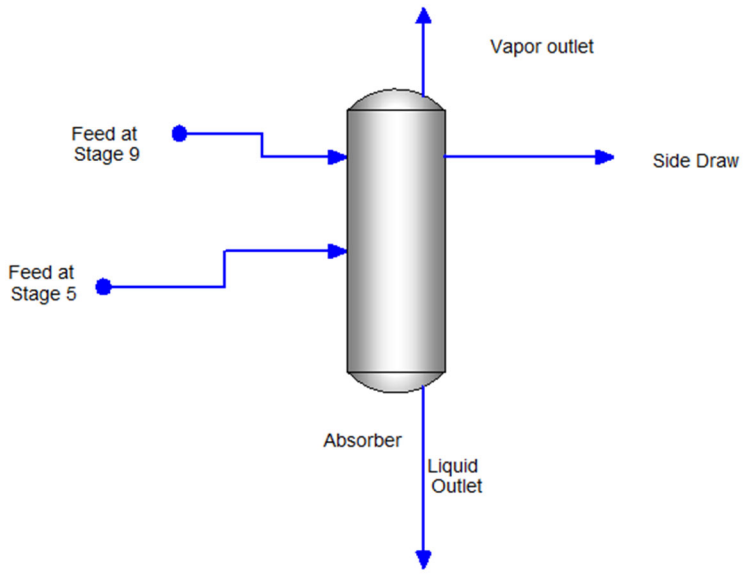
This facility allows the user to add or delete extra inlet streams to the unit and is accessed via the Properties Pane. An additional six feeds may be defined if required.

4.4.4. Guidelines

When additional streams are to be added, the user must first ensure the minimum data requirements for the unit are specified prior to adding new streams.

Absorber Unit

This is a multi-stage conventional or environmental process unit which allows species in a vapor feed to be absorbed by a countercurrent liquid stream. The unit can hold up to a maximum of 50 stages and up to a maximum of 10 feed and 10 product streams.



Data Requirement

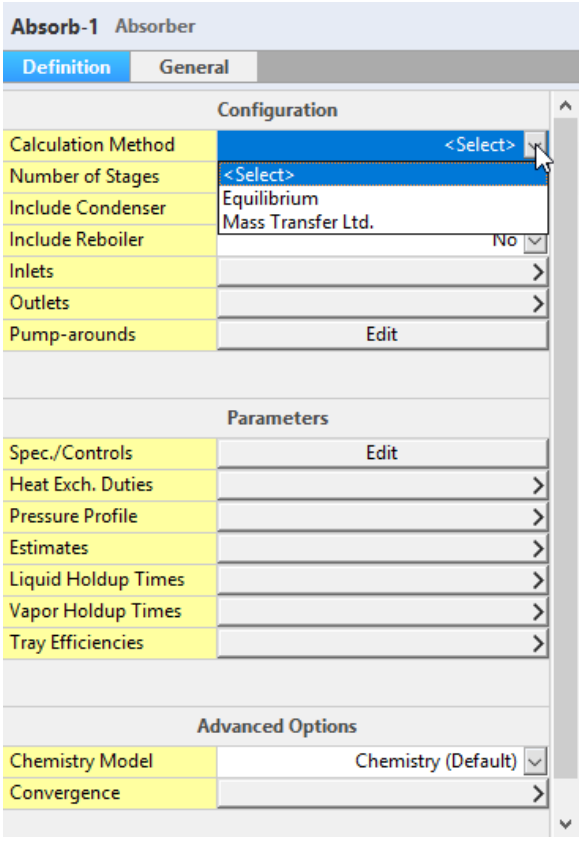
A minimum of one liquid stream entering the top of the column and one vapor stream entering the bottom of the unit must be specified. The respective feed stream temperature, pressure, flow, and composition must be defined by the user or be a product stream from another Process Block.

When defining the feed stream, the temperature and pressures of each stream should be such that the species components reside in the correct phase for the respective stream.

The column exit vapor and liquid streams must be named, in addition to various column parameters.

Column Configuration

Column parameters can be defined, via the Properties Pane. Seven options are available:



- **Calculation Method:**
  Equilibrium
  Mass transfer Ltd.

  Number of Stages: The default number is 10 stages.

  Include condenser/reboiler: This option allows the user to delete, or insert, these respective units from/to the column. Initially, the process block does not include the two heat exchanger units.

  Inlets: This function is optional and allows the user to specify up to 8 additional feed streams to the column.

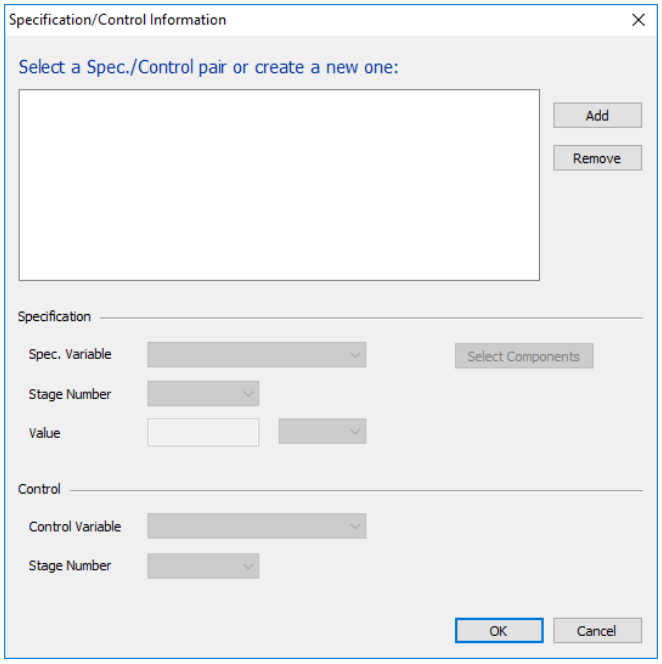
- **Outlets**: This function is optional and allows the user to specify up to 8 additional product streams from the column.

- **Pumparounds**: This function is optional and allows the user to specify side stream pumparounds if required. Pumparounds must be from a lower to a higher stage of the column and the flow rate must be defined.

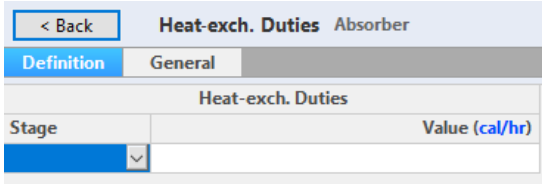
Column Parameters

The column operating parameters are accessed using Properties Pane. Eight options are available:

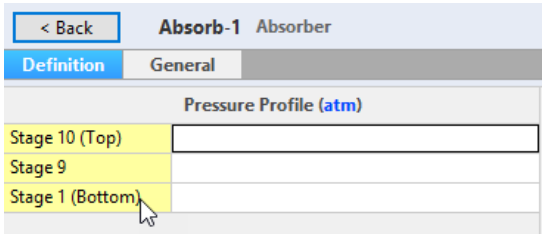
Spec/Controls: This function is optional and allows the user to manipulate parameters (e.g., heat exchange duty) to meet specifications in the column operation. For example, vapor and/or liquid composition specifications, stage operating temperature and vapor and/or liquid stream component flow rate specifications can all be achieved.



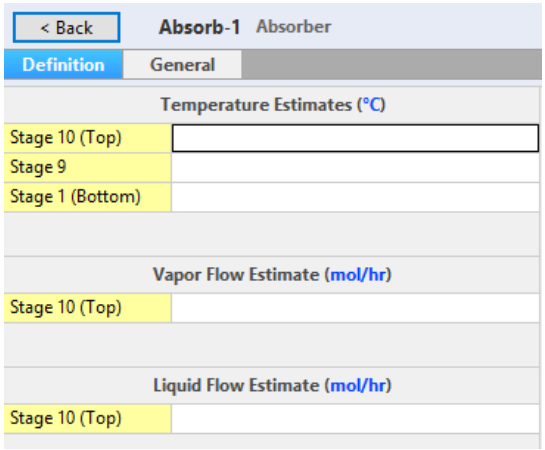
Heat Exchanger Duties: This option allows column heat exchanger duties to be specified. For columns using a condenser and/or reboiler the user must define duties for the respective units.



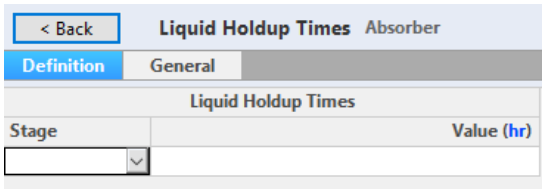
Pressure Profile: This option allows an accurate pressure profile to be specified. This is done by specifying top and bottom stage pressures, taking the reboiler and condenser into account. If only one stage pressure is given, a zero-pressure drop is assumed through the column.



Column Estimates: This option allows stage operating temperatures, vapor distillate and liquid reflux flow estimates to be specified. The estimates for top and bottom stage temperature, as well as vapor distillate and liquid reflux flow rates must all be specified by the user.



Liquid/Vapor Hold-Up Volumes: This function is required for columns whose Chemistry Model contains rate-limited reactions. This facility allows the user to specify both liquid and vapor hold-up volumes for specific column stages.



Tray Efficiencies: This function is enabled when the calculation method chosen is Equilibrium. This function is optional and allows the user to specify Murphree efficiencies for the column stages. If no data is entered the stage efficiency is assumed to be 1.0.

< Back

Definition | General

Specify murphree efficiency for each stage

Enter efficiency as a fraction between 0 and 1.

Stage	Value
10 (Top)	1.0
9	1.0
8	1.0
7	1.0
6	1.0
5	1.0
4	1.0
3	1.0
2	1.0
1 (Bottom)	1.0

Mass Transfer: This function is enabled when the calculation method chosen is the Mass transfer Ltd. This option allows the user to specify vapor-liquid mass and heat transfer coefficients on each stage of the column. The coefficients are overall coefficients and apply to all components. The interfacial transfer area must also be specified. If the same coefficients are used throughout the column, the coefficient may be varied to meet a composition specification by means of the spec/control parameters.

< Back **Absorb-1** Absorber

Definition | General

Mass Transfer Column Type

Column Type	Packed Column

Mass Transfer Parameters

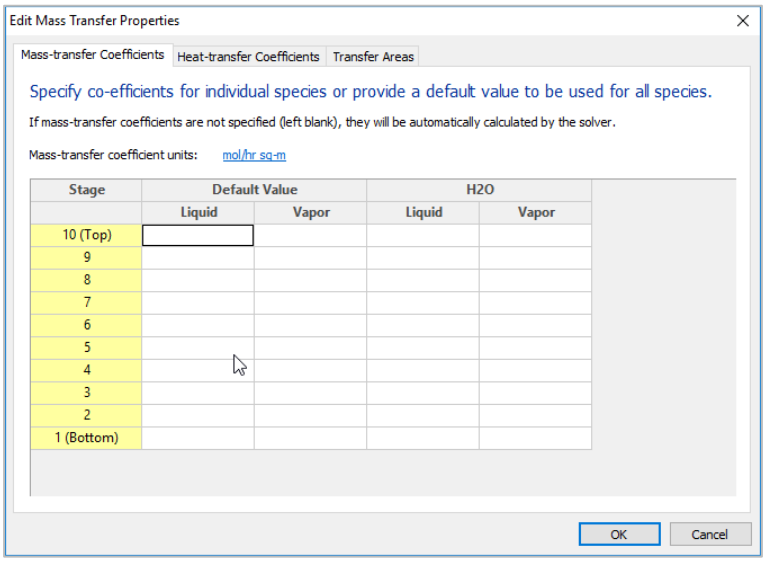
Stage Height (cm)	
Column Diameter (cm)	
Packing Type	Pall Ring
Packing Material	Metal
Packing Size (mm)	50
Packing Characteristics (Billet & Schultes)	
N (1/m3)	6242.0
a (m2/m3)	112.6
e (m3/m3)	0.951
Cs	2.725
Cfl	1.58
C2	0.784
Cp	0.763
Cl	1.192
Cv	0.41

Advanced

Advanced Parameters	Edit
No. of Liq. Interface Film Segments	1

In the mass transfer parameters panel, the user also has the option for advanced parameters:

Enter mass transfer coefficients for each stage.
Enter heat transfer coefficient for each stage.
Specification of transfer areas



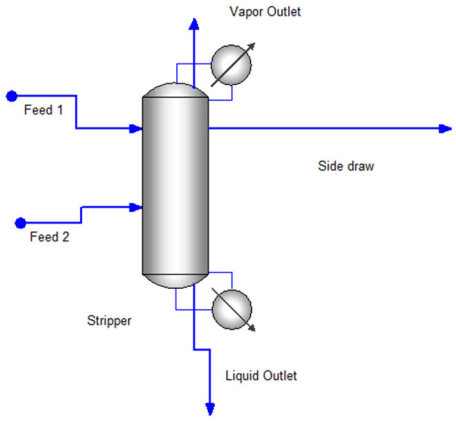
Guidelines

When defining column parameters, a zero-liquid reflux (i.e., distillate) rate should be defined. This is because the distillate flow exiting the unit must only exist in the vapor phase.

Distillation/Stripper Unit

This is a multi-stage unit allowing species in a liquid to be separated either by distillation, or by the action of a countercurrent vapor stream (i.e., stripper). The unit can hold a maximum of 50 stages, 10 feed streams, and 10 exit streams.

When this block is selected the user can choose either an electrolyte column or a non-electrolyte column (if a non-electrolyte model was created). In the case of an electrolyte column, an aqueous phase must be present in every liquid stream. The liquid feed and/or liquid product can contain both an aqueous and non-aqueous liquid phase, or just an aqueous phase alone. In the case of a non-electrolyte column, only the non-electrolyte liquid phase exists (electrolyte chemistry is not considered).



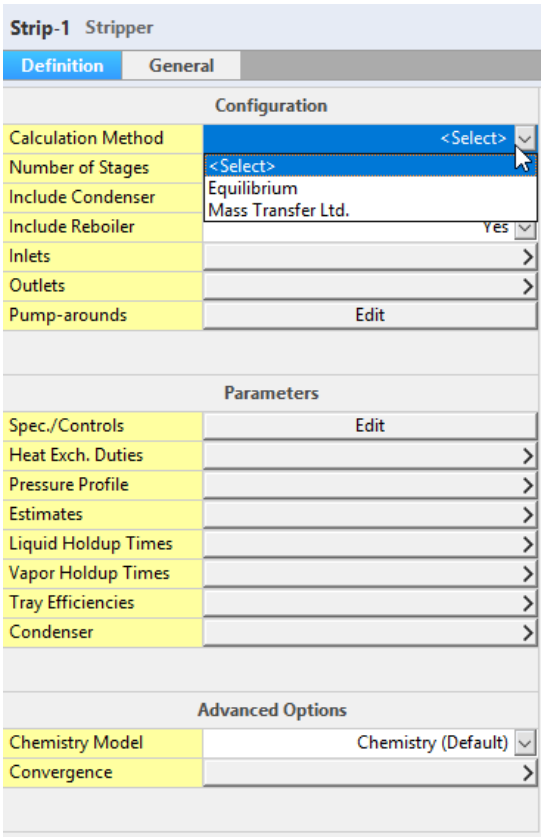
Data Requirement

A minimum of one feed stream and two exit streams (i.e., distillate and bottoms) must be named when using the unit for distillation. An additional feed must be added when using the unit as a stripper. The feed stream temperature, pressure, flow, and composition data must be specified by the user or be a product stream from another Process Block. The number of stages will default to 10 and appear that way on the

initial screen. The user may override this value. If there is a condenser or reboiler, these will count as stages. Additionally, various column operating parameter information must be supplied by the user.

Column Configuration

Additional column parameters can be defined, via configuration pane. Seven options are available:



- **Calculation Method:**
  Equilibrium
  Mass transfer Ltd.

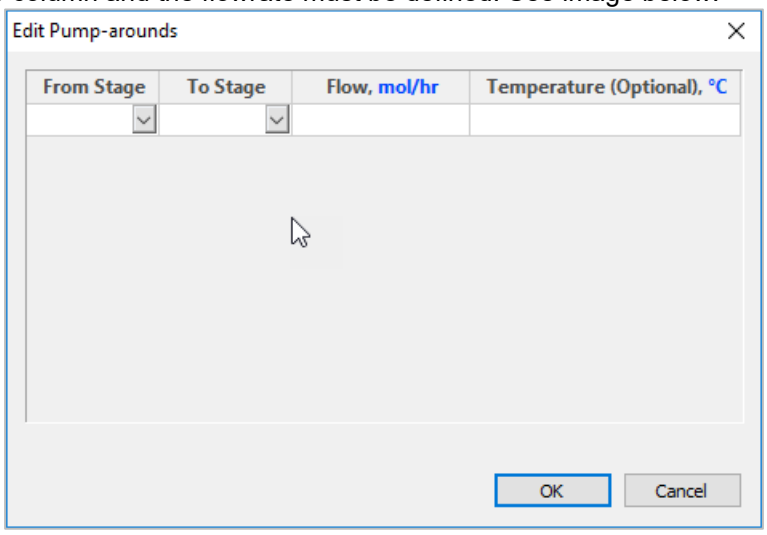
  Number of Stages: The default number is 10 stages.

  Include condenser/reboiler: This option allows the user to delete, or insert, these respective units from/to the column. Initially, the process block includes the two units on the display.

  Inlets: This function is optional and allows the user to specify up to 8 additional feed streams to the column.

- **Outlets**: This function is optional and allows the user to specify up to 8 additional product streams from the column.

- **Pumparounds:** This function is optional and allows the user to specify side stream pumparounds if required. Pumparounds must be from a lower to a higher stage of the column and the flowrate must be defined. See image below:

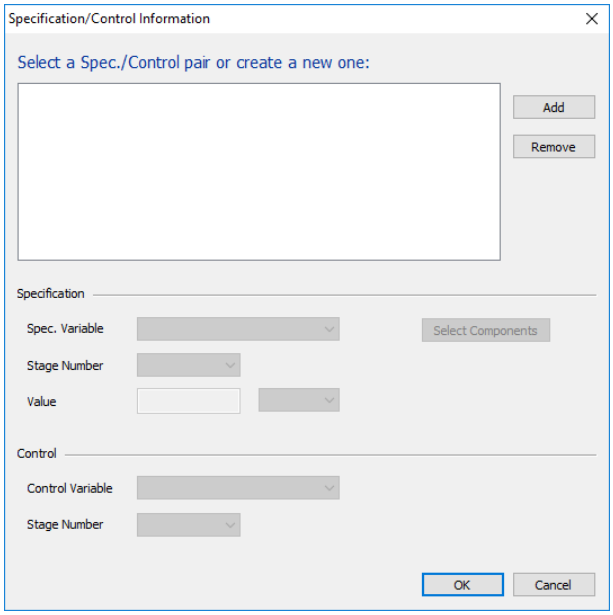


Column Parameters

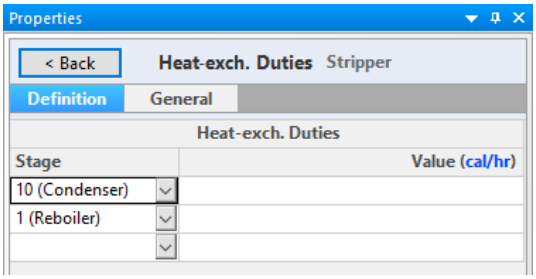
The column operating parameters are accessed using the Action Key and then by selecting the parameters facility. Eight options are available:

Spec/Controls: This function is optional and allows the user to manipulate parameters (e.g., heat exchanger duty) to meet specifications in the column operation. For example, vapor and/or liquid

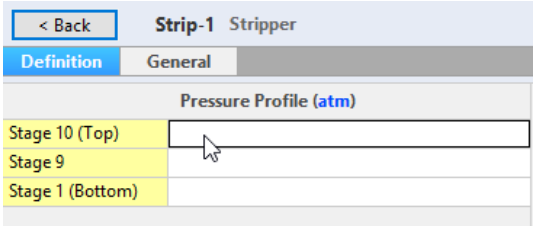
composition specifications, stage operating temperature, and vapor and/or liquid stream flowrate specifications can all be achieved.



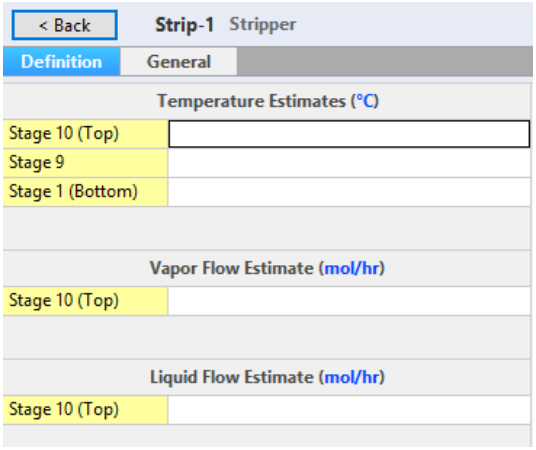
Heat Exchanger Duties: This option allows column and pumparound heat exchanger duties to be specified. For columns using a condenser and/or reboiler, the user must define duties for the respective units. Negative heat duties imply heat removal.



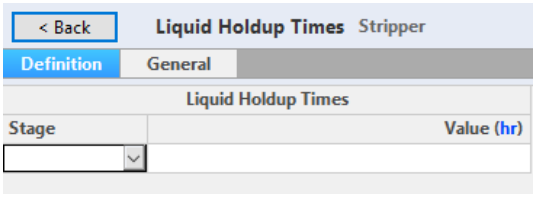
Pressure Profile: This option allows an accurate pressure profile to be specified. This is done by specifying top and bottom stage pressures, taking the reboiler and condenser into account. If only one stage pressure is given, a zero pressure drop through the column is assumed. If no values are given, the entire column is assumed to operate at atmospheric pressure.



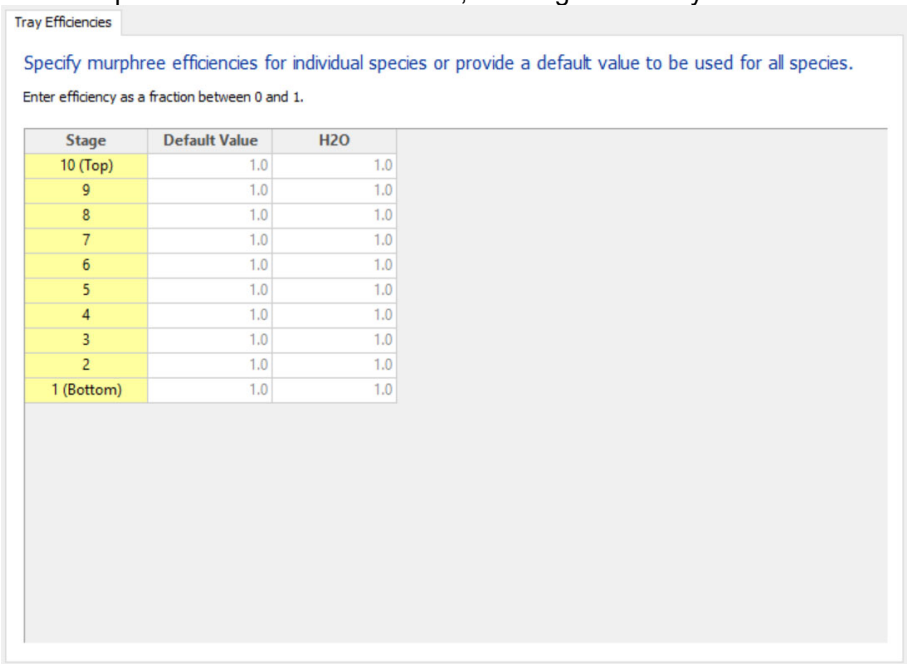
Estimates: This option allows stage operating temperatures, vapor distillate and liquid reflux flow estimates to be specified. The estimates for top and bottom stage temperature, as well as the vapor distillate rate and liquid reflux flowrates, must all be specified by the user.



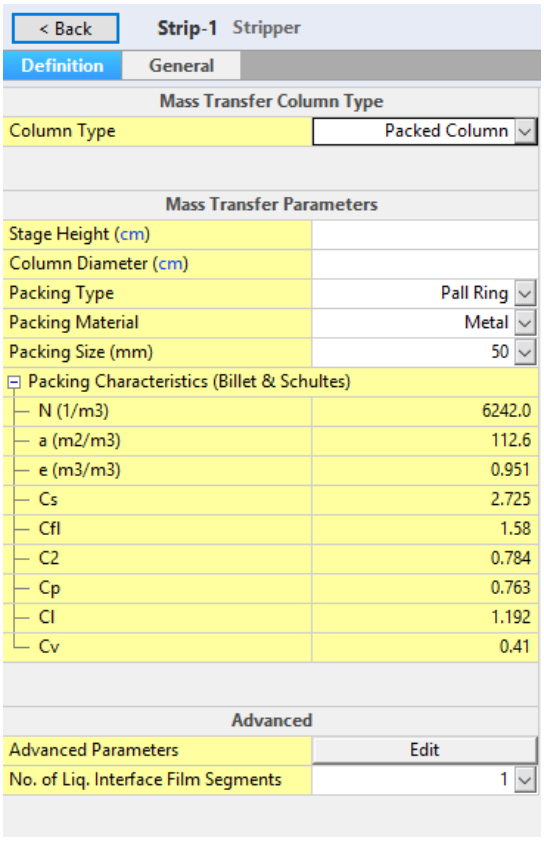
Liquid/Vapor Hold-Up Volumes: This function is required for columns whose chemistry contains rate-limited reactions. This facility allows the user to specify both liquid and vapor hold-up volumes for specific column stages.



Tray Efficiencies: This function is enabled when the calculation method chosen is Equilibrium. This function is optional and allows the user to specify Murphree efficiencies for the column stages and individual components. If no data is entered, the stage efficiency is assumed to be 1.0.

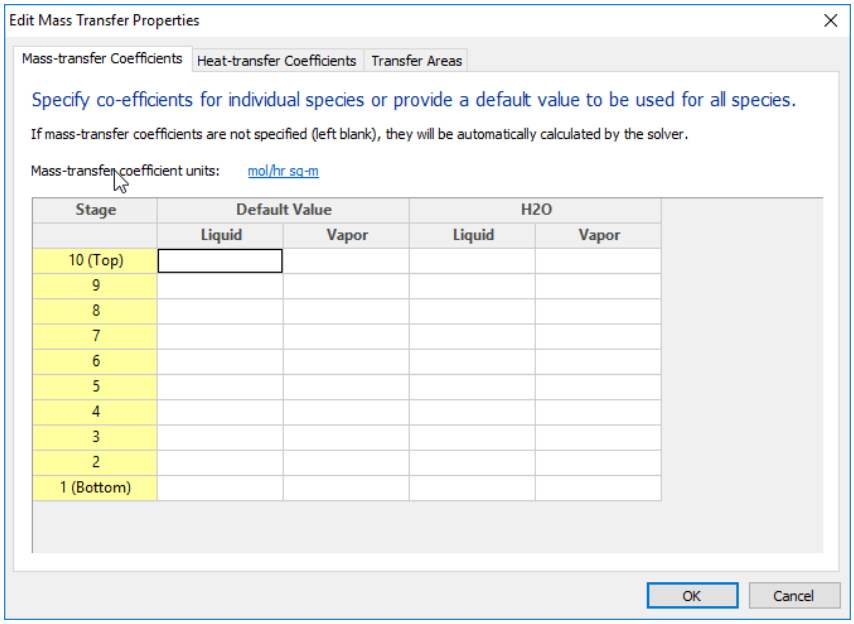


- **Mass Transfer:** This function is enabled when the calculation method chosen is Mass Transfer Ltd. This option allows the user to specify vapor-liquid mass and heat transfer coefficients on each stage of the column. The coefficients are overall coefficients and apply to all components. The interfacial transfer area must also be specified. If the same coefficients are used throughout the column, the coefficient may be varied to meet a composition specification by means of the spec/control parameters.



In the mass transfer parameters panel, the user also has the option for advanced parameters:

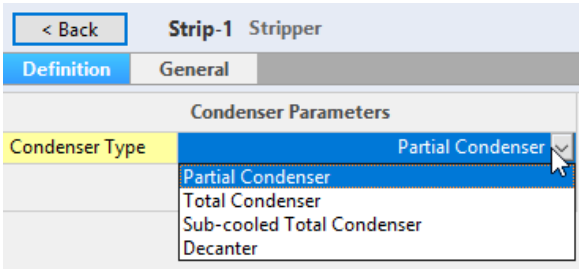
Enter mass transfer coefficients for each stage.
Enter heat transfer coefficient for each stage.
Specification of transfer areas



- **Condenser:** This function is optional and allows the user to specify the type of condenser. If no data is entered, the condenser is assumed to be partial condenser.

Four types of condensers can be selected:

- Partial condenser
- Total condenser
- Sub-cooled Total condenser
- Decanter



Guidelines

For columns with condenser and/or reboiler units the heat duty estimates defined by the user must be such that a vapor flow exists on the bottom stage and a liquid phase flow exists on the top stage of the column, respectively.
The column can only operate if two (or optionally three) phases exist on every stage of the column.

For columns without a condenser and/or reboiler unit, a feed stream must be specified entering at the respective position of the omitted unit. The phase of this stream must be correctly defined. A liquid phase feed stream is required as an alternative to a column condenser, and a vapor phase stream in place of a reboiler unit (i.e., the column must have two phases flowing to and from every stage).

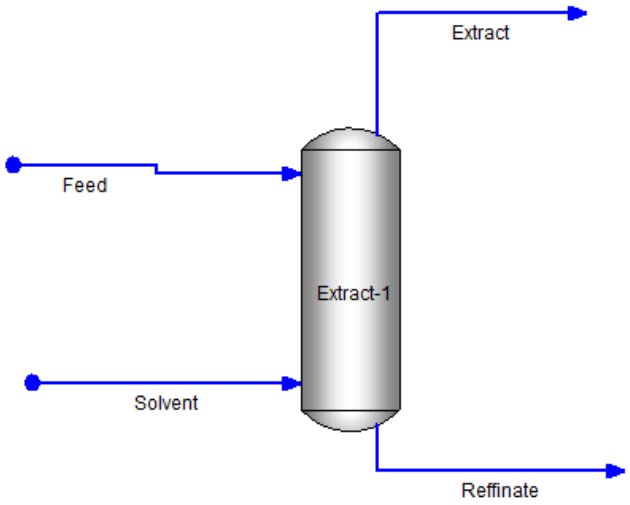
When defining a stripper unit, an all-liquid feed stream must be specified entering the top of the column and the stripping vapor must enter the bottom of the unit.

When defining stripper column parameters, a zero-liquid reflux (i.e., distillate) flow must be made. This is because the distillate flow exiting the unit must only exist in the vapor phase.

All column stages are numbered from bottom to top.

If a feed stream contains both a vapor and a liquid phase, the liquid goes to the feed tray specified by the user and the vapor goes to the stage above.

Extractor Unit



Data Requirement

A minimum of one aqueous feed stream must be defined entering the top of the column, and one solvent stream entering the bottom of the unit. The respective feed streams temperatures, pressures, flows and compositions must be specified, or be a product stream from another Process Block, and the unit outflows named. Additionally, various column operating parameter information must be specified by the user.

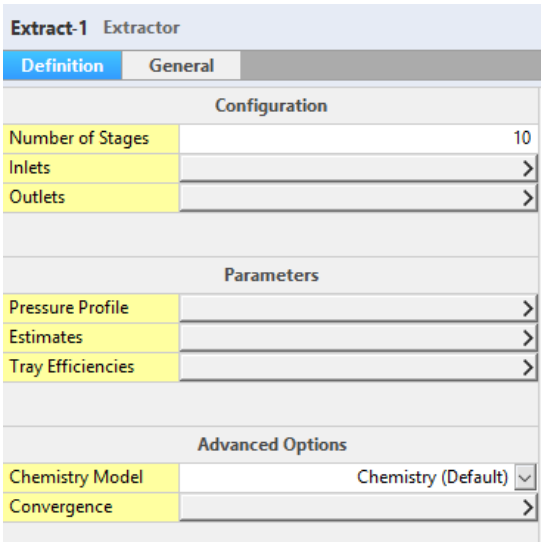
Column Configuration

Additional column parameters can be defined, via the Action Key and selecting the Config facility. Five options are available:

- **Number of Stages:** The default number is 10 stages.

Feed Streams: This function is optional and allows the user to specify up to 8 additional feed streams to the column.

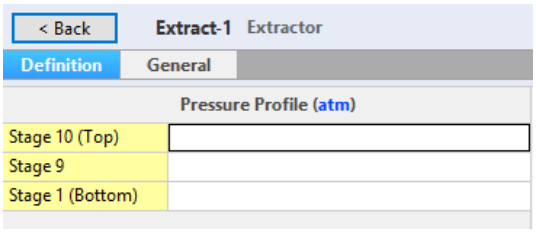
- **Inlets:** This function allows the user to specify up to 8 additional inlets to the column.
- **Outlets:** This function allows the user to specify a Second Liquid Outlet and Aqueous outlet from the column.



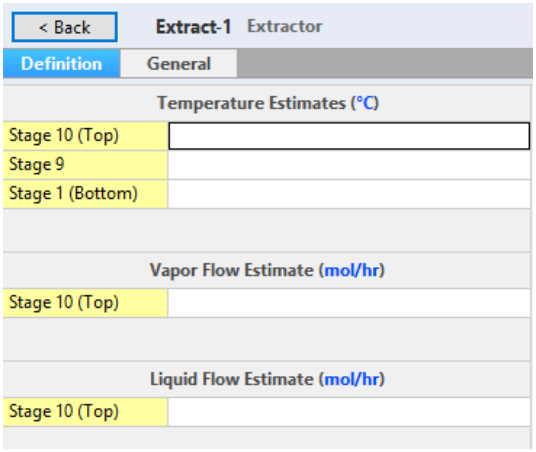
Column Parameters

The column operating parameters are accessed using the Action Key and selecting the Parameters facility. The options available are:

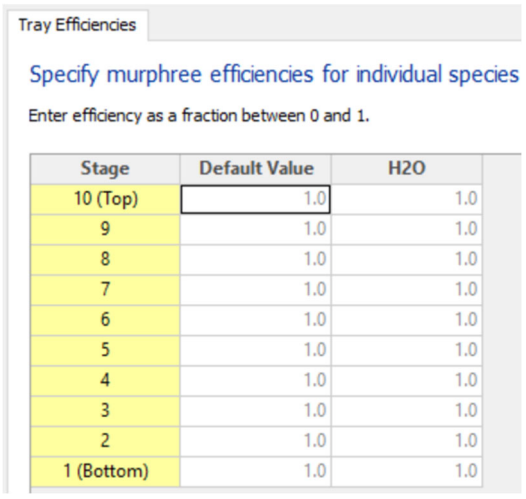
- **Pressure Profile:** This option allows an accurate pressure profile to be specified. This is done by specifying top and bottom stage pressures. If only one stage pressure is given, a zero-pressure drop is assumed through the column.



- **Column Estimates:** This option allows stage operating temperatures, organic distillate and liquid flow estimates to be specified. The estimates for top and bottom stage temperatures, as well as organic distillate and liquid flowrates must all be specified by the user. The End or Quit Key is used to change displays.



- **Tray efficiencies:** This option allows to enter the Murphree efficiency for each tray.



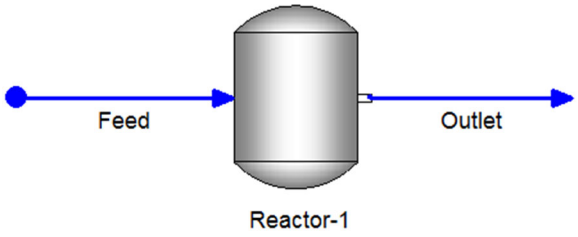
Reactor Unit

This is a process unit which determines the phase separation and intra-phase speciation for a Chemistry Model which can include both equilibrium and rate-limited reactions. The various types of phenomena that can be modeled include ion exchange, kinetics, and redox reactions.

The following types of reactors are available:

Kinetics
Stoichiometric Conversion
Gibbs

Workout examples for each type of reactor can be found in Chapter 6, sections 6.1.

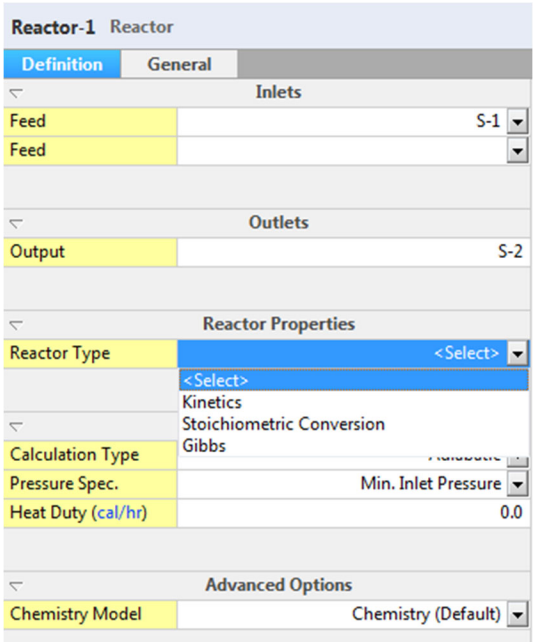


Data Requirement

A minimum of one feed stream entering the reactor must be named, along with the stream temperature, pressure, total flowrate, and composition data defined by the user or be a product stream from another Process Block. Also, the product stream exiting the unit must be named. Additionally, the reactor operating parameters must be specified.

Reactor Configuration

Reactor parameters can be defined in the Reactor Properties pane. Three different reactors can be selected, and this will define the additional parameters needed.

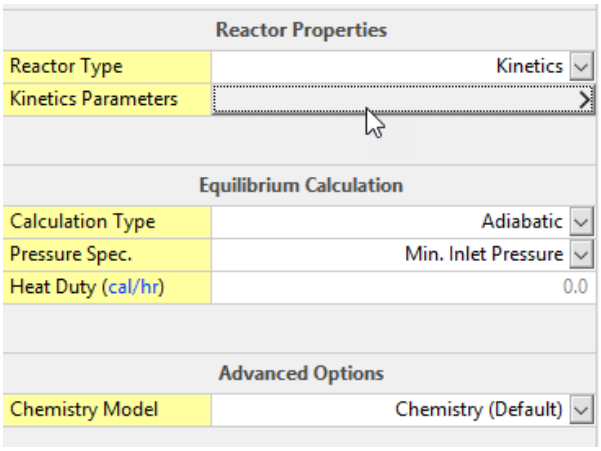


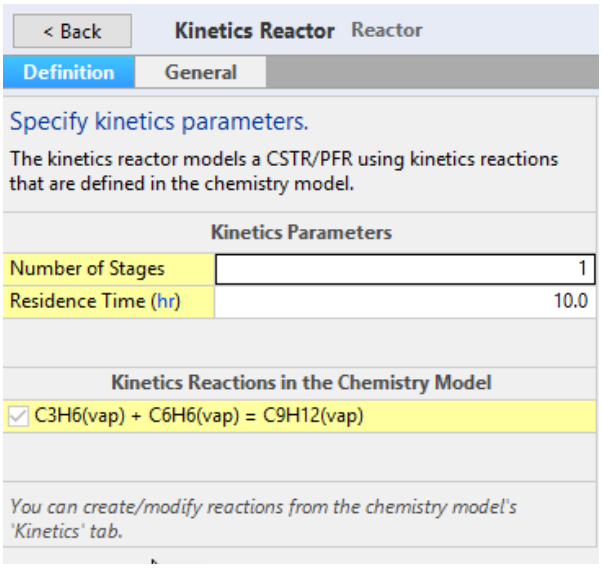
Kinetics Reactor

The chemical kinetics of the reaction are described by the Arrhenius Equation which is specified in the Chemistry Model.

Reactor Properties

For the Kinetics reactor you can specify kinetics parameters.

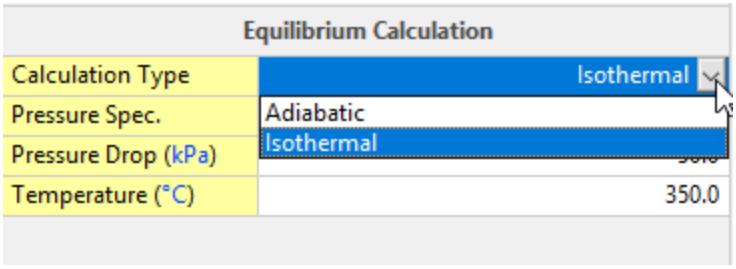




Equilibrium Calculations

Several options are given in this panel:

Calculation Type: Can be Adiabatic or Isothermal
Pressure Spec.: Can be Min. inlet pressure, absolute pressure, and pressure drop.
Pressure Drop: Specify the pressure drop within the block.
Temperature: If the calculation is isothermal
Heat duty: If the calculation is adiabatic

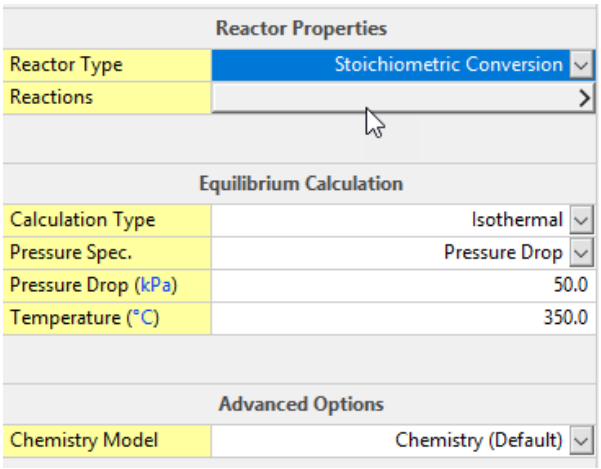


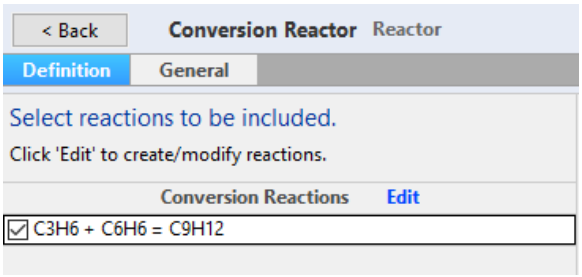
Stoichiometric Conversion Reactor

Stoichiometric reactors use a simple stoichiometric relationship between reactants and products. There is no time factor for these reactions.

Reactor Properties

For the Conversion Reactor you can specify Reactions.

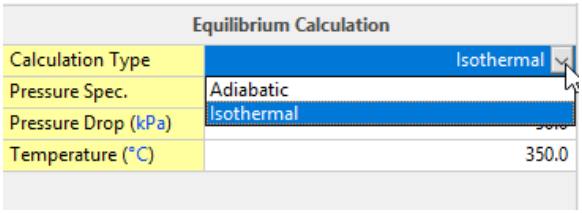




Equilibrium Calculations

Several options are given in this panel:

Calculation Type: Can be Adiabatic or Isothermal
Pressure Spec.: Can be Min. inlet pressure, absolute pressure, and pressure drop.
Pressure Drop: Specify the pressure drop within the block.
Temperature: If the calculation is isothermal
Heat duty: if the calculation is adiabatic

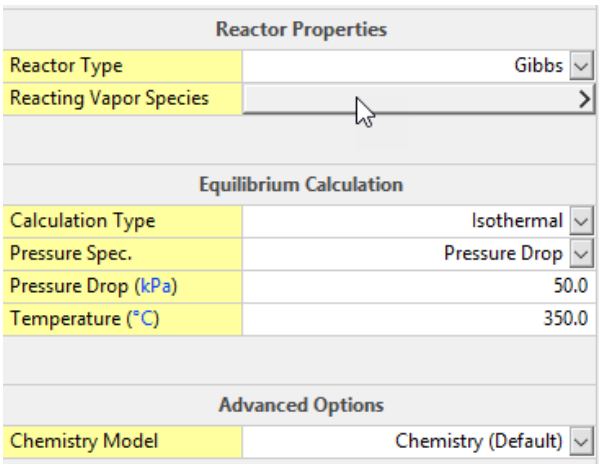


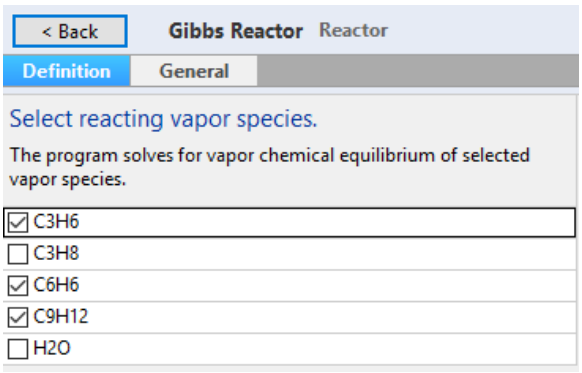
Gibbs Reactor

A Gibbs reactor is a special type of reaction in OLI Flowsheet: ESP in that it does not evaluate the standard equilibrium equations found in the chemistry model. Rather it minimizes the Gibbs Free Energy at a given temperature and pressure or maximizes entropy at a given pressure and enthalpy. It is important to point out that this reactor can be used only for reactions that occur in the vapor phase.

Reactor Properties

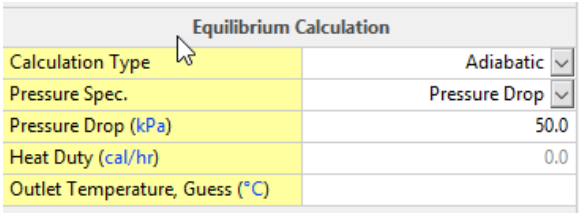
For the Gibbs Reactor you can specify Reacting Vapor Species.





Equilibrium Calculations

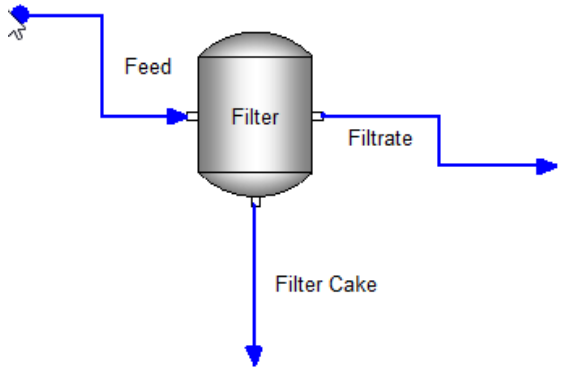
Several options are given in this panel:



Calculation Type: Can be Adiabatic or Isothermal
Pressure Spec.: Can be Min. inlet pressure, absolute pressure, and pressure drop.
Pressure Drop: Specify the pressure drop within the block.
Temperature: If the calculation is isothermal
Heat Duty: If the calculation is adiabatic
Outlet Temperature, Guess: Enabled for adiabatic calculations.

Filter Unit

This is a crystallization process unit which models the separation of the liquid portion of the feed stream from the solid portion of the feed stream. The liquid and solid are divided between the filtrate and filter cake (or solids) streams based upon specified fractions or flows.

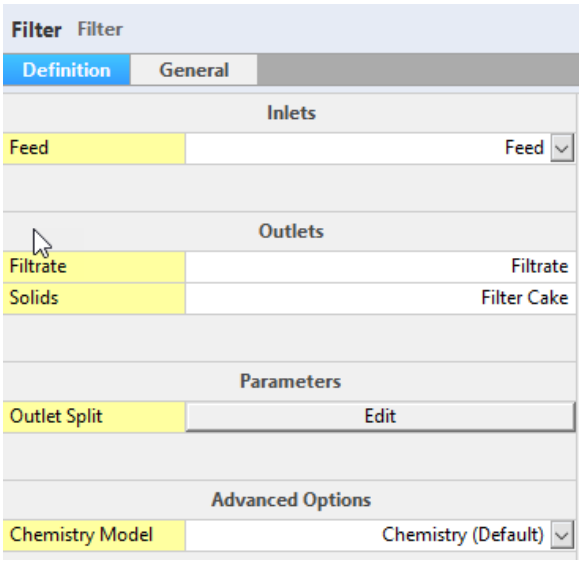


Data Requirement

One feed stream entering the Filter must be named, along with the stream temperature, pressure, total flowrate, and composition data defined by the user or be a product stream from another Process Block. Also, the outlet (filtrate and filter cake) streams exiting the unit must be named. The filter operating parameters must be specified.

Unit Parameters

The Filter operating conditions are specified using the Edit button.



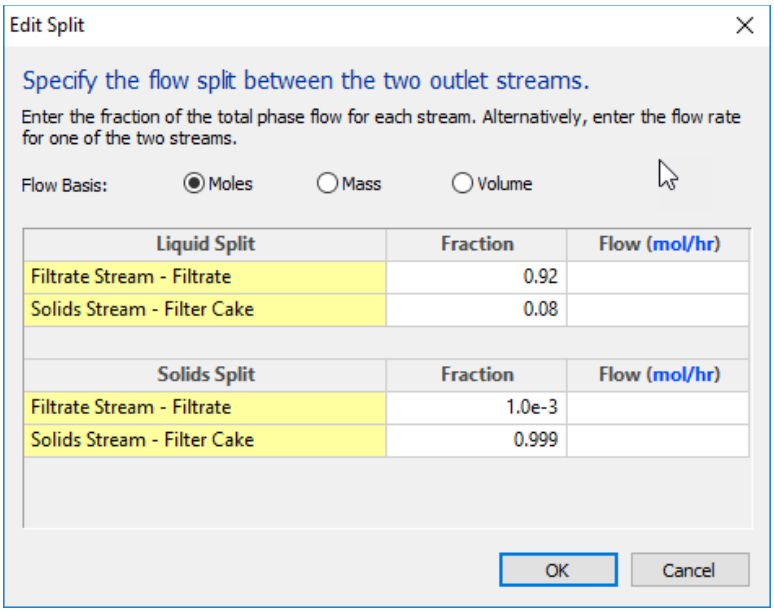
Two basic conditions must be specified:

Split of the total liquid to the filtrate and solids streams, and
Split of the solid between the filtrate and solids streams.

The total liquid may be split by using fractions or flows. Once one fraction is specified (e.g., the fraction of the total liquid split to the filtrate stream), the other is known and cannot be specified (e.g., the fraction of liquid split to the solids stream).

The total liquid may be split by specifying the flow of liquid in moles/hr, grams/hr or m^3/hr to one of the outlet streams. Likewise, once one flow is specified, the other is known and cannot be specified.

The same procedure is followed when specifying the split of the solid to each of the outlet streams.



Guidelines

1. The only inlet stream allowed is the feed stream.

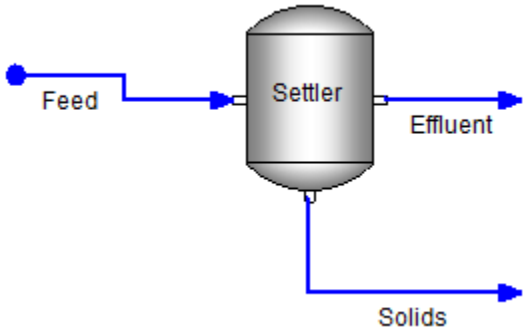
2. The entire liquid is split by fraction or flow to the two outlet streams, filtrate and solids.

3. The entire solid is split by fraction or flow. Individual solid species may not be selected. Thus, the makeup of the solid in the filtrate stream will be the same as the makeup of the solid in the solids stream.

4. Once the fraction or flow of liquid to the filtrate or solids stream is specified, the fraction and flow to the other stream is fixed and may not be specified. The same is true for the solid.

Settler Unit

This is a crystallization process unit which models the separation of the liquid portion of the feed stream from the solid portion of the feed stream. The liquid and solid are divided between the filtrate and solids outlet streams based upon specified fractions or flows. The solid may be split as a total solid or, differentially, split by individual solid species.

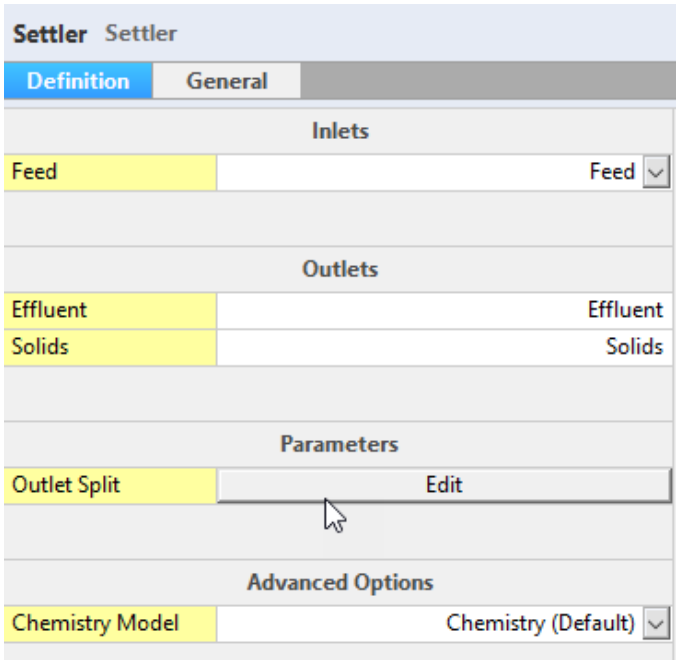


Data Requirement

One feed stream entering the Settler must be named, along with the stream temperature, pressure, total flowrate, and composition data defined by the user or be a product stream from another Process Block. Also, the outlet (effluent and solids) streams exiting the unit must be named. Additionally, the Settler operating parameters must be specified.

Unit Parameters

The Filter operating conditions are specified using the Edit Button.



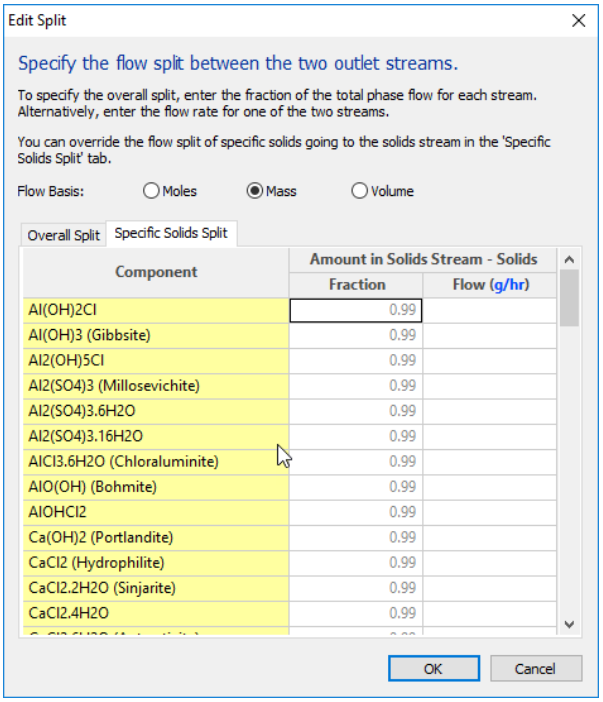
Two basic conditions must be specified:

split of the total liquid to the filtrate and solids streams, and
split of the solid, or individual solid species, between the filtrate and solids streams.

The total liquid may be split by using fractions or flows. Once one fraction is specified (e.g., the fraction of the total liquid split to the filtrate stream), the other is known and cannot be specified (e.g., the fraction of liquid split to the solids stream). The total liquid may be split by specifying the flow of liquid in moles/hr, grams/hr or m^3/hr to one of the outlet streams. Likewise, once one flow is specified, the other is known and cannot be specified.

The Settler also offers the option to split specific solids from a solid stream.

The total solid may be split by using fractions or flows or the solid may be split by specifying the fraction or flow of specific solid species to each of the outlet streams. A combination of the two may also be used. That is, you may split one or more individual solid species by fraction or flow and then split the remainder of the solid by an overall fraction or flow. Since the solid may be split by individual solid species, the resulting solid portion of each of the outlet streams are not necessarily of the same makeup.



Guidelines

The only inlet stream allowed is the feed stream.

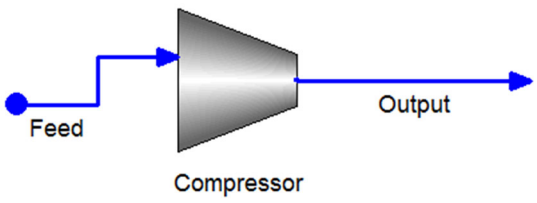
The entire liquid is split by fraction or flow to the two outlet streams, filtrate and solids.

When splitting the solid, individual solid species may be selected. Any solid species not selected will be split using the overall solid split fraction or flow. Thus, the makeup of the solid in the filtrate stream will be the same as the makeup of the solid in the solids stream.

Once the fraction or flow of liquid to the filtrate or solids stream is specified, the fraction and flow to the other stream is fixed and may not be specified. The same is true for the solid.

Compressor Unit

This is a conventional process block which allows the compression of 1-7 feed streams into a single product stream. The compression can be carried out on either an isentropic or polytropic basis. The resulting phase separation and speciation within each phase is computed.



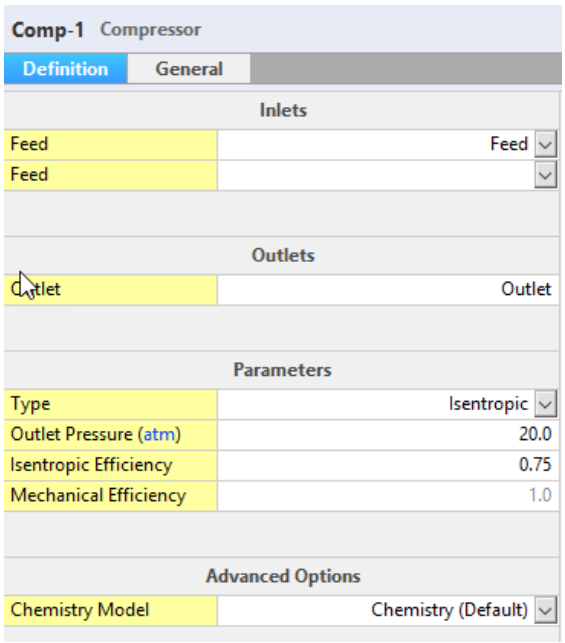
Data Requirement

The unit's stream inflows and exit flow must be given distinct names. This enables streams and units to be recognized and linked together when building a complex process. A minimum of one feed stream, together with its conditions must be defined by the user or said stream must be a product stream from another process block.

Unit Parameters

The parameters available to define the compressor are as follows:

Parameter	Value	Comment
Compressor	Isentropic or polytropic	Must provide
Outlet Pressure	User	Must provide
Isentropic Efficiency	User (0.0 to 1.0)	Default = 0.72
Polytropic Efficiency	User (0.0 to 1.0)	Default = 0.72
Mechanical Efficiency	User (0.0 to 1.0)	Default = 1.0



Unit Configuration

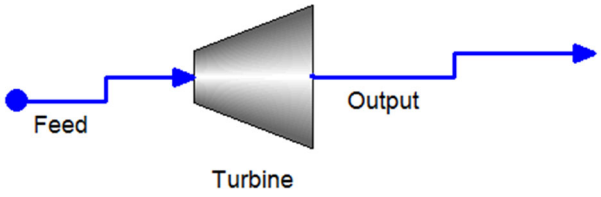
This unit allows the user to add or delete extra feed streams. An additional six inlet streams may be defined if required.

Guidelines

When additional streams are to be added to the unit, the user must first ensure the minimum data requirements for the unit are specified prior to adding new streams.

Turbine Unit

This is a conventional process block which allows the expansion of 1-7 feed streams into a single product stream. The turbine block works on either an isentropic or polytropic basis. The resulting phase separation and speciation within each phase is computed.



Data Requirement

The unit's stream inflows and exit flow must be given distinct names. This enables streams and units to be recognized and linked together when building a complex process. A minimum of one feed stream, together with its conditions must be defined by the user or said stream must be a product stream from another process block.

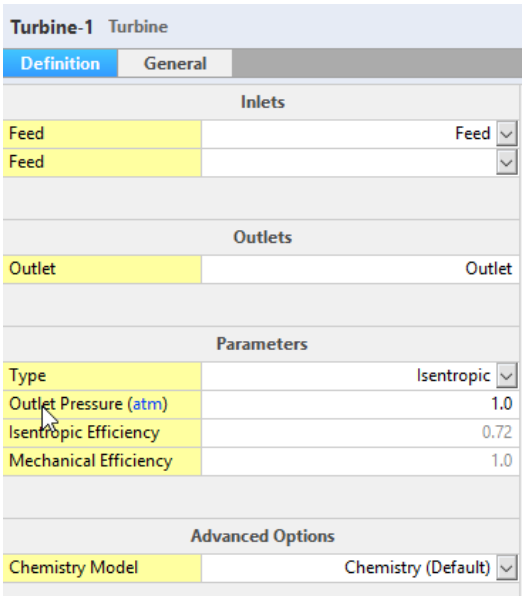
Unit Parameters

The parameters available to define the compressor are as follows:

Parameter	Value	Comment
Turbine	Isentropic or polytropic	Must provide
Outlet Pressure	User	Must provide
Isentropic Efficiency	User (0.0 to 1.0)	Default = 0.72
Polytropic Efficiency	User (0.0 to 1.0)	Default = 0.72
Mechanical Efficiency	User (0.0 to 1.0)	Default = 1.0

Unit Configuration

This unit allows the user to add or delete extra feed streams. An additional six inlet streams may be defined if required.

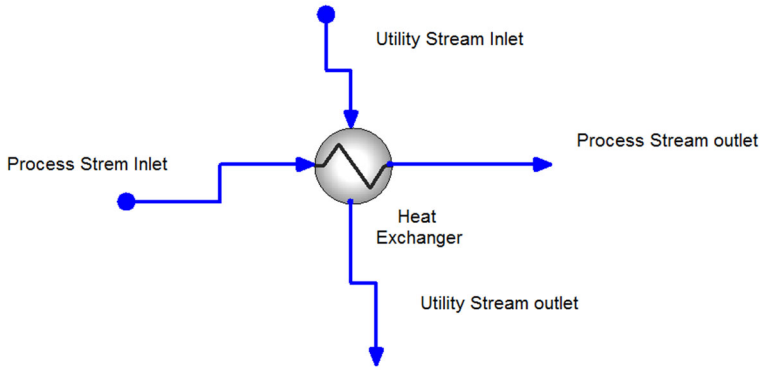


Guidelines

When additional streams are to be added to the unit, the user must first ensure the minimum data requirements for the unit are specified prior to adding new streams.

Heat Exchanger Unit

This is a conventional process unit which allows energy to be added to, or removed from, a single stream, or transferred between a process stream and a utility stream.

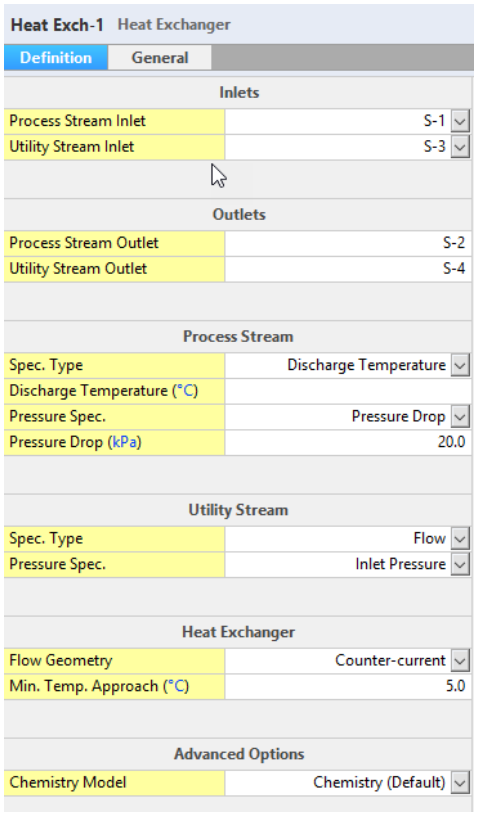


Data Requirement

A minimum of one inlet, and corresponding exit stream must be named for the unit. Optionally, when simulating heat transfer between two streams, the utility inlet and outlet flows must also be identified. The inlet stream(s) temperature, pressure, flows and composition data must also be defined by the user. Additionally, the unit operating conditions must be specified.

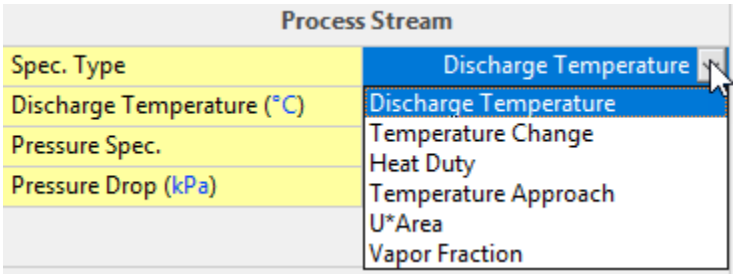
Unit Parameters

The unit operating conditions are specified in the definition panel.



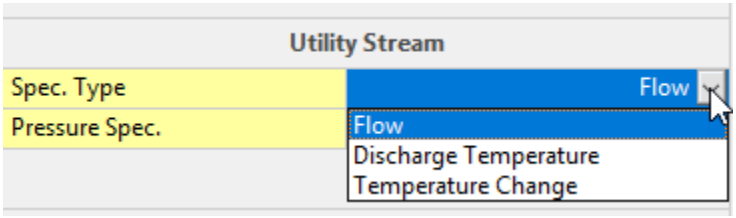
Six options are available for defining the Process Exit Stream requirements:

Discharged Temperature
Temperature Change
Heat Duty
Temperature Approach
U*Area
Vapor Fraction



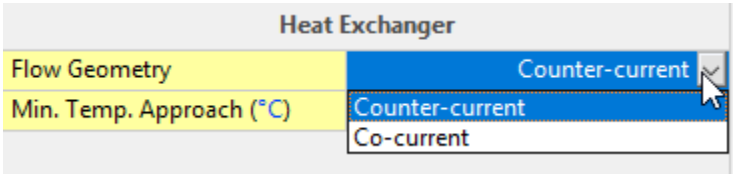
For systems in which a utility stream is defined, the option is also available to specify:

Flow rate
Discharge Temperature
Temperature Change



For definitions in which the utility stream exit temperature, or change in temperature, is specified, the utility stream flowrate is automatically modified. The initial user-defined value is changed in order to meet the required temperature operating requirements. Conversely, if the utility stream flowrate is defined its respective exit temperature is determined in order to comply with the process stream duty requirements.

The Heat Exchanger flow geometry can be either co-current or counter-current, and a minimum temperature approach can be specified.

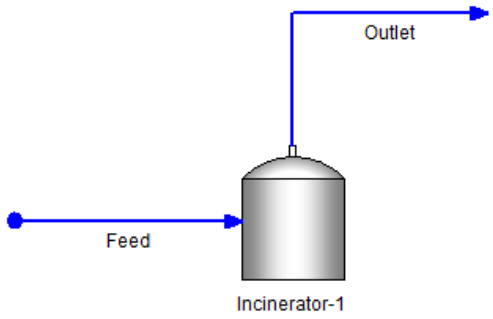


Guidelines

1. Additional inlet streams cannot be defined for this unit.

2. Process streams from other process units can be used as the utility stream if required. However, for this type of operation only the outlet temperature can be specified by the user.

Incinerator



Data Requirement

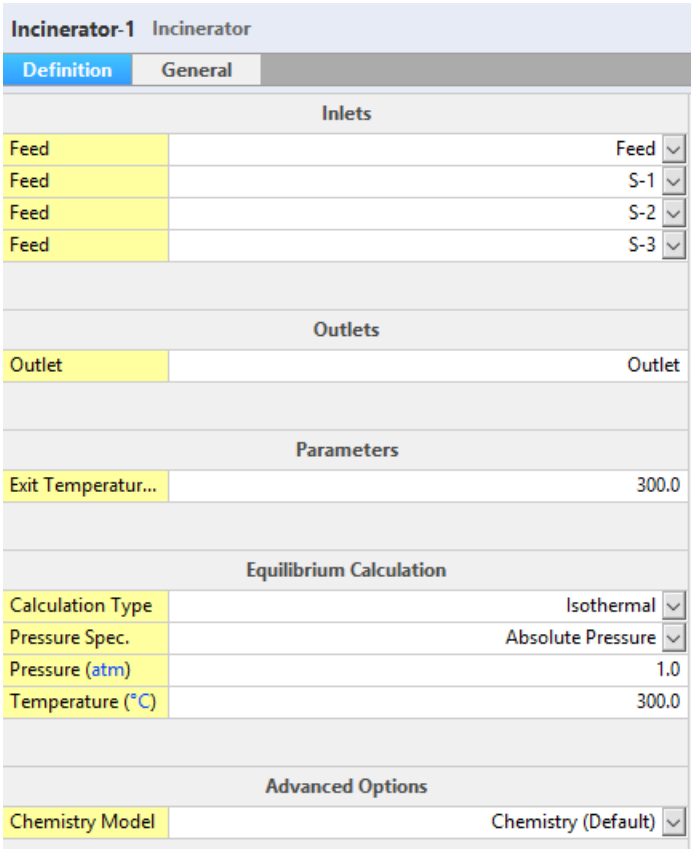
A minimum of one feed stream to the unit must be defined, and its temperature, pressure, total flowrate and composition data should be specified by the user or be the product stream from another Process Block. Note that the oxidation vapor stream composition (i.e., the air being used to burn the feed) must also be included as part of the feed stream(s) definition. The outlet (waste gas stream exiting the unit) must also be identified.

Unit Parameters

This unit can operate adiabatically or isothermally, one of which must be selected. For isothermal operation, the incinerator operating temperature must be supplied by the user.

Unit Configuration

This facility allows the user to add or delete extra inlet streams to the unit. An additional 3 feeds may be defined if required.



Guidelines

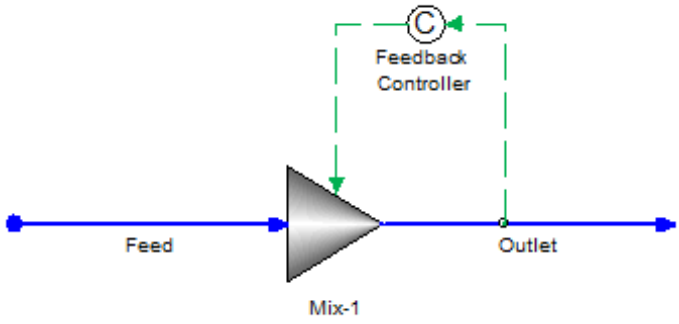
When using this unit, the user must ensure a Non-Electrolyte Chemistry Model.

For clarification purposes it is advised that the oxidation vapor stream is specified as a separate inlet flow to the unit, rather than as part of the feed stream composition.

Species that may form through a reduction/oxidation process and be in the outlet stream must be named as a species in the Chemistry Model (e.g., NOx compounds, SO2, etc.).

Feedback Controller

This is a Control Block which allows the user to specify a particular stream property by adjusting a block parameter of another process block.

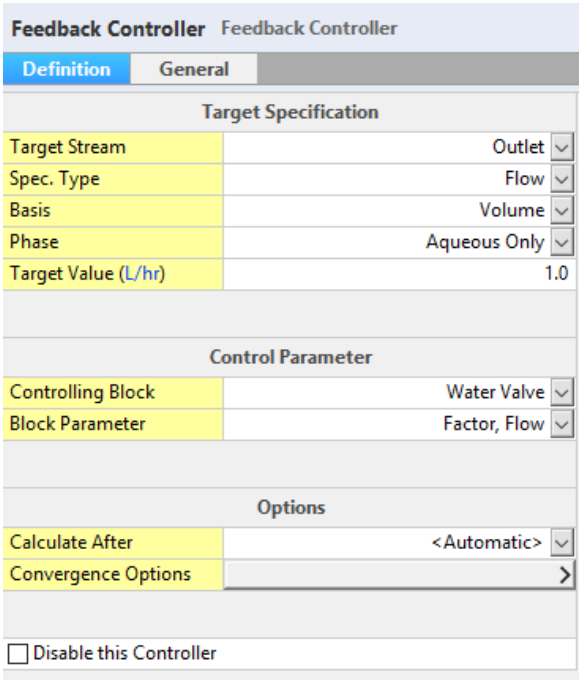


Data Requirement

The Controller definition can be divided into two parts: defining the stream specification and defining the block parameter of the process block to be varied to meet the stream specification.

Defining the Target Specification

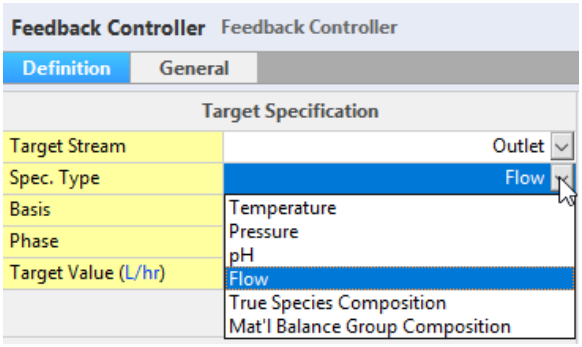
The target stream is chosen from the streams already defined in another process block. Only streams which have been defined can be named in the Controller Block.



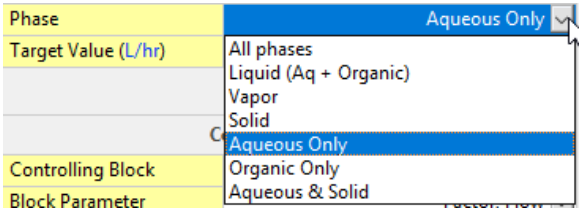
The stream's specification type is then selected from a list, which include:

Temperature
Pressure
pH
Flow (When flow is selected as a specification, the phase and the units can be named)

True species composition of the stream (when composition is selected as a specification, the phase and units of the composition can also be named)
Material Balance Group Composition (the target composition can be named in terms of either the species in the solution (e.g., CaCO3), or in terms of the material balance groups in the solution e.g., Ca (+2), C (+4), or O (-2)).



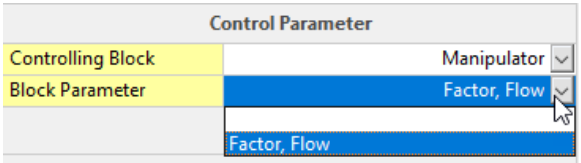
The Feedback controller basis needs to be specified. It can be either volume, mass or moles.
Different phases can also be specified:



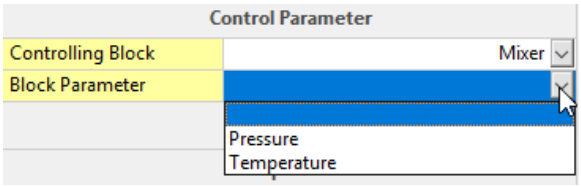
Defining Control Parameter

The controlling block, which will be varied to meet the stream specification, is selected from a list of process blocks already defined. Once the controlling block is selected, the parameters available for that block are listed.

For example:

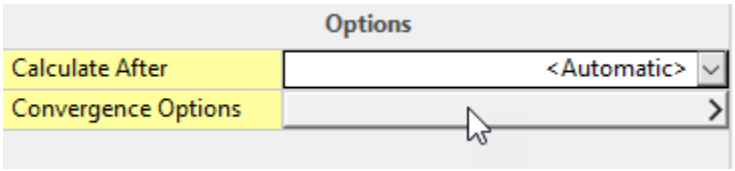


Or



Unit Parameters

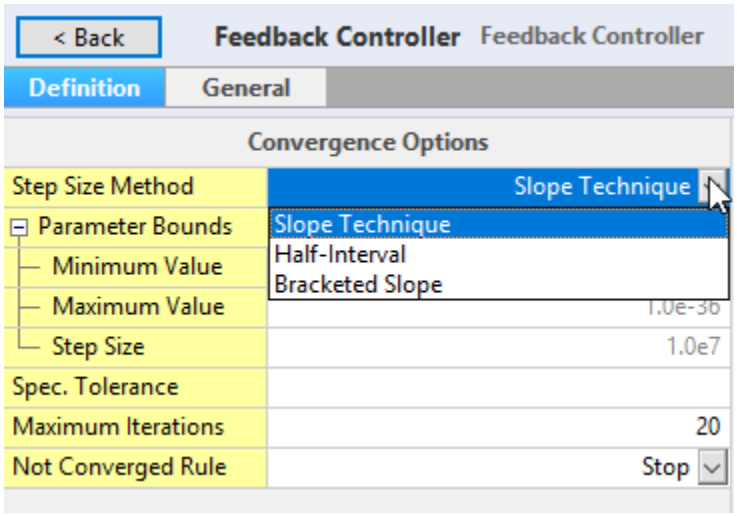
Controller parameters can be set which guide the convergence of the Controlling Block. These optional parameters are accessed in the Convergence Options.



The parameters which can be set are:

Step Sized Method: Which are divided into three different methods. One of three calculation step size methods can be selected. The Slope Technique is the default

Slope Technique: The slope between the last two guesses determines the next guess unless the step size minimum or maximum is exceeded. This is the fastest technique provided there are no large differences in slopes (as there are in titration curves, or precipitation curves).



Half Interval: A new minimum or maximum is computed each iteration, and the new guess is based on (min + max)/2. This is a conservative technique, but a solution is assured for unimodal functions.

Bracketed Slope: As with the Half Interval technique, a new minimum and maximum is computed each iteration. The slope is then used to calculate the next guess (rather than (min + max)/2).

Bounds - The upper and lower limits of the process block parameter and the step size can be set. The default step size for the first iteration is 1%. The default for subsequent iterations is:
50% for general process variables
20 ºC for temperature
25% for duty

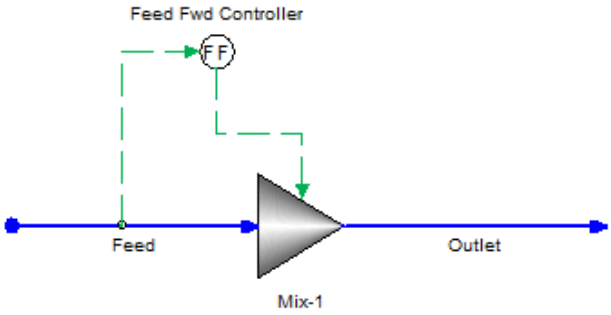
Spec. Tolerance: Tolerance given by user.

Max Iterations: The number of iterations can be changed from the default of 20 iterations.

Not Converged Rule: The default rule in OLI ESP FS for non-convergence is to stop execution. This rule can be changed to continue execution.

Feedforward Controller Unit

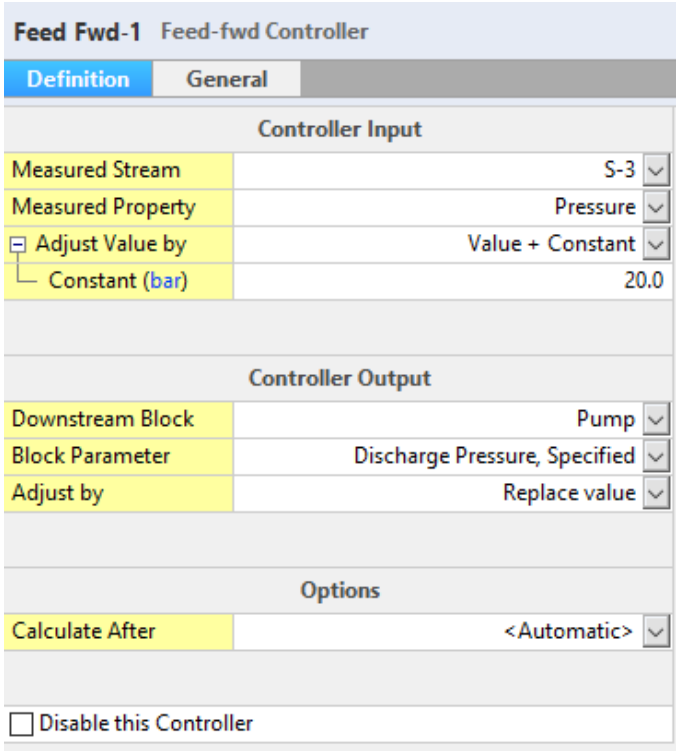
This is a Control Block which allows the measured value of a stream property or of a block parameter to be passed, or transferred, to a downstream block.



Data Requirement

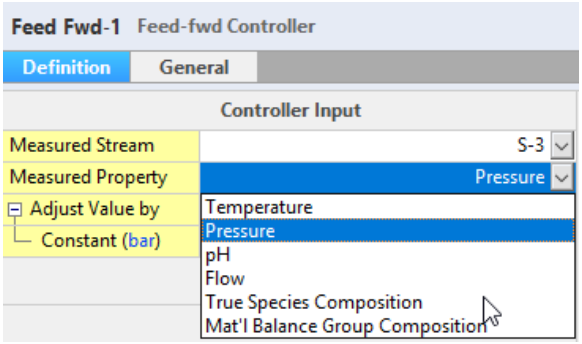
The Feedforward definition is divided into two parts: Controller Input and Controller Output.

The Controller Input defines the measured stream and measured property value that will be transferred. The Controller Output defines the downstream block or block parameter which will receive the value.



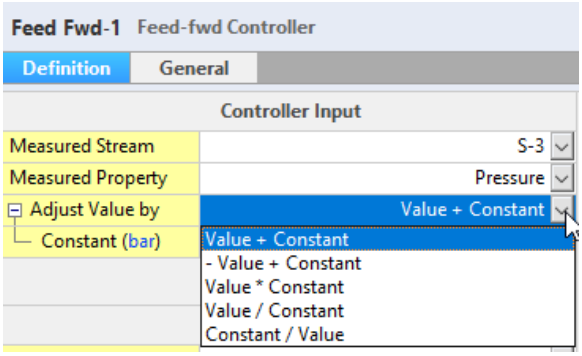
Defining the Controller Input (Transfer Value)

The Measured Property of the Measured Stream is chosen as the property to be transferred. The stream is chosen from those already defined in the process. The stream property is then selected from a list of possible names. For streams, this list includes temperature, pressure, pH, flow, or the composition of the stream (True Species Composition or Material Balance Group Composition).



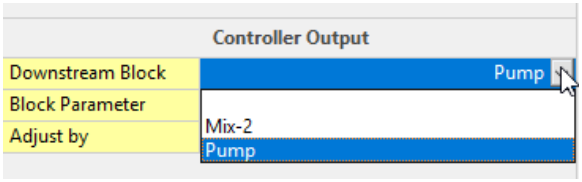
Finally, the value of the selected stream property can have an adjustment applied to it. Possible adjustments include:

Value + Constant
-Value + Constant
Value * Constant
Value / Constant
Constant / Value

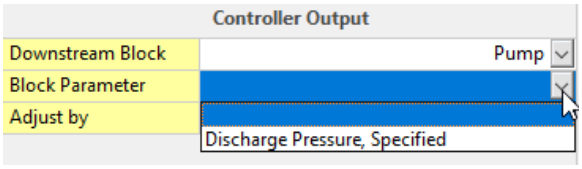


Defining the Controller Output (Block Parameter)

The process block parameter which will receive the transferred value is named as Downstream Block. The process block is selected from a list of process blocks already defined.



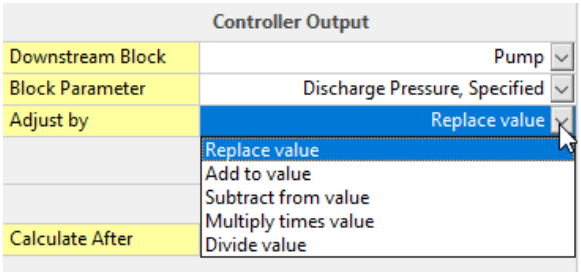
Once the process block is selected, the allowed parameters for that block are available.



Finally, the value of the selected Block Parameter can have an adjustment applied to it. Possible adjustments include:

Replace value
Add to value
Subtract from value

Multiply times value
Divide value



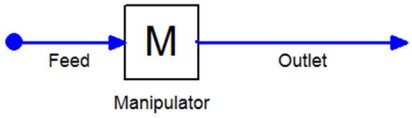
Guidelines

1. Avoid trying to control a variable which is discontinuous. For example, avoid trying to reach the saturation point of a solution with respect to a solid.

2. OLI Flowsheet: ESP allows for controlling and tearing the same stream.

Manipulator Unit

This is a Control Block which allows the mixing of up to 7 feed streams adiabatically. Either the resulting flow or individual components can be multiplied by a factor. The resulting phase separation and speciation within each phase of the outlet stream is computed.

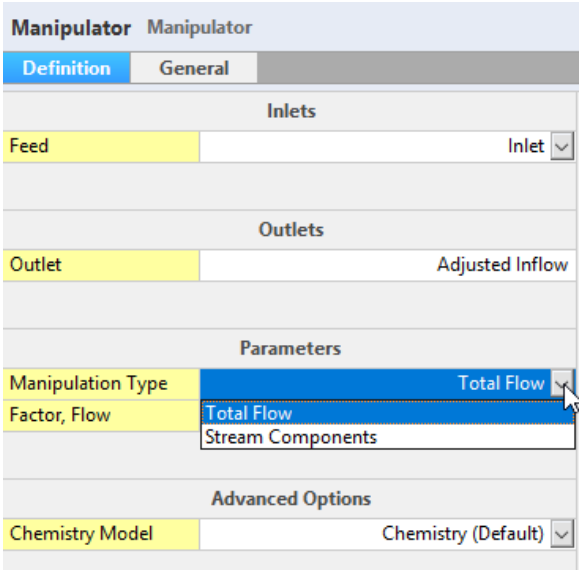


Data Requirement

The Feed and Outlet streams must all be given distinct names. This enables streams and units to be recognized and linked together when building a complex process. A minimum of one feed stream and their respective temperature, pressure, flow and composition must be defined by the user.

Unit Parameters

The Properties pane allows the user to specify the factors by which either the Total Flow or Stream Component composition of the exit stream can be multiplied.



Unit Configuration

This facility allows the user to add or delete extra feed streams to the unit and is accessed via the Properties Pane. An additional six inlet streams may be defined if required.

Guidelines

When additional streams are to be added to the unit, the user must first ensure the minimum data requirements for the unit are specified prior to using the Properties Pane.

This block is generally used in conjunction with the other ESP Control Blocks (e.g., Controller) to adjust the flow of a stream or a composition in the stream.

Direct Stream Manipulation

This feature allows the same functionality as a manipulator block. Either the resulting flow or individual components in a stream can be directly multiplied by a factor by the feedback controller. The resulting phase separation and speciation within each phase of the outlet stream is computed. Streams can now also be connected to feed forward controller.

Data Requirement

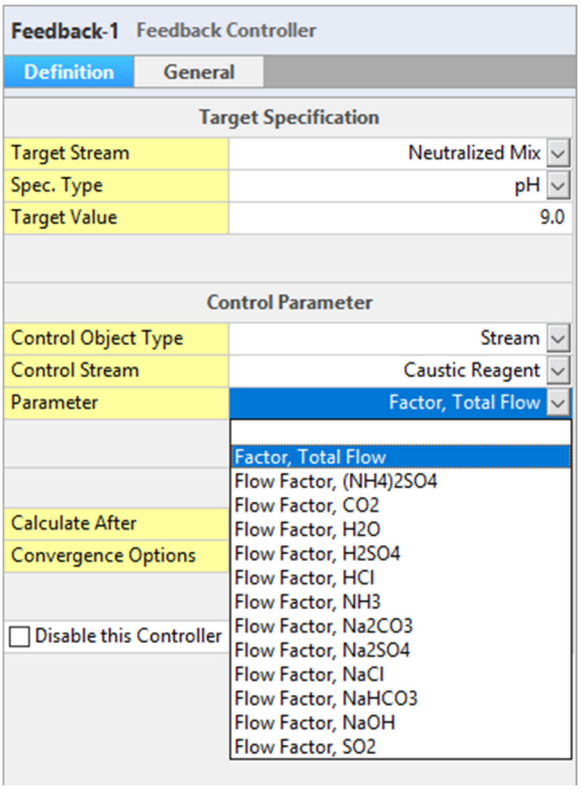
1. For the stream: A minimum of one feed stream and their respective temperature, pressure, flow and composition must be defined by the user

2. For the feedback controller: Target specification and control parameter must be selected.

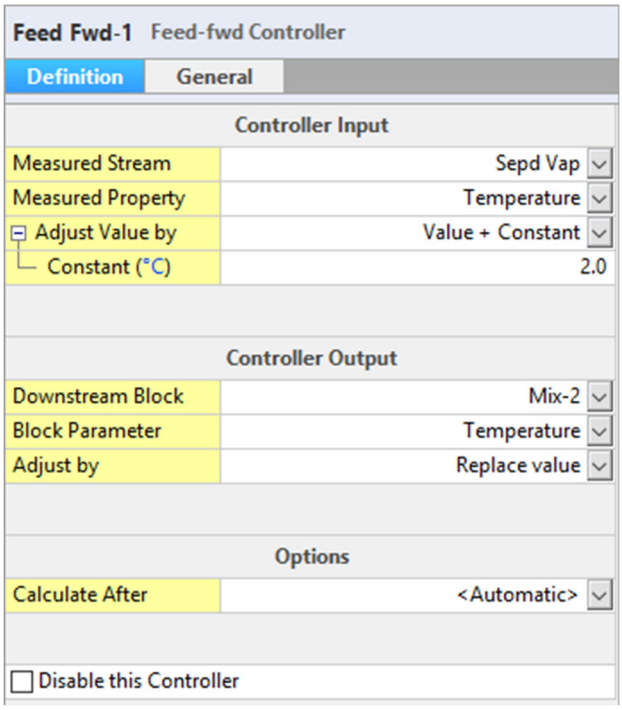
3. For the feedforward controller: The input and output parameters must be the same

Unit Parameters

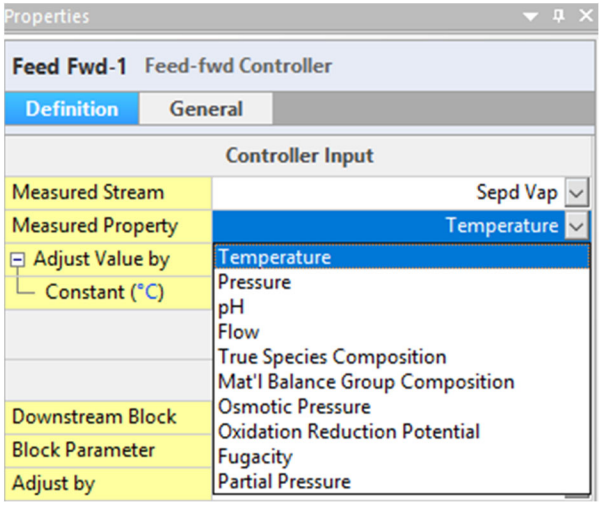
1. For the feedback controller: The Properties pane allows the user to specify the factors by which either the Total Flow or Stream Component composition of the exit stream can be multiplied.



2. For the feedforward controller:

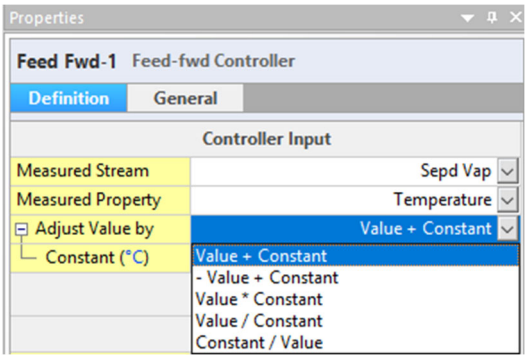


The Measured Property of the Measured Stream is chosen as the property to be transferred. The stream is chosen from those already defined in the process. The stream property is then selected from a list of possible names. For streams, this list includes temperature, pressure, pH, flow, or the composition of the stream (True Species Composition and Material Balance Group Composition) along with additional parameters like Osmotic Pressure, Oxidation Reduction Potential, Fugacity, Partial Pressure.



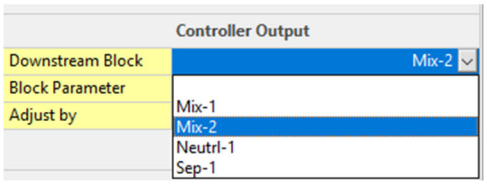
Finally, the value of the selected stream property can have an adjustment applied to it. Possible adjustments include:

Value + Constant
-Value + Constant
Value * Constant
Value / Constant
Constant / Value

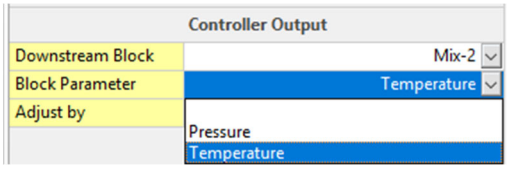


Defining the Controller Output (Block Parameter)

The process block parameter which will receive the transferred value is named as Downstream Block. The process block is selected from a list of process blocks already defined.

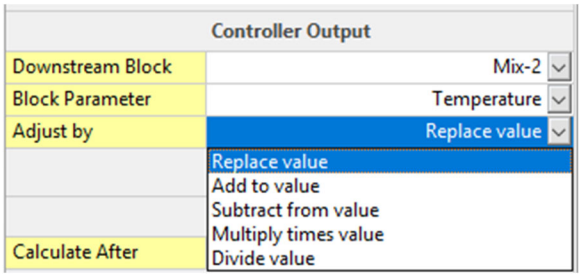


Once the process block is selected, the allowed parameters for that block are available. It is important to select the same input parameter as the output parameter for direct manipulation of streams. In this case we have selected temperature as the parameter to manipulate.



Finally, the value of the selected Block Parameter can have an adjustment applied to it. Possible adjustments include:

Replace value
Add to value
Subtract from value
Multiply times value
Divide value



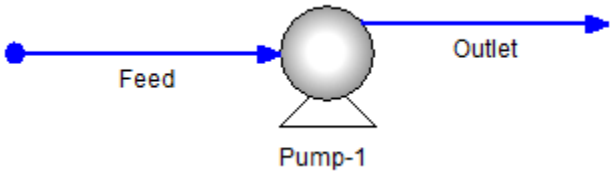
Guidelines

User must first ensure the minimum data requirements for the stream are specified prior to connecting the stream to a controller.

This block is generally used in conjunction with the other ESP Control Blocks (e.g., Controller) to adjust the flow of a stream or a composition in the stream or to feed manipulate the values of downstream blocks.

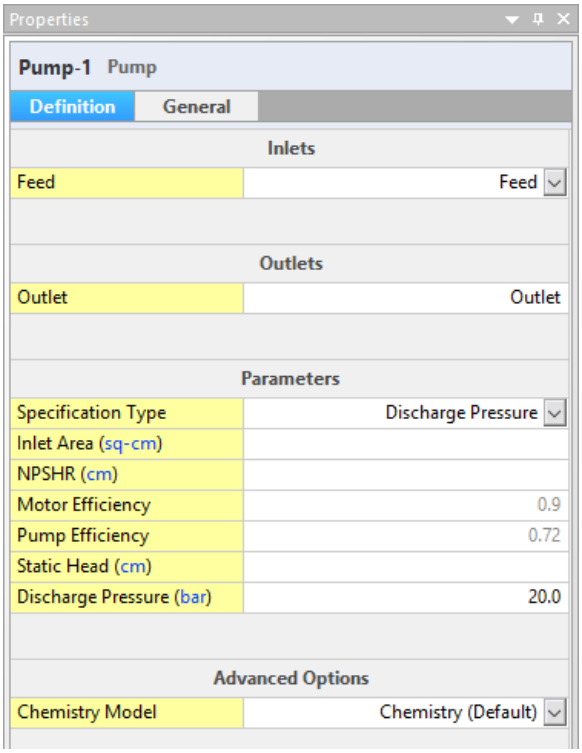
Pump

This is a conventional process block which allows the change of the discharged pressure of 1 feed stream.



Data Requirement

The unit's stream inflow and exit flow must all be given distinct names. This enables streams and units to be recognized and linked together when building a complex process. The feed stream and their respective temperature, pressure, flow and composition must be defined by the user.



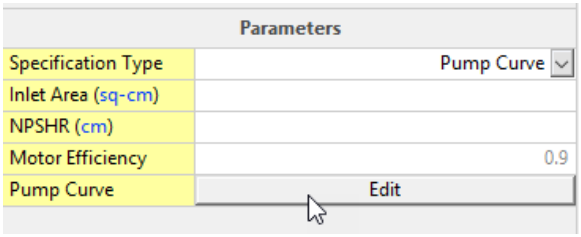
Unit Parameters

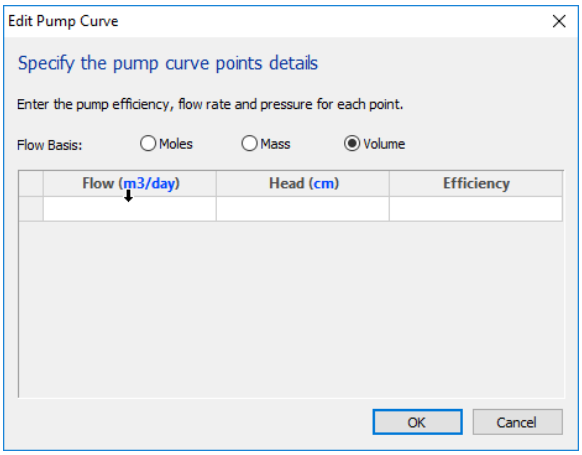
The parameters available to define the pump are as follows:

Parameter	Value	Comment
Specification Type	Discharged Pressure or Pump Curve	Must provide
Inlet Area	User	Optional
NPSHR*	User	Optional
Motor Efficiency	User (0.0 to 1.0)	Default = 0.9
Pump Efficiency	User (0.0 to 1.0)	Default = 0.72
Static Head	User	Optional
Discharge Pressure	User	Must provide
Pump Curve	User	Must provide

**Net Positive Suction Head Required*

To add a Pump Curve, go to Edit Button:





RO Membranes (Reverse Osmosis)

This is a process block which allows for the separation of salts from a single process feed stream using a semi-permeable membrane. As a result of this separation, two product streams result one called the “concentrate stream” and the other called the “permeate stream.” The specification of a permeate inlet stream is optional.

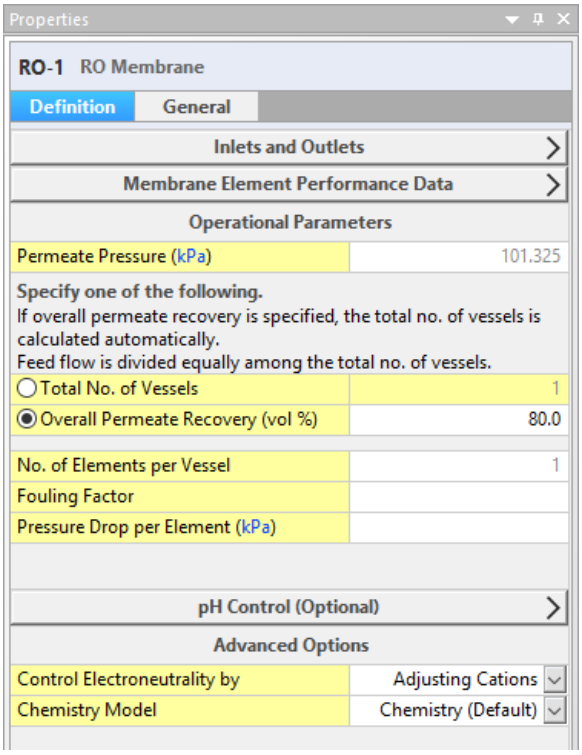
Data Requirement

The unit’s stream inflow(s) and exit flows must be given distinct names. This enables streams and units to be recognized and linked together when building a complex process. A minimum of one conventional feed stream and one additional, optional permeate feed stream, together with their conditions must be defined by the user or said stream must be a product stream from another process block.

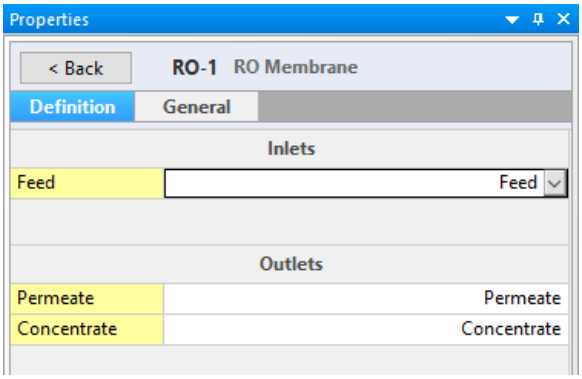
Unit Parameters

The parameters available in the Properties Panel are divided into the following:

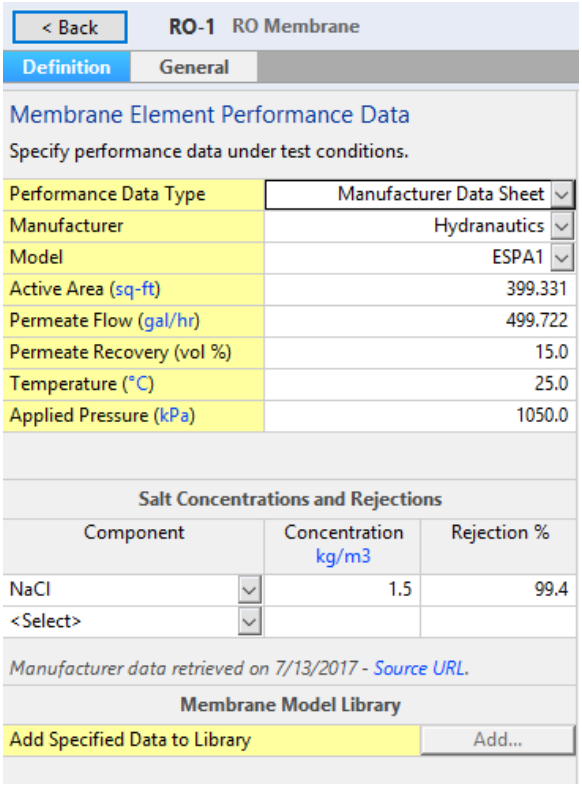
Inlets and Outlets
Membrane Element Performance Data
Operation Parameters
pH Control (Optional)
Advanced Options



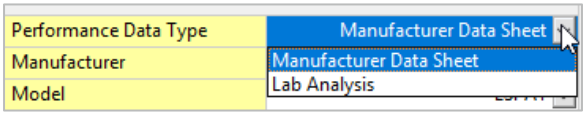
Inlets and Outlets: Clicking the inlets and outlets button, it will bring a new pane where the connections in and out of the RO block can be modified.



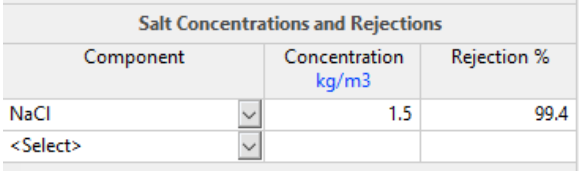
Membrane Element Performance Data: Clicking on the Membrane Element Performance Data button, it will bring a new pane where you can input the following information:



In this option, you can select either Manufacturer Data Sheet or Lab analysis. When Manufacturer Data Sheet is selected the user needs to specify the Manufactures and the Model of the membrane. Different options for manufacturer and model will be displayed. Additionally, active area, permeate flow, permeate recovery, temperature and applied pressure values must be provided.



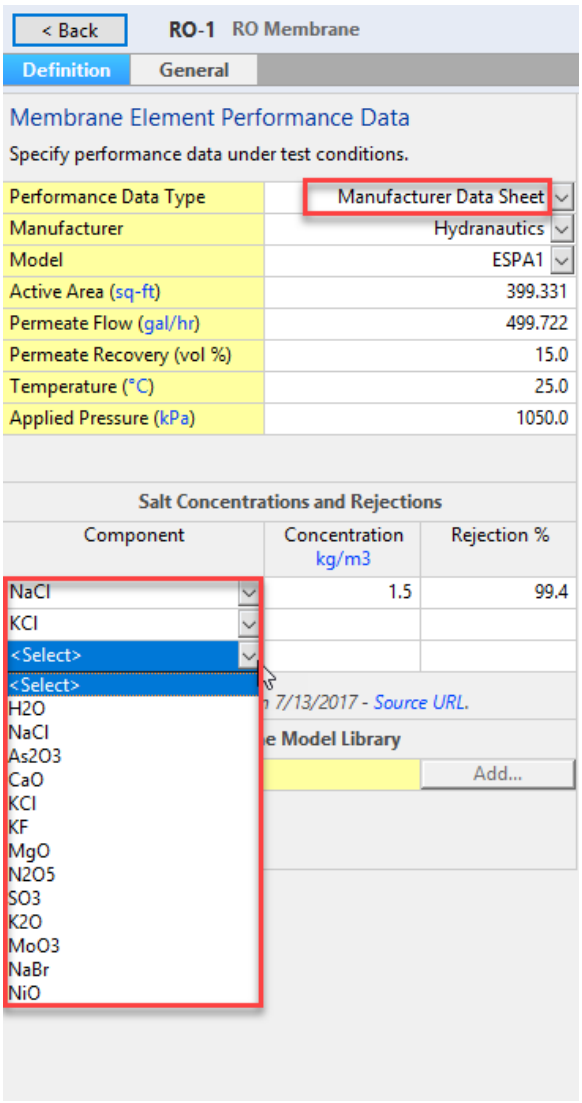
Salt Concentration and Rejections: The user has the option to select specific salts and define their concentration and rejection percentage.

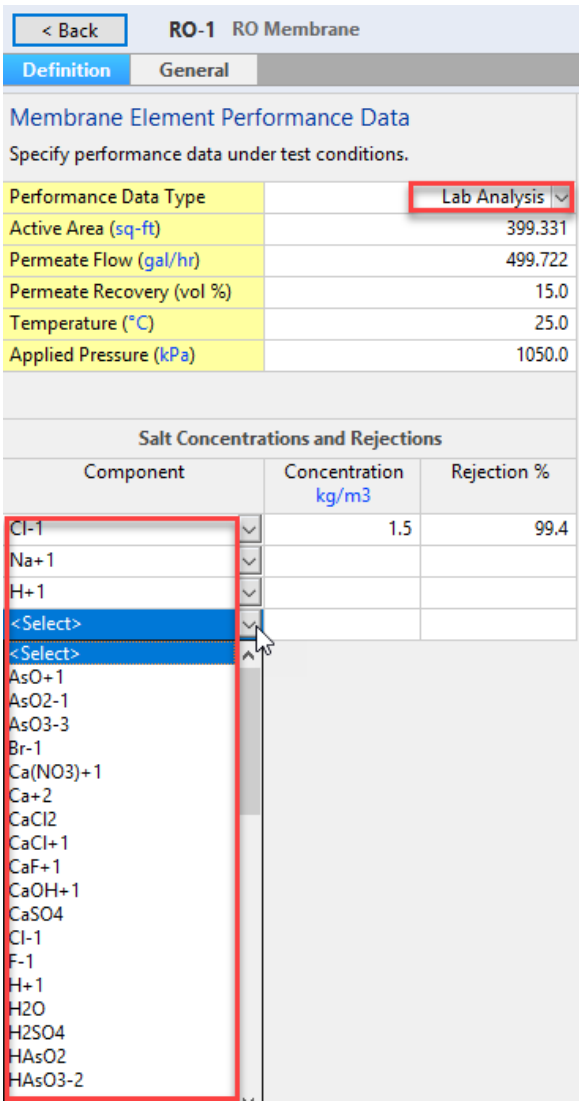


Membrane Model Library: This option allows the user to save the specified data to Library.

Note: If the user has selected the Manufacturer Option, the test rejection components will have species selection as a Molecular format. On the other hand, if the user selects the Lab Analysis Option, the salt concentration and rejection components will have species selection as Ionic format.

For “Manufacturer” option “Salt Concentrations and Rejections” section requires at least one molecular test species entry. On the contrary, “Lab Analysis” option “Salt Concentrations and Rejections” section requires at least one cation test species and one anion test species entry.


< Back
RO-1 RO Membrane
Definition
General
Membrane Element Performance Data
Specify performance data under test conditions.
Performance Data Type
Manufacturer Data Sheet
Manufacturer
Hydranautics
Model
ESPA1
Active Area (sq-ft)
399.331
Permeate Flow (gal/hr)
499.722
Permeate Recovery (vol %)
15.0
Temperature (°C)
25.0
Applied Pressure (kPa)
1050.0
Salt Concentrations and Rejections
Component
Concentration kg/m3
Rejection %
NaCl
1.5
99.4
KCl
<Select>
<Select>
H2O
NaCl
As2O3
CaO
KCl
KF
MgO
N2O5
SO3
K2O
MoO3
NaBr
NiO
7/13/2017 - Source URL.
e Model Library
Add...


< Back
RO-1 RO Membrane
Definition
General
Membrane Element Performance Data
Specify performance data under test conditions.
Performance Data Type
Lab Analysis
Active Area (sq-ft)
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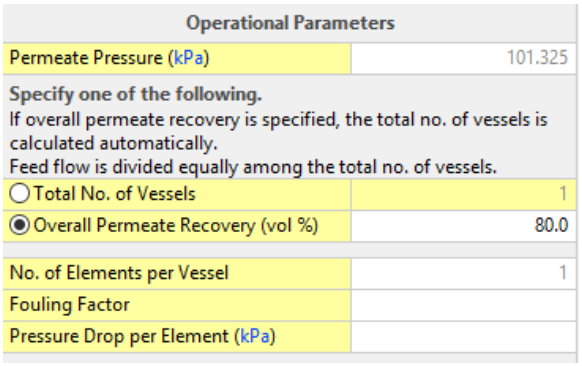
Permeate Flow (gal/hr)
499.722
Permeate Recovery (vol %)
15.0
Temperature (°C)
25.0
Applied Pressure (kPa)
1050.0
Salt Concentrations and Rejections
Component
Concentration kg/m3
Rejection %
Cl-1
1.5
99.4
Na+1
H+1
<Select>
<Select>
AsO+1
AsO2-1
AsO3-3
Br-1
Ca(NO3)+1
Ca+2
CaCl2
CaCl+1
CaF+1
CaOH+1
CaSO4
Cl-1
F-1
H+1
H2O
H2SO4
HAsO2
HAsO3-2

Operational Parameters

The following parameters need to be defined:

- Permeate Pressure
- Total Number of Vessels
- Overall Permeate Recovery (vol %)
- Fouling Factor
- Pressure Drop per Element



Note: Definitions of these different operation parameters can be found in the Appendix.

A more detailed description of the parameters needed in the Operational Parameters is given below:

Permeate Pressure: This calculates the pressure differential across membrane (e.g., difference between the feed pressure and permeate pressure). Pressure differential needs to overcome the osmotic pressure differential of your feed for reverse osmosis to take place.

Total Number of Vessels: When the number of total vessels is given, the overall permeate recovery is calculated automatically.

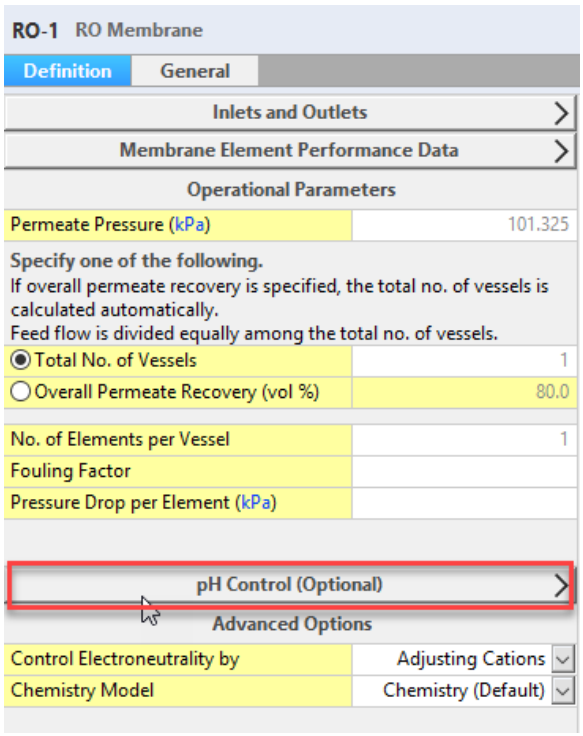
Overall Permeate Recovery: When the overall permeate recovery is given, the total number of vessels is calculated automatically.

Number of Elements per vessel: Number of elements is by default 1, however could be maximum 5. This subdivides the total area of the membrane assembly by the elements entered and calculates each subdivision (or mini-membrane block or element) individually. However, it is important to note that in this option (if your number of elements is greater than 1), the permeates are collected in the common permeate duct after each element, and the residue or concentrated stream from mini-membrane block 1 (or element 1) will be fed to the feed side of the mini-membrane block 2 (or element 2) and so on.

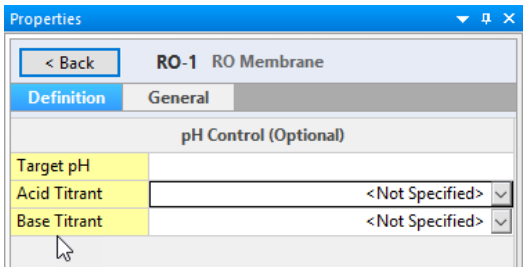
Fouling Factor: Optional. Generally, manufacturers provide the value to the customer in their product sheet.

Pressure Drop per element: Feed side pressure may reduce during operation resulting in a decrease of the hydraulic pressure difference across membrane. Thus, the feed pressure of the 2^{nd} element (e.g., residue pressure of 1^{st} element) may decrease. Users can specify the pressure drop per element. In the absence of the user specified value, software will calculate the pressure drop.

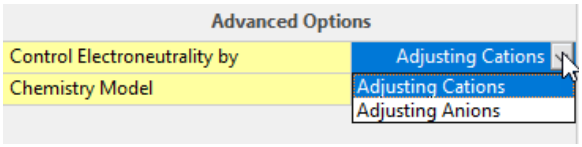
pH control (Optional): This option is turned off by default. If user wants to operate the RO Membrane at a given pH it can be done with this option. Generally, membrane manufactures recommend the pH for specific membrane. For example, a pH 4.5-11.0 may be reasonable for some membranes.



Clicking on pH Control (optional) button, the user can specify the target pH, and the acid and base titrants needed to reach the target pH.



Advanced Options: Under advance options, the user can control the electroneutrality by adjusting either cation or anions. By default, the software adjusts cations.



Guidelines

1. The membrane test methods or specifications are a set of test conditions previously known to membrane users. They would either have this data provided to them by the manufacturer or through lab analysis. These set of test conditions are the conditions at which the membranes are tested. They include, temperature, applied pressure, unit permeate flow rate, recovery vol% and unit active area for the membrane to be used.

2. The next set of values that the user must provide are test rejections. These involve the inflow concentration of the species and their manufacturer provided rejection rate.

3. The user can specify the desired operational specifications for the membrane he/she wants to simulate, such as permeate pressure and permeate recovery. The user also needs to configure the membrane with a specific number of elements/vessel and a total number of vessels. Number of elements per vessel is a fixed number. Currently maximum number of elements is set at 5.

4. It is up to the user to configure the vessel and element numbers and input it in the software, however the software can calculate that number if it is not provided. In that case, the user must provide the

permeate recovery volume. After all these conditions are met, the user can simulate the block to see the block report which contains calculated number of vessels, total membrane area, total water flux along with membrane solute permeabilities and rejection rates in fractions.

Virtual Stream Portal

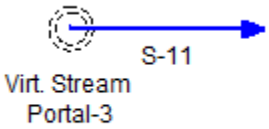
Data Requirement

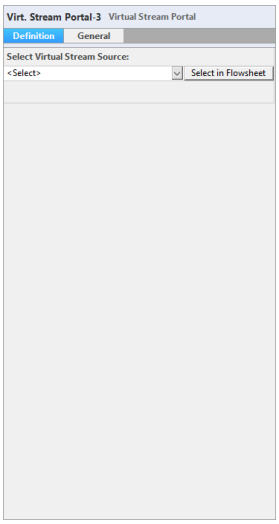
The Virtual Stream Portal allows for a stream to be “Live-copied” to another stream. Live-copied means that the exact parameters of a stream are copied to another stream. If the original stream parameters are updated (either by the user or by the software) then the live-copied stream is also updated.

This differs from a direct-copied stream where the copy takes place only once. In a direct-copied stream, if the original stream is updated the copied stream is not updated.

To use the Virtual Stream Portal a stream must already be defined in the flowsheet.

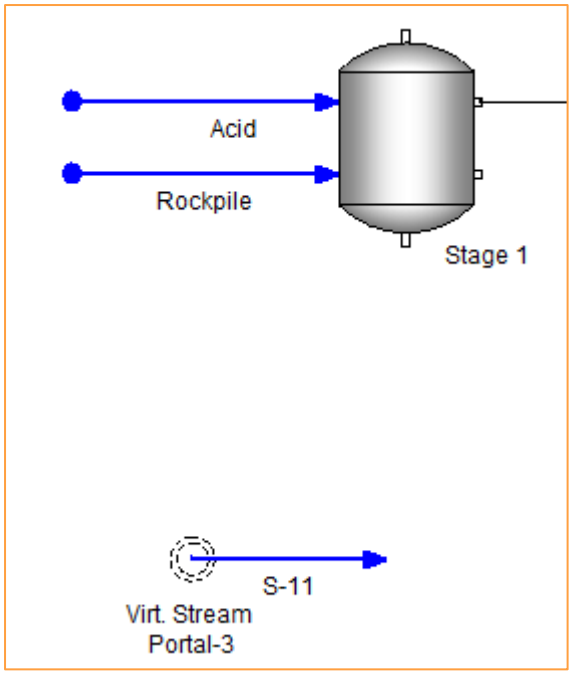
Unit Parameters



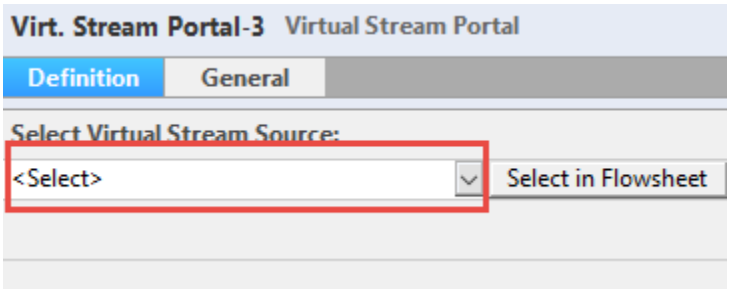


The Virtual Stream Portal has only two inputs. The user can select from a drop-down list of existing stream or select one by clicking the flowsheet diagram.

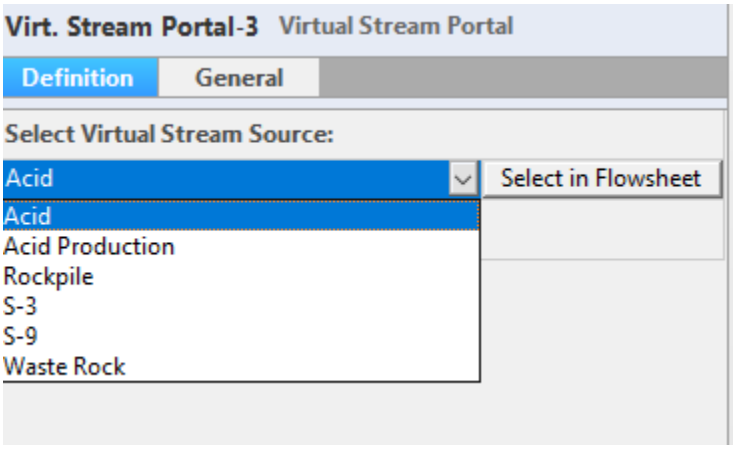
In this example we have a very simple process.



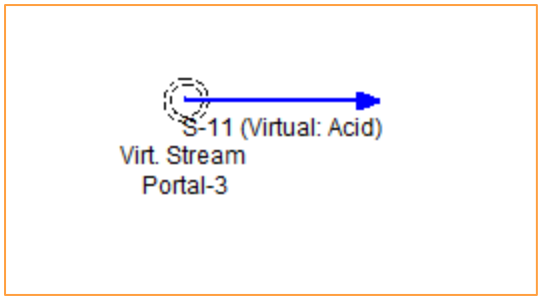
The Virtual Stream Portal can specify the stream by selecting it via the drop-down box



Click the drop-down box and select a stream from the list. Here we are selecting the stream “Acid”

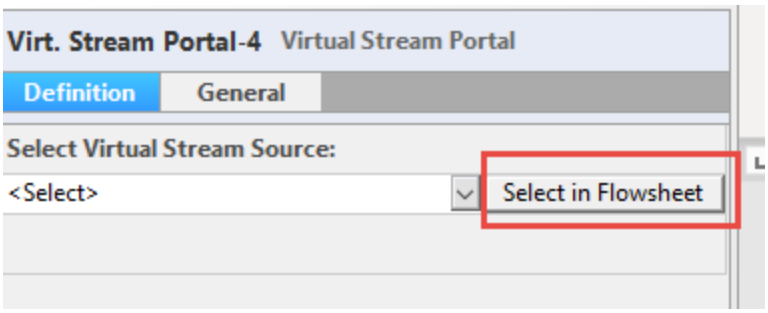


This updated the flowsheet diagram:

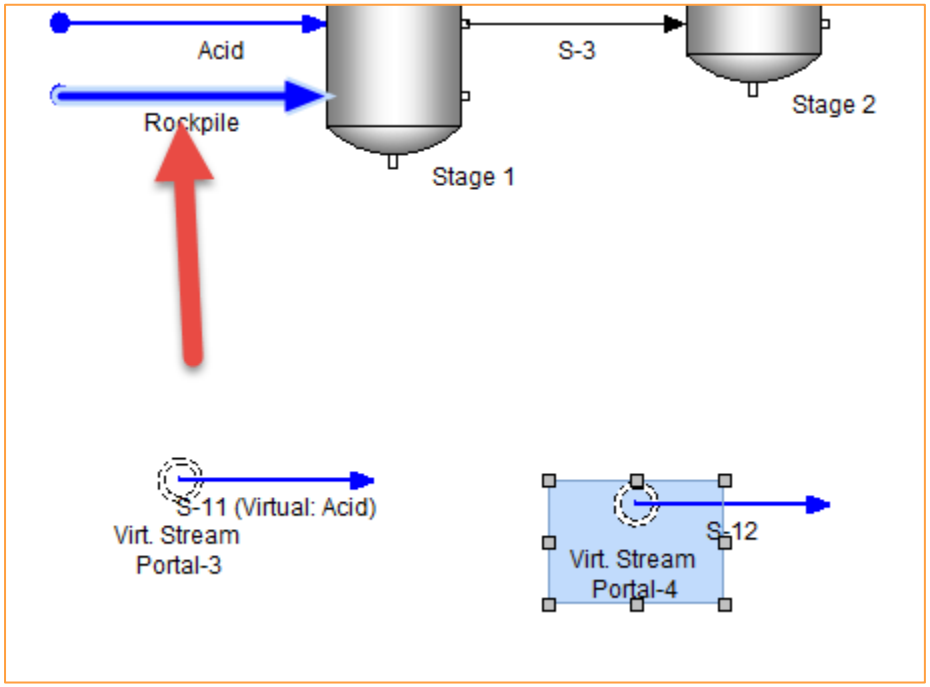


This is now a live copy of the original steam “Acid”

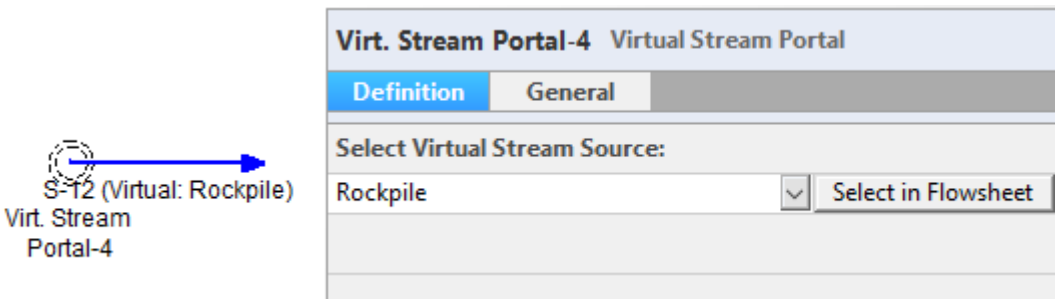
You can also use the diagram to select a virtual stream:



Click the button then click on the desired stream in the flowsheet diagram:

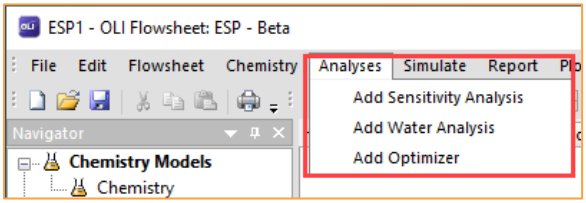


The selected stream is darkened to show that it is selected.


S-12 (Virtual: Rockpile)
Virt. Stream
Portal-4
Virt. Stream Portal-4 Virtual Stream Portal
Definition
General
Select Virtual Stream Source:
Rockpile
Select in Flowsheet

Chapter VI – Analyses Tab

In this section, we will explore how to set up the different Analyses available in OLI Flowsheet: ESP, these are: Sensitivity Analysis, Water Analysis, and the Optimizer tool.



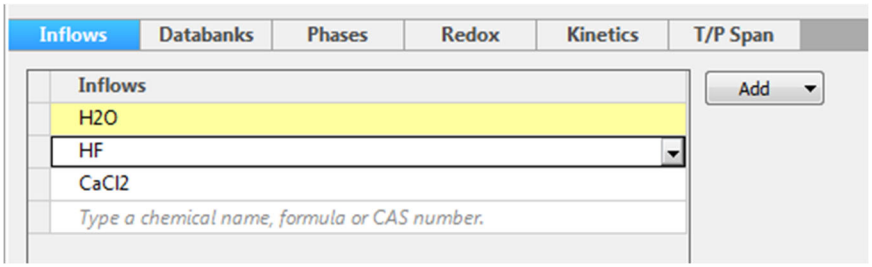
Sensitivity Analysis

HF Titration

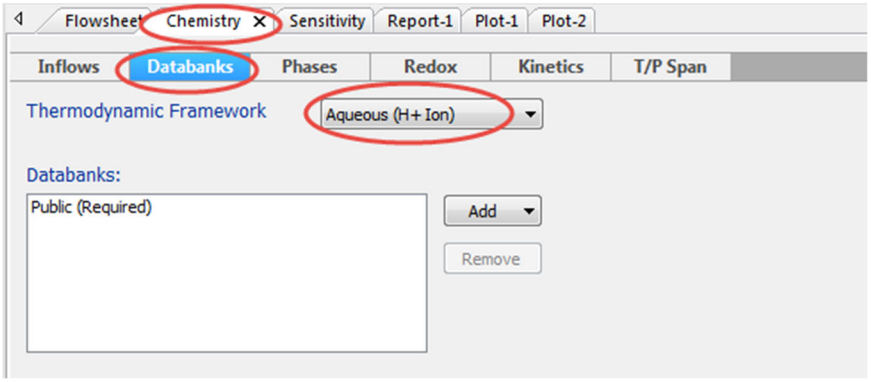
When a stream containing HF is mixed with a stream containing CaCl2, a retrograde effect on pH can be observed. To perform this sensitivity analysis, please follow the procedure listed below.

Chemistry and Thermodynamic Framework

Add HF and $CaCl_2$ in the chemistry model under the chemistry tab:

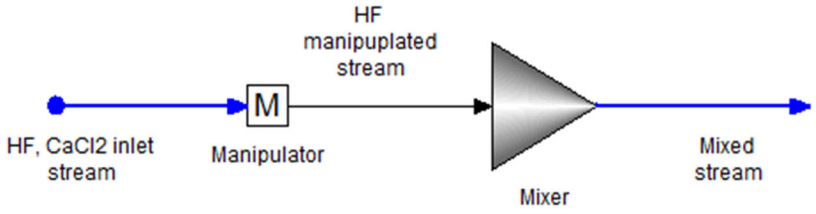


The framework we will be selecting for this example is the AQ framework. If you click on the Databanks tab as shown in the image below, you would be able to select the preferred databank:



Flowsheet

To see the effect of the $CaCl_2$ flow rate on the pH of the mixed stream, a manipulator block is needed for controlling the $CaCl_2$ stream composition.



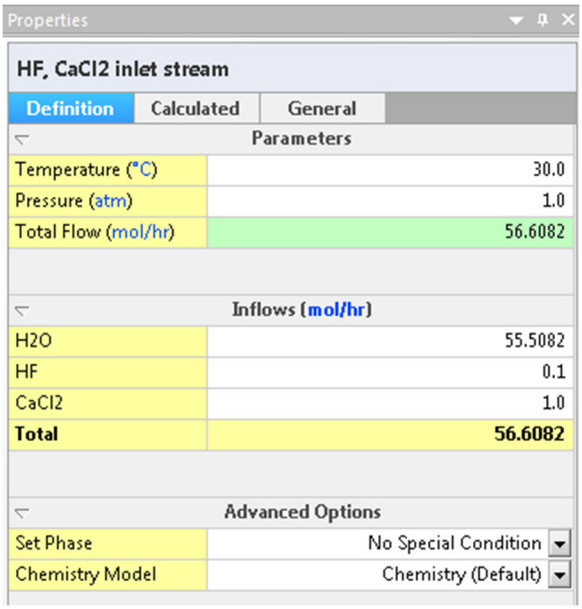
Composition and setup

Input the following set of conditions for the Inflows and the Parameters.

Temperature (°C)	30
Pressure (atm)	1.0
Total Flow (mol/hr)	56.6082
H2O (mol/hr)	55.5082
HF (mol/hr)	0.1
CaCl2 (mol/hr)	1.0

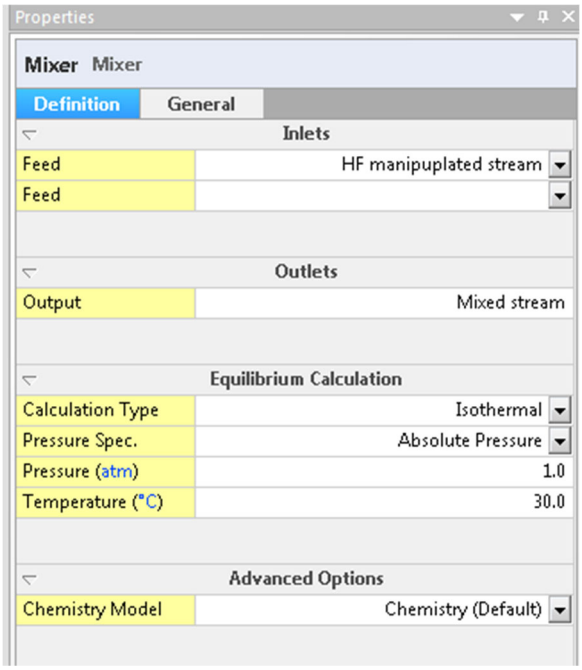
Properties Tab

Definition of HF, CaCl2 inlet stream



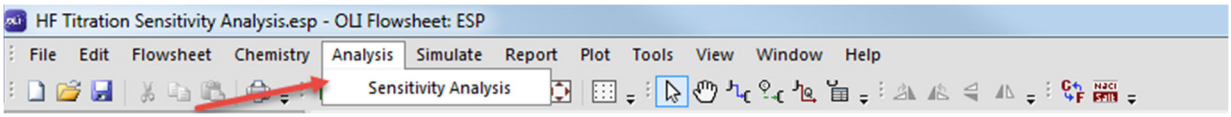
Mixer specifications

This is an Isothermal calculation type with 30°C temperature and 1 atm absolute pressure.

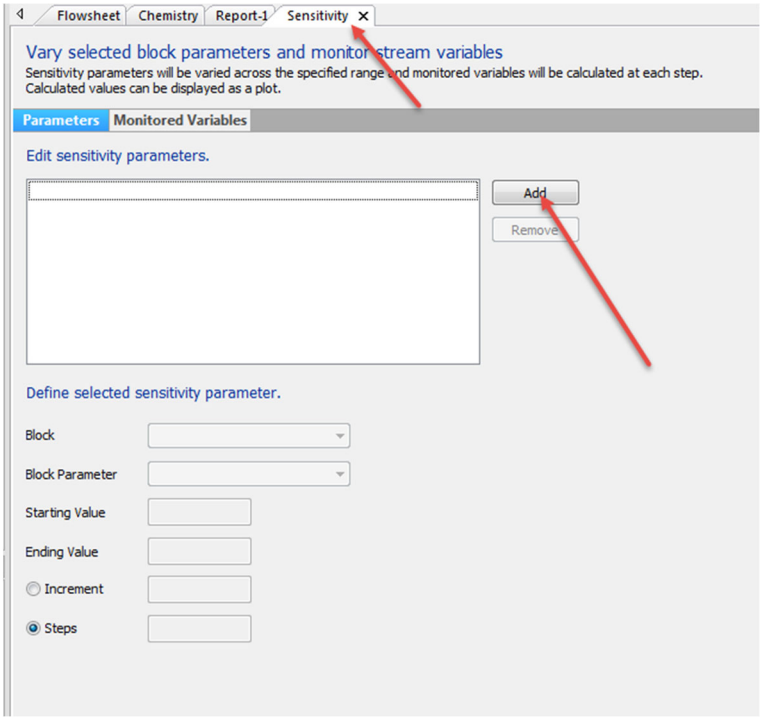


Create Analysis

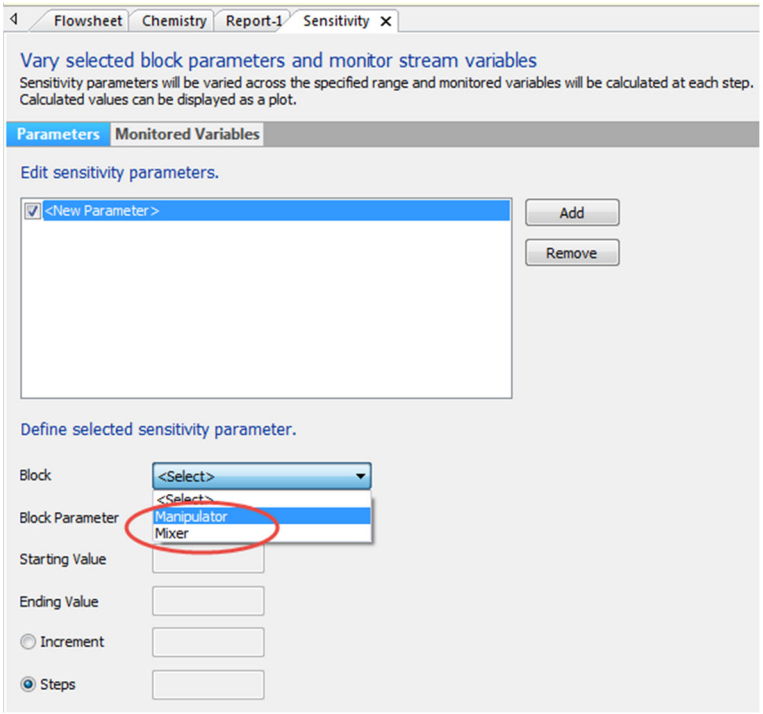
Click on the Analysis option at the top toolbar:



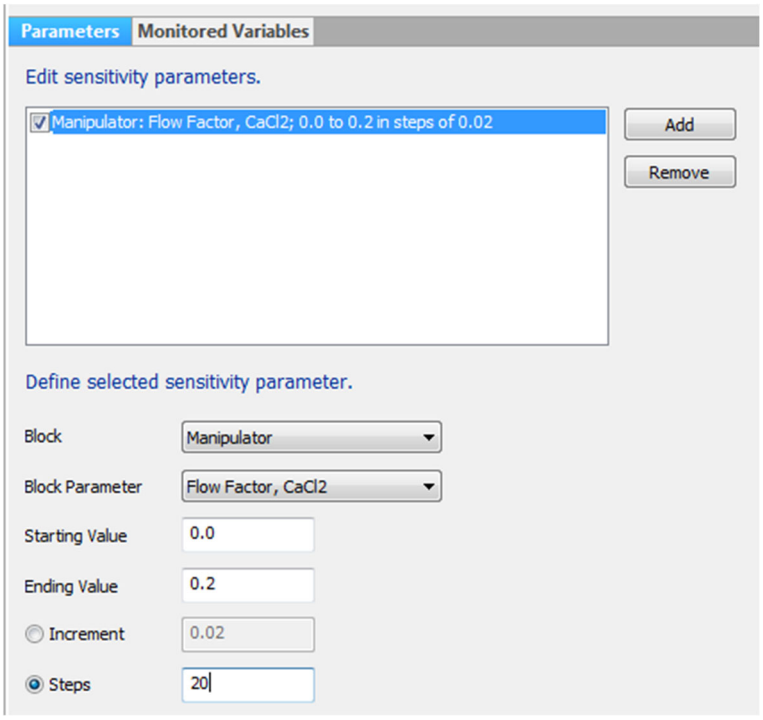
You will see the following screen:



Click on the Add button and select the Block to be Manipulator block.

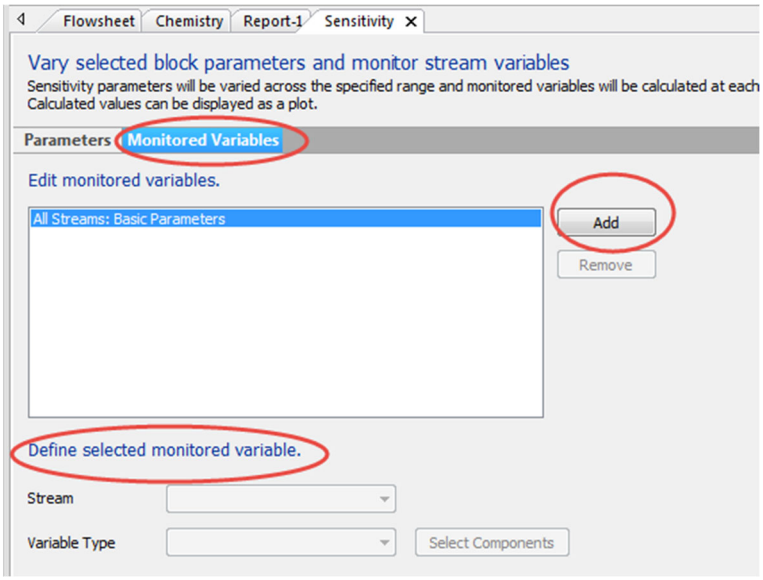


Drop down on the Block Parameter and select the Flow Factor, $CaCl_2$. Your final screen with the starting value 0.0 and ending value 0.2 with 20 steps specification should match the following image:

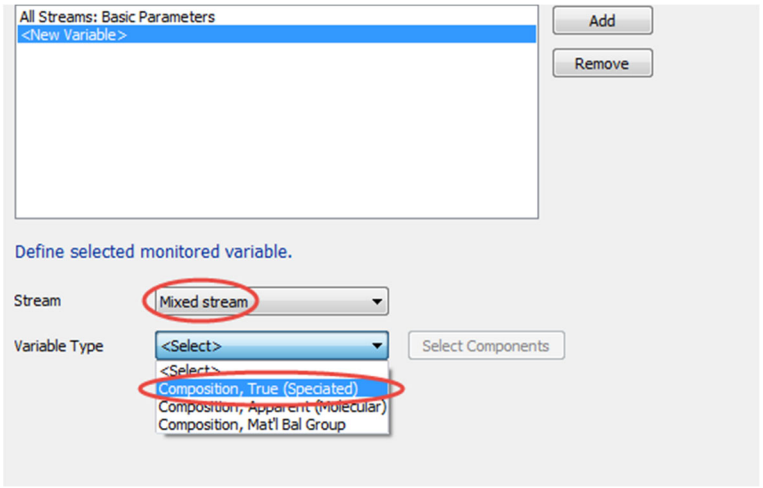


Monitored Variables

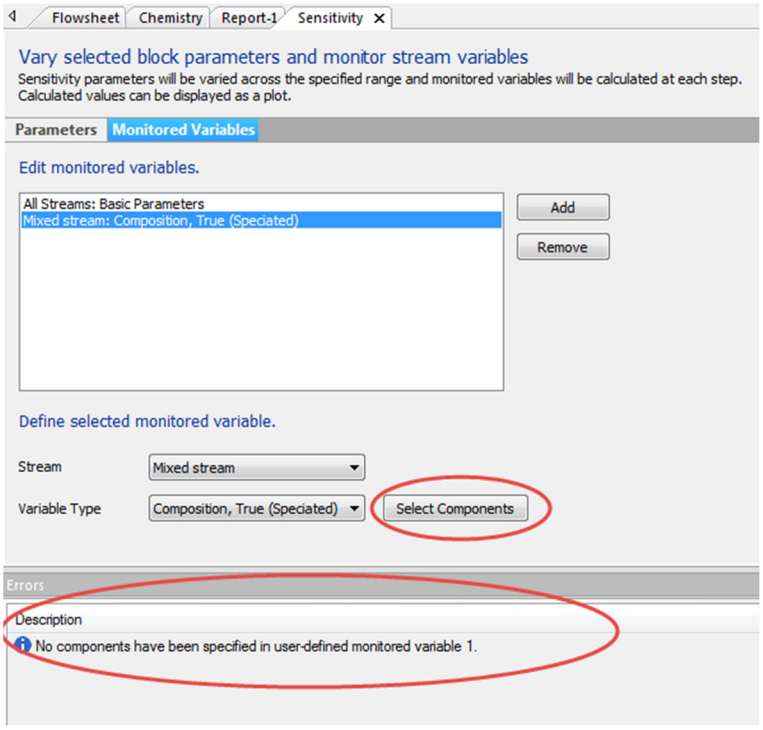
Now that we have selected the parameters to vary, we would need to select the monitored variables to create the plot. If you click on the Monitored Variables tab, you will see the following screen, click on the Add button:



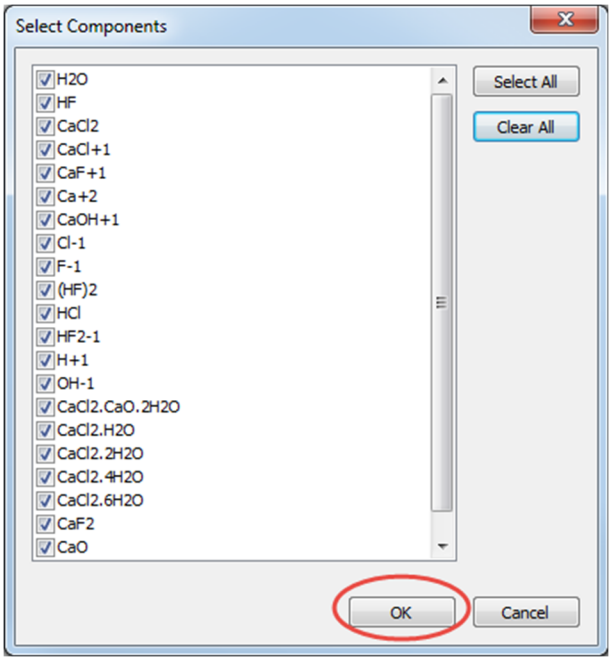
Select the Mixed Stream and the Variable type as Composition, True (Speciated):



You will see the following error message after you make your selection, which will need you to select a specific component/s for the plot:



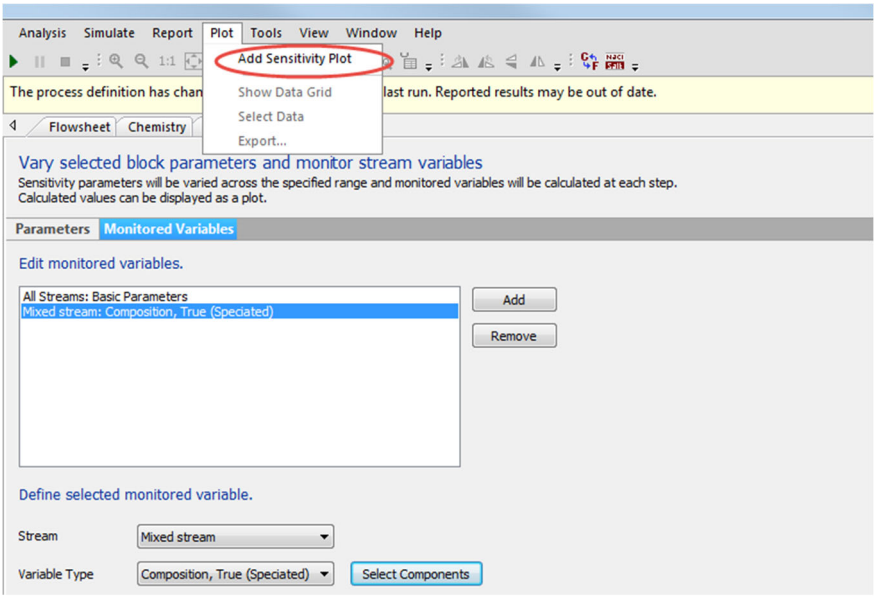
Click on the encircled Select Components option as shown in the image above which will bring you to the following pop-up window. Depending on the case you could either select individual components or in this case all components.



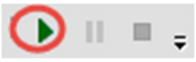
Click **OK**.

Add Sensitivity Plot

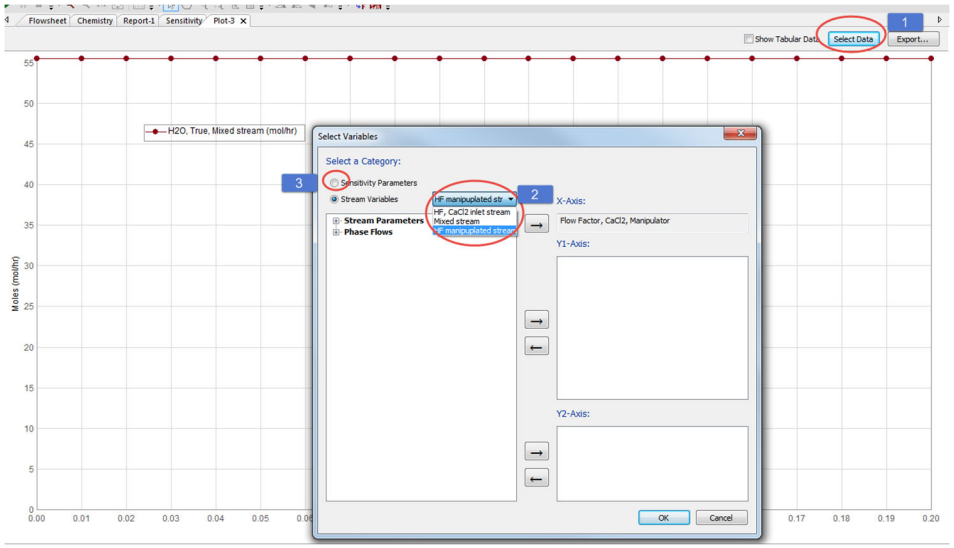
The plot needs to be added manually by going to the top toolbar again and clicking on the Plot option-> Add Sensitivity Plot.



Now you will need to run the file by clicking the Run button or using a shortcut F9.



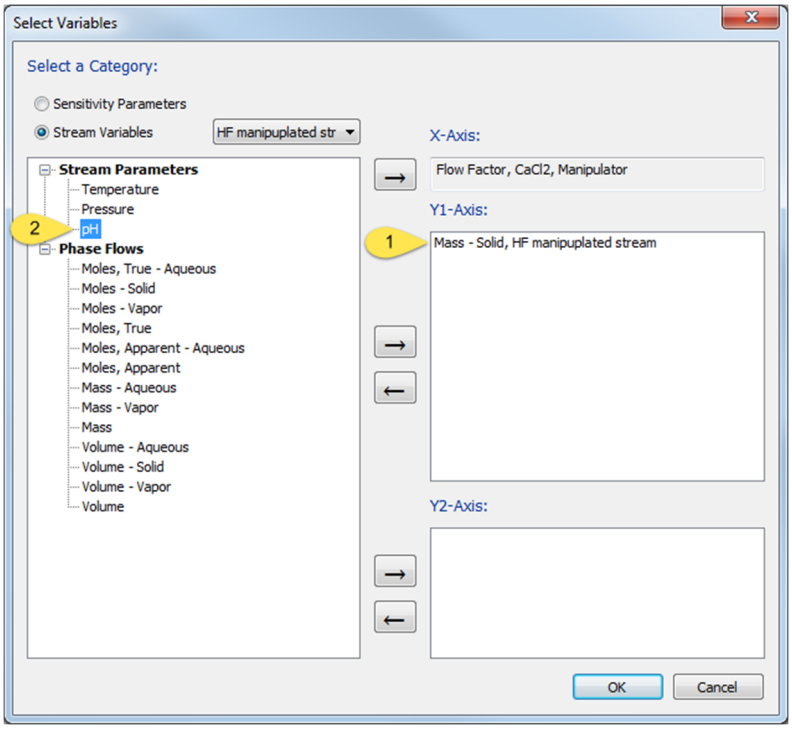
The default plot has H2O Mixed Stream on Y axis, and you will need to click on Select Data button to customize the plot view.



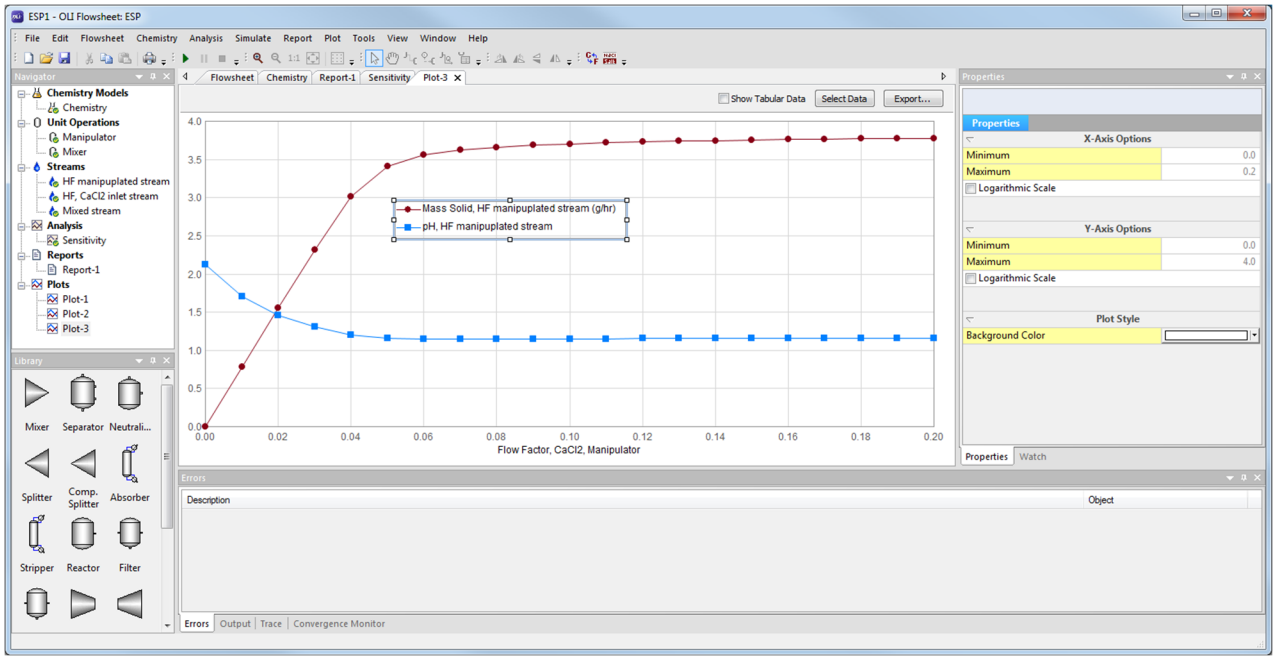
Click on Select Data

Select the Stream that you want to plot the stream variables for, in this case, since we are interested in the pH of the mixed stream, we will select the HF manipulated stream.

Add Mass of Solid phase for the manipulated stream and the pH as shown below:



We can see from the plot below that the pH drops as the solid starts forming:



As you can see in the Properties Pane, X-axis and Y-axis can be manipulated.

You can download a worked example of this case from here: [HF Titration Sensitivity Analysis]

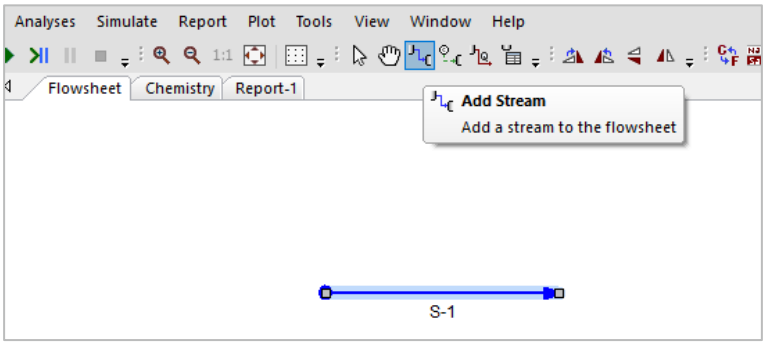
Water Analysis (Ionic Input)

OLI Flowsheet: ESP also allows the user to enter a stream as an ionic input. In this section, we will input dissolved species concentrations and other measured properties into a *Water Analysis* to model a hypothetical water sample. We will also explain the different reconciliation options available in the *Water Analysis.*

The table below shows the hypothetical water that we will create as an example.

Water Analysis							
Cations, mg/L		**Anions, mg/L**		**Neutrals, mg/L**		**Measured Properties**	
Na+1	36000	Cl-	57000	CO2	15	Temperature	25 ºC
K+1	300	SO4-2	250	H2S	5	Pressure	1 atm
Ca+2	600					pH	6.67
Mg+2	150					Alkalinity	600
Sr+2	80					Density	1.064 g/ml
Ba+2	5					Total Dissolved Solids	96280 mg/L

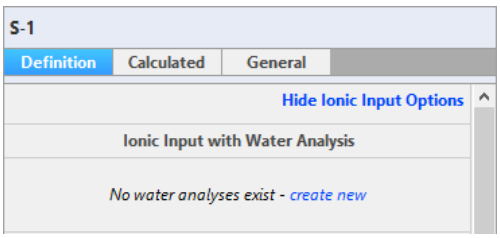
Create a **Stream** in the Flowsheet



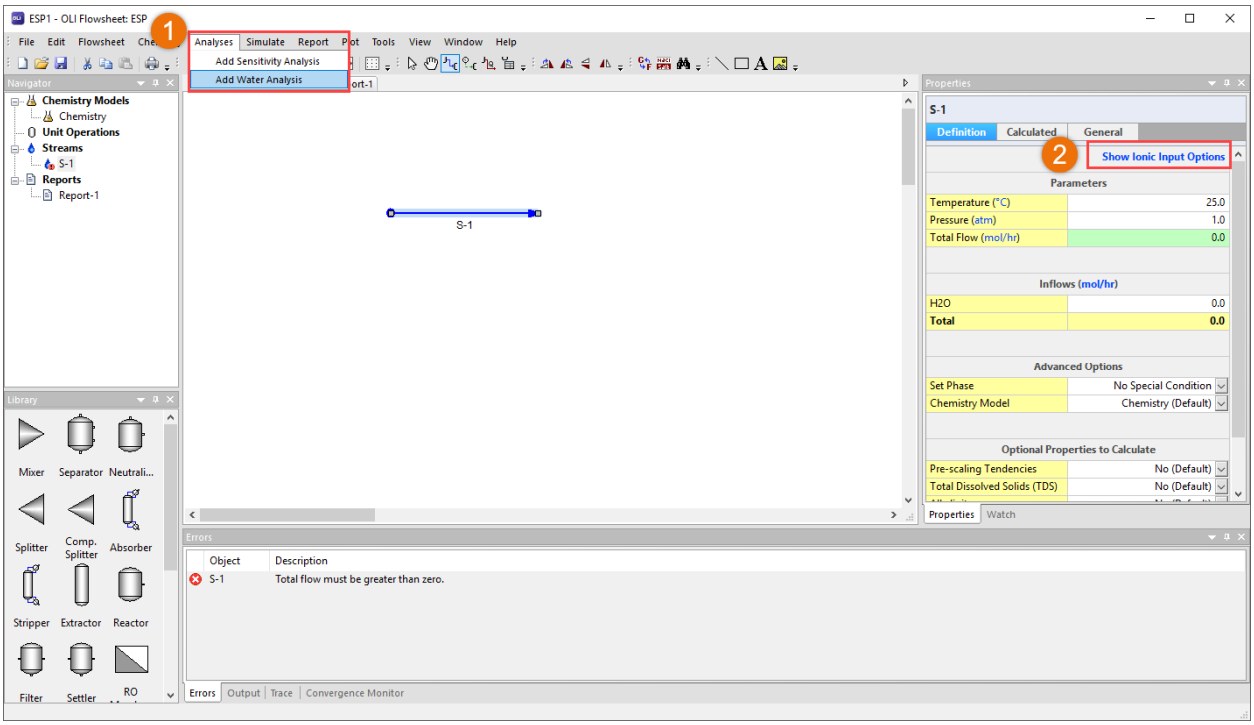
Add a Water Analysis. You have two options:

Option 1 – In the **Menu** Bar go to Analyses>Water Analyses, or

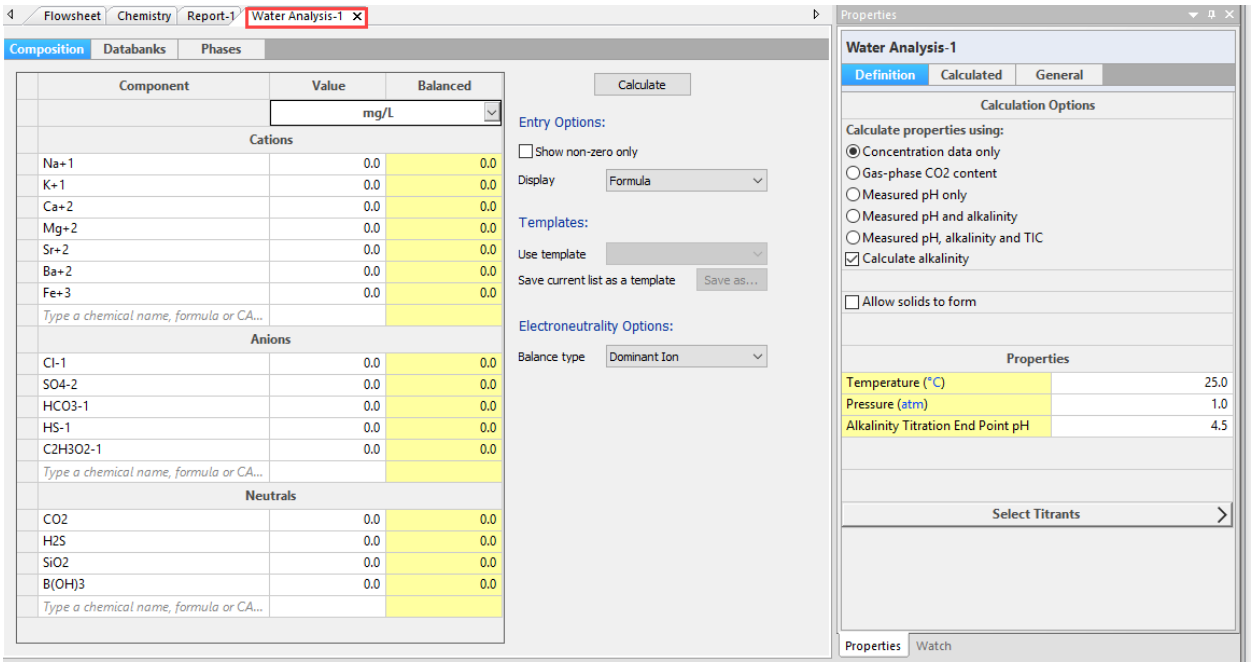
Option 2 – In the **Properties** panel, click on **Show Ionic Input Options.** Then, click on *create new*, since a water analysis has not been created yet.



The two options for ionic input are show in the figure below.



For this example, we will use **Option 1** – **Menu Bar** > Analyses > Water Analyses. This should open a new tab named **Water Analysis**.



Enter the composition of the Water Analysis given in the table above. Make sure to enter the concentration of cations, anions, and neutrals, as well as the conditions at which the properties of the solution (such as pH, alkalinity, density, etc.) were measured.

Reconciliation Options

When reconciling a Brine Analysis, there are five options for reconciliation:

%□揉□檬¡溢 **Concentration Data Only:** The software will run an electroneutrality reconciliation only, and then compute the water properties such as pH, density, etc., based on the entered concentration of neutral, cations, and anions species. In the **Concentration Data Only** option you may allow the program to pick the species to adjust for electroneutrality or you may manually choose the species to perform the adjustment.

Use Concentration Data Only when:

- Species concentrations are accurate
- Need to calculate properties using concentration data only
- Good for what-if iterations

%□揉□檬¡溢 **Gas-phase CO2 content (mole%):** Frequently it is simpler and more stable to measure the gas-phase CO_2 that is separated from the brine at the sampling point. When matched with another measured variable, usually alkalinity, the concentration of the carbonate species and the pH can be calculated. OLI Flowsheet: ESP performs a CO_2 gas fraction calculation by taking the P_{CO2} and the calculated alkalinity (based on the water analysis data) to reconcile the system for pH and carbonate properties. The CO_2 is adjusted to match a saturated gas composition.

Use Gas Phase CO2 Content (mole%) or Fix CO_2 Fraction in Gas when:

P_{CO2} in produced gas is known
Need to calculate at T/P under which the gas measurement was taken
ScaleChem adjusts $CO2_T$, until the calculated P_{CO2} equals the entered value

%□揉□檬¡溢 **Measured pH Only:** Many brine analyses report a measured pH. This pH may or may not match the pH calculated by the software. The cause may be an incomplete and/or inaccurate brine description. The software will run both an electroneutrality and pH reconciliation. This type of reconciliation will match your recorded pH. Additionally, the software will compute the water properties such as, density, electrical conductivity, etc. The pH of the solution is automatically adjusted by the software by adding either HCl or NaOH, or you may select your preferred acids and bases to adjust the pH.

Use Measured pH Only when:

pH is accurate
Need to calculate at T/P that the pH was taken
ScaleChem adjusts H^+, Cl^-, until the calculated pH matches the measured value

%□揉□檬¡溢 **Measured pH and Alkalinity:** The purpose of the Measured pH and Alkalinity reconciliations is to match the computed pH and alkalinity values with those you measured. The software will run an electroneutrality, pH and alkalinity reconciliation. Additionally, the software will compute the water properties such as density, electrical conductivity, etc. The pH of the solution is automatically adjusted by the software by adding either HCl or NaOH or you may select your preferred acids and bases to adjust the pH. The Alkalinity is automatically calculated by the software, using CO_2 as the alkalinity titrant, H_2SO_4 as the alkalinity pH titrant and 4.5 as the alkalinity end point pH. You can also change a different alkalinity titrant if you prefer.

Use Measured pH and Alkalinity when:

pH and alkalinity data are accurate
Need to calculate at T/P that the pH was taken
ScaleChem adjusts H^+, Cl^-, and CO_2 until the calculated pH/alkalinity equals measured values

%□揉□檬;盎 **Measured pH, Alkalinity, TIC:** The purpose of this reconciliation is to match the measured pH, total alkalinity, and the total inorganic carbon (TIC). The Total Inorganic Carbon (TIC) is adjusted using CO_2 as the alkalinity titrant, H_2SO_4 as the alkalinity pH titrant and 4.5 as the alkalinity end point pH. The software adjusts the acetate concentration (organic acids) to match the total Alkalinity value by adding or removing acetic acid. You cannot however change the CO_2 or acetic acid for the alkalinity adjustment. These are fixed by the software. The target pH is obtained simultaneously by HCl or NaOH. You may select your preferred acids and bases to adjust the pH instead of the default HCl and NaOH.

Use Measured pH, Alkalinity, and TIC when:

pH, alkalinity, and TIC data are accurate
Calculate at T/P that the pH was taken
ScaleChem adjusts H+, Cl-, CO2 and Acetic Acid until the calculated pH/alkalinity/TIC equals measured values

Additionally, there is the option to **Calculate Alkalinity**: It is important to note, that this is only an alkalinity calculation based on the concentration entered, it is not an alkalinity reconciliation.

Optimizer Analysis

Note: *The optimizer tool requires an add-on license*

This section of the manual is under constant revision. Please see the latest updated information and examples at https://wiki.olisystems.com/wiki/OLI_Flowsheet:_Optimizer_Documentation_and_Examples

In this example, we will use the Optimizer Analysis tool (hereafter referred to as the Optimizer) to determine the minimum amount of wash water needed to prevent under-deposit corrosion in an overhead crude distillation unit. The basic application of the under-deposit corrosion has been found in many places in the OLI literature.

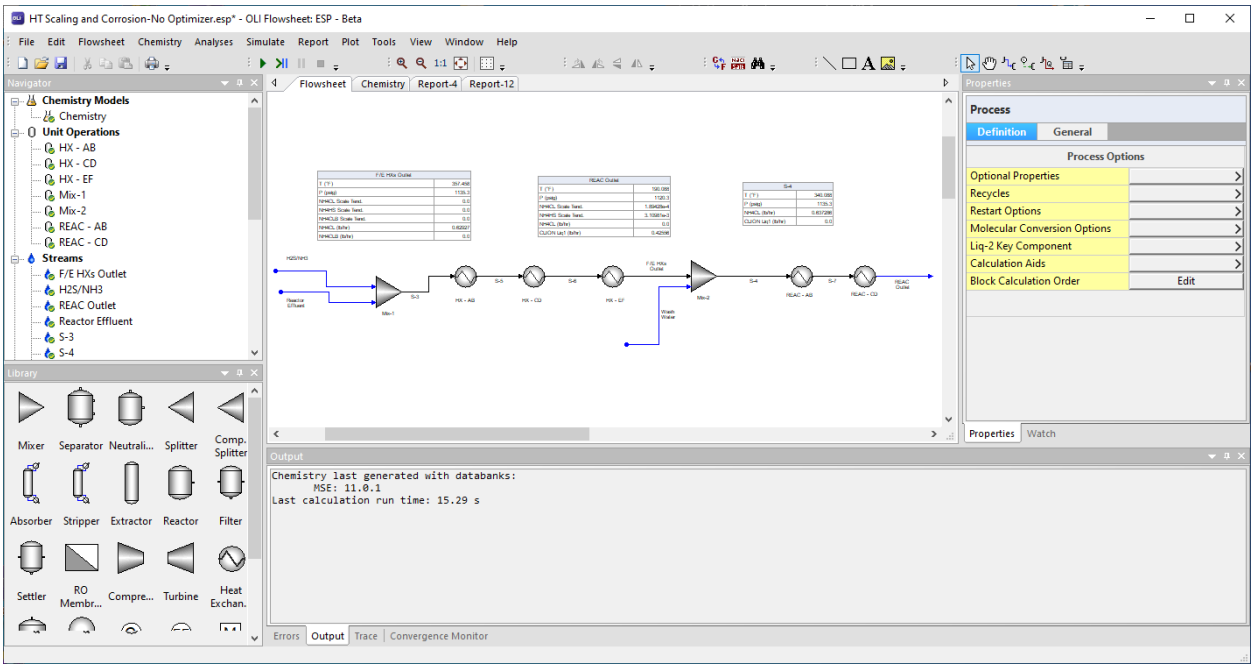
Describing the Sample Case

Please download the case file without the optimizer added. The case can be found here:

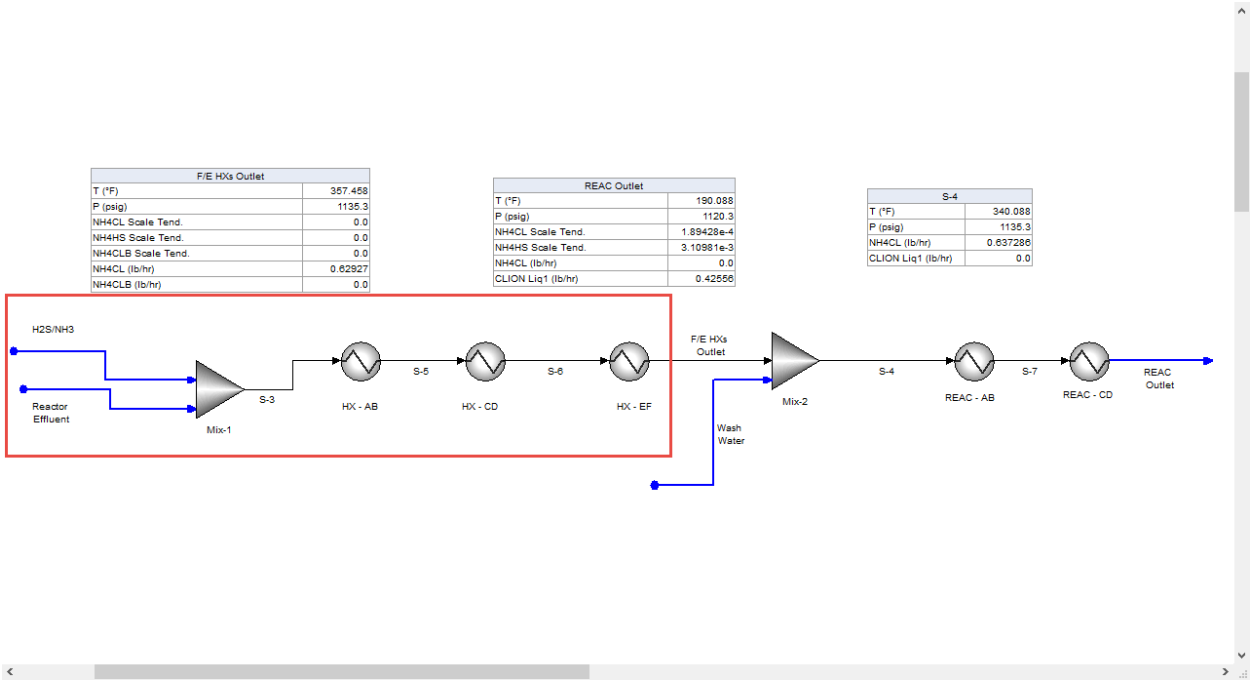
https://wiki.olisystems.com/wiki/images/7/71/HT_Scaling_and_Corrosion-No_Optimizer.zip

Unzip the file into a working folder and then open the case file with OLI Flowsheet: ESP version 11.0 or later.

You should see the following:

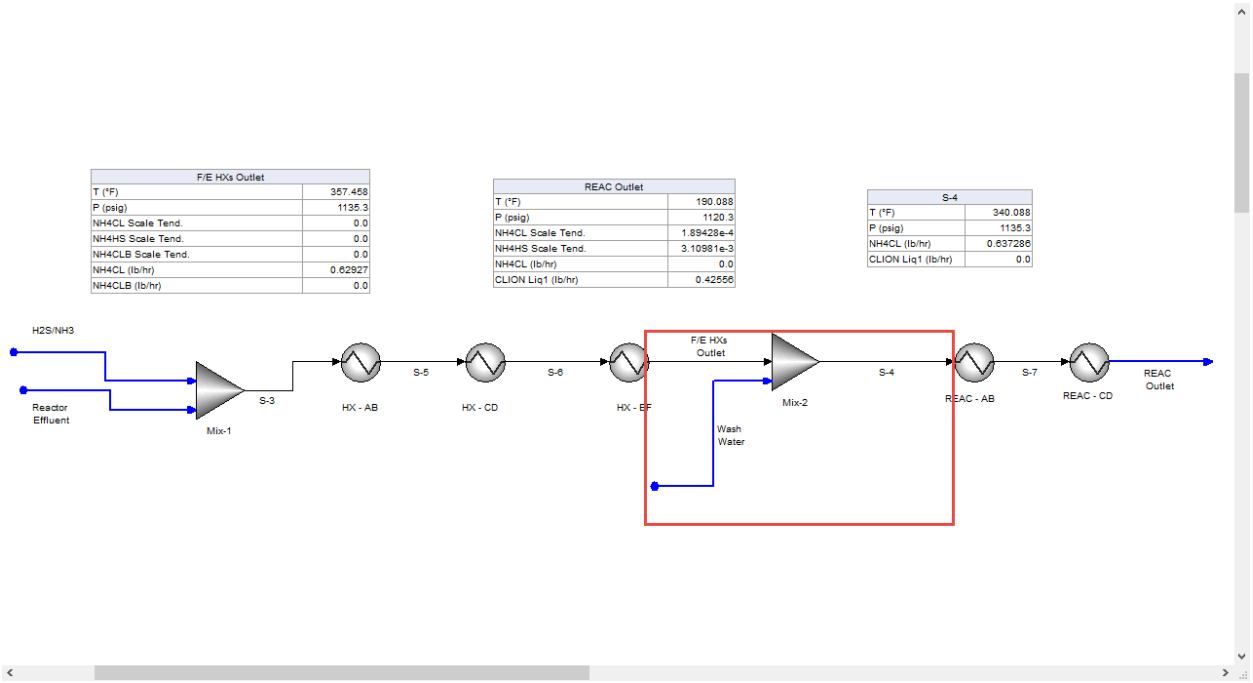


Let us describe the process in a bit more detail.



This section of the process represents the top of the crude column. The vapor distillate and the neutralizing amines (in this case it is just ammonia – NH_3) are mixed and then cooled in a series of steps. This represents natural cooling of the overhead line exposed to the environment.

It is known from experience that at a particular temperature a solid phase can condense out of the vapor phase and this solid will adhere to the surface of the overhead line. In this case the solid of concern is ammonium chloride (NH_4Cl). These solids are hydroscopic and can result in grabbing water and forming corrosion hotspots. Operators usually inject some wash-water to dissolve these deposits and thus protect the overhead lines.



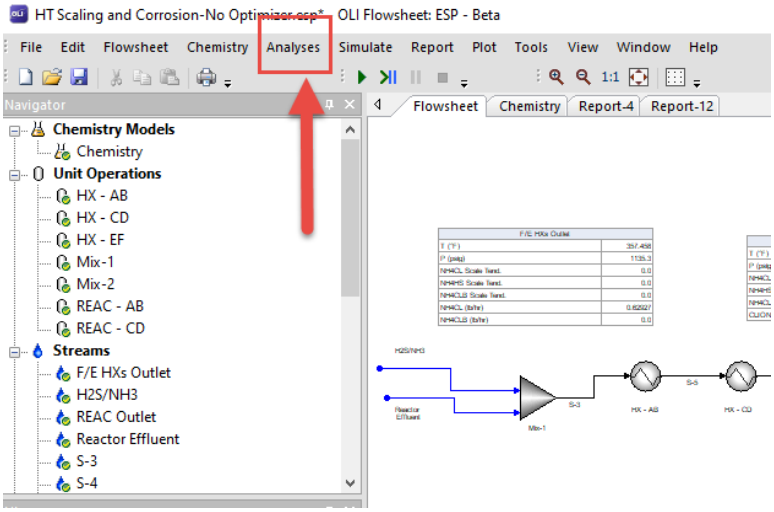
This section represents the injection of the wash-water. This will also result in a further cooling of the line before it reaches the air coolers just downstream. Water is expensive and can cause degradation of the

product so it will eventually have to be removed. It will be required to remove this added water later in the process. It would be of great benefit to allow the program to optimize the amount of wash-water to be added to just minimize the formation of the under-deposit solids.

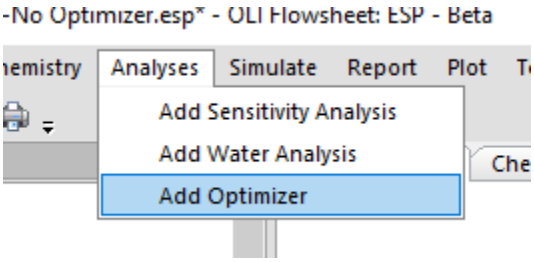
The OLI Flowsheet: ESP program can accomplish this for us.

Adding the Optimizer Analysis

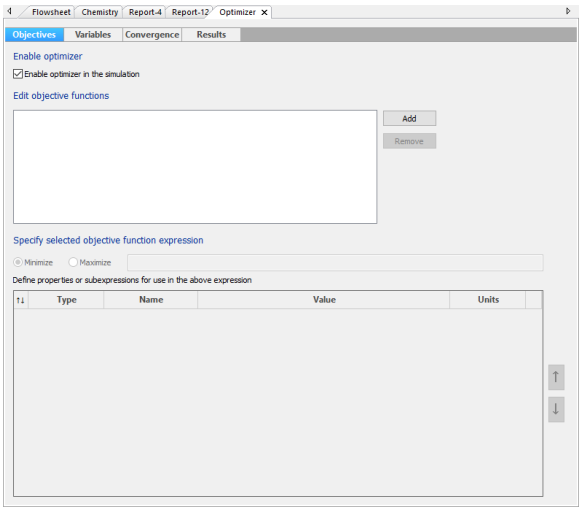
We start by adding a new type of analysis called an optimizer. Select a new optimizer from the **Analyses** menu item:



And then select *Add Optimizer*

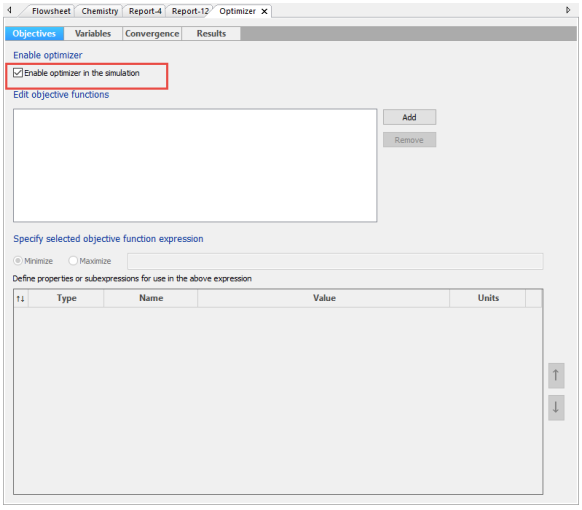


The initial panel looks like this:



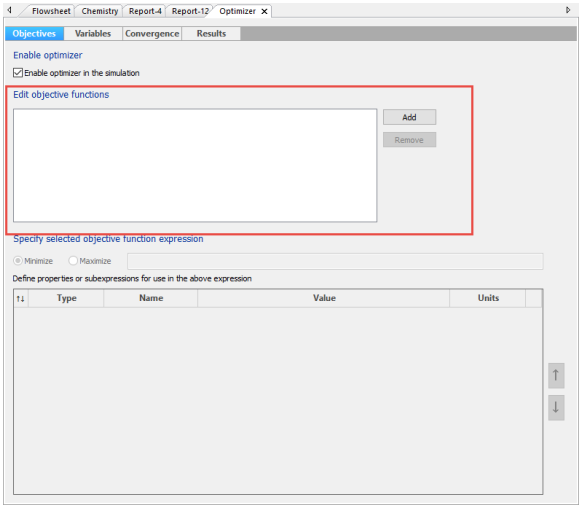
There is quite a bit of new features here so each should be discussed in turn.

Enable optimizer



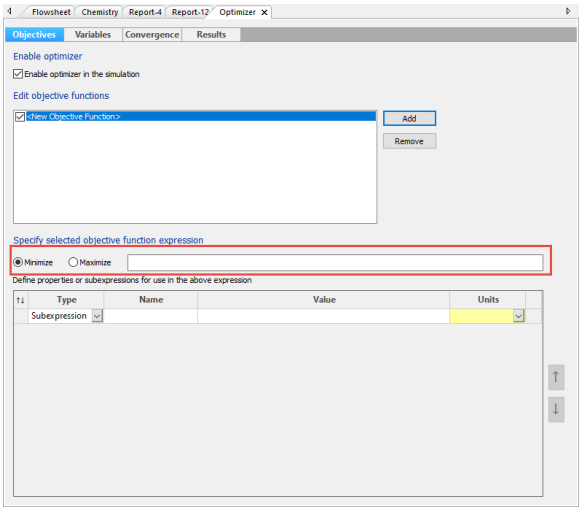
Check this box to enable the optimizer for this document. Once you have optimized this function you can update the process file with the new value(s) and continue to run your optimization. Since it is already optimized at that point you can disable the optimizer code. For now, we will leave this checked.

Edit objective functions



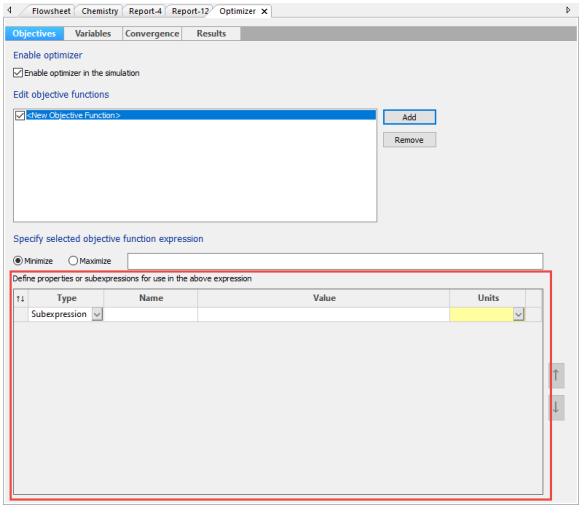
In this box we will add our objective functions. These functions are as varied as your imagination. OLI will continue to post new techniques as we develop them on our wiki page (see above). We will fill out this panel in the next section. To enable this panel, we would click the **Add** button. Do so now.

Specify the selected objective function expression



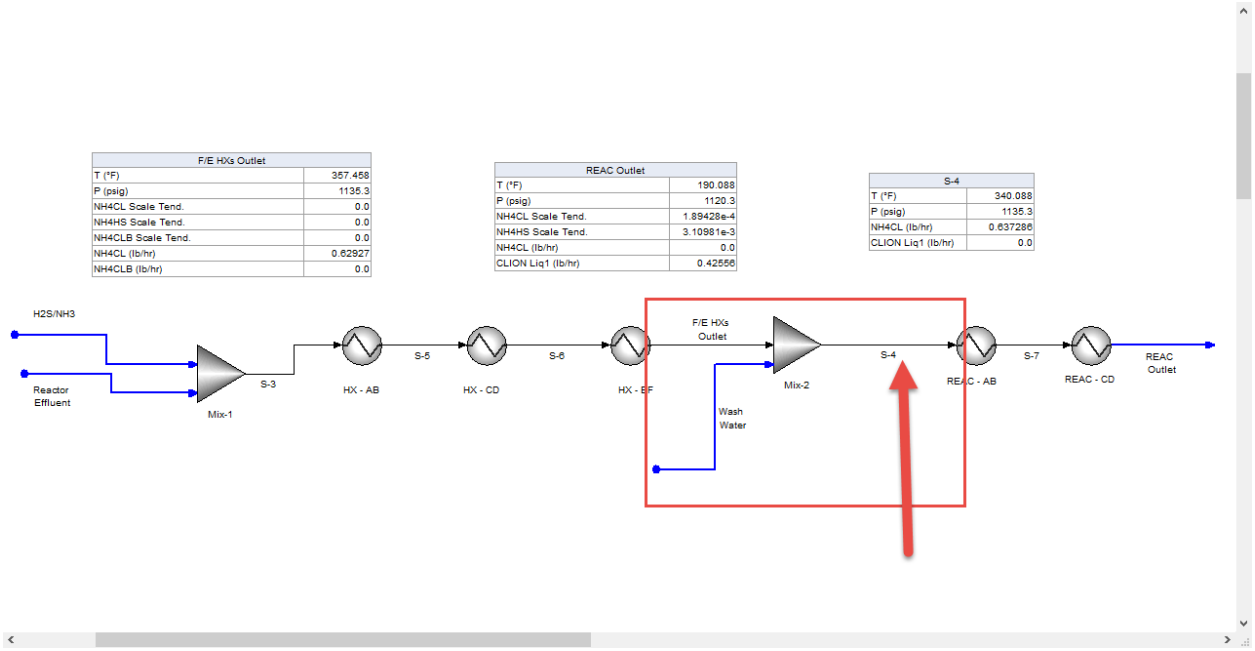
You will eventually define whether to minimize or maximize the objective function. This will become clearer in a minute.

Define properties or subexpressions for use in the above expression



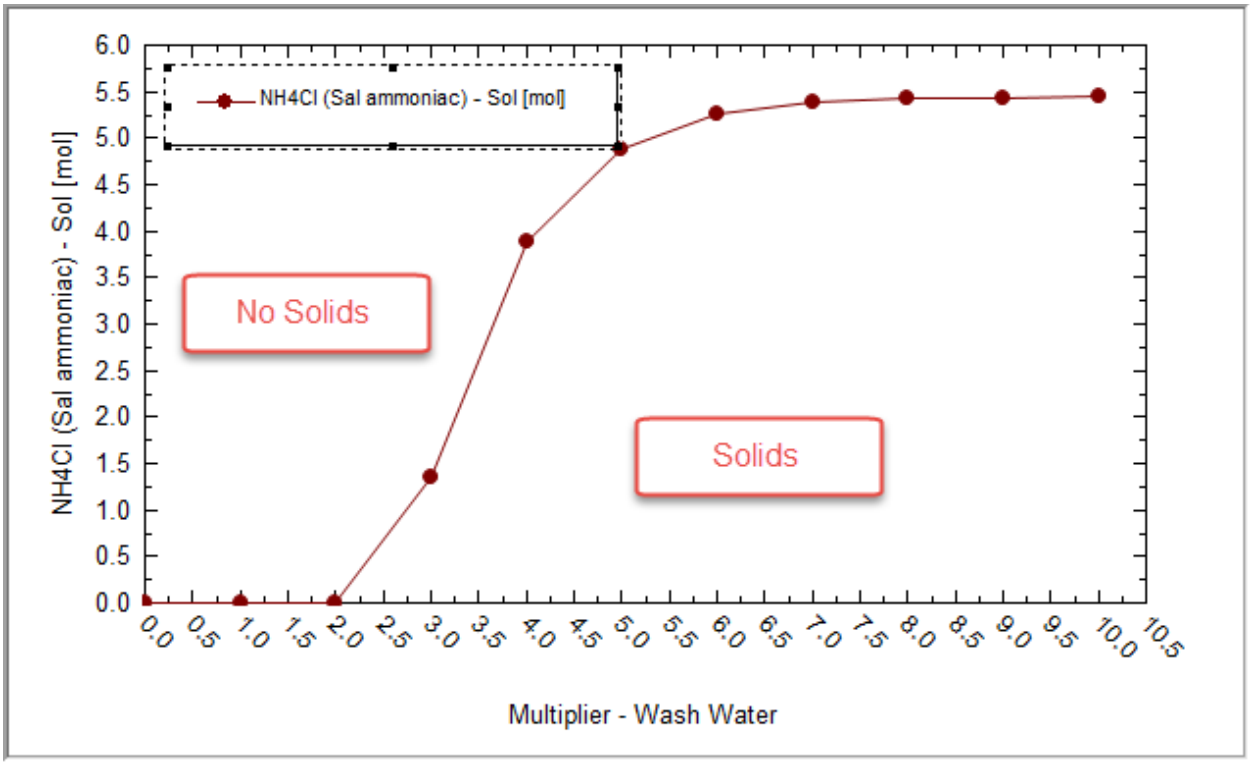
Here is the meat of the optimizer. We will create a series of expressions and variables that allow us to have something to optimizer.

Let us dig into this further.



Our objective is to add just enough “Wash Water” to make sure we have no solids in stream “S-4”. This is a round-about way of saying we want to minimize the amount of wash water.

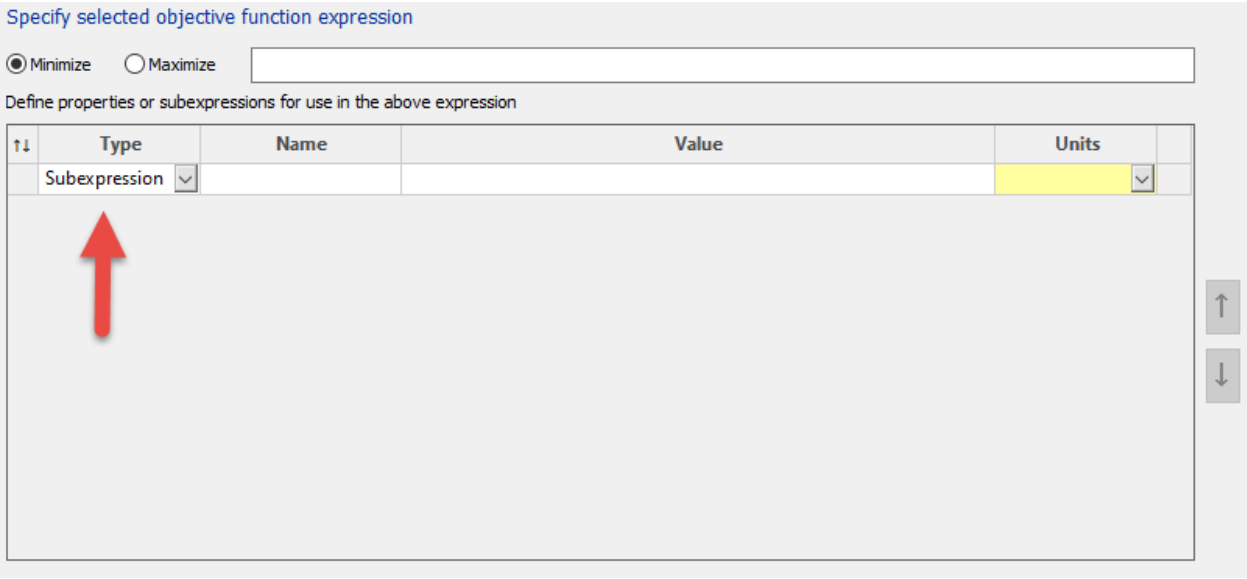
We now must discuss some things that are unique to OLI Flowsheet: ESP. Imagine a plot where we have solids on one side of a break point and no solids on the other. Here is such an example (using OLI Studio Studio on this case).



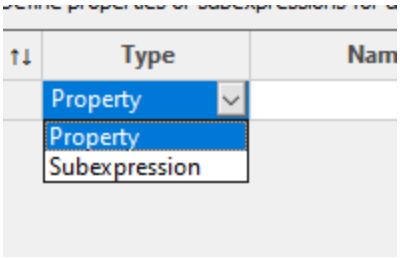
The question you may have is: “Why not use a controller to find the minimum amount of wash water?” There are two answers, 1-a controller only finds a set point which the operator needs to define which may or may not be a minimum value and 2-when the controller accidently solves in the “No Solids” region, there is no slope to the curve to find its way back to a solution.

This is where writing your own objective function works so well. We are going to define a variable which will be the sum of all the chloride species (both liquid, organic and solid phases) which is a continuous function in the numerical space.

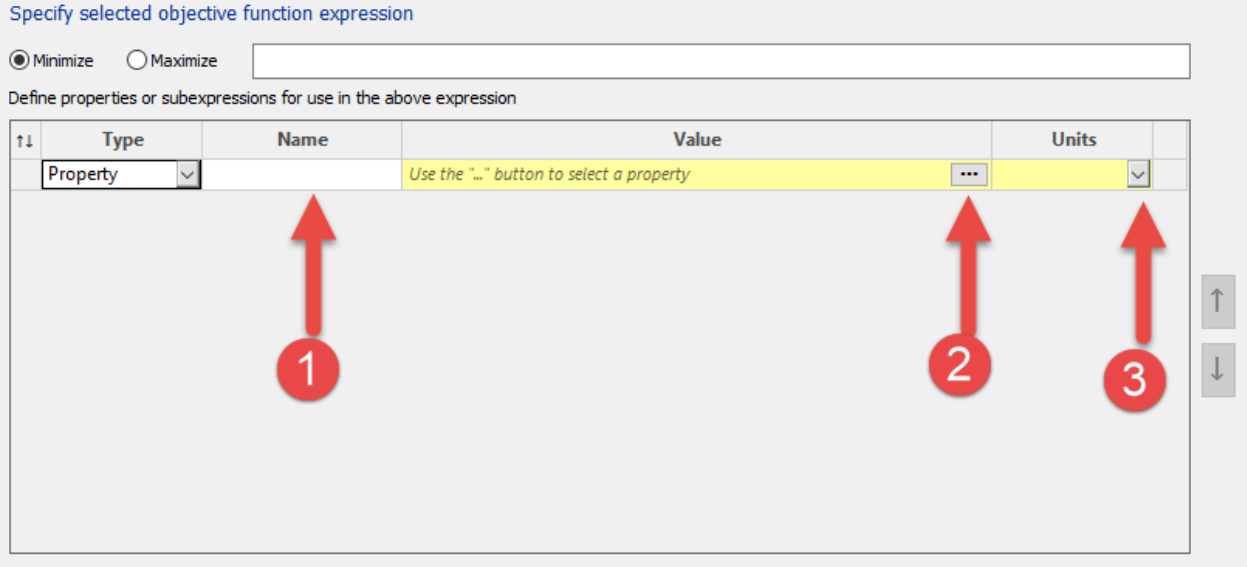
We are first going to define a variable which is the amount of chloride species in the liquid phase of our target stream “S-4”.



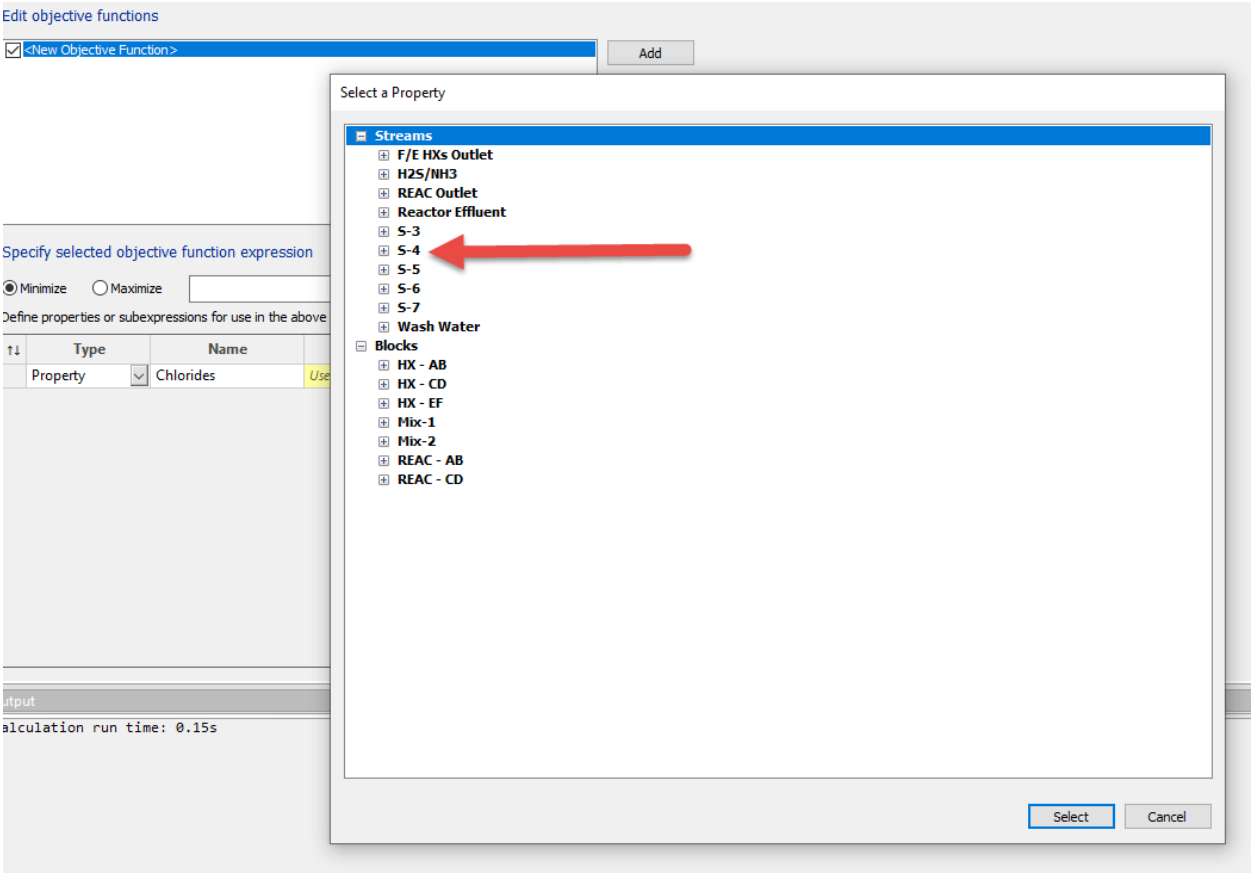
Change the drop-down box from ***Subexpression*** to ***Property***



We will now start to enter our first variable

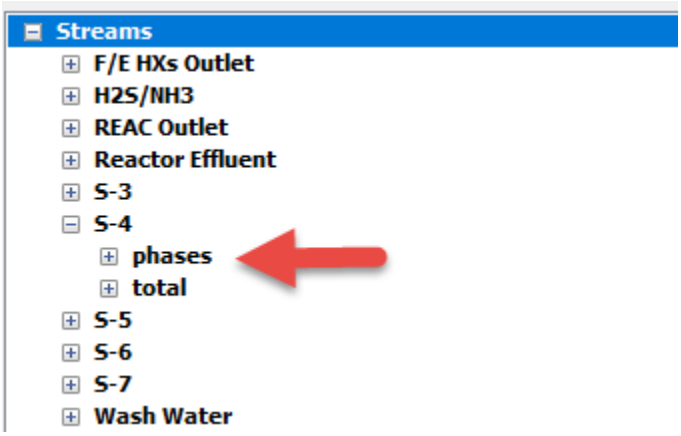


In the box #1 enter the name “Chlorides” then click the “…” box (#2) to enter the expression and then finally enter the units in Box #3 when it becomes active.

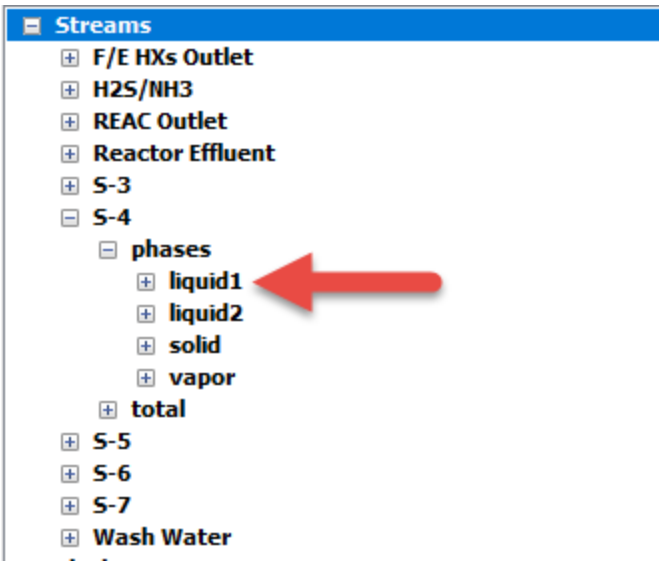


This is what the dialog looks like after clicking the "…" box

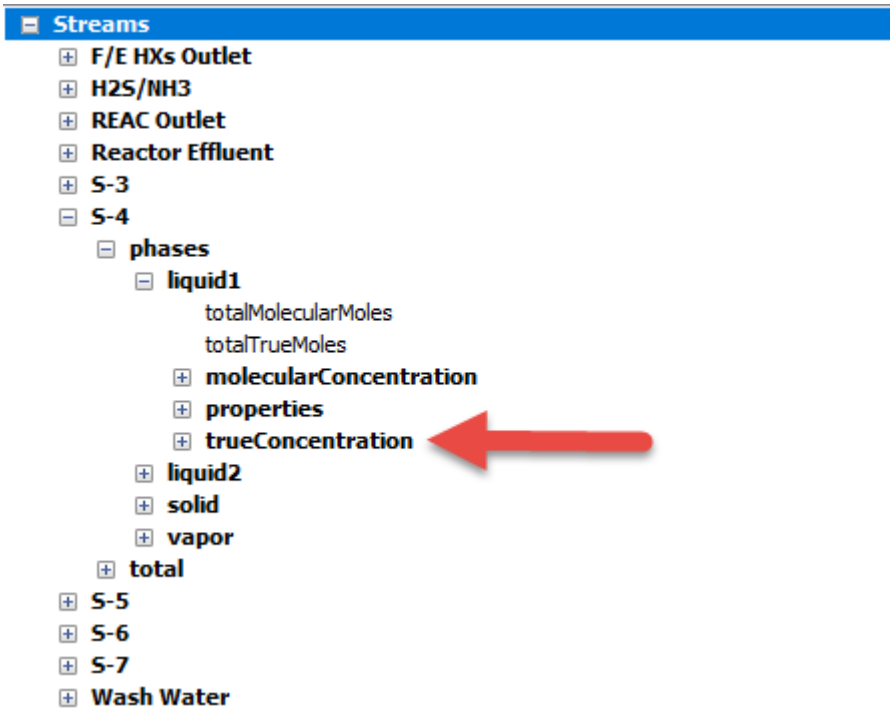
Expand the stream "S-4"



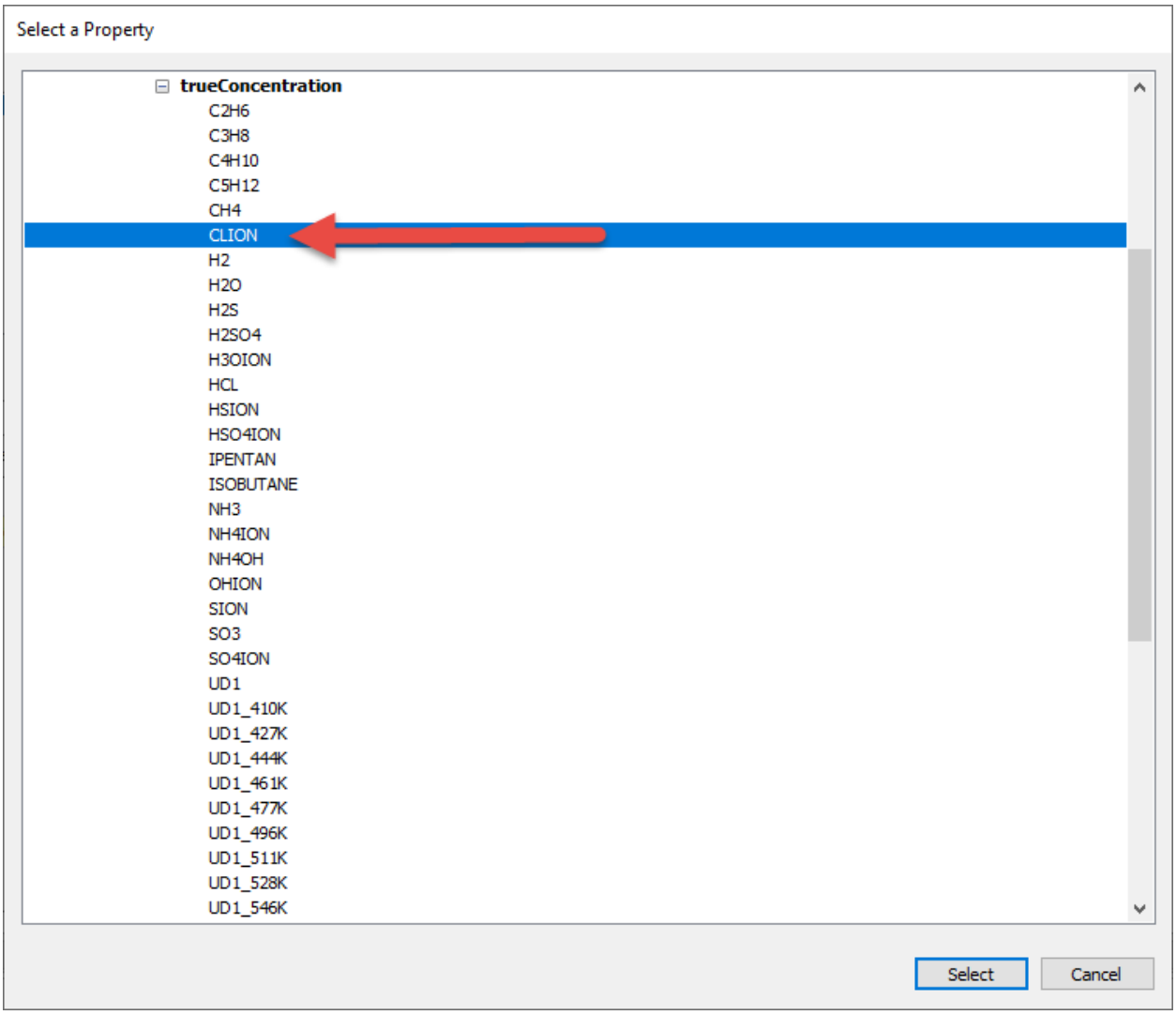
Now expand "phases" since we only want the liquid phase components.



Now expand “liquid1” which is the traditionally water-rich (aqueous) phase.



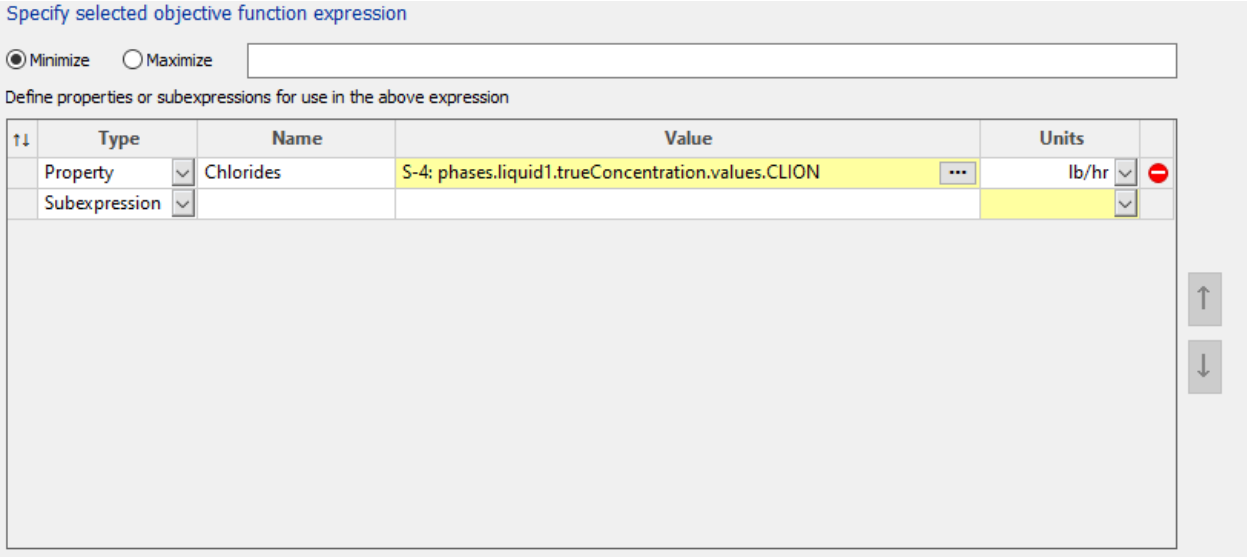
Now expand “trueConcentration” to see the actual species. This differs from what is called “molecularConcentration” which is defined in other OLI documents.



Select all the species that contain a chloride ion. Fortunately for this example only species contains the chloride ion and that is CLION[5]

Press the **Select** button.

[5] The syntax here is the OLI Tag name. This can be confusing to sort out if the species is heavily renamed. You can use the OLI Data Locator to help you sort out the name. This limitation will be relieved in future versions.

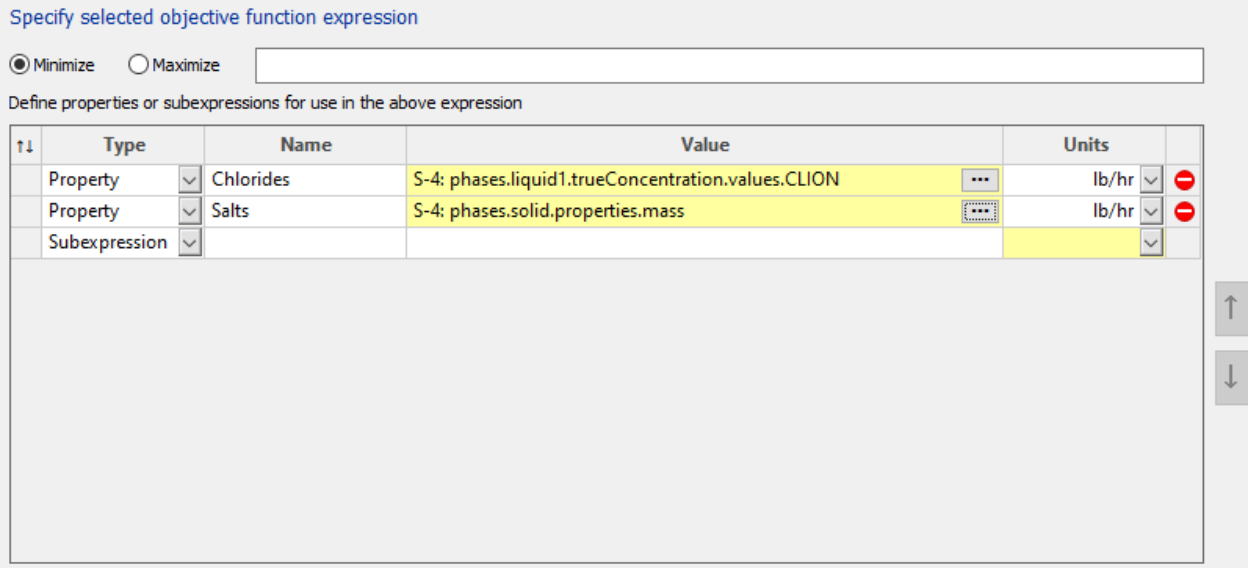


We have just entered our first variable. We will use the default unit set which is derived from the document.

Please repeat the steps for a new property called “Salts.” Here we just outline the steps

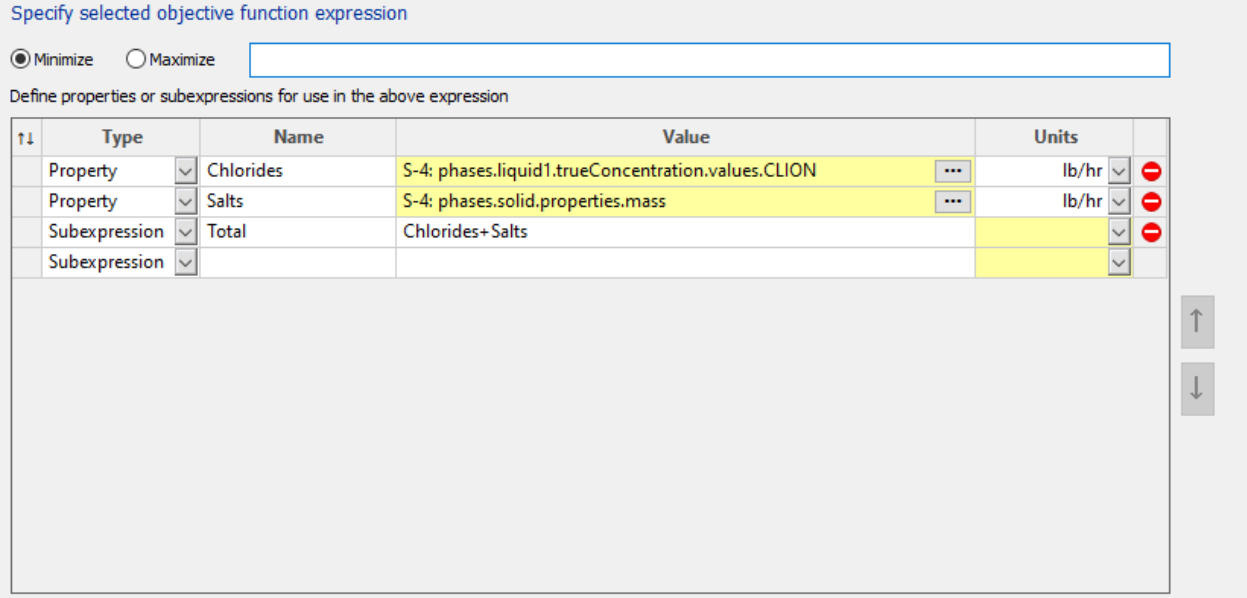
Change the **Type** drop-down box to Property
Enter the name “Salts”
Click the “…” button
Select Stream “S-4
Select “Phases”
Select “Solid”
Select “properties”
Select “mass”
Click the **Select** button

The panel should look like this:



You will now enter your sub-expression. This is very simple; it is a function of the properties you have just defined. You can also perform mathematical operations in the sub-expressions, but you will need to see a list of supported functions. See Appendix-2 on page 242

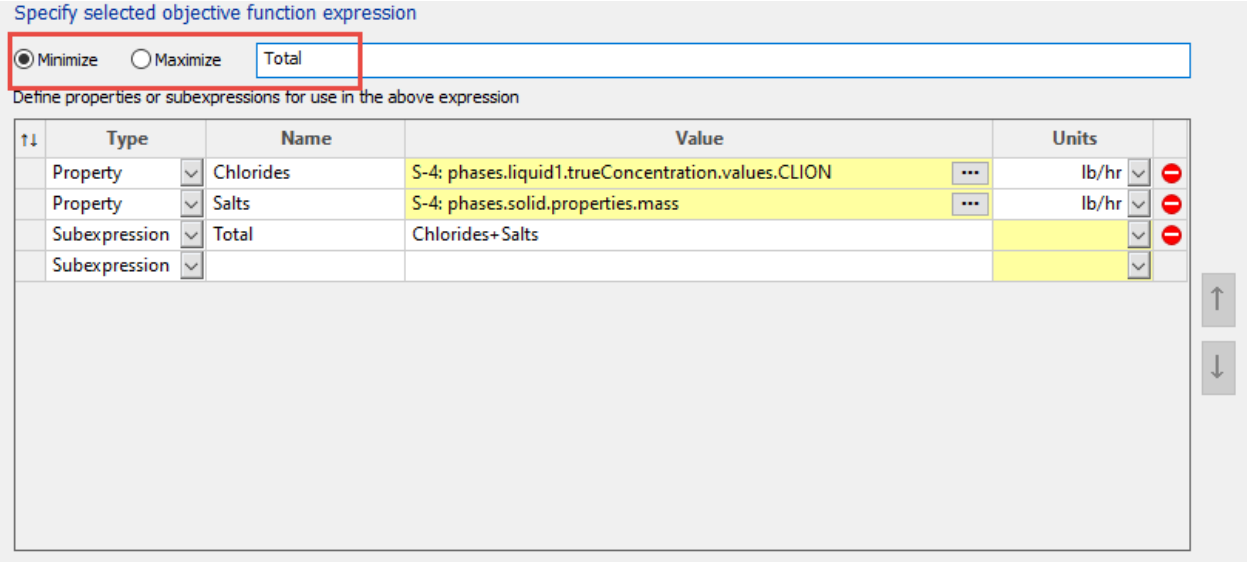
Enter a subexpression Total = Chlorides + Salts, when done your panel should look like this:



A few notes here, if you made a mistake in your property values you can edit them via the "…" button. If you want to delete them click the red "-", and the value is deleted.

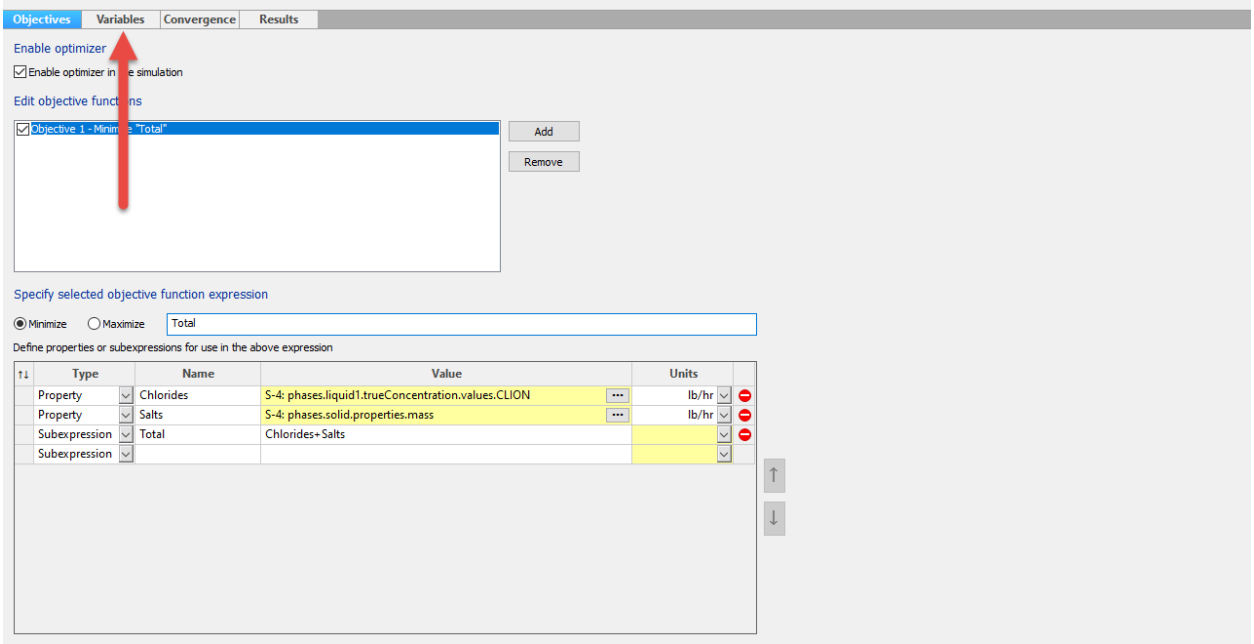
The sub-expression is order dependent. That means all variables that the expression use must be previously defined above the expression. There is no "Insert" function so if you missed a variable you need to add it to the end of the list and then use the arrows on the right to move them as needed.

The final step on this panel is to enter the objective function expression.

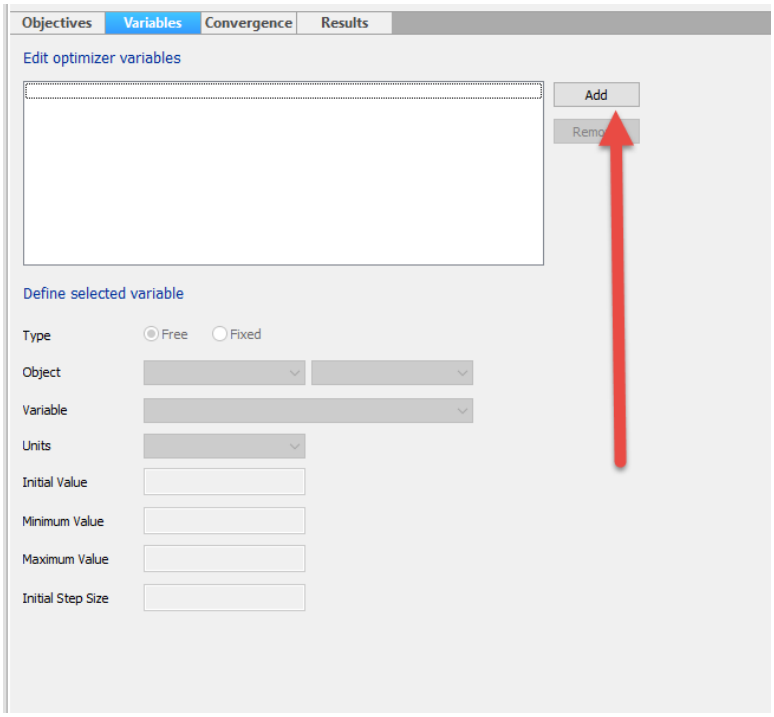


You could have saved a step and entered the value directly into the box, but this method is better if you need to debug the process.

We are not yet done; we need to define the variables which will be adjusted which will be the "Wash Water" flowrate.

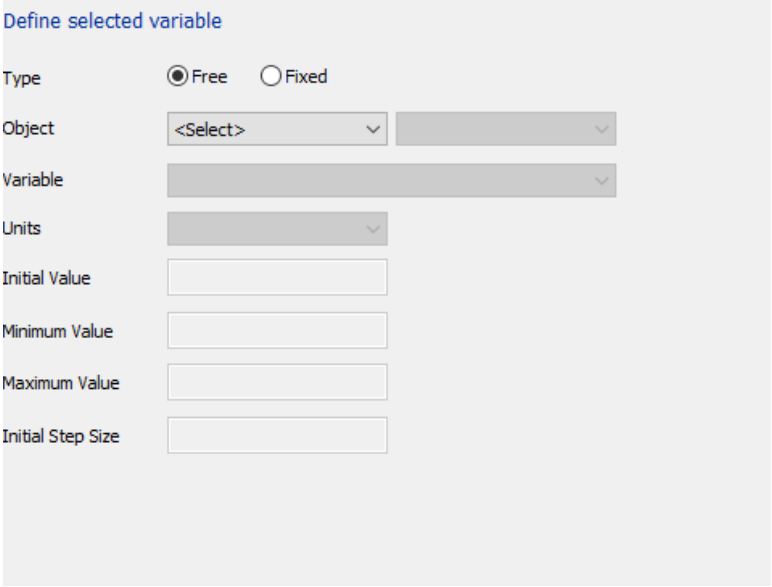


Click on the **Variables** tab.



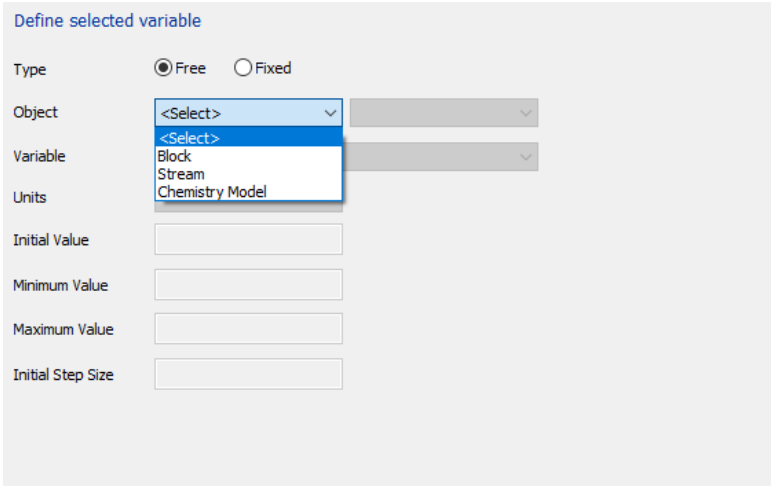
This is the panel where we define the variables that will be adjusted during the optimizer process. We will go through each option in turn.

Click the **Add** button



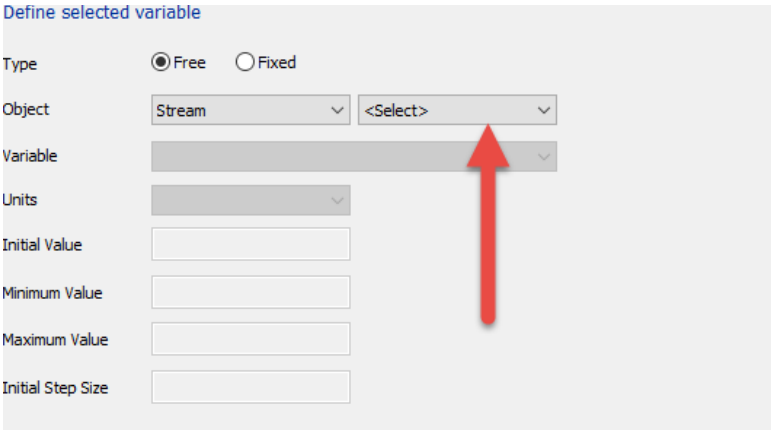
When the “add” button is clicked, the parameters become live. The parameters can be “Free” which means the parameter will be adjusted or “Fixed” which means the parameter is a set value. Normally this option is set to “Free”

Click the drop-down box next to object to select the type of parameter.

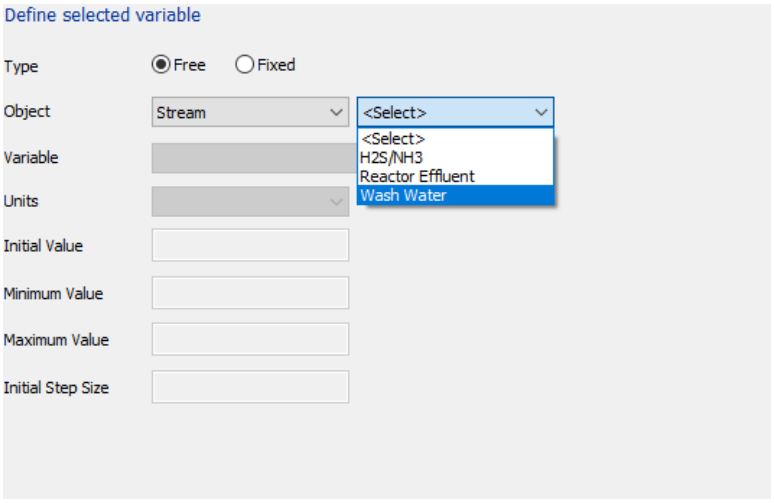


You can select block parameters such as duty or stream parameters such as flow (which is what we will do in this example). You can also adjust thermodynamic parameters which will be discussed on our wiki page.

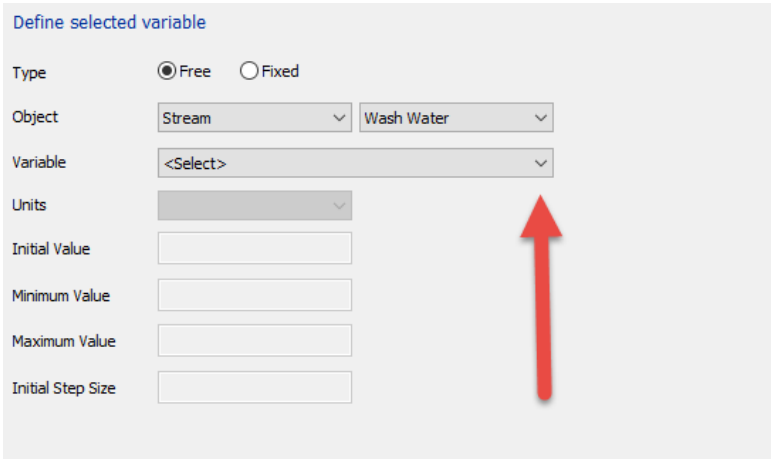
Select **Stream**.



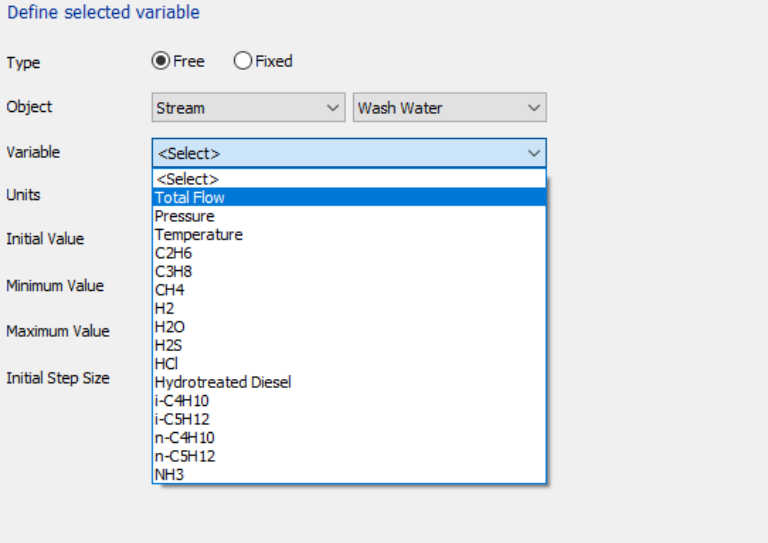
You can now select from any stream in the process. We will use the “Wash Water” stream. Click the drop-down box to find and select “Wash Water”



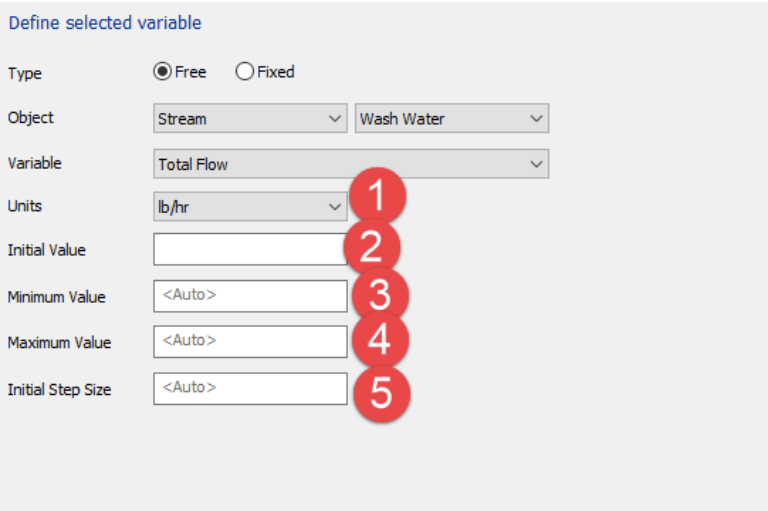
There are several parameters unique to the stream variable.



From this drop-down list find and select “Total Flow”



We are now ready to enter some initial values and boundary conditions



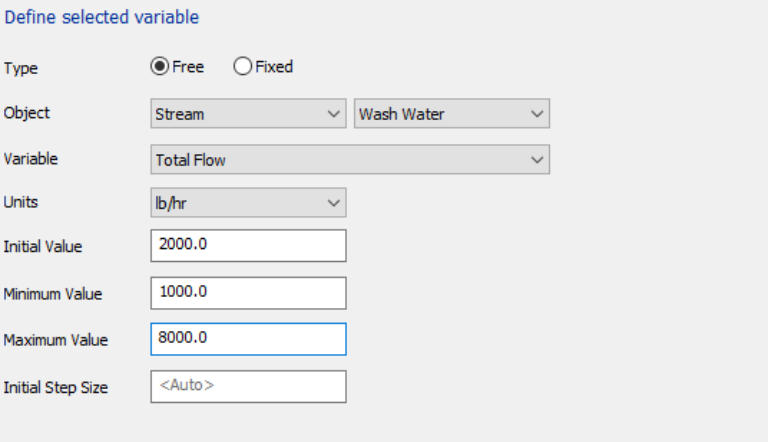
#1 The units are pulled from the actual units for the stream. These can be changed, within reason, to other units. For this example, we will use the defaulted value.

#2 We need an initial value. This is the initial value for the “Wash Water” stream. Currently, this value is 1500 lb/hr (review the flowsheet) but you can set it to whatever value is required. Enter 2000 for this value.

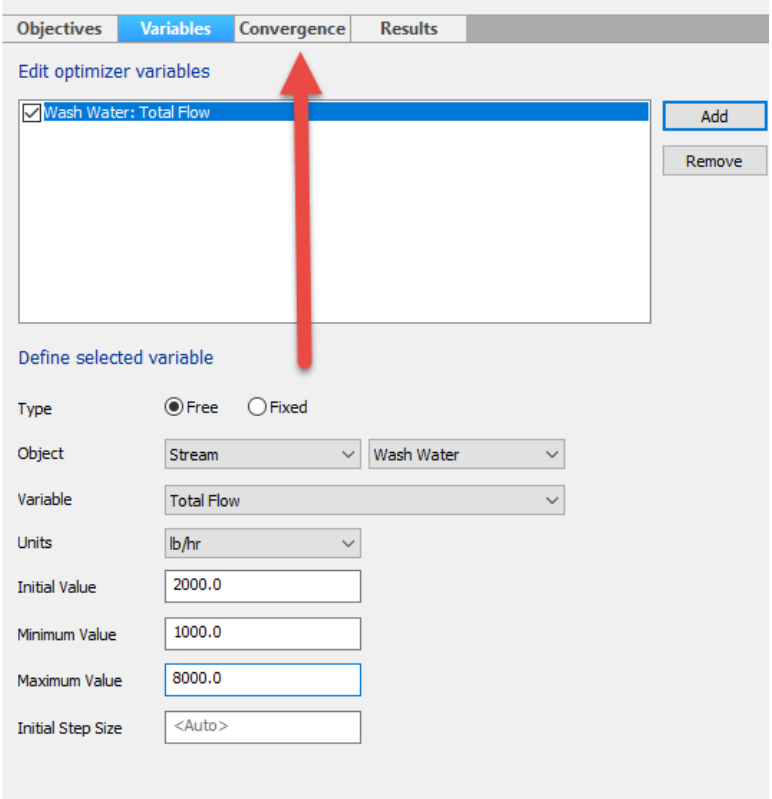
#3 We know that at 1500 lb/hr that there are solids so we should not need to go below this value. For our example let’s be sure and set this minimum value to 1000

#4 We are sure that the solids will be dissolved with 8000 lb/hr of water so we do not need to go above this value. Enter 8000

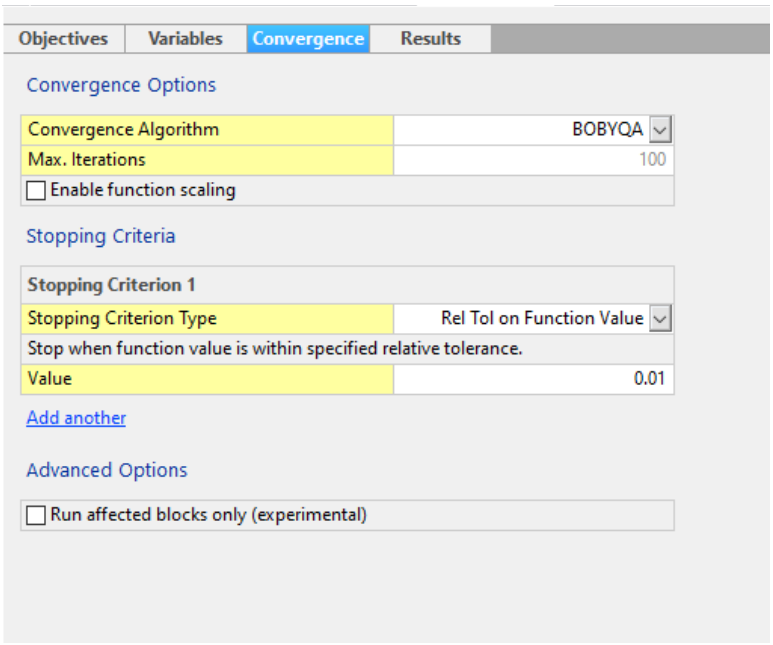
#5 Steps, please leave this set to auto. The panel should now look like this.



We are almost done.



Click on the **Convergence** tab.



Here is where the conditions for convergence are set for the optimizer.

Convergence Options

The first parameter is **Convergence Algorithm** which must be specified. Currently the only algorithm which can be used is BOBYQA.

What is BOBYQA? Simply put, BOBYQA is an iterative algorithm for finding a minimum of a function $F(x), x \in R^n$, subject to the simple bounds

$$a_i \leq x_i \leq b_i, \quad i = 1, 2, 3, \ldots\ldots, n$$

on the variables, F being specified by a "black box" that returns the value $F(x)$ for any feasible x. Each iteration employs a quadratic approximation *Q* to *F* that satisfies

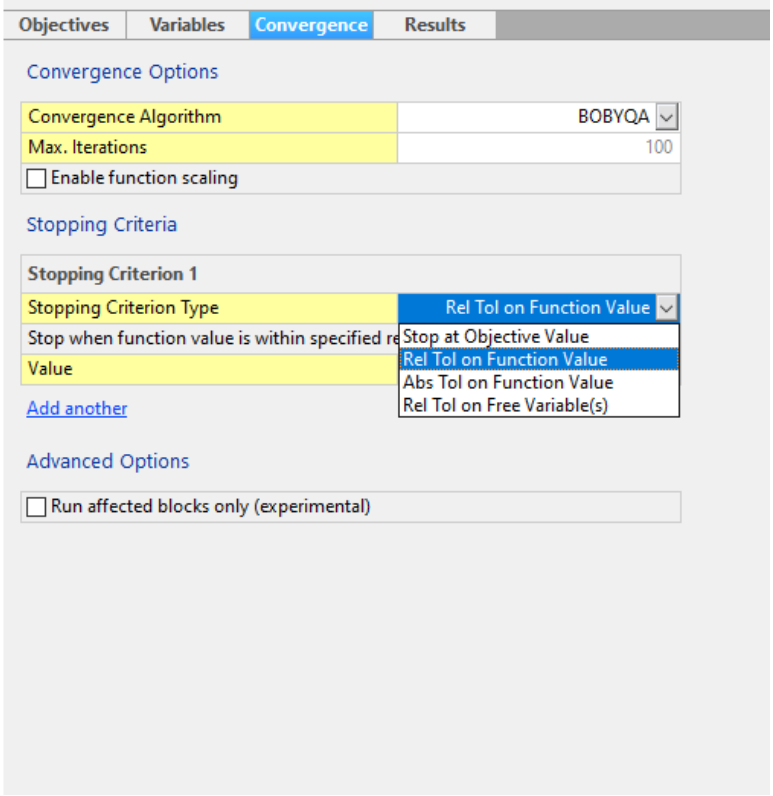
$$Q(y_j) = F(y_j), \quad j = 1, 2, 3, \ldots\ldots, m$$

the interpolation points y_j being chosen and adjusted automatically, but m is a prescribed constant. These conditions leave much freedom in *Q*, taken up when the model is updated by the highly successful technique of minimizing the Frobenius norm of the change to the second derivative matrix of *Q*. Thus, no derivatives of *F* are required explicitly. Most changes to the variables are an approximate solution to a trust region subproblem, using the current quadratic model, with a lower bound on the trust region radius that is reduced cautiously, to keep the interpolation points well separated until late in the calculation, which lessens damage from computer rounding errors. The name BOBYQA is an acronym for Bound Optimization BY Quadratic Approximation.

Max Iterations is the maximum number of iterations the optimizer will use to reach convergence. It defaults to100

Stopping Criteria

This defines convergence. You may have more than one stopping criteria if you have more than one objective function. Select the **Stopping Criterion Type** "Rel Tol on Function Value"



Each of these values are straight forward to define.

$$Rel\ Tol\ on\ Function\ Value = \left|\frac{Current\ Value - Previous\ Value}{Previous\ Value}\right|$$

$$Abs\ Tol\ on\ Function\ Value = |Current\ Value - Previous\ Value|$$

$$Relative\ Tol\ on\ Free\ Value = \left|\frac{Current\ Free\ Value - Previous\ Free\ Value}{Previous\ Free\ Value}\right|$$

If the value that is calculated is less than the specified value, then the optimizer is converged. Each type has its place in optimization. The “Rel Tol on Function Value” is the most common. This looks for a fractional change in the calculated function value. This is useful when your function has a very large dynamic range of values.

The “Abs Tol on Functional Value” is for the absolute difference between two iterations in the optimizer. This is useful when tight tolerances are required, and the dynamic range of the calculated functions is small.

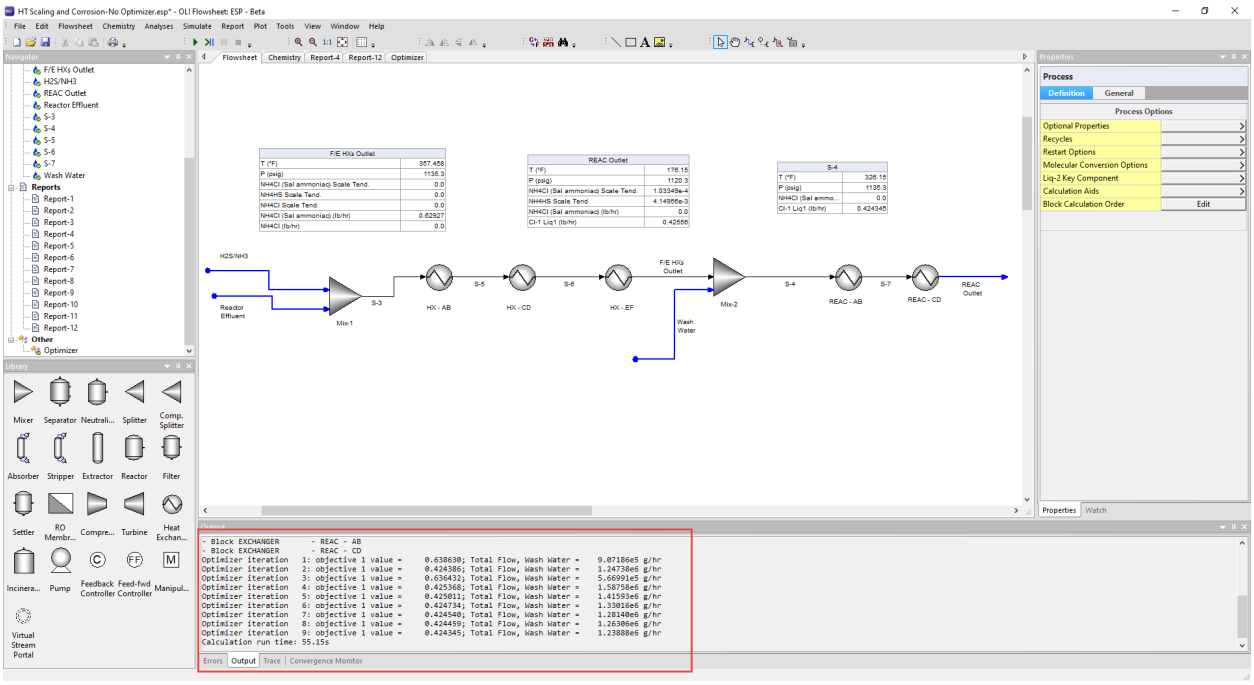
The “Relative Tol on Free Value” is when a free type of optimizer function is used. This is infrequently used.

The default value is 0.01 which is suitable for this example.

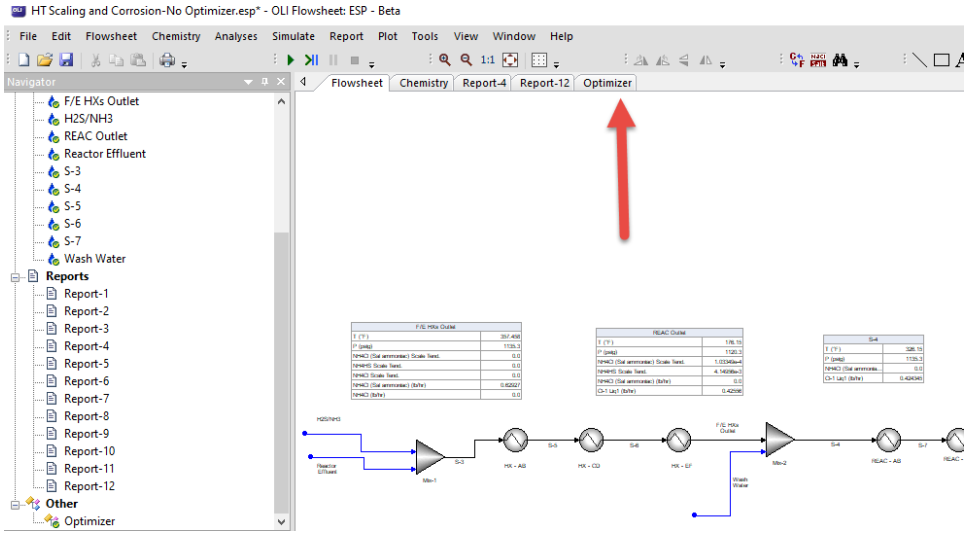
Running the optimizer

The optimizer is completely set up. You can now run the simulation.

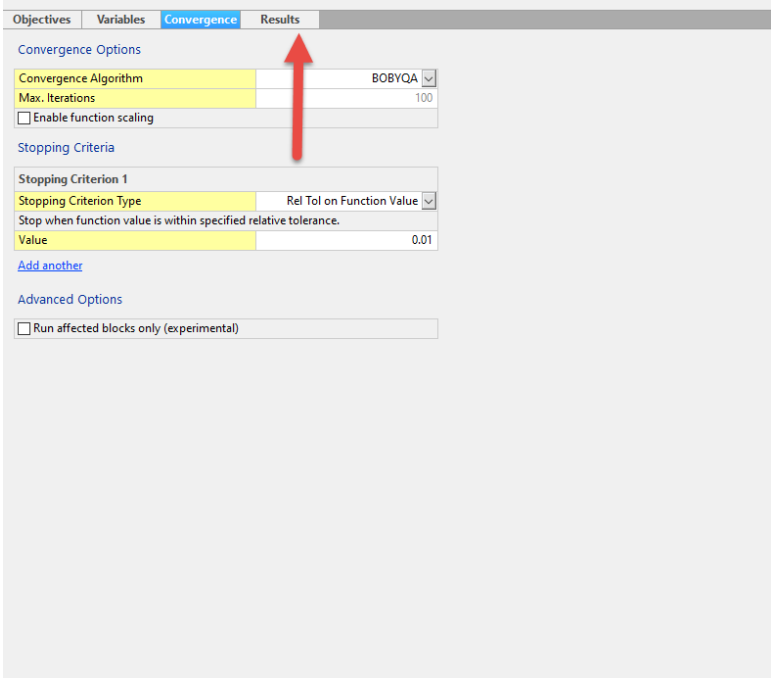
After the run converges you will see the output screen:



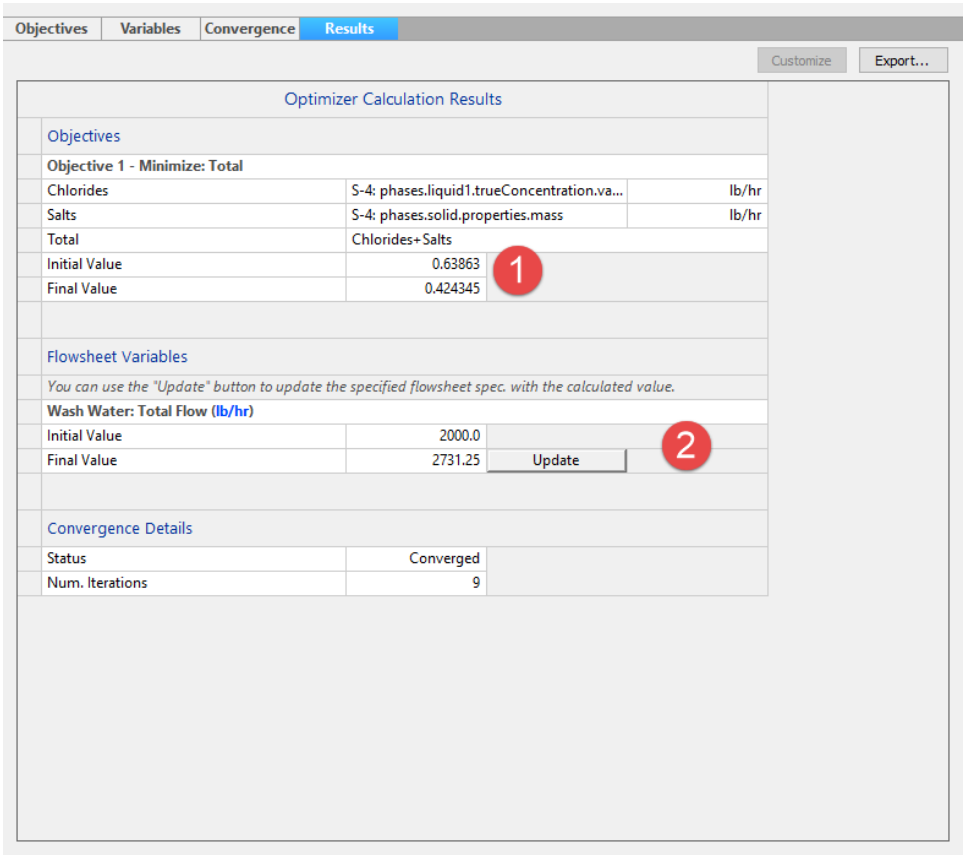
The output panel shows the trace of the optimizer. To see the results, click back on the optimizer tab:



You will probably be returned to the panel you left when you ran the simulation:



Click the results tab:



#1 shows the initial value of the objective function (approximately 0.638) and the final value of objective function (0.424). This can help you determine if you used the correct objective function.

#2 shows the initial value of the objective variable (the stream “Wash Water” flowrate) which was 2000 lb/hr and the final value of 2731.25 lb/hr. This is the minimum flowrate necessary to minimize the amount of chlorides and solids in the stream “S-4”.

The **Update** button will automatically update the variable in the stream “Wash Water”. At that point the optimizer analysis can be disabled so further studies can be made.

Final Note:

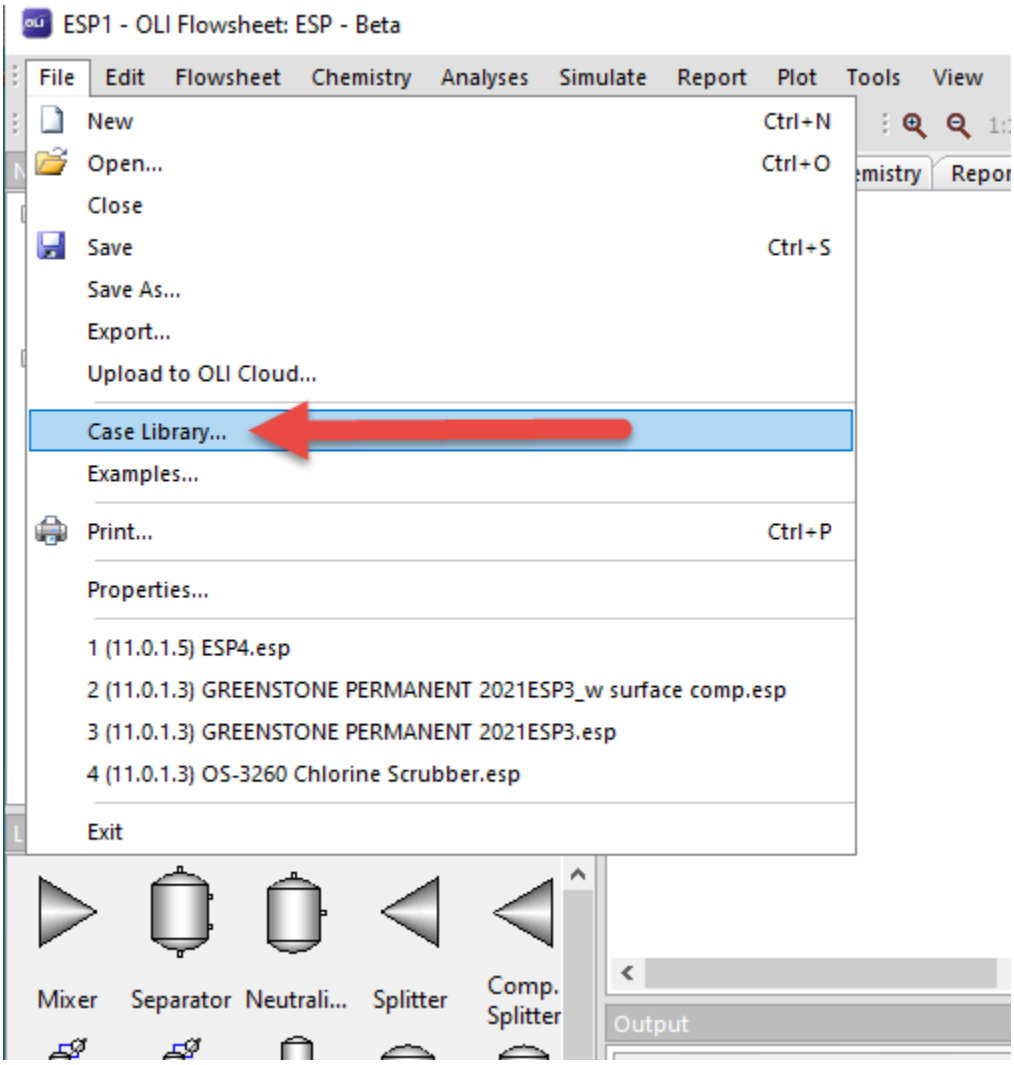
During the development of this example, the authors ran into non-convergence issues. This was debugged to find that spelling and capitalization counts. The authors used the word “Chlorides” in the Property field but the misspelled work “Chorides” in the sub-expression. A future version will trap this spelling error.

A more insidious error is that the Property Field “Salts” was represented as “salts” in the subexpression. This was taken to be a new variable and caused convergence errors. When the spelling and capitalization errors were fixed the program converged.

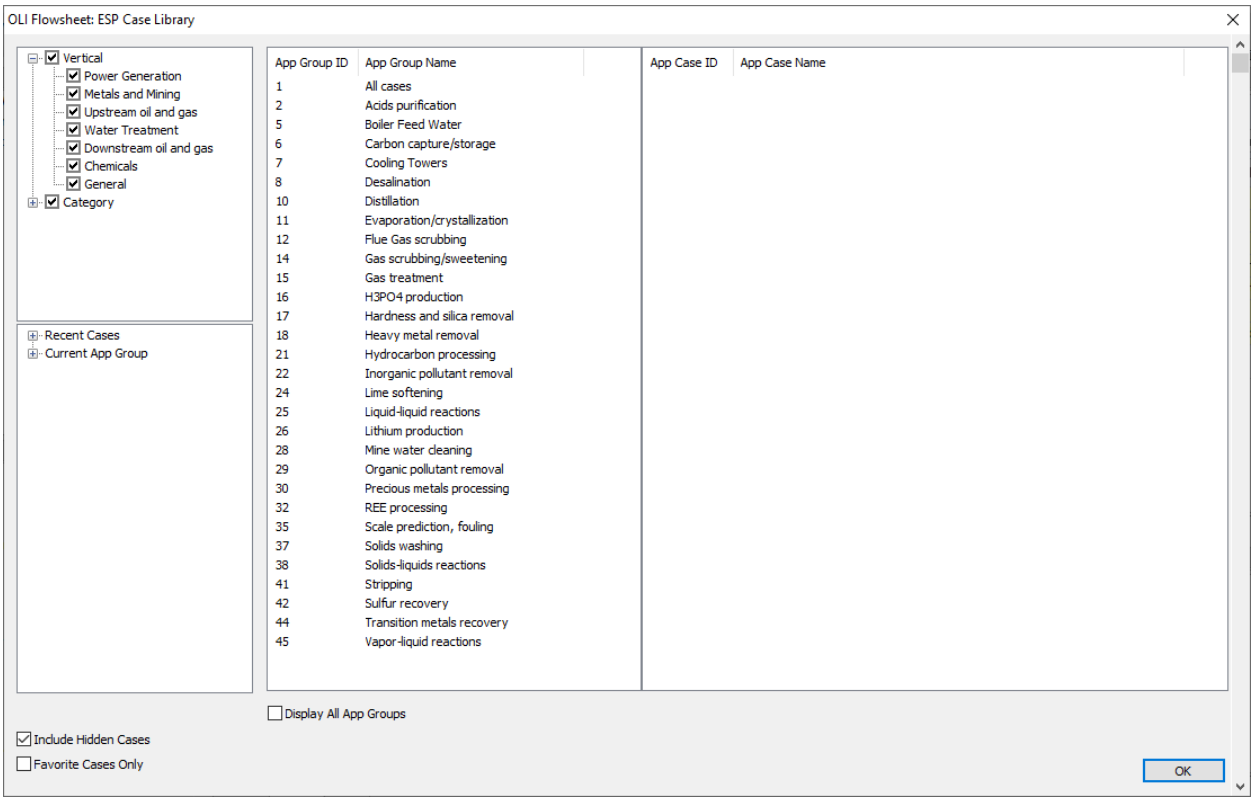
Chapter VII – Case Library

The Case Library gives the user access to several detailed cases that are built into flowsheet and contains 60+ flowsheet cases that are part of different industries.

To access the **Case Library,** select **File** from the menu and then ***Case Library***

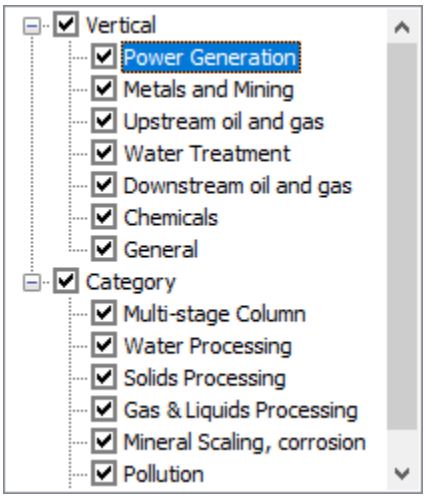


This will display the Case Library menu



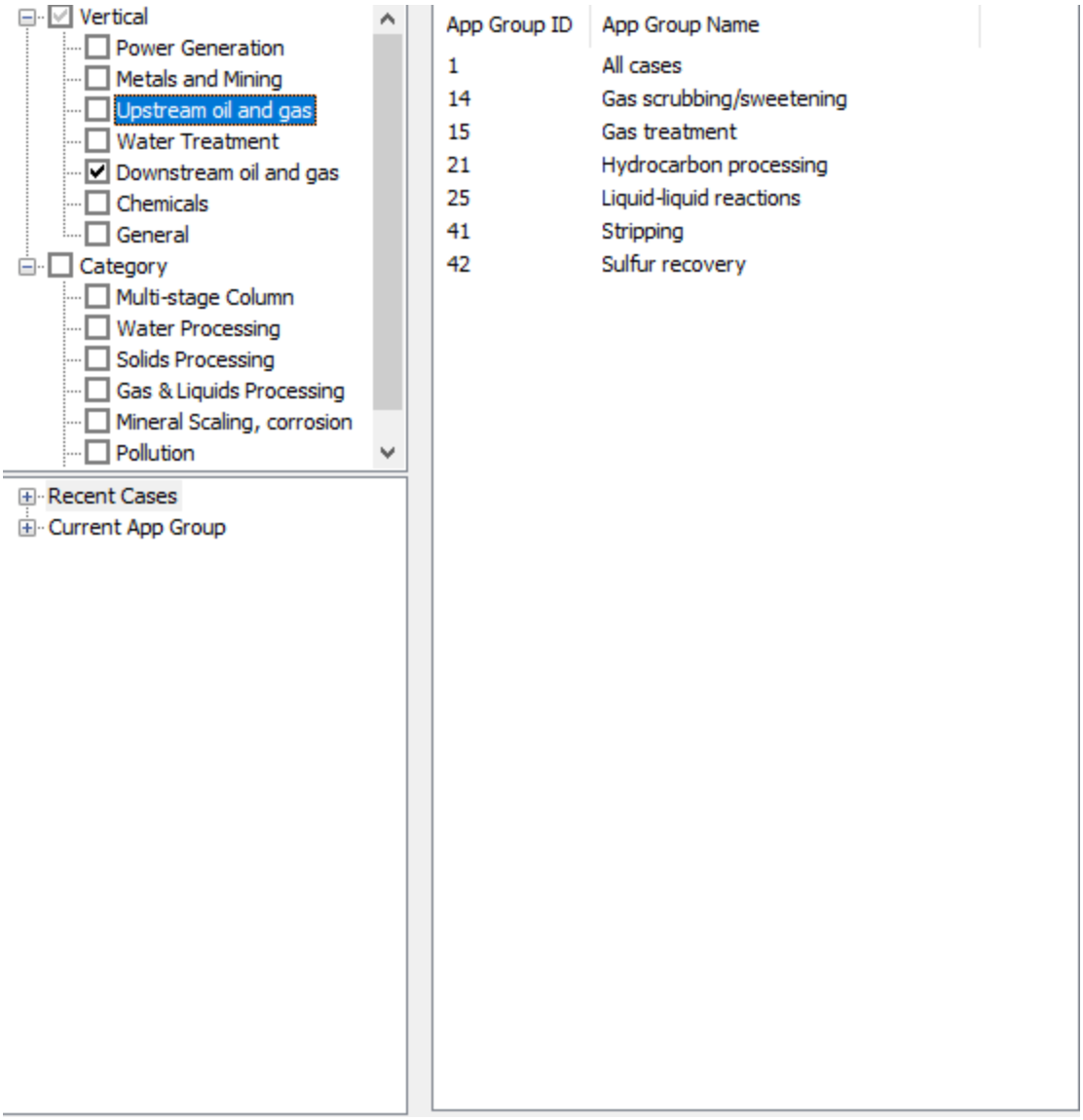
We will discuss each panel individually.

Category



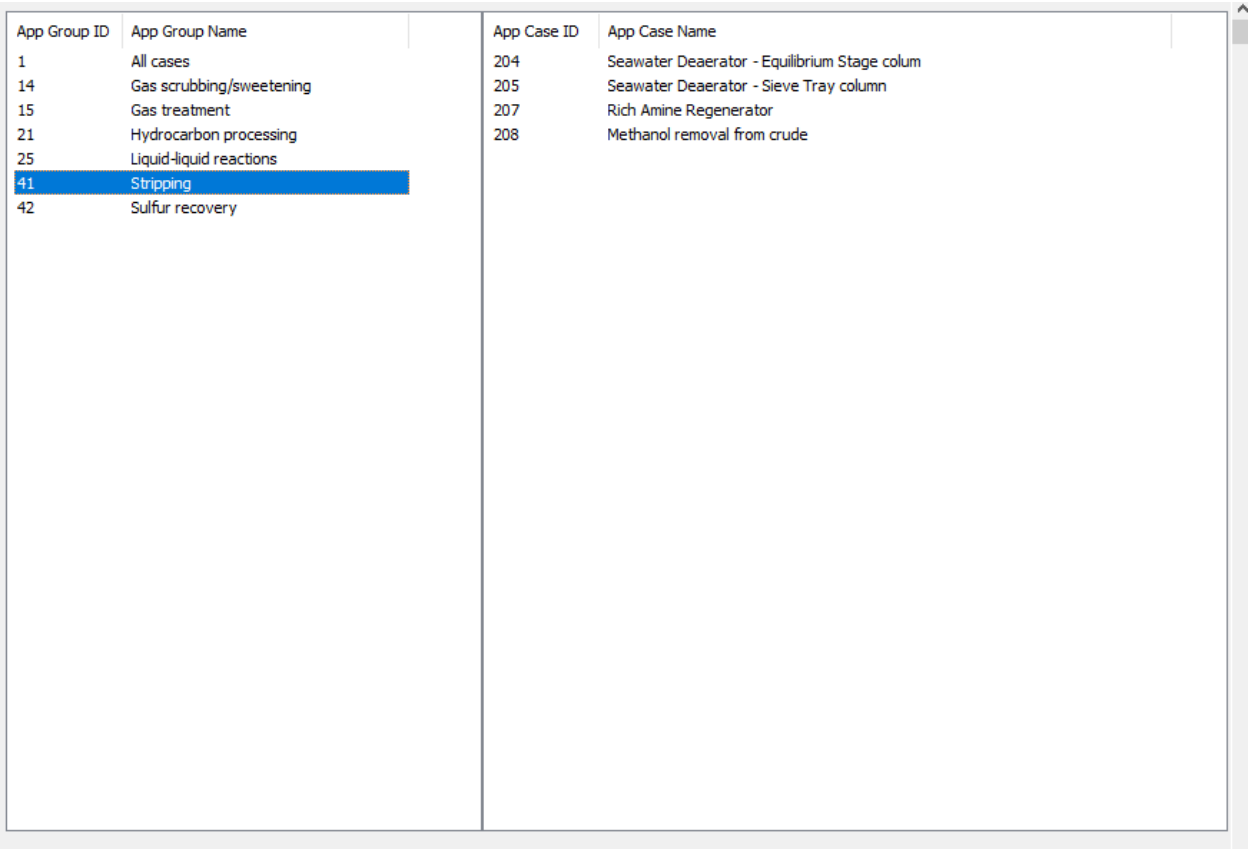
This panel is affected by your license. If you or your organization only licensed a subset of database segments, then some of these verticals will not be displayed.

This panel shows the different industry verticals that contain examples. Uncheck these verticals if you do not want to search them. The panel also shows the case files by the type of application.



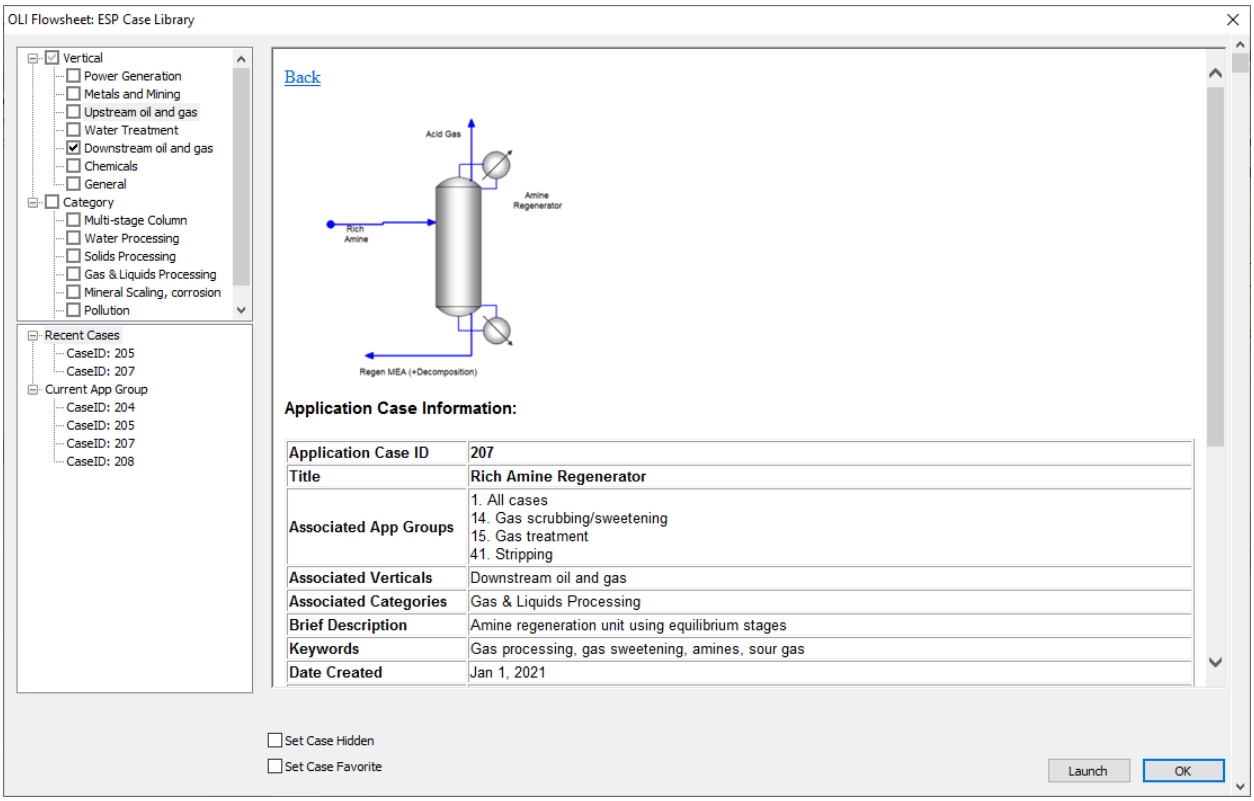
The Application group is displayed next to the vertical/category panel. You can see in the example that only the **Downstream oil and gas** vertical has been selected so only those case files are displayed.

For this example, we will select group ***41 Stripping*** to see what happens.

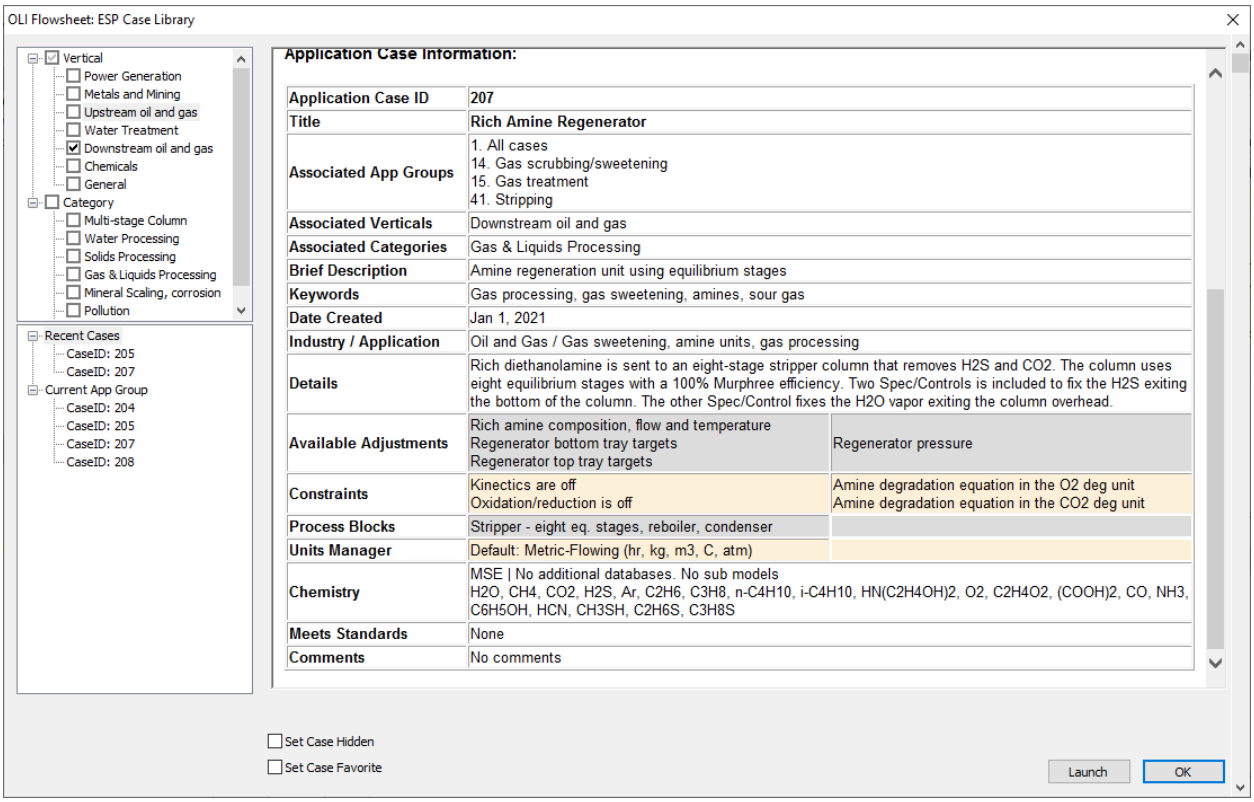


You can see that case files pertaining to “Stripping” are now displayed

For this example, we will select “207 Rich Amine Regenerator”



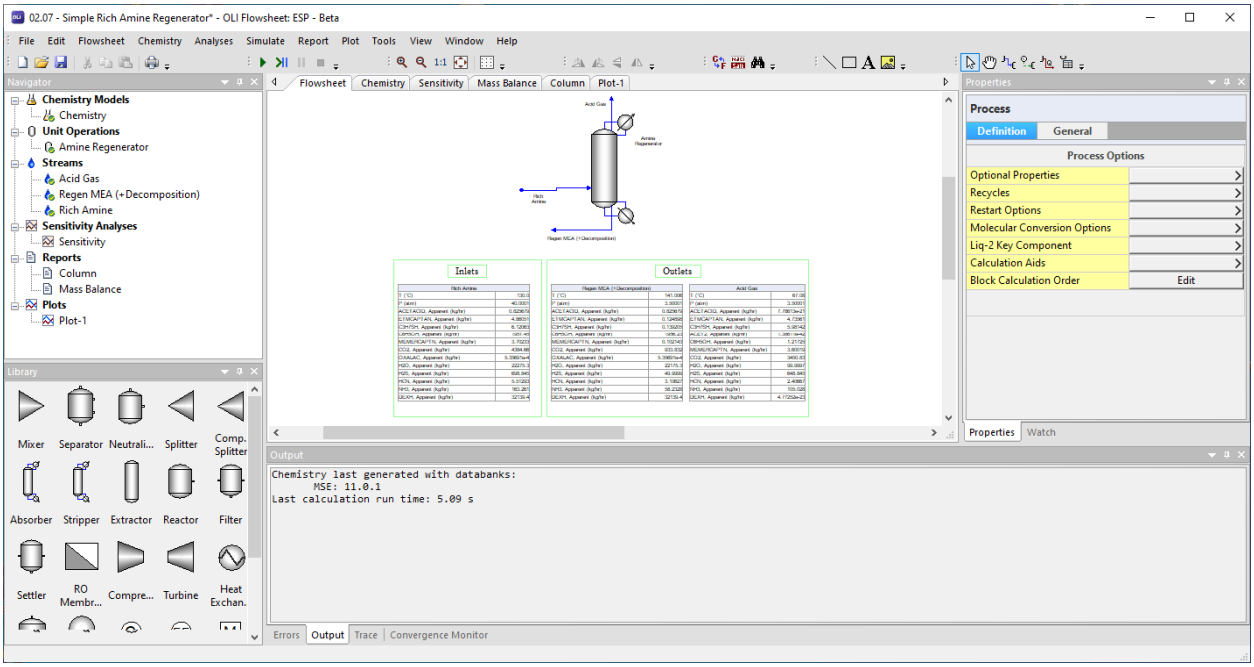
This panel now displays some additional information about this case. There is information below this panel so scrolling down is required.



After scrolling down, you can read more information about this case.

To use this case as is, click the **Launch** button. To see different case and return to the library click the **Back** hyperlink.

After clicking the **Launch** button, you will need to close the Case Library.



This case was previously run, and you can see the results. This is a saved file in the system, and you cannot overwrite it. Clicking Save will open a new save as dialog.

Chapter VIII – Process Applications

In this section, we will have examples of various process applications which illustrate the use of the unit operations in OLI Flowsheet: ESP.

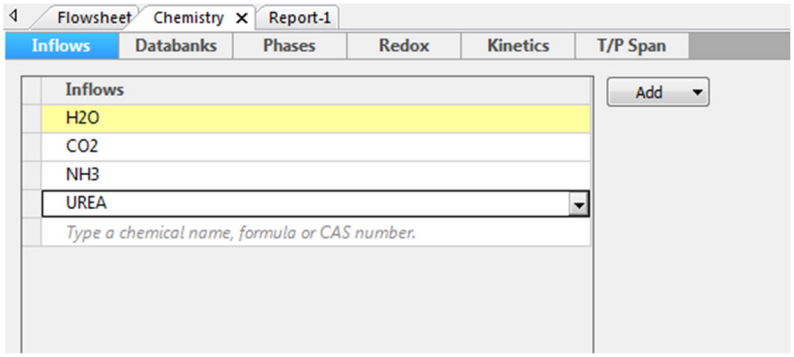
Reactor Block Examples

Standard Reaction Kinetics

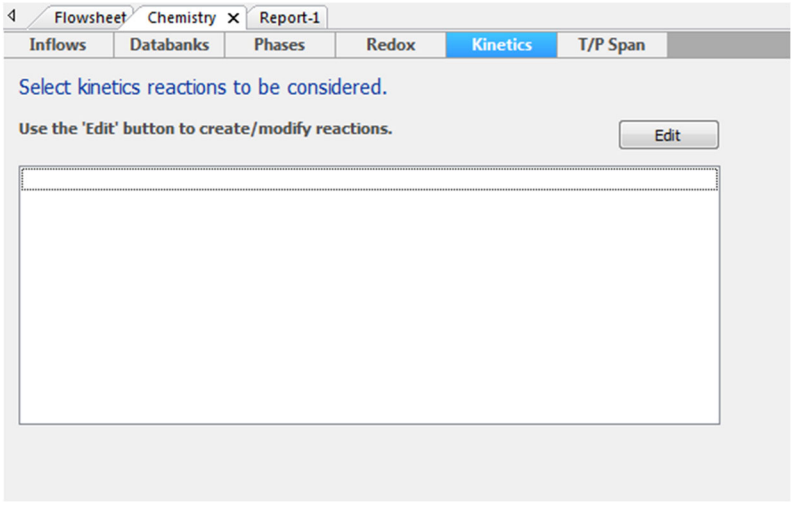
This example shows the implementation of standard reaction kinetics. It is about the hydrolysis of urea. Create a new flowsheet with the following input chemistry using the AQ thermodynamic framework.

Species	Formula	OLI Tag Name
Water	H_2O	H2O
Carbon dioxide	CO_2	CO2
Ammonia	NH_3	NH3
Urea	NH_2CONH_2[6]	UREA

When complete your chemistry model section should look like the following:



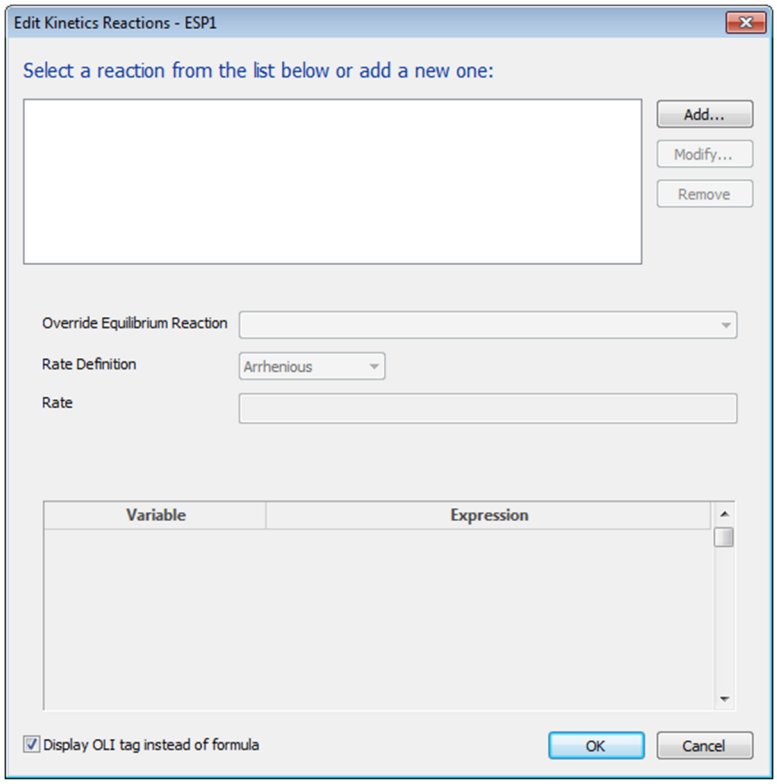
Click on the **Kinetics** tab.



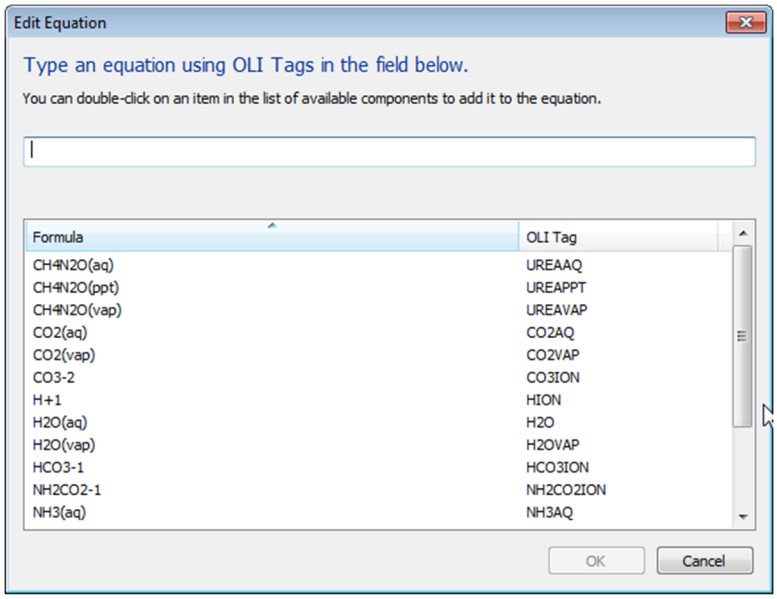
[6] This may also be represented as CH4N2O

This will display the reaction kinetics editor. Now, there is nothing displayed.

Click the **Edit** button.



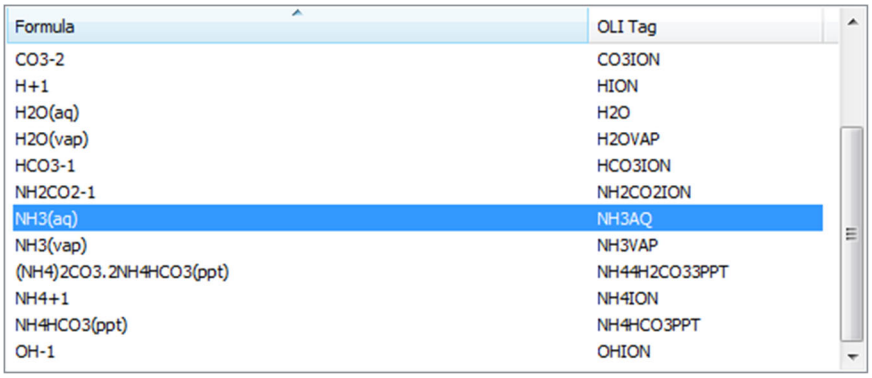
This is the reaction kinetics editor. To add the hydrolysis of urea we need to click the **Add** button.



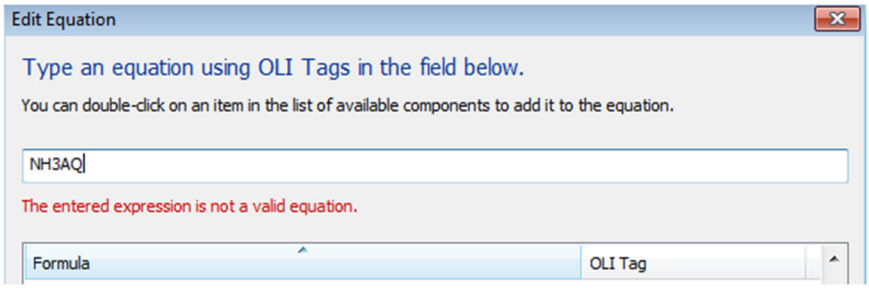
These are all the components currently in the chemistry model. Our reaction equation must contain these species. The reaction we want is the following:

$$2NH3AQ + CO2AQ = NH2CONH2AQ + H2O$$

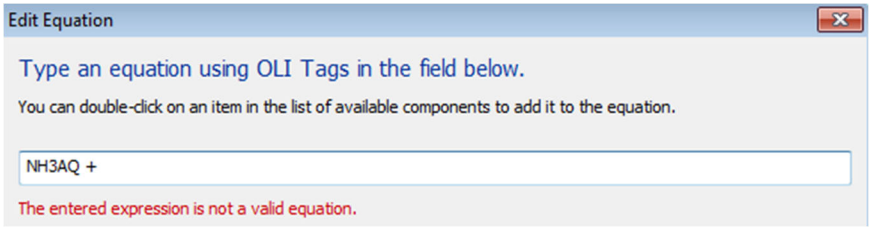
Let's start by locating NH3(AQ) from the list:



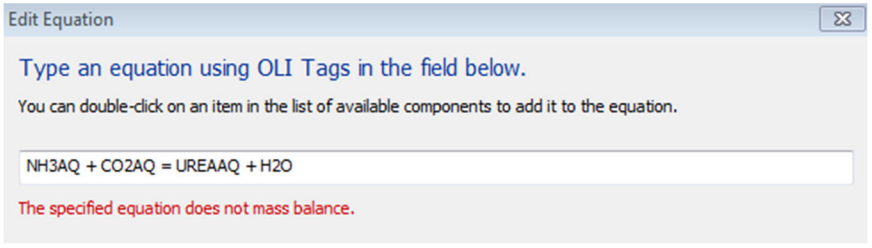
Double-click the component to add it to the equation.



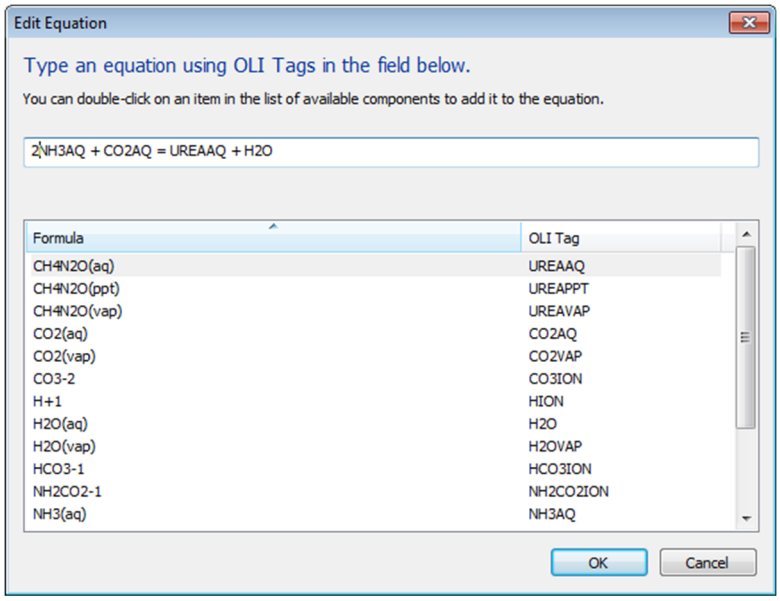
You can see that we have entered the component but there is an error message. This is ok for now since we haven't completed the equation. We now need to add the plus sign "+" to add the next component:



Now locate CO2(AQ) from the list and add it in the same manner. After that complete the equation so it looks like the following:

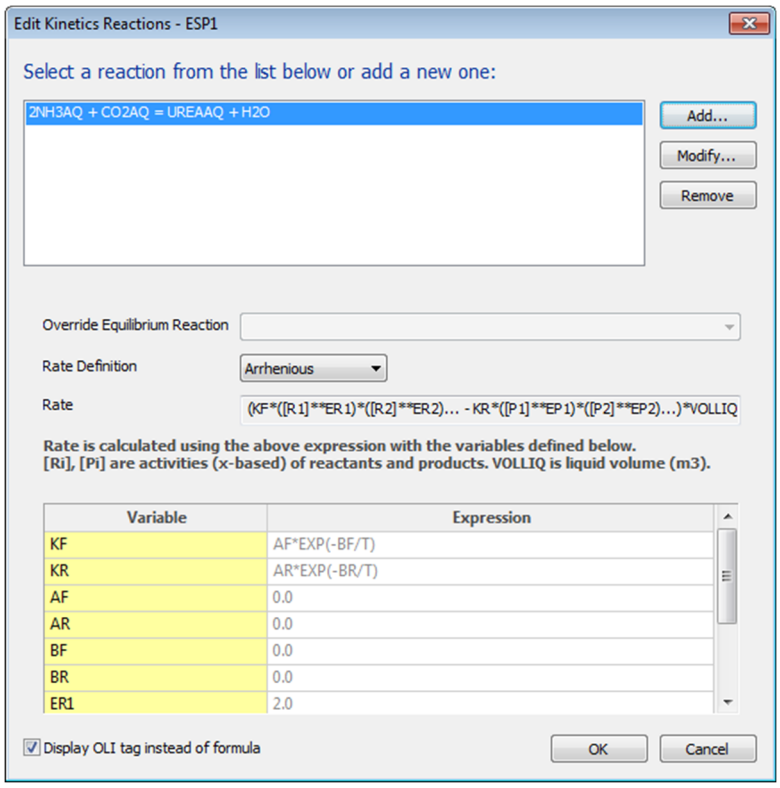


There seems to be a problem. The program will check to see if the equation mass-balances and in this case, it does not. This is because it takes two molecules of ammonia to make urea. You can add the "2" in front of the NH3AQ variable:



Click the OK button to close the editor.

We now have a reaction in the model. We now must change some constants which we get from the literature.



We do have some data to enter. The rate function has been determined to be:

$$Rate = K_f[NH_3]^2\,[CO_2] - K_r\,[NH_2CONH_2]$$

Where:

Rate [moles/h]

K_f = forward reaction equilibrium constant = 20

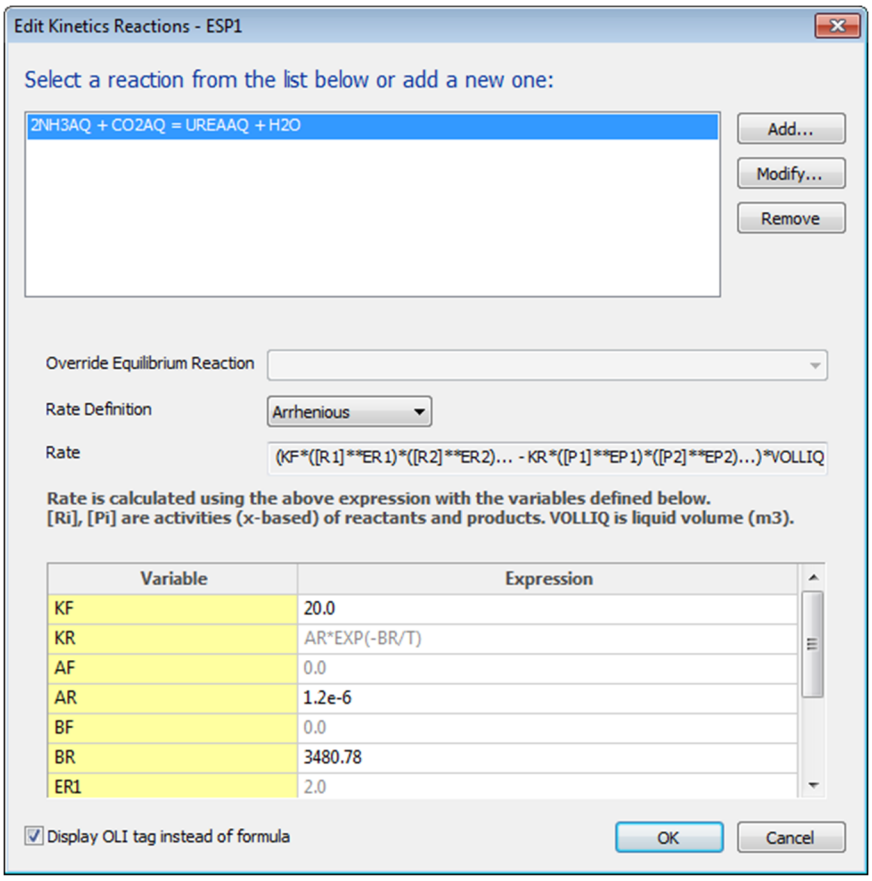
[a] = concentration of species a

K_r = reverse reaction equilibrium constant determined by Arrhenius Equation

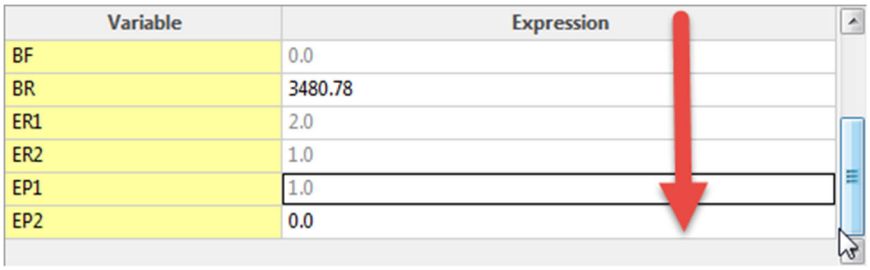
$$K_f = 1.2E-06\,EXP[-28939.9/8.3142 \times T]$$

Thus,

$$BR = -(-28939.9/8.3142) = 3480.78$$

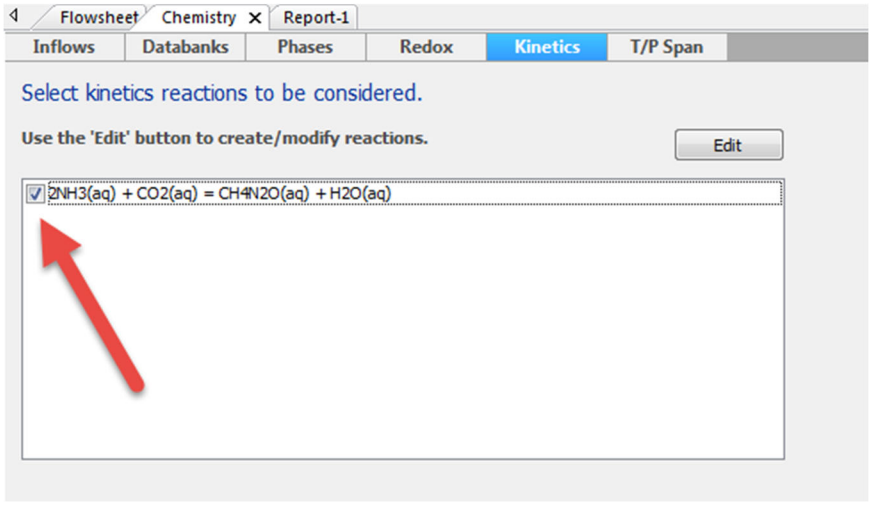


Scroll down to enter EP2



Click OK when done.

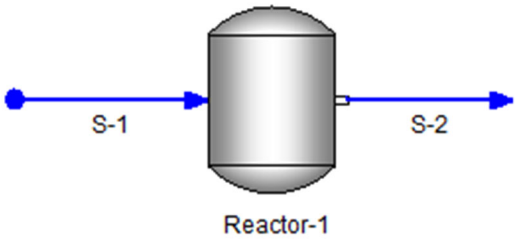
Now enable the added reaction kinetics.



Check the box if it is not already checked.

Now click on the **Flowsheet** tab to begin entering the blocks and streams.

Create a flowsheet with a rector block with a single feed stream and a single product stream such as the following:



Enter the following feed parameters given in the table below:

Feed Stream Parameters	
Feed Stream Name	S-1
Temperature	25 °C
Pressure	1 atm
Total Flow	100 mole/hr
H2O	1.0 mole/hr
CO2	0.1 mole/hr
NH3	0.35 mole/hr
Urea	0.0 mole/hr

Enter the following reactor block parameters given in the table below:

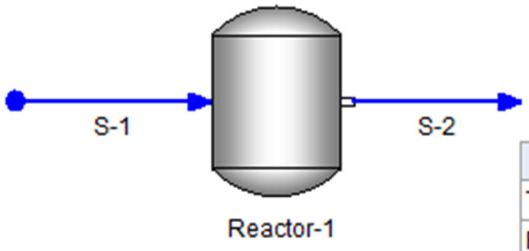
Reactor Block Parameters		
Reactor Type		Kinetics
Kinetic Parameters *(flyout dialog)*		
	Number of Stages	10
	Residence Time (hr)	100
Calculation Type		Isothermal
Pressure Spec.		Min. Inlet Pressure
Temperature (°C)		35.0
Chemistry Model		Default

Once entered, run the process and then review the output. We have added call-outs to show you the formation of urea (albeit a small amount).

To add callouts, right click on the streams and select add callout.

Your simulation should look like the image below:

S-1	
T (°C)	25.0
P (atm)	1.0
pH	10.0567
UREAAq (mol/hr)	0.0



S-2	
T (°C)	35.0
P (atm)	1.0
pH	9.74381
UREAAq (mol/hr)	1.41575e-7

Non-Standard (User Defined) Reaction Kinetics

In this example, we are using non-standard reaction kinetics to hydrolyze ammonia. The overall reaction is:

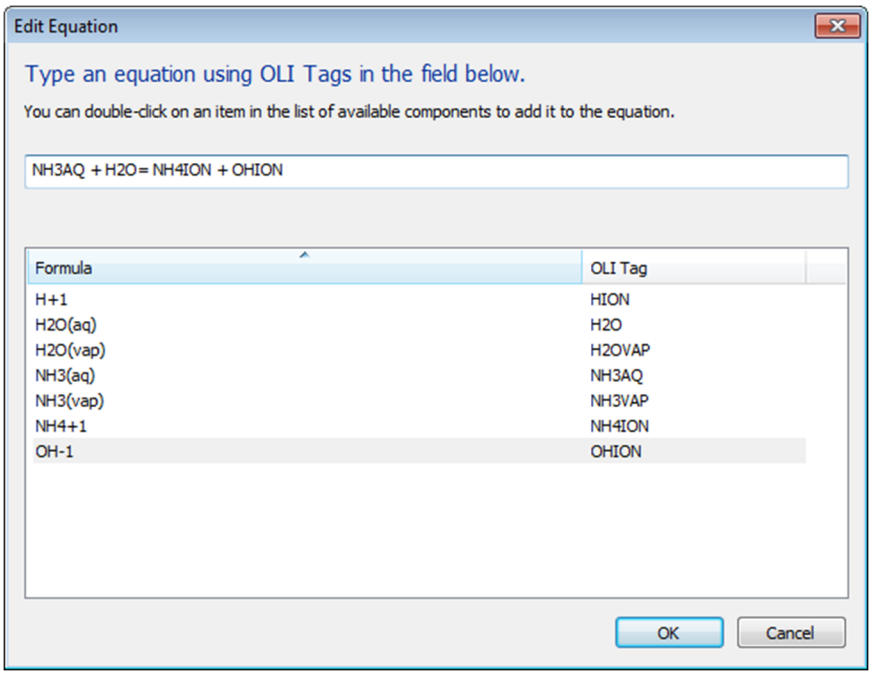
$$NH_{3(aq)} + H_2O \rightleftharpoons NH_4^+ + OH^-$$

We know the forward rate constant (and hence the forward reaction rate) but we wish to constrain the forward and reverse reaction rates to the thermodynamic equilibrium constant stored in the OLI Databases.

Create a chemistry section with the following information:

Non-Standard Reaction Kinetics		
Thermodynamic Framework	Aqueous (H+ Ion)	
Additional Databanks	None	
Phases	Default	
Redox	Off	
Inflows	Formula	OLI Tag Name
Water	H_2O	H2O
Ammonia	NH_3	NH3

Using the techniques from the previous section, add the kinetics reaction for the reaction shown above.



The reaction mechanism has been previously determined. It is beyond the scope of the document to instruct you how to determine that mechanism, only to add the mechanism to the program.

$$R_f = k_f \gamma_{NH_{3(aq)}} [NH_{3(aq)}] \gamma_{H_2O} [H_2O]$$

$$R_r = k_r \gamma_{NH_4^+} [NH_4^+] \gamma_{OH^-} [OH^-]$$

Where,

$$k_f = 3$$

$$k_r = \frac{k_f}{Keq}$$

Thus, the rate can be defined as:

$$rate = \left(k_f e^{R_f} - k_r^{R_r}\right) \times \frac{volume}{100}$$

We now need to turn these values into "OLI" terms[7].

FXRATE=LNH3AQ+ANH3AQ+LH2O+AH2O

RXRATE=LNH4ION+ANH4ION+LOHION+AOHION

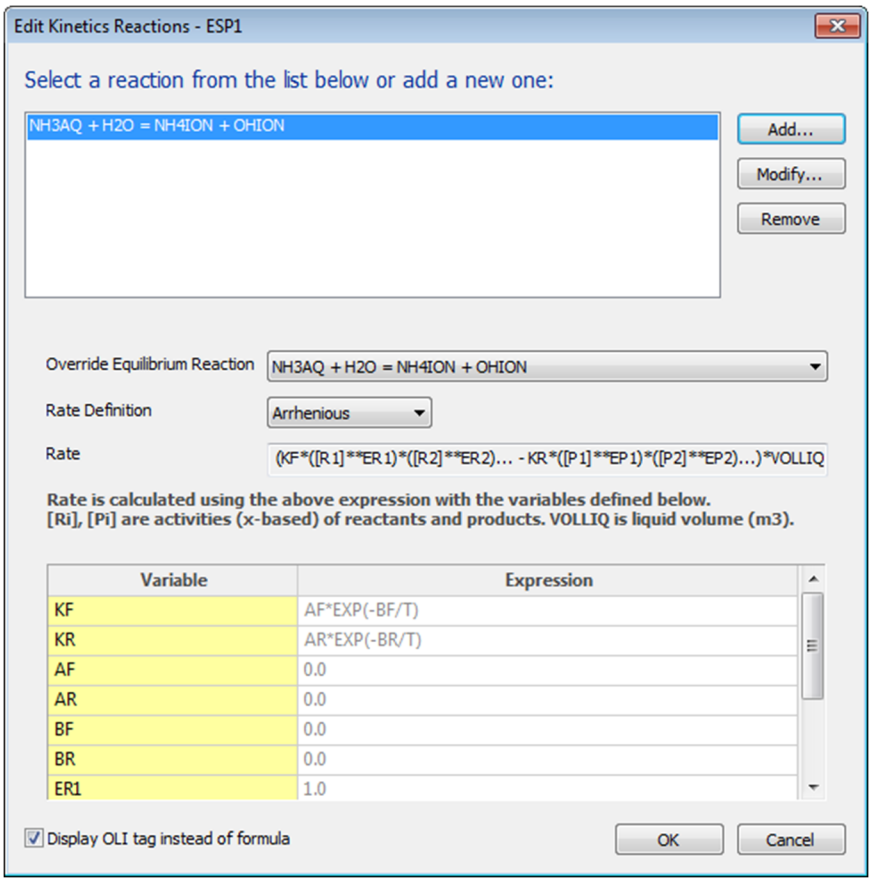
KF1=3

KR1=KF1/KEQ

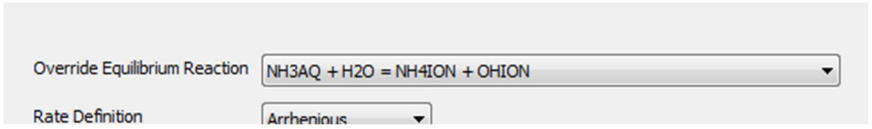
RATE=(KF1*EXP(FXRATE)-KR1*EXP(RXRATE)) *VOLLIQ/1000.

Clicking OK will return you to the editor:

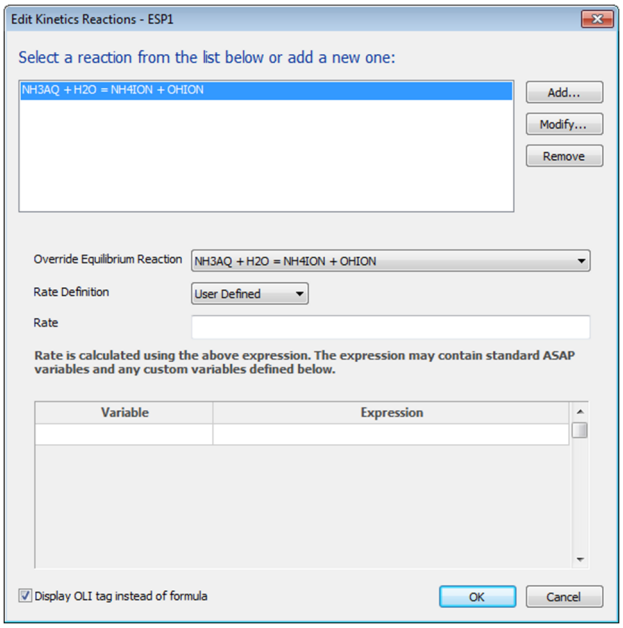
[7] Commonly referred to as ASAP variables.



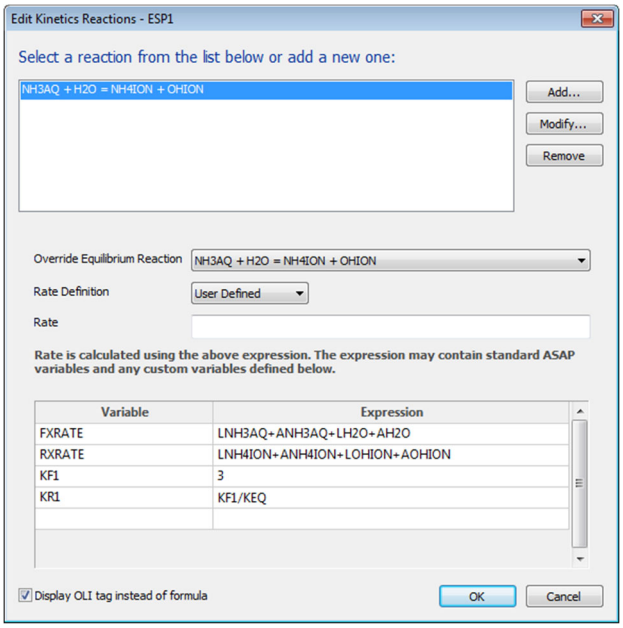
You will notice that we are replacing an existing equilibrium equation with reaction kinetics (unlike the previous example where we created a new equation.)



The reaction kinetics we have for this example is not Arrhenius. Change the **Rate Definition** button to **User Defined.**

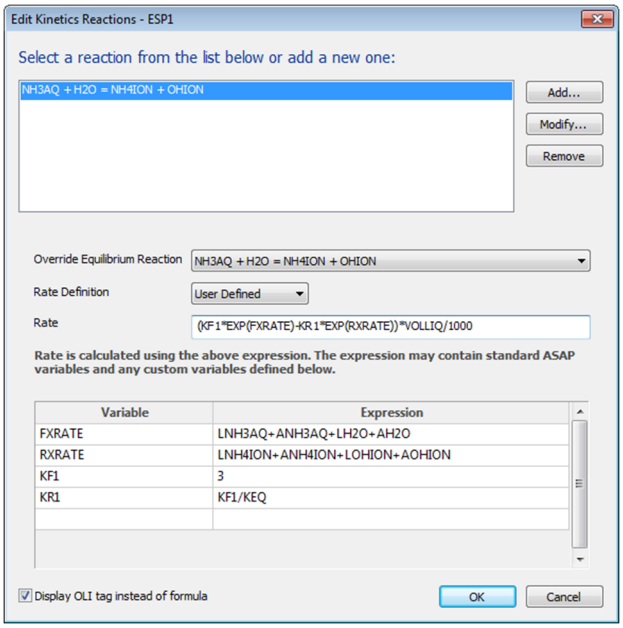


We first must enter our variables and expressions in the lower half of the dialog. Each variable must be on a separate row.



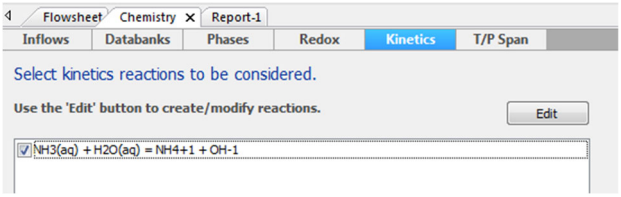
You now must enter the overall rate expression in the box marked **Rate**.

Click ok to accept this information.

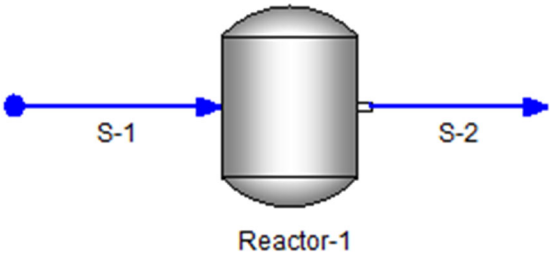


Enable the kinetics reaction by checking the box.

Return now to the flowsheet.



Create a flowsheet with a rector block with a single feed stream and a single product stream such as the following:



Enter the following for the feed stream parameters:

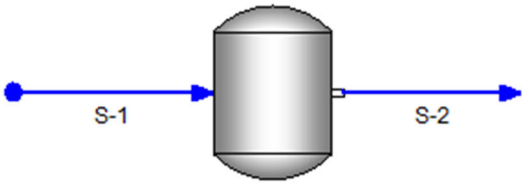
Feed Stream Parameters	
Feed Stream Name	S-1
Temperature	25 °C
Pressure	1 atm
Total Flow	Automatic
H2O	55.5087 mole/hr
NH3	0.1 mole/hr

Enter the following for the Reactor block parameters:

Reactor Block Parameters		
Reactor Type		Kinetics
Kinetic Parameters *(flyout dialog)*		
	Number of Stages	10
	Residence Time (hr)	100
Calculation Type		Isothermal
Pressure Spec.		Min. Inlet Pressure
Temperature (°C)		25.0
Chemistry Model		Default

Run the process.

Here we have displayed the output of the process using callouts:



S-1	
T (°C)	25.0
P (atm)	1.0
pH	6.99709
NH3 Aq, True (mol/hr)	0.1
NH4ION Aq (mol/hr)	0.0
OHION Aq (mol/hr)	1.0071e-7
HION Aq (mol/hr)	1.0071e-7

S-2	
T (°C)	25.0
P (atm)	1.0
pH	10.6921
NH3 Aq, True (mol/hr)	0.0994881
NH4ION Aq (mol/hr)	5.11867e-4
OHION Aq (mol/hr)	5.11867e-4
HION Aq (mol/hr)	2.08544e-11

The stream S-1 represents the equilibrium condition. The stream pH is approximately 7.0. The stream S-2 represents the condition with reaction kinetics limiting the reforming of ammonia from the ammonium ion. The pH is much higher at approximate 10.7 which shows that it is not at equilibrium.

Stoichiometric Reactors (CONV)

Stoichiometric reactors in the ESP Original program were called CONV reactors (conversion). These reactors used a simple stoichiometric relationship between reactants and products. There is no time factor for these reactions.

In this example, we will mimic the bio-remediation of phenol (C_6H_5OH) using aerobic degradation. The reaction we are simulating is:

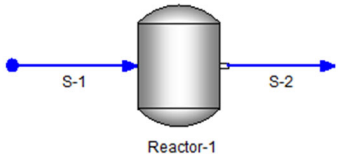
$$C_6H_5OH + 7O_2 \rightarrow 3H_2O + 6CO_2$$

Start OLI Flowsheet: ESP and create the following chemistry:

Stoichiometric Reactor		
Thermodynamic Framework	Aqueous (H+ Ion)	
Additional Databanks	None	
Phases	Default	
Redox	Off	
Inflows	Formula	OLI Tag Name
Water	H_2O	H2O
Phenol	C_6H_5OH	C_6H_5OH
Oxygen	O_2	O_2
Carbon Dioxide	CO_2	CO_2

Unlike previous reactors, we do not define the stoichiometric parameters in the chemistry section. Create a flowsheet with the following block and streams:

Create a flowsheet with a rector block with a single feed stream and a single product stream such as the following:



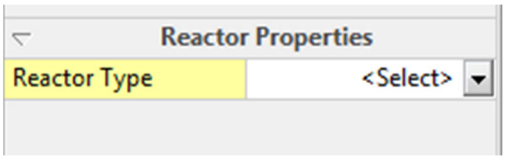
Enter the following feed stream parameters:

Feed Stream Parameters	
Feed Stream Name	S-1
Temperature	25 °C
Pressure	200.0 atmosphere
Total Flow	Automatic
H2O	55.0 mole/hr
C6H5OH	1.0 mole/hr
O2	7.0 mole/hr

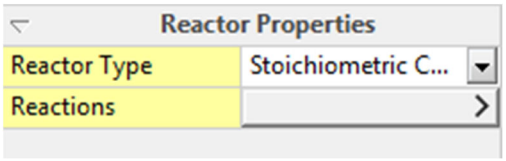
Now enter the block parameters:

Reactor Block Parameters		
Reactor Type		Stoichiometric Conversion
Reactions		
	Conversion Reaction (edit)	C6H5OH + 7O2 = 3H2O + 6CO2
	Key Component	C6H5OH
	Conversion factor	0.4
Calculation Type		Isothermal
Pressure Spec.		Min. Inlet Pressure
Temperature (°C)		25.0
Chemistry Model		Default

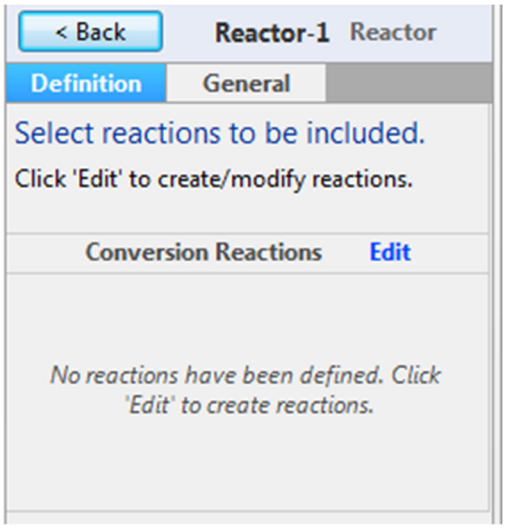
Here are the individual steps for this type of reactor. Click on the reactor you have added. This will display the properties dialog for the block:



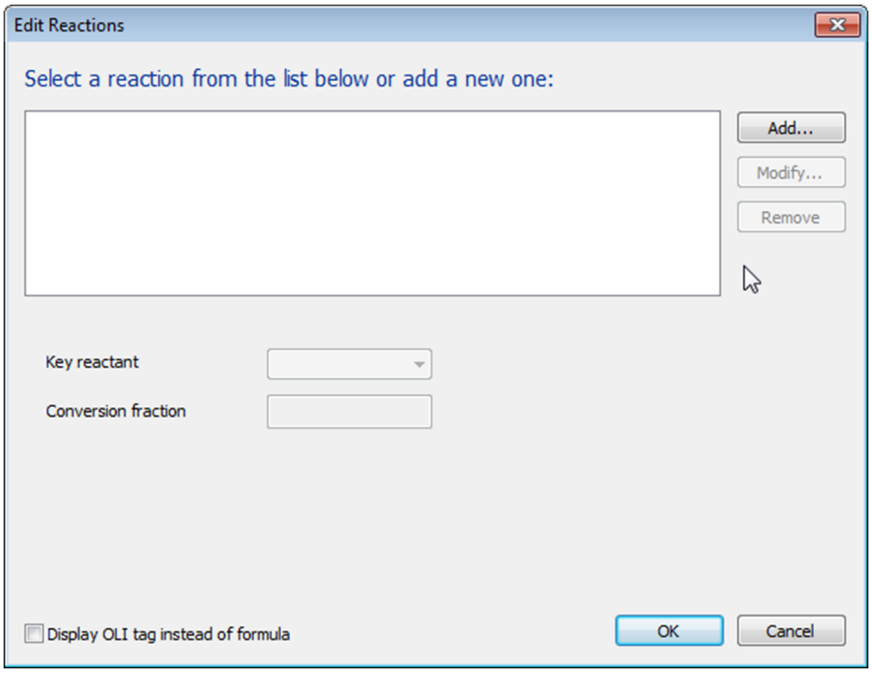
Change the type of reactor to **Stoichiometric Conversion**.



Click on the **Reactions** button. This will display a fly-out dialog.



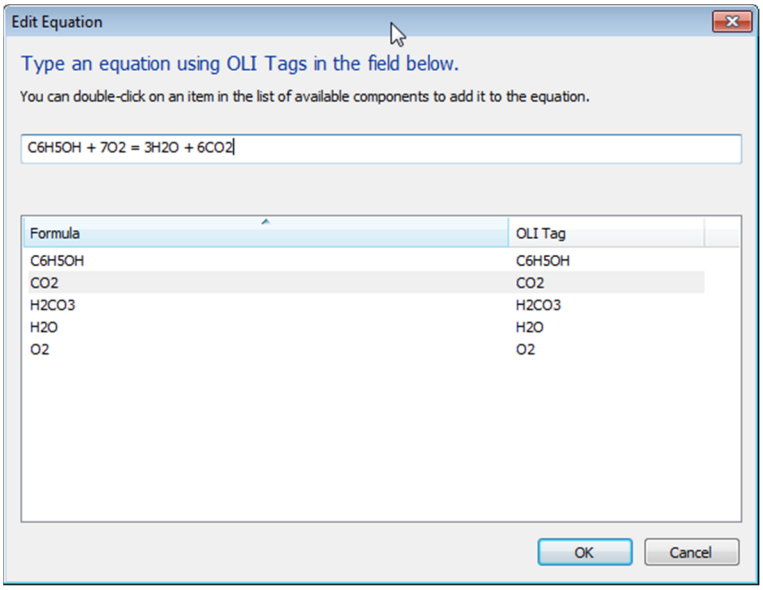
This brings up a familiar dialog. Normally we used this dialog in the chemistry section but now we are using the same dialog in the block.



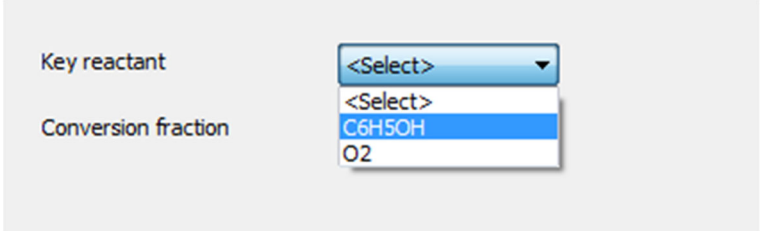
Click the **Add** button.

As we did in the previous section, we will now add the equation from above.

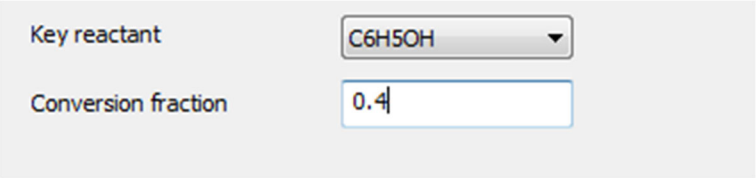
Click **OK**



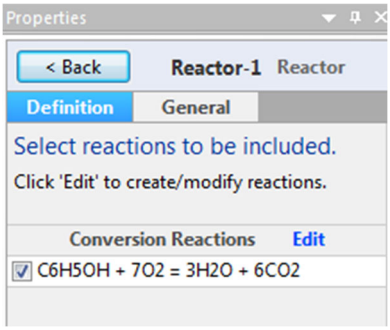
We now must define the key reactant. This is what the conversion is based on. Select phenol (C_6H_5OH).



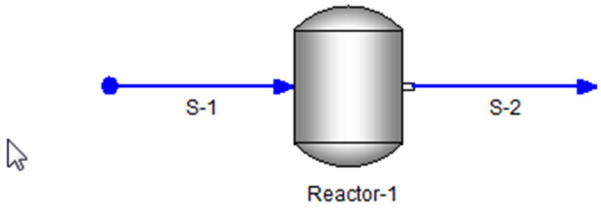
For our purposes we are converting 40% (on a mole basis) so enter 0.4



Click **OK** to continue.



We have run our sample process at very high pressure to force the oxygen into solution. Here are the results:



S-1	
T (°C)	25.0
P (atm)	200.0
C6H5OH Aq, Apparent (mol/hr)	0.999932

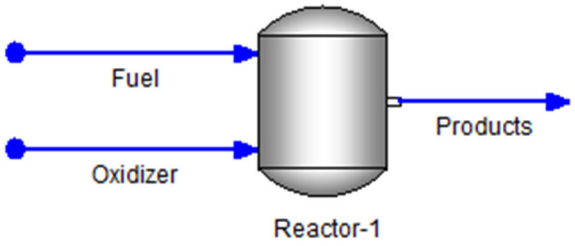
S-2	
T (°C)	25.0
P (atm)	200.0
C6H5OH Aq, Apparent (mol/hr)	0.599854

We started with 1.0 mole of phenol (0.999932 is close to 1.0 moles) and have 0.599854 moles. This is means we have reacted 40% of the phenol which is exactly to what the conversion factor was set.

Gibbs Reactor

A Gibbs reactor is a special type of reaction in OLI Flowsheet: ESP in that it does not evaluate the standard equilibrium equations found in the chemistry model. Rather it minimizes the Gibbs Free Energy at a given temperature and pressure or maximizes entropy at a given pressure and enthalpy. The latter is usually what is calculated in OLI Flowsheet: ESP.

Create a flowsheet with the following configuration:



Create the chemistry model with the following parameters:

Gibbs Reactor		
Thermodynamic Framework	MSE (H3O+ Ion)	
Additional Databanks	None	
Phases	Default	
Redox	Off	
Inflows	Formula	OLI Tag Name
Water	H_2O	H2O
Methane	CH_4	CH4
Oxygen	O_2	O2
Carbon Dioxide	CO_2	CO2
Nitrogen	N_2	N2
Carbon Monoxide	CO	CO

Enter the parameters for each inlet stream:

Feed Stream Parameters		
Feed Stream Name	Fuel	
Temperature	25	°C
Pressure	1.0	Atm
Total Flow	1 m3/hr	m3/hr
H2O	0.0 mole/hr	mole/hr
CH4	100.0	mole/hr
O2	0	mole/hr
CO2	0	mole/hr
N2	0	mole/hr
CO	0	mole/hr

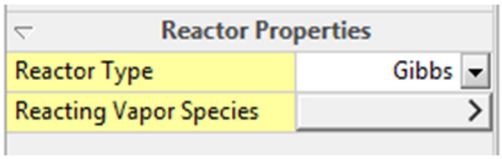
Feed Stream Parameters		
Feed Stream Name	Oxidizer	
Temperature	25	°C
Pressure	1.0	Atm
Total Flow	0.1 m3/hr	m3/hr
H2O	0.0 mole/hr	mole/hr
CH4	0.0	mole/hr
O2	20	mole/hr
CO2	0	mole/hr
N2	80	mole/hr
CO	0	mole/hr

Enter the block parameters for the reactors. We will describe the details about the new parameters after the table.

Reactor Block Parameters		
Reactor Type		Gibbs
Reacting Vapor Species		
	CH4	Enabled
	CO	Enabled
	CO2	Enabled
	H2O	Enabled
	N2	Disabled
	O2	Enabled
Calculation Type		Adiabatic
Pressure Spec.		Min. Inlet Pressure
Heat Duty		0.0
Chemistry Model		Default

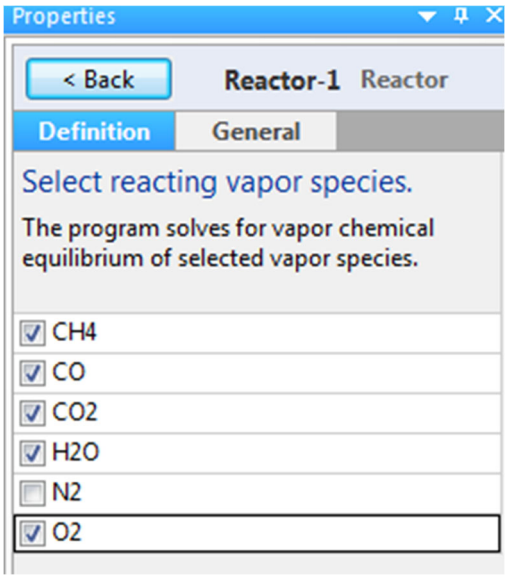
This type of reactor requires the user to specify which vapor species can react. In this case, we are simulating a combustion reaction, so we do not require Nitrogen gas to be reactive. After specifying the reactor type we need to enable the gasses.

Click the fly-out button next to **Reacting Vapor Species**.



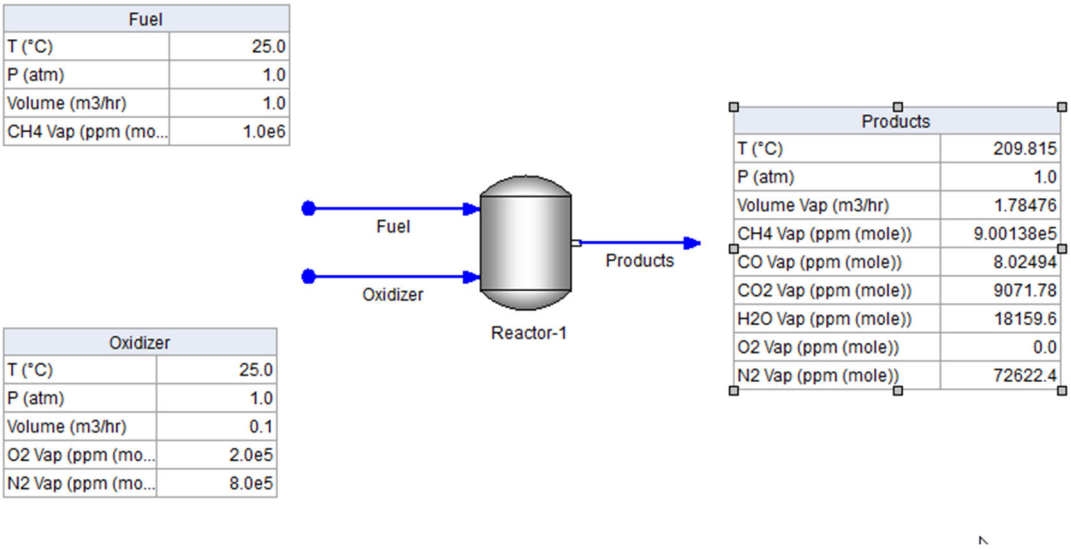
Check the following components:

CH4CO
CO2
H2O
O2



Click the **Back** button and then run the calculation.

The simulation results are presented in the callout tables.

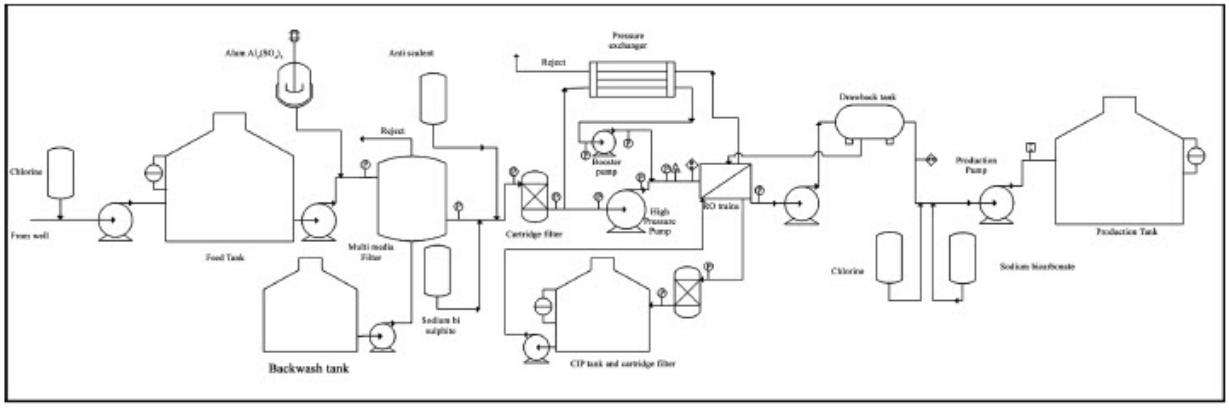


You can see that we have reacted methane with oxygen and have formed the traditional combustion products of carbon dioxide and water. We also have some incomplete combustion and have formed some carbon monoxide at approximately 8 ppm. There has also been a temperature increase.

RO Membranes (Reverse Osmosis) Example

Overview of RO

This example of an RO membrane compares the OLI Flowsheet: ESP simulation with a real-world application. In this case, we are simulating a desalination plant located in the Middle East and built to World Health Organization standard. The overall process flowsheet is shown in the image below:



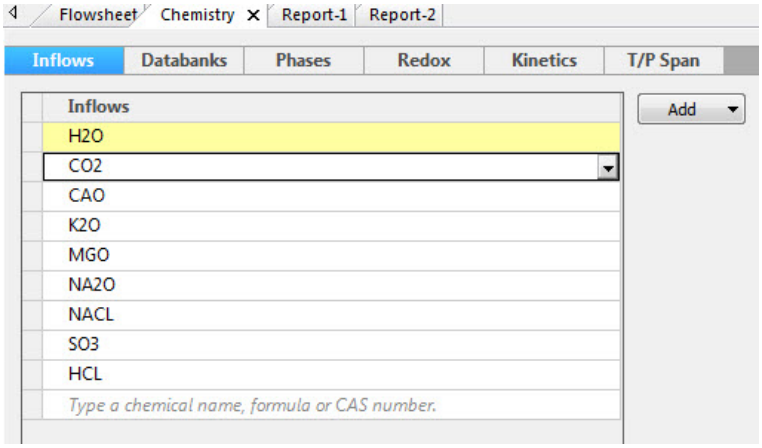
Flowsheet RO plant[8]

The goal of this simulation is to confirm that the objective of having a permeate flowrate of a minimum of 3600 m^3/day with a TDS (total dissolved solids) less than 100 ppm. The brackish feedwater is over 10,000 TDS.

In this simulation we will concentrate on only the pH pretreatment section and the RO membrane itself.

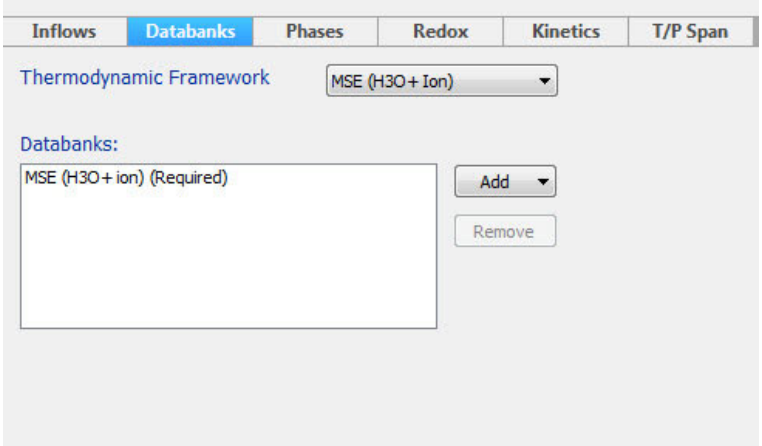
Defining the Chemistry Model

For this simulation we are assuming you already know how to use OLI Flowsheet: ESP. We need to first define the chemistry for this process. Start OLI Flowsheet: ESP and click on the Chemistry Tab.



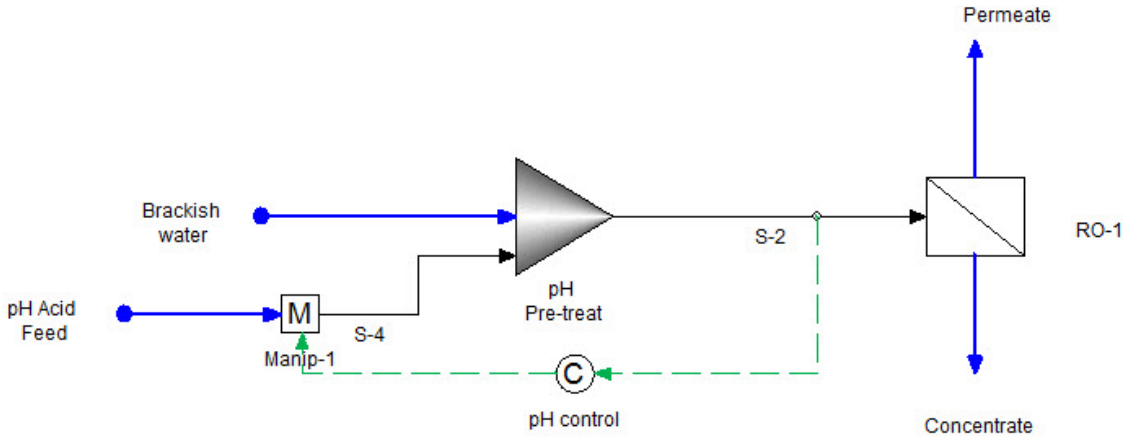
Click on the databanks tab to select MSE

[8] Source: Abdel-Fatah, M.A., El-Gendi, A and Ashour, F. (2016) Performance Evaluation and Design of RO Desalinatino Plant: Case Study. *Journal of Geoscience and Environment Protection,* **4**, 53-63



Defining the Flowsheet

The following diagram shows the partially completed flowsheet. Please enter the blocks from the palette and arrange as shown.



Entering the stream and block parameters (except the RO membrane).

We have shown you how to do this before, so we will just summarize the parameters in table form:

Feed Stream Parameters		
Feed Stream Name	pH Acid Feed	
Temperature	25	ºC
Pressure	1.0	Atm
Total Flow	1.0	m3/day
H2O	99.0	mass %
CO2	0	mass %

CAO	0	mass %
K2O	0	mass %
MGO	0	mass %
NA2O	0	mass %
NACL	0	mass %
SO3	0	mass %
HCL	1.0	mass %

Feed Stream Parameters		
Feed Stream Name	Brackish water	
Temperature	25	°C
Pressure	1.0	Atm
Total Flow	7200	m3/day
H2O	1323.38	mol/day
CO2	0.176125	mol/day
CAO	0.220969	mol/day
K2O	0.139955	mol/day
MGO	0.16293	mol/day
NA2O	0.0196066	mol/day
NACL	1.6363	mol/day
SO3	0.502502	mol/day
HCL	0.0	mass %

The TDS has been calculated for this stream to be approximately 7400 mg/L

Block Parameters		
Block Type		Manipulator
Block Name		Manip-1
Streams		
	Inlet	pH Acid Feed
	Outlet	S-4
Parameters		
	Manipulator Type	Total Flow
	Factor, Flow	1.0
Chemistry Model		Default

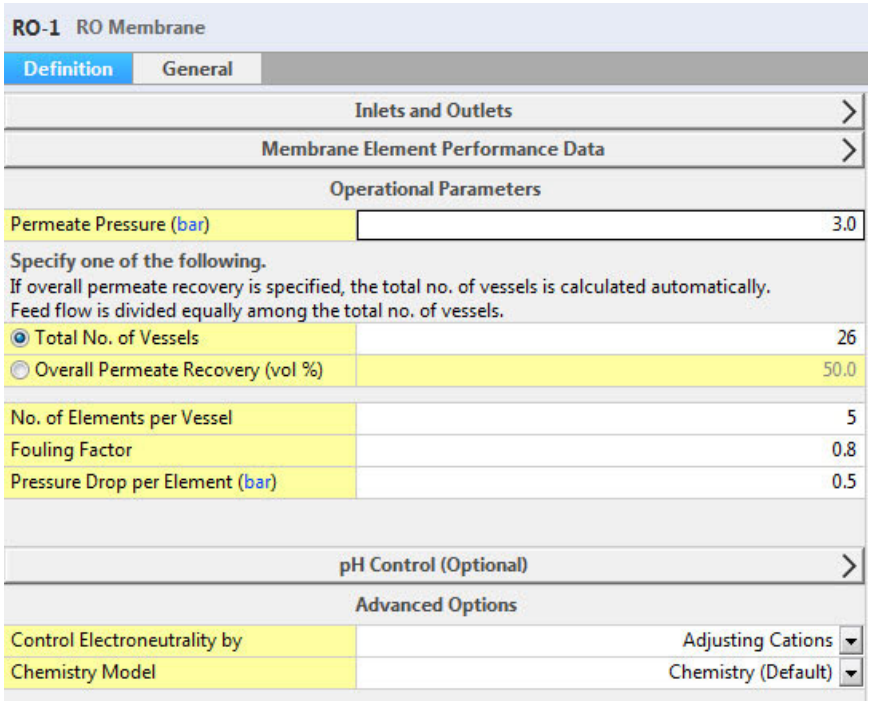
Block Parameters		
Block Type		Mixer
Block Name		pH Pre-Treat
Streams		
	Inlet	Brackish Water
	Outlet	S-2
Parameters		
	Calculation Type	Adiabatic
	Pressure Spec.	Absolute Pressure
	Pressure (Bar)	21.6
	Heat Duty (cal/hr)	0
Chemistry Model		Default

Block Parameters

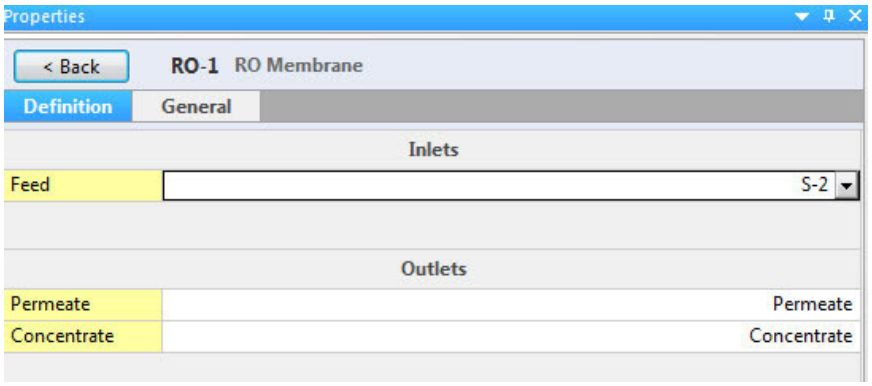
Block Type		Feedback Controller
Block Name		pH Control
Parameters		
	Target Stream	S-2
	Spec Type	pH
	Target Value	6.0
	Heat Duty (cal/hr)	0
Control Parameters		
	Controlling Block	Manip-1
	Block Parameter	Factor, Flow
Options		
	Calculate After	<automatic)
	Disable this Controller	No (unchecked)

Defining the RO Membrane Block

The RO Membrane block is a relatively complicated block. For this simulation we are using the parameters of a real membrane. The membrane under consideration is DOW FILMTEC™ BW30-400 Element[9].



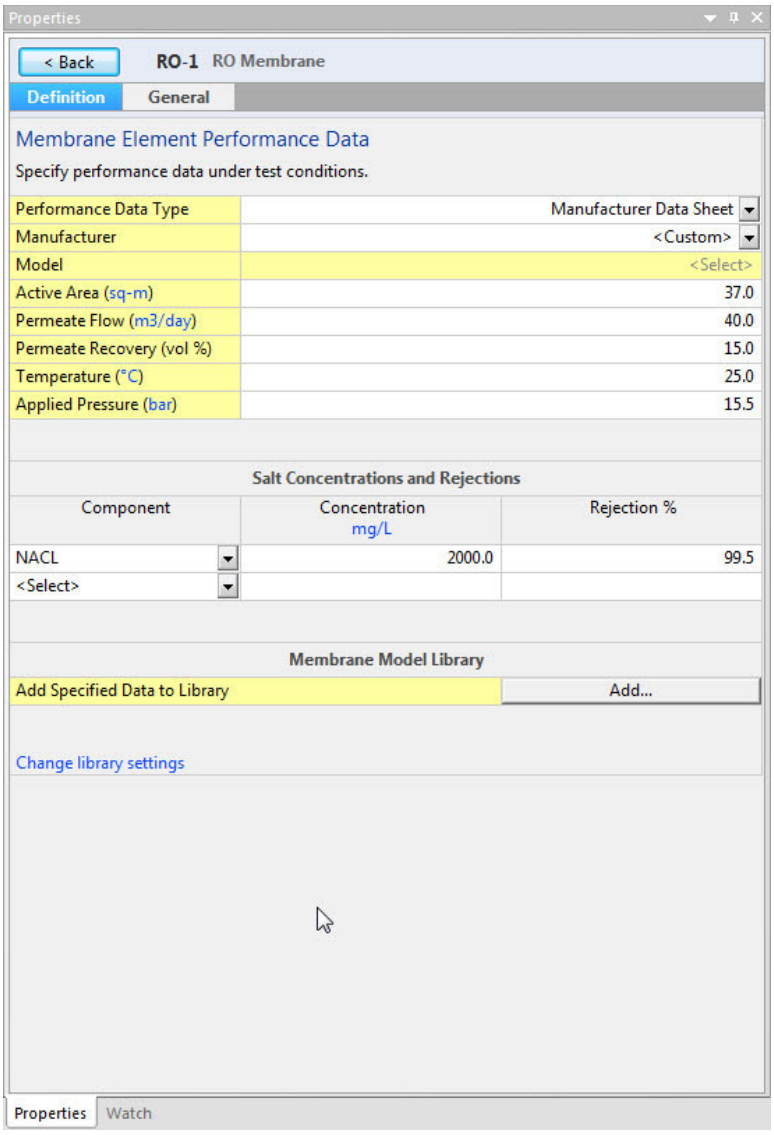
There is a lot of data to enter for this simulation. The first is to confirm the **Inlets and Outlets**.



Click the **Back** button.

Now, we need to define our RO membrane parameters. Click the **Membrane Element Performance Data** button.

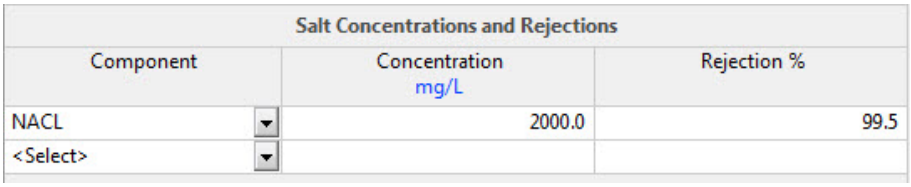
[9] DOW FILMTEC is a registered trademark of the DOW Chemical Company. The parameters were taken from the paper referenced earlier in this section.



The most common source of data will be from a manufacturer's data sheet. From data sheet we have the following values.

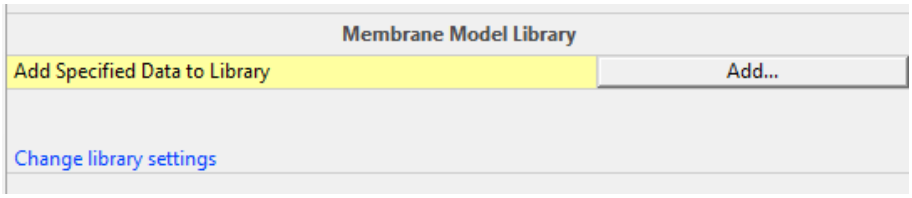
RO Element Data	
Active Area (m^2)	37.0
Permeate Flow (m^3/day)	40
Permeate Recovery (vol %)	15
Temperature (°C)	25
Applied Pressure (bar)	15.5

These values were developed by the manufacturer at a test condition. In this case the manufacturer has provided the test data.

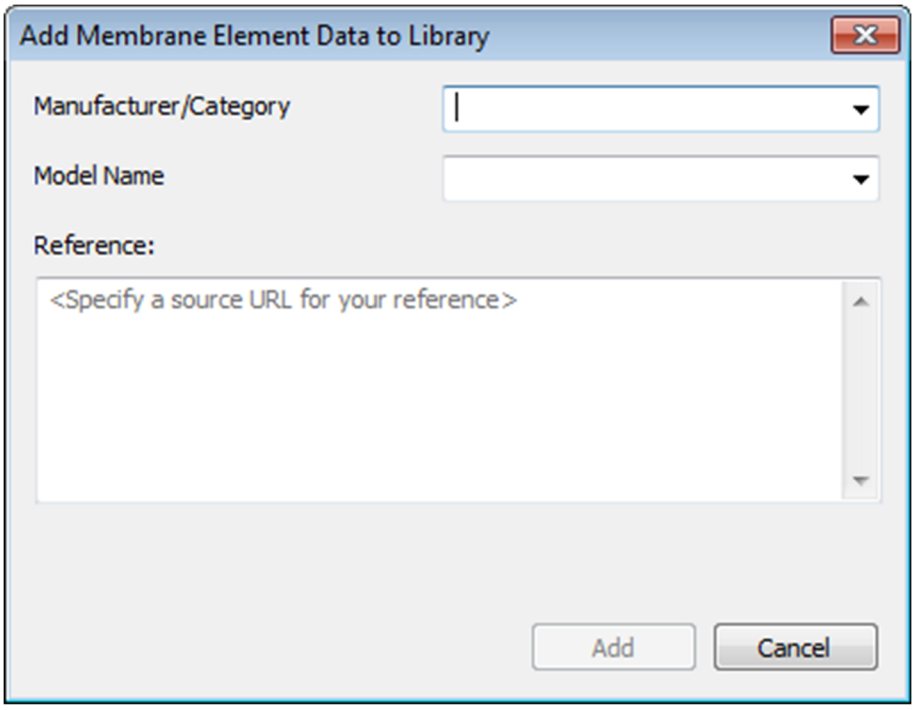


It is important to note that these conditions are required to simulate the RO Membrane. However, your actual feed solution may contain different amounts of NaCl as well as other minerals. OLI has developed correlations for how these membranes will respond with various ions at varying concentrations.

You can also save this membrane for use in later simulations by clicking the **Add…** button.

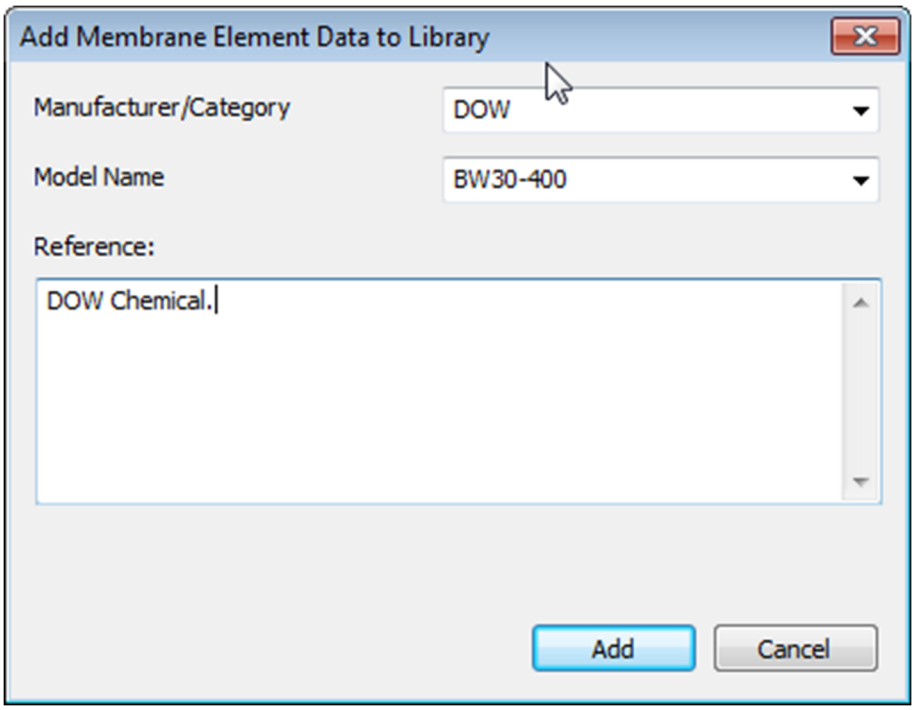


Clicking the **Add** button will display a new dialog:



The **Manufacturer/Category** allows you to select the company that provided the data.

Here we have added the name “DOW” and the model number:



Click the **Add** button.

You will notice that the Data grid has updated.

Click the **Back** button.

Now we need to specify the **Operational Parameters**.

Operational Parameters	
Permeate Pressure (bar)	3.0
Specify one of the following. If overall permeate recovery is specified, the total no. of vessels is calculated automatically. Feed flow is divided equally among the total no. of vessels.	
Total No. of Vessels	26
Overall Permeate Recovery (vol %)	50.0
No. of Elements per Vessel	5
Fouling Factor	0.8
Pressure Drop per Element (bar)	0.5
pH Control (Optional)	
Advanced Options	
Control Electroneutrality by	Adjusting Cations
Chemistry Model	Chemistry (Default)

The Permeate Pressure is the pressure on the downstream side of the membrane and is usually determined by other operational considerations. The total number of vessels are the actual RO units under consideration. The number of vessels was set by the authors of the reference mentioned previously (Abdel-Fatah, et.al.)

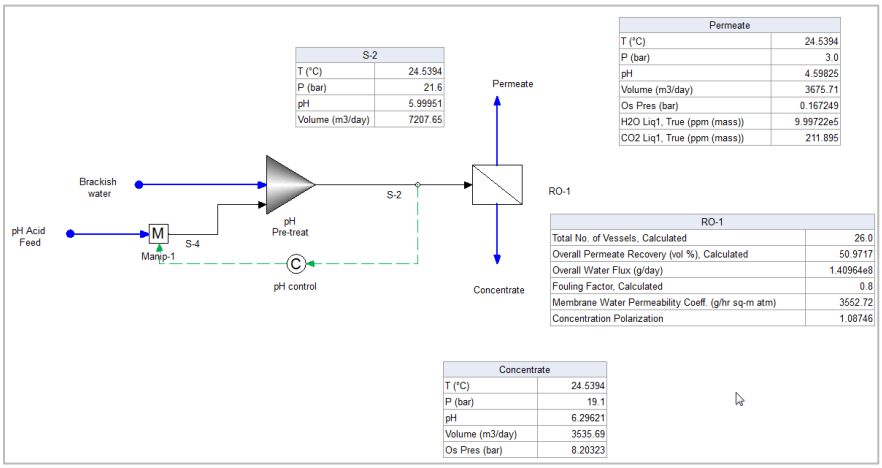
The number of Elements per Vessel was set to 5. The authors used 6 but that number is outside the range permitted by OLI. The authors set a fouling factor of 0.8 and a pressure drop per element of 0.5 bar.

As the ions move across the membrane there is a mathematical imbalance in electrical charge. The user can specify if the imbalance is corrected by adding/removing cations or anions. Cations are the default value.

At this point the membrane is fully defined and we are ready to run the simulation.

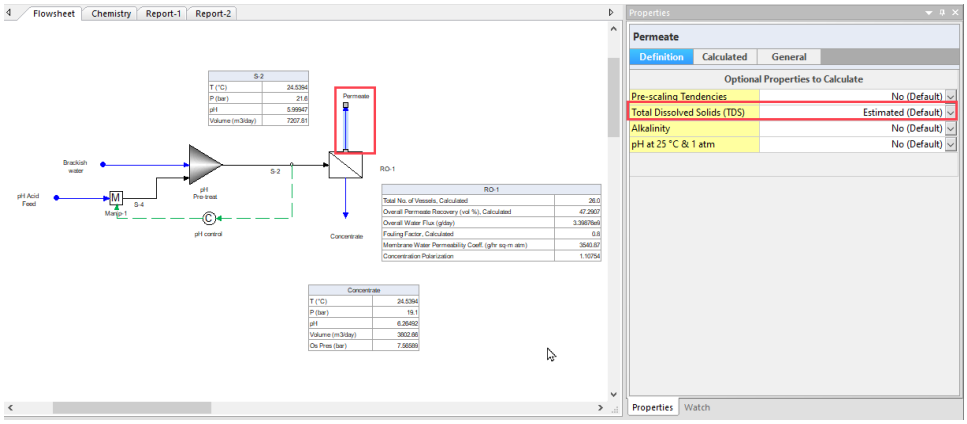
Running the simulation

The simulation was run without any additional tweaks. We have added some call-outs to make analyzing the simulation easier.



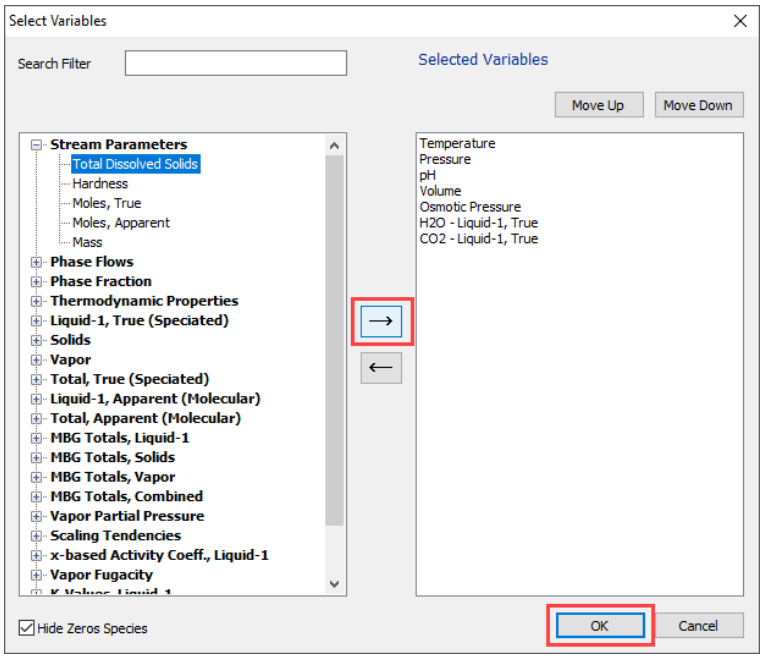
The brackish water has a TDS of approximately 7400 mg/L. Remember the World Health Organization wants a TDS of less than 100 mg/L. Reviewing the ***Permeate*** stream we can see some values that are of use to us.

To report the TDS value, we need to turn on this calculation. **Select** the **Permeate Stream**, go to the **Definition** tab, and enable the **Total Dissolved Solids Calculation (TDS) Estimated.**

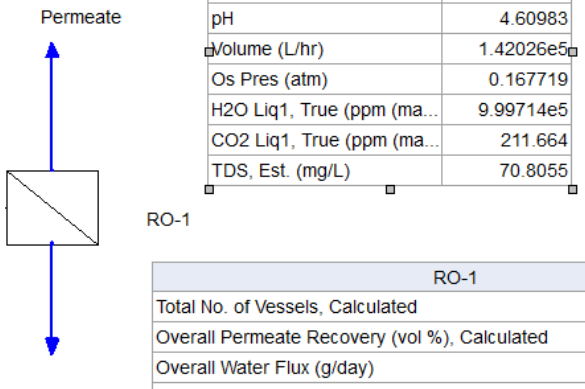


Run the simulation.

Double-click on the **Permeate Callout**. This will open a new window. Go to the **Stream Parameters section,** click on the '+' icon, and select **Total Dissolved Solids. Double-click** it or use the → arrow to put this variable under the *Selected Variables* window. Then click **OK.**



The calculated TDS value is ~ 70.8 mg/L.



Permeate	
T (°C)	24.5394
P (atm)	2.96077
pH	4.60983
Volume (L/hr)	1.42026e5
Os Pres (atm)	0.167719
H2O Liq1, True (ppm (ma...	9.99714e5
CO2 Liq1, True (ppm (ma...	211.664
TDS, Est. (mg/L)	70.8055

RO-1	
Total No. of Vessels, Calculated	26.0
Overall Permeate Recovery (vol %), Calculated	47.2907
Overall Water Flux (g/day)	3.39876e9
Fouling Factor, Calculated	0.8
Membrane Water Permeability Coeff. (g/hr sq-m atm)	3540.87
Concentration Polarization	1.10754

This certainly achieves the World Health Organization specification of less than 100 mg/L. The authors also wanted to have a permeate flowrate of more than 3600 m^3/day and we are reporting slightly more at 3675 m^3/day.

This shows that the OLI RO Membrane matches a peer reviewed academic project.

You can download a worked copy of this example from here: RO Membranes.

Appendix-1 Reverse Osmosis Technology

OLI MEMBRANE TECHNOLOGY: SIMULATOR FOR REVERSE OSMOSIS PROCESS

Summary

To model the transport mechanism inside the membrane, solution-diffusion approach has been incorporated. In the solution-diffusion model, it is proposed that transfer of ions and water through polymeric membranes occurs via a solution diffusion mechanism because of dissolution of permeates in the membrane materials [1]. The water flux through the membrane is a function of water permeability coefficient, hydrodynamic pressure difference and osmotic pressure difference across the membrane, whereas, the solute flux through the membrane is a function of solute permeability constant and solute concentration gradient across the membrane [2]. Molecular size of the ions strongly affects the transport characteristics of the ions due to the sieving action of the membranes. However, in water environment, different number of water molecules surround each cation and anion. Thus, the real radius of an ion is the one that considers the water molecules around it (i.e., the hydrated ion radius) rather than the absolute ionic crystal radius. Regardless of membrane type, the type of experiment, and the membrane configuration, the salt permeabilities are inversely proportional to the hydrated radii of the ions [3]. In OLI membrane model, permeability of ions has been correlated with their hydration numbers.

In general, the typical order of rejection of cations by reverse osmosis membranes follow $Fe^{3+} > Ni^{2+} \approx Cu^{2+} > Mg^{2+} > Ca^{2+} > Na^{+} > K^{+}$, and $PO_4^{3-} > SO_4^{2-} > HCO_3^{-} > Br^{-} > Cl^{-} > NO_3^{-} \approx F^{-}$ for anions [4]. The permeability of cations and anions calculated as a function of hydration numbers follow the typical trends. For some organics with same homologous group (i.e., alcohols, phenols, acids), the rejections have been correlated by calculating the topological parameters characterizing molecular structure [5]. For other neutrals, self-diffusivities relative to water have been used to correlate the permeability.

Commercial membrane manufacturers provide product specification sheet for each type of membranes. In addition to physical dimensions (i.e., membrane area), the product sheet also reports performance of the membrane (i.e., permeate flux, recovery and rejection percentage for NaCl or other solutes) at specific test conditions. User entered test conditions data are the key information for calculating the permeability coefficients of water and the test solute for the membrane element. These calculated permeability coefficients along with the above-mentioned correlations are used to estimate the permeability coefficients of other species present. The advantage of this method is that a reasonable and preferential order of permeabilities for the membrane regardless of membrane type can be correctly estimated.

In the current OLI membrane development, users can enter number of membrane elements per vessel and total number of vessels in the assembly. Alternatively, users can estimate total number of vessels required (or total membrane area) for a specific recovery. Concentration polarization is approximated using Peclet number and intrinsic enrichments [4]. Flow factor (sometimes referred as fouling factor) is estimated from the water activity reduction unless specified by the users. Users may specify feed side pressure drop per element if available. There are options for conditioning the feed to a specific pH by choosing a pH acid titrant or base titrant.

Model Development

Water flux in RO membrane is a function of membrane permeability of water, applied pressure and the feed water osmotic pressure. According to solution-diffusion model, water flux can be calculated from the following equations:

$$J_w = AP_w(\Delta P - \Delta\pi); \text{ For water} \quad (1)$$

$$J_{si} = AP_{si}(C_{si} - C_{pi}); \text{ For } i = 2, n \text{ (water is not included)} \quad (2)$$

where J_w, P_w, $\Delta P, \Delta\pi$ and A represent water flux through membrane, water permeability, membrane pressure gradient, osmotic pressure gradient and membrane area, respectively. J_{si}, P_{si}, C_{si} and C_{pi} represent species i flux through membrane, permeability, concentration at the membrane surface and concentration at the permeate side, respectively. It is to be noted that n represents total number of aqueous and ionic species in the system.

$$\Delta P = P_f - P_{pd} - P_p \quad (3)$$

where P_f, P_{pd} and P_p represent feed side pressure, pressure drop at the concentrate (residue) side and permeate pressure, respectively.

$$P_{pd} = 0.005Q_{avg}^{1.7} \quad (4)$$

$$Q_{avg} = \frac{Q_f + Q_c}{2} \quad (5)$$

where Q_f, Q_c and Q_{avg} represent feed, concentrate and average concentrate (residue) side flow rate, respectively.

$$\Delta\pi = \pi_{avg} - \pi_p \quad (6)$$

$$\pi_{avg} = \frac{\pi_f + \pi_c}{2} \quad (7)$$

where π_f, π_p, π_c and π_{avg} represent feed side osmotic pressure, permeate side osmotic pressure, concentrate (residue) side osmotic pressure and average concentrate (residue) side osmotic pressure, respectively.

The salt concentration adjacent to the membrane surface is higher than the bulk solution concentration because reverse osmosis membranes preferentially permeate water and retain salt. Water and salt are brought toward the membrane surface by the flow of solution through the membrane. Water and a little salt permeate the membrane, but most of the salt is rejected by the membrane and retained at the membrane surface. Salt accumulates at the membrane surface until a sufficient gradient has formed to allow the salt to diffuse to the bulk solution [4]. The increase or decrease of the concentration at the membrane surface relative to the bulk solution concentration determines the extent of concentration polarization.

$$CP = \frac{e^{PK}}{1 + E_0(e^{PK} - 1)} \quad (8)$$

$$PK = {J_v \delta}/{D_v} \tag{9}$$

where CP, PK, E_0, J_v, δ and D_v represent concentration polarization modulus, Peclet number, enrichment factor, typical flux through membrane, boundary layer thickness and typical diffusion coefficient, respectively.

$$C_{si} = C_{pi} + CP(C_{fi} - C_{pi}) \tag{10}$$

where C_{si} and C_{fi} represent concentration at the membrane surface and feed side bulk concentration for the species, respectively.

The fouling factor is applied to membrane due to loss of permeability by compaction and scale fouling. Typically, a fouling factor less than 1.0 is applied depending on the membrane life. A correlation was developed for fouling factor which considers the water activity reduction at the membrane surface due to permeation relative to the fresh membrane under the test conditions.

$$FF = function\,(T_c, \pi_{avg}) \tag{11}$$

where FF, T_c and π_{avg} represent fouling factor, concentrate (residue) side temperature and average concentrate (residue) side osmotic pressure, respectively.

The osmotic pressure, self-diffusivity and densities are calculated in OLI Systems' Mixed-Solvent Electrolyte (MSE) or Aqueous (AQ) framework.

Equations (1-11) constitute the solution of the RO membrane and are simultaneously solved to calculate J_w, J_{si}, C_{pi}, C_{si}, CP and FF.

Permeability Estimate

In water rich environment, hydration numbers refer to the number of water molecules in the vicinity of the ion. Thus, real radius of an ion is the one that considers the water molecules around it (i.e., the hydrated ion radius) rather than the absolute ionic crystal radius. The water molecules that these hydration number pertain to presumably move together with the ions and are sufficiently firmly attached to them by ion-dipole interactions and hydrogen bonding to constitute a fairly stable entity [6]. Stokes radii are calculated as a function of ionic limiting conductivities and charge of species. The Stokes radii are corrected to relate Van Der Waals ionic sizes [7, 8]. The hydration numbers are calculated as a function of corrected Stokes radii, ionic limiting standard molar volume and molar volume of water. Membrane specific permeation behavior found in open literature were analyzed and from the analyzed data, a correlation was developed for permeability as a function of hydration numbers. It is worth mentioning that regardless of membrane type, the type of experiment, and the membrane configuration, the salt permeabilities are inversely proportional to the hydrated radii of the ions [3]. However, for regressing the water permeability and key components (test solutes) permeabilities, a modified subset of equations (1-11) were formulated and simultaneously solved based on the performance data provided. After calculating water and key components permeabilities, an update (but preserving the trend) in the aforementioned correlation was achieved, and the permeabilities of the rest of the ionic species were calculated from the updated correlation. The advantage of this technique is that a reasonable and preferential order of permeabilities for the membrane regardless of membrane type can be correctly estimated.

For some organics with same homologous group (i.e., alcohols, phenols, acids), the rejections were correlated by calculating the topological parameters characterizing molecular structure [5]. For other neutrals, self-diffusivities relative to water were used to correlate the permeability. These calculated permeabilities remain constant unless there is a change in temperature.

References

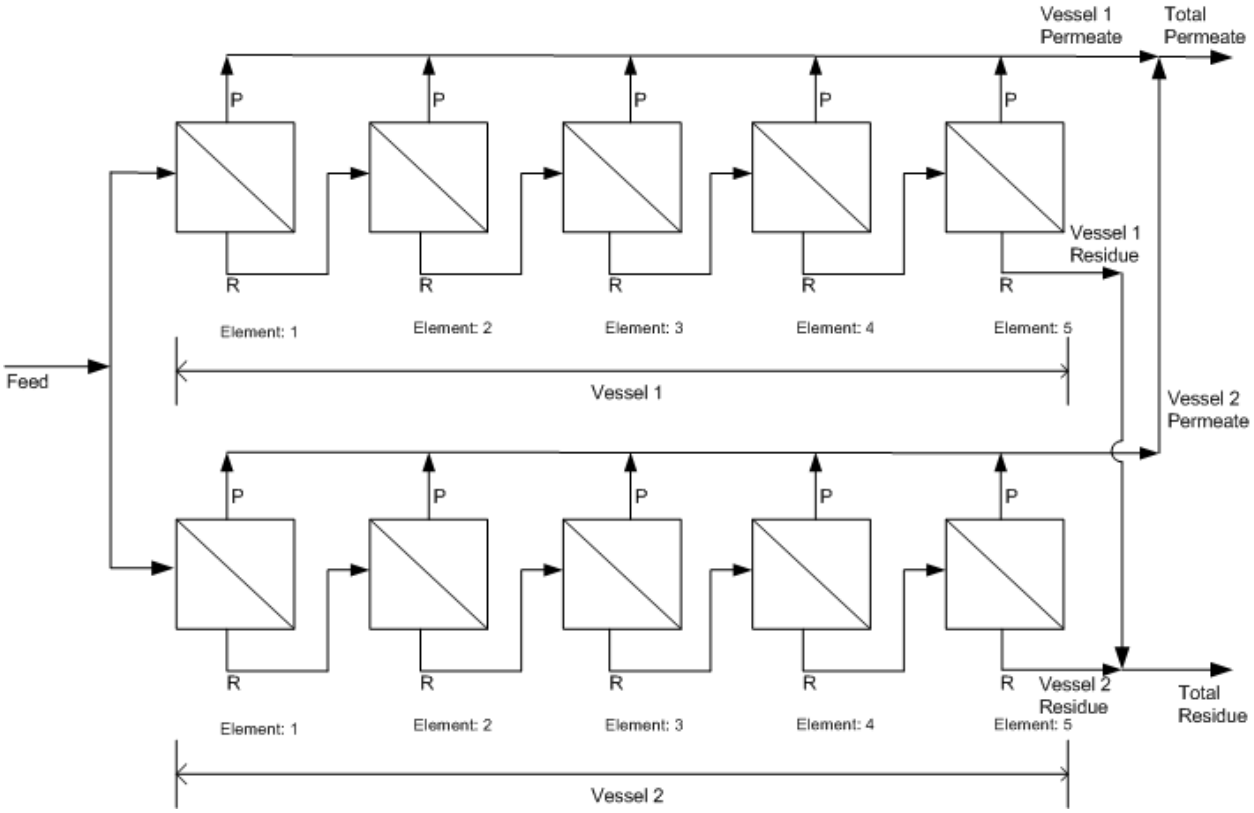
[1] S.M.J. Zaidi, F. Fadhillah, Z. Khan, and A.F. Ismail. Salt and water transport in reverse osmosis thin film composite seawater desalination membranes. Desalination, 368 (2015) 202.
[2] P. Mukherjee, A. Sengupta. Ion exchange selectivity as a surrogate indicator of relative permeability of ions in reverse osmosis processes. Environ. Sci. Technol., 37 (2003) 1432.
[3] S.M.S. Ghiu, Mass transfer of ionic species in direct and reverse osmosis processes, Doctoral dissertation, University of South Florida, 2003.
[4] R.W. Baker, Membrane technology and applications, 2nd Ed., Chichester, England: Wiley, 2004.
[5] A. Książczak, A. Anderko. A chemical approach to the prediction of thermophysical properties of associating compounds. Berichte der Bunsengesellschaft für physikalische Chemie, 92 (1988) 496.
[6] Y. Marcus. Ion properties, 1st Ed., New York: Marcel Dekker, 1997.
[7] Y. Marcus. Ion solvation, 1st Ed., New York: John Wiley & Sons, 1985.
[8] R.E. Nightingale. Phenomenological theory of ion solvation: Effective radii of hydrated ions, J. Phys. Chem., 63 (1959) 1381.

Definitions

Number of Elements/Vessel and Total Number of Vessels

An Element is the building block (e.g., a single membrane unit operation block) of the membrane assembly. Many elements are connected together to form a vessel.

Below is a diagram of 5 Elements/Vessel and a total of 2 Vessels membrane assembly. The feed will be equally divided among the vessels.



Fouling Factor

Fouling factor represents the resistance to flow through the membrane, hence sometimes termed as flow factor. The fouling factor is defined as the fraction of the water permeability of the membrane relative to a membrane with nominal flow specification. Hydranautics suggests a fouling factor of 1 in the projection is used to calculate the performance of new elements with exactly nominal flow rate. A fouling factor < 1 should be applied when making a design for long-term operation.

Concentration Polarization

When a component is enriched at the membrane surface, then mass balance dictates that a second component is depleted at the surface. Because the feed mixture components permeate at different rates, concentration gradients form in the fluids at the boundary layer. This phenomenon is called concentration polarization. Unless the solutions are extremely well stirred, concentration gradients form in the solutions on either side of the membrane. Concentration polarization is the measure of the intensity of concentration gradients occurring at the surface relative to the total absence of concentration polarization (value 1).

Pressure Drop Per Element

Feed side pressure may reduce during operation resulting in a decrease of the hydraulic pressure difference across membrane. Thus, the feed pressure of the 2nd element (e.g., residue pressure of 1st element) may decrease. Users can either specify the pressure drop per element. In absence of the user specified value, software will calculate the pressure drop.

Control Electroneutrality

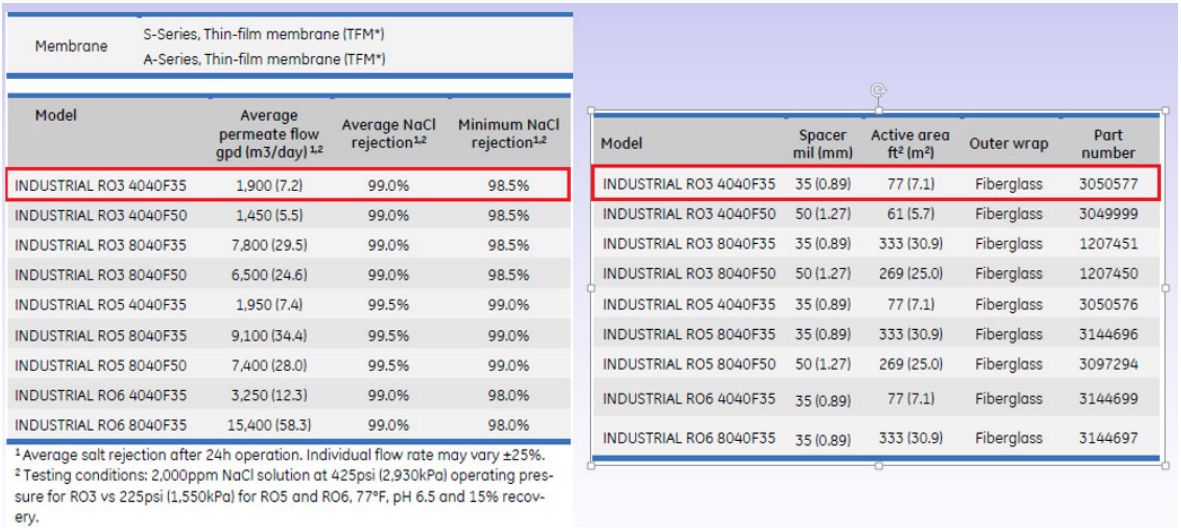
Since the permeation rates of the species are different, there could be imbalance of the associated ions. An electroneutrality balance must be achieved on both sides of the membrane. This option controls how the electroneutrality balance will be achieved any time you are out of balance in the solver. By default, it is Cation Control. Currently we follow “Prorate Cations and Prorate Anions” selection as you’ve seen in OLI Studio. Electroneutrality balance by adjusting cations or anions should result in the same flux across membrane.

Manufacturer Data Sheet for RO Membranes

Membrane manufactures provide a technical sheet for each type of membrane. In addition to physical dimensions (such as membrane area, spacer arrangement, tube diameter and so on), the technical sheet also reports results of a standard experimental measurement of the membrane, that is, permeate flux, recovery and rejection percentage for NaCl (or other salts) aqueous solution at 25 ºC. These are the data we will use to calibrate membrane properties.

The following are standard product sheet information from different manufactures.

Example 1: GE



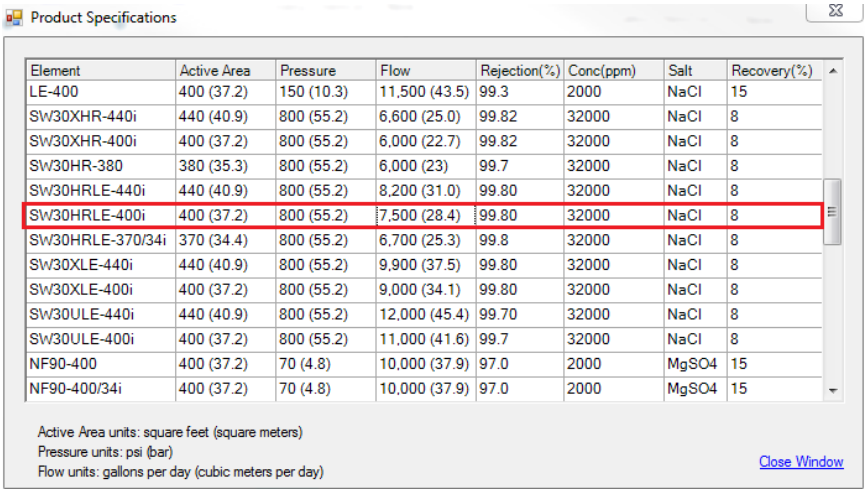
Membrane	S-Series, Thin-film membrane (TFM*) A-Series, Thin-film membrane (TFM*)

Model	Average permeate flow gpd (m3/day)[1,2]	Average NaCl rejection[1,2]	Minimum NaCl rejection[1,2]
INDUSTRIAL RO3 4040F35	1,900 (7.2)	99.0%	98.5%
INDUSTRIAL RO3 4040F50	1,450 (5.5)	99.0%	98.5%
INDUSTRIAL RO3 8040F35	7,800 (29.5)	99.0%	98.5%
INDUSTRIAL RO3 8040F50	6,500 (24.6)	99.0%	98.5%
INDUSTRIAL RO5 4040F35	1,950 (7.4)	99.5%	99.0%
INDUSTRIAL RO5 8040F35	9,100 (34.4)	99.5%	99.0%
INDUSTRIAL RO5 8040F50	7,400 (28.0)	99.5%	99.0%
INDUSTRIAL RO6 4040F35	3,250 (12.3)	99.0%	98.0%
INDUSTRIAL RO6 8040F35	15,400 (58.3)	99.0%	98.0%

[1] Average salt rejection after 24h operation. Individual flow rate may vary ±25%.
[2] Testing conditions: 2,000ppm NaCl solution at 425psi (2,930kPa) operating pressure for RO3 vs 225psi (1,550kPa) for RO5 and RO6, 77°F, pH 6.5 and 15% recovery.

Model	Spacer mil (mm)	Active area ft² (m²)	Outer wrap	Part number
INDUSTRIAL RO3 4040F35	35 (0.89)	77 (7.1)	Fiberglass	3050577
INDUSTRIAL RO3 4040F50	50 (1.27)	61 (5.7)	Fiberglass	3049999
INDUSTRIAL RO3 8040F35	35 (0.89)	333 (30.9)	Fiberglass	1207451
INDUSTRIAL RO3 8040F50	50 (1.27)	269 (25.0)	Fiberglass	1207450
INDUSTRIAL RO5 4040F35	35 (0.89)	77 (7.1)	Fiberglass	3050576
INDUSTRIAL RO5 8040F35	35 (0.89)	333 (30.9)	Fiberglass	3144696
INDUSTRIAL RO5 8040F50	50 (1.27)	269 (25.0)	Fiberglass	3097294
INDUSTRIAL RO6 4040F35	35 (0.89)	77 (7.1)	Fiberglass	3144699
INDUSTRIAL RO6 8040F35	35 (0.89)	333 (30.9)	Fiberglass	3144697

Example 2: Hydranautics



Product Specifications

Element	Active Area	Pressure	Flow	Rejection(%)	Conc(ppm)	Salt	Recovery(%)
LE-400	400 (37.2)	150 (10.3)	11,500 (43.5)	99.3	2000	NaCl	15
SW30XHR-440i	440 (40.9)	800 (55.2)	6,600 (25.0)	99.82	32000	NaCl	8
SW30XHR-400i	400 (37.2)	800 (55.2)	6,000 (22.7)	99.82	32000	NaCl	8
SW30HR-380	380 (35.3)	800 (55.2)	6,000 (23)	99.7	32000	NaCl	8
SW30HRLE-440i	440 (40.9)	800 (55.2)	8,200 (31.0)	99.80	32000	NaCl	8
SW30HRLE-400i	400 (37.2)	800 (55.2)	7,500 (28.4)	99.80	32000	NaCl	8
SW30HRLE-370/34i	370 (34.4)	800 (55.2)	6,700 (25.3)	99.8	32000	NaCl	8
SW30XLE-440i	440 (40.9)	800 (55.2)	9,900 (37.5)	99.80	32000	NaCl	8
SW30XLE-400i	400 (37.2)	800 (55.2)	9,000 (34.1)	99.80	32000	NaCl	8
SW30ULE-440i	440 (40.9)	800 (55.2)	12,000 (45.4)	99.70	32000	NaCl	8
SW30ULE-400i	400 (37.2)	800 (55.2)	11,000 (41.6)	99.7	32000	NaCl	8
NF90-400	400 (37.2)	70 (4.8)	10,000 (37.9)	97.0	2000	MgSO4	15
NF90-400/34i	400 (37.2)	70 (4.8)	10,000 (37.9)	97.0	2000	MgSO4	15

Active Area units: square feet (square meters)
Pressure units: psi (bar)
Flow units: gallons per day (cubic meters per day)

Close Window

Example 3: Koch

PRODUCT DESCRIPTION	**Membrane Chemistry:**	Proprietary TFC® polyamide
	Membrane Type:	TFC® HR membrane
	Construction:	Spiral wound with fiberglass outerwrap
	Applications:	High rejection for brackish water treatment

SPECIFICATIONS

Part Number	Model	Permeate Flow		Chloride Rejection	Active Membrane Area		Feed Spacer
		gpd	(m^3/d)	percent	ft^2	(m^2)	mil (mm)
8882234	8040-HR-375	10,200	(38.6)	99.55	375	(34.8)	31 (0.8)

Test Conditions: 2,000 mg/l NaCl solution at 225 psi (1,550 kPa) applied pressure, 15% recovery, 77°F (25°C) and pH 7.5

Appendix-2 Optimizer Mathematical Functions

Table 2 Optimizer mathematical functions to write subexpressions

Mathematical functions	**Uses**
math.abs(x)	Return the absolute, or non-negative value of x.
math.exp(x)	Returns the the value e^x.
math.pow(x,y)	Returns x^y, you can also use the expression x^y to compute this value.
math.sqrt(x)	Returns the square root of x, you can also use the expression x^0.5 to compute this value.
math.log(x)	Returns the natural logarithm of x.
math.log10(x)	Returns the base-10 logarithm of x.
math.pi	Returns the value of PI.
math.ceil(x)	Returns the smallest integer larger than or equal to x.
math.floor(x)	Returns the largest integer smaller than or equal to x.
math.fmod(x, y)	Returns the remainder of the division of x by y that rounds the quotient towards zero.
math.max(x, …)	Returns the maximum value among its arguments.
math.min(x, …)	Returns the minimum value among its arguments.
math.sin(x)	Returns the sine of x (assumed to be in radians).
math.sinh(x)	Returns the hyperbolic sine of x.
math.asin(x)	Returns the arc sine of x (in radians).

Lua defines/objective function NAMING rules:

names should not have spaces in between (e.g., Calculated pH)
names should not start with numbers (e.g., 123ABC), or names with only numbers are not allowed (e.g., 007)
special characters in the names are better to avoid (e.g., XYZ(6), XYZ$)
+/-/* should be avoided in names (e.g., XYZ-6, Calculated-pH)
underscore is acceptable in names (e.g., Calculated_pH)
could start with an underscore even (e.g., _XYZ)