



INTRODUCTION TO
OLI Engine for Aspen Hysys



think simulation



getting the
chemistry right

Introduction to OLI Engine for Aspen Hysys

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OLI Engine for Aspen Hysys

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Other useful links and resources are:



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Disclaimer

This manual was produced using the OLI Engine 12.0.0.6 for Aspen Hysys 14

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.

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Overview

The OLI Engine for Aspen HYSYS interface greatly enhances Aspen HYSYS' capability to model electrolyte systems. A rigorous and self-consistent thermodynamic framework is employed to tame the mathematically stiff equations commonly found in electrolyte systems. Also, a database of over 10,000 components is available.

The OLI model is available as a property set within Aspen HYSYS. This "Getting Started" guide will show you how to create the electrolyte chemistry for a simple case and then create a simple flowsheet in Aspen HYSYS.

Assumptions

The following assumptions are made for this guide:

1. Aspen HYSYS is currently installed and running on your computer.
2. The license manager for Aspen HYSYS is currently set up.
3. The OLI Engine for Aspen HYSYS product has been installed.
4. The OLI security model is running.
5. Aspen HYSYS V14 is being used.
6. The user is expected to know how to run Aspen HYSYS.

Application

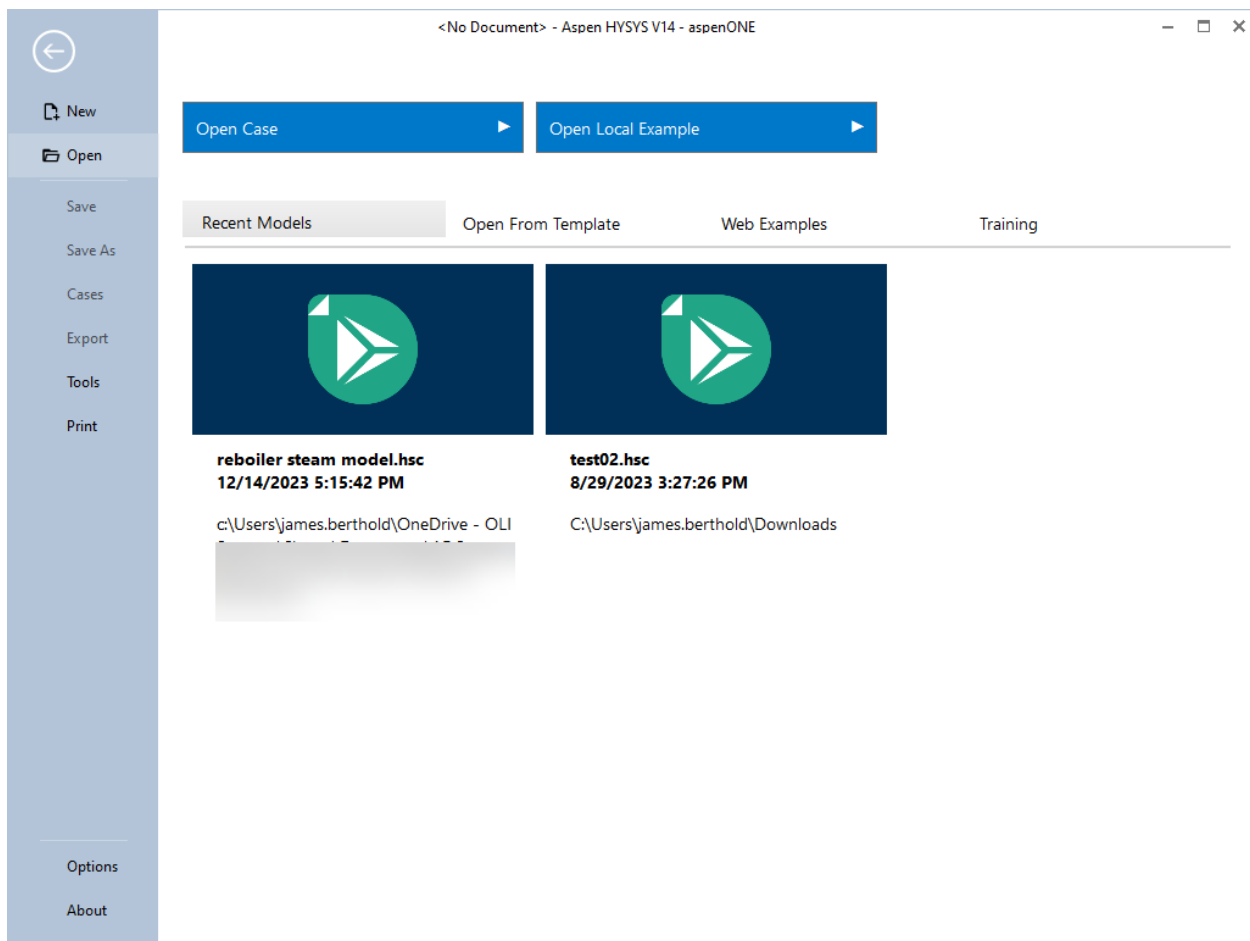
This application will take an acid stream and titrate it against a basic stream to see the resultant pH changes. Some heat and vapor are expected to be evolved.

Using the OLI Engine for Aspen HYSYS

Start Aspen Hysys in the normal manner. A splash screen will display and then disappear.



This will now display the Aspen HYSYS development environment.



Entering the Chemistry and fluid packages

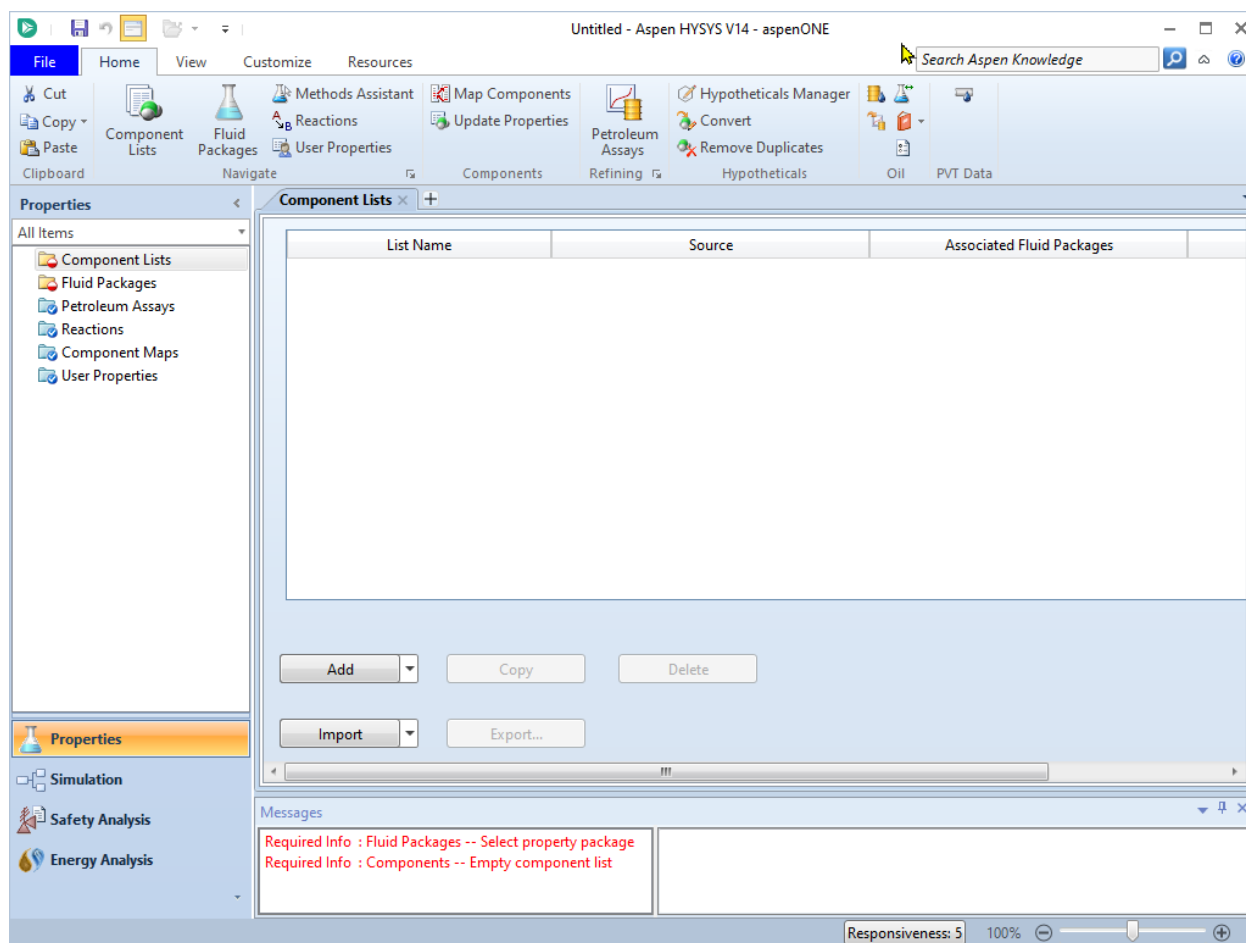
Select **New** and then **Create New Case**

The screenshot shows the Aspen HYSYS V14 software interface. On the left, a vertical menu is open, with the 'New' option selected. A yellow arrow points to the 'New' option. To the right of the menu, a blue button labeled 'Create New Case' is highlighted with a yellow arrow. Below this button, the 'New Case From Template' section is visible, featuring three options: 'New Template', 'Column', and 'Reformer'. Each option has a corresponding icon and a brief description.

New Case From Template

Option	Description
New Template	Create a new template.
Column	Create a new column template.
Reformer	Create a new

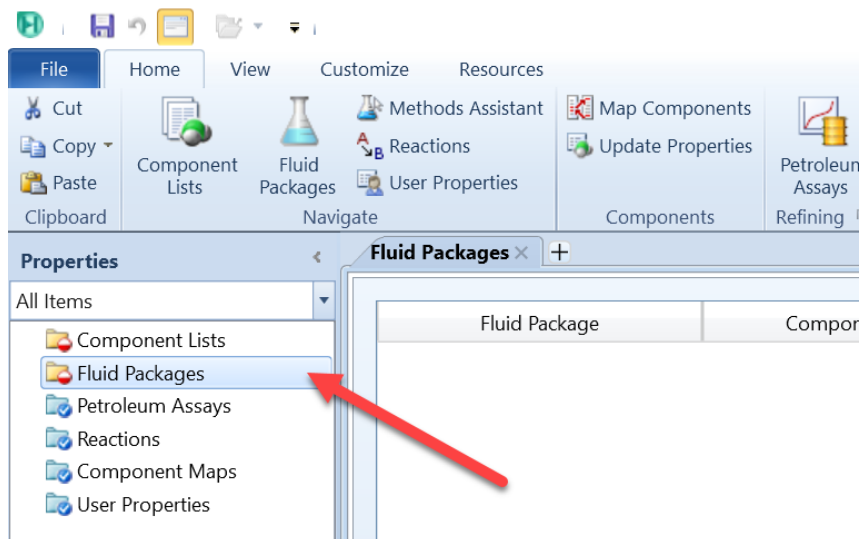
This will bring up the **Simulation Environment**.



Selecting Fluid Packages

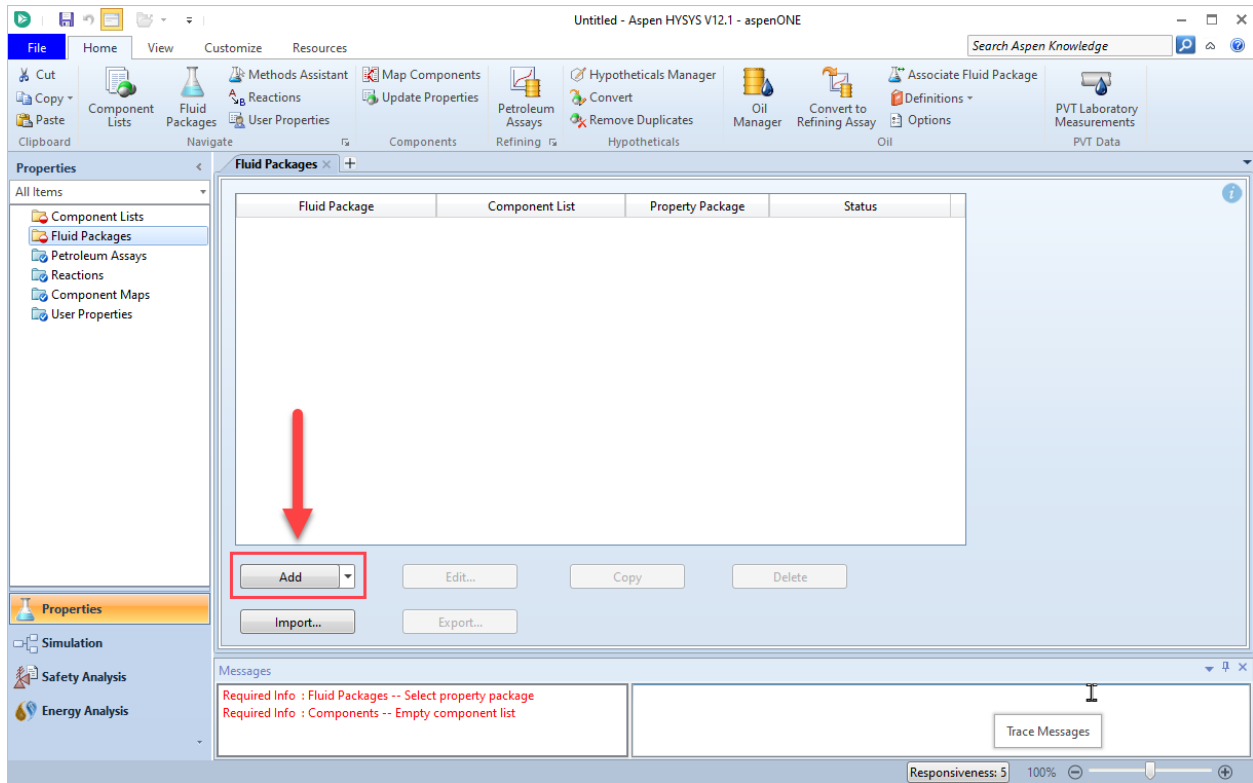
OLI recommends starting with adding a fluid package.

Select *Fluid Packages*

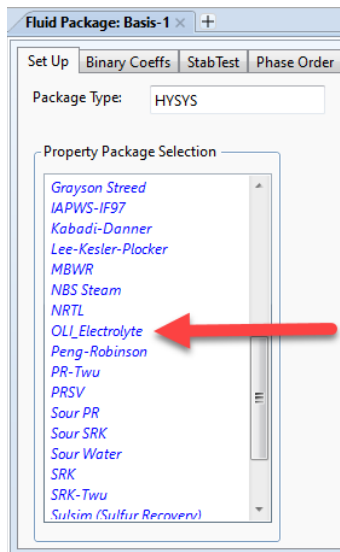


There are no fluid packages currently defined for this simulation. We need to add a package.

Click the **Add** button

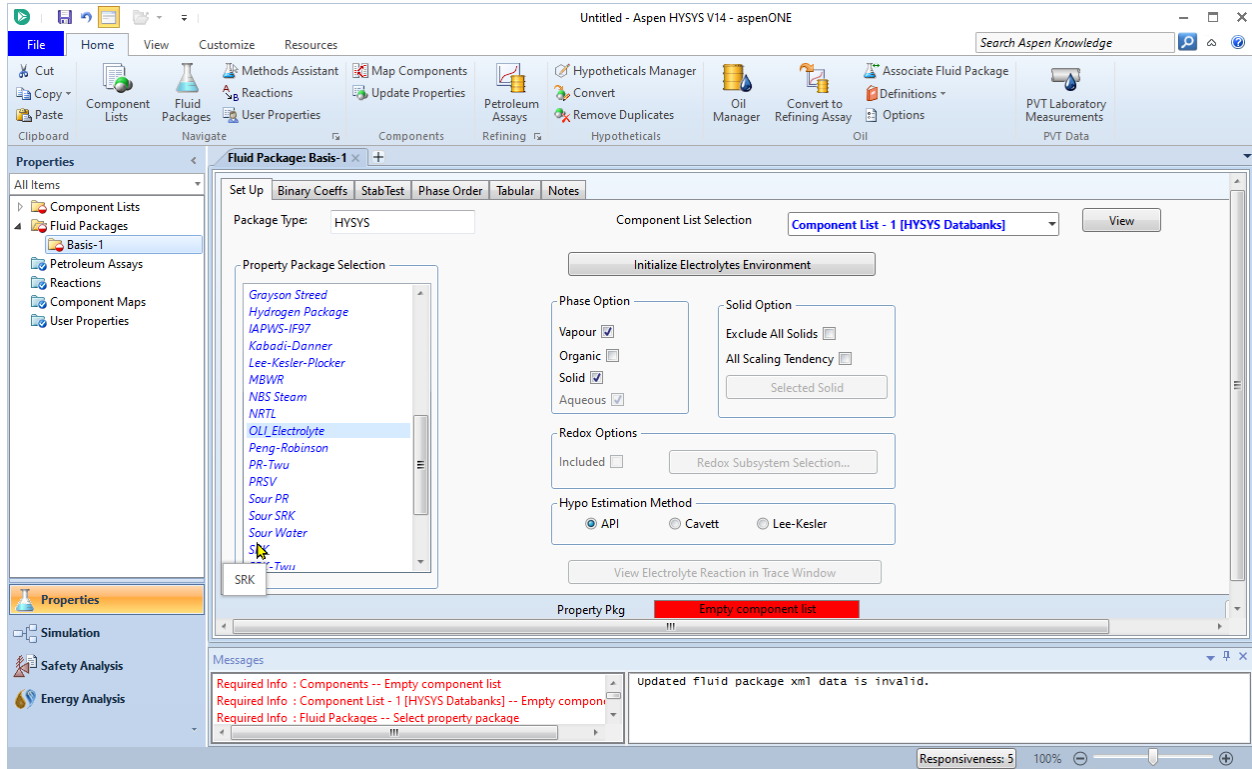


Scroll down the window to find **OLI_Electrolyte**

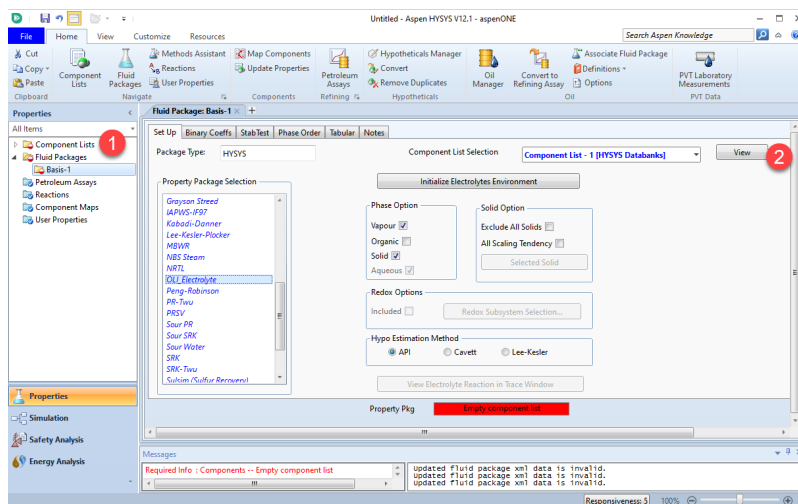


Highlight the object **OLI_Electrolyte**.

The window changes to display some OLI specific options. It is beyond the scope of this document to explain those options currently. Notice that the name of the component list is **Component List -1**.



You have two options to see the component list. Either click the Component List in the navigator (options 1) or click the View Button next to the list (option 2)



Here we are choosing Option 1, In the tree-view, click on **Component Lists**.

Click the small arrow to expand the list. This will expand the list to display all the component lists.

Select **Component List -1**

The screenshot shows the Aspen HYSYS V12.1 interface. The left sidebar contains a tree view with 'Component Lists' expanded, and 'Component List - 1' selected. The main window displays a table of components with columns for Simulation Name, Full Name / Synonym, and Formula. A red arrow points to the 'Component List - 1' item in the tree view.

Simulation Name	Full Name / Synonym	Formula
Methane	C1	CH4
Ethane	C2	C2H6
Propane	C3	C3H8
i-Butane	i-C4	C4H10
n-Butane	n-C4	C4H10
i-Pentane	i-C5	C5H12
n-Pentane	n-C5	C5H12
n-Hexane	C6	C6H14
n-Heptane	C7	C7H16
n-Octane	C8	C8H18
n-Nonane	C9	C9H20
n-Decane	C10	C10H22

Entering Components

A new basis set has been defined. We can now specify the components.

Aspen HYSYS categorizes the components according to function and type. OLI Components are no different. Expand the drop-down list from the **Select** box.

The screenshot shows a software interface with the following elements:

- Select:** A dropdown menu set to "Pure Components".
- Filter:** A dropdown menu set to "All Families".
- Search for:** An empty text input field.
- Search by:** A dropdown menu set to "Full Name/Synonym".
- Table:** A table with the following data:

Simulation Name	Full Name / Synonym	Formula
Methane	C1	CH4
Ethane	C2	C2H6
Propane	C3	C3H8
i-Butane	i-C4	C4H10

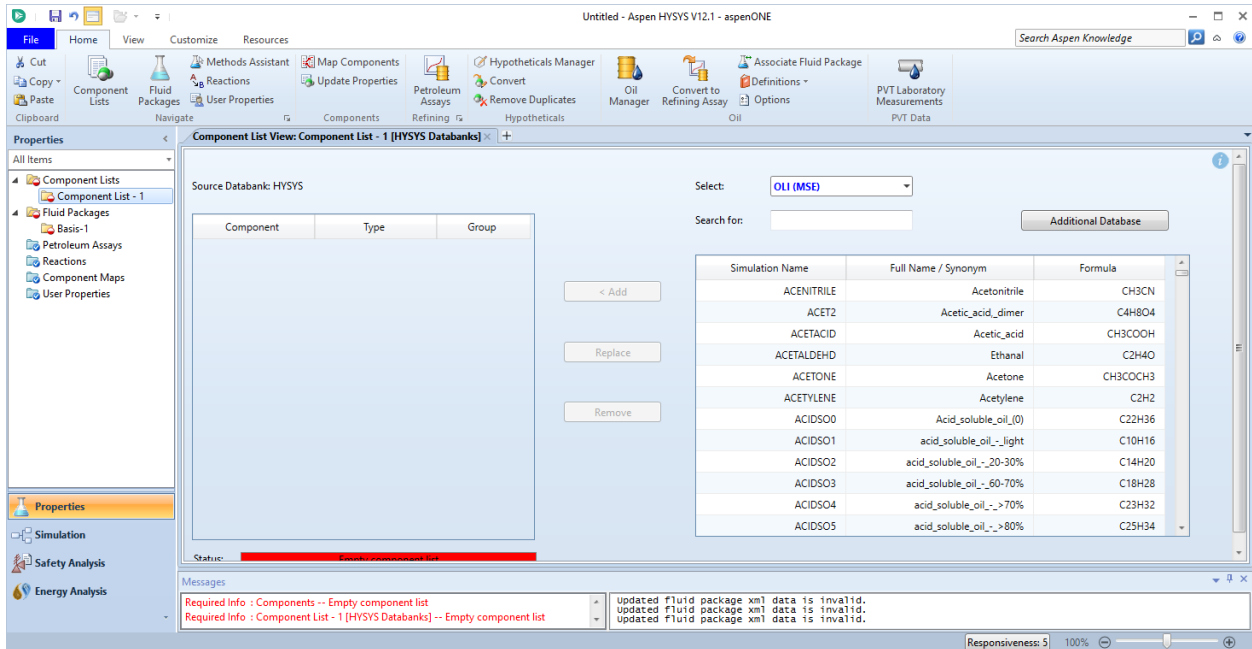
This will display several options:

The screenshot shows the "Select:" dropdown menu expanded, displaying the following options:

- Pure Components
- OLI (Aqueous)
- OLI (MSE)
- Hypothetical
- Hypothetical Solid

The "OLI (MSE)" option is highlighted by the mouse cursor. The background shows the same search filters and table as the previous screenshot.

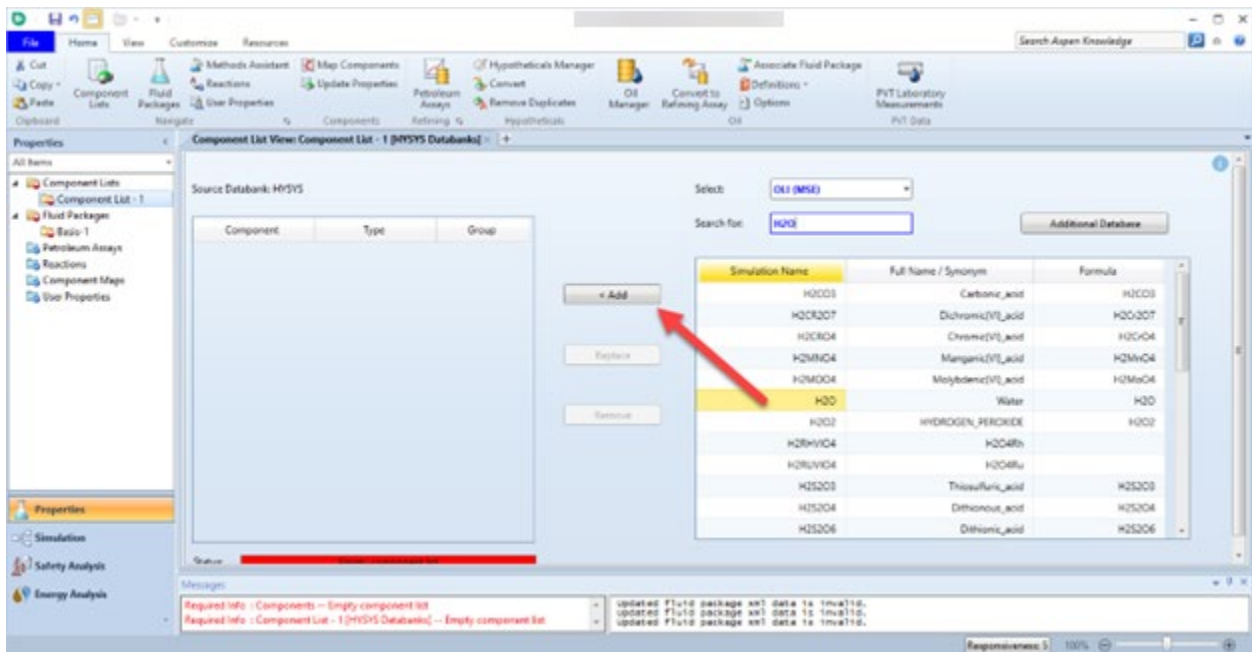
For this example, we will use **OLI (MSE)**



We can now begin to select our components from the OLI supplied species. You can either scroll down the rather large list or enter your species into the **Search For:** box.

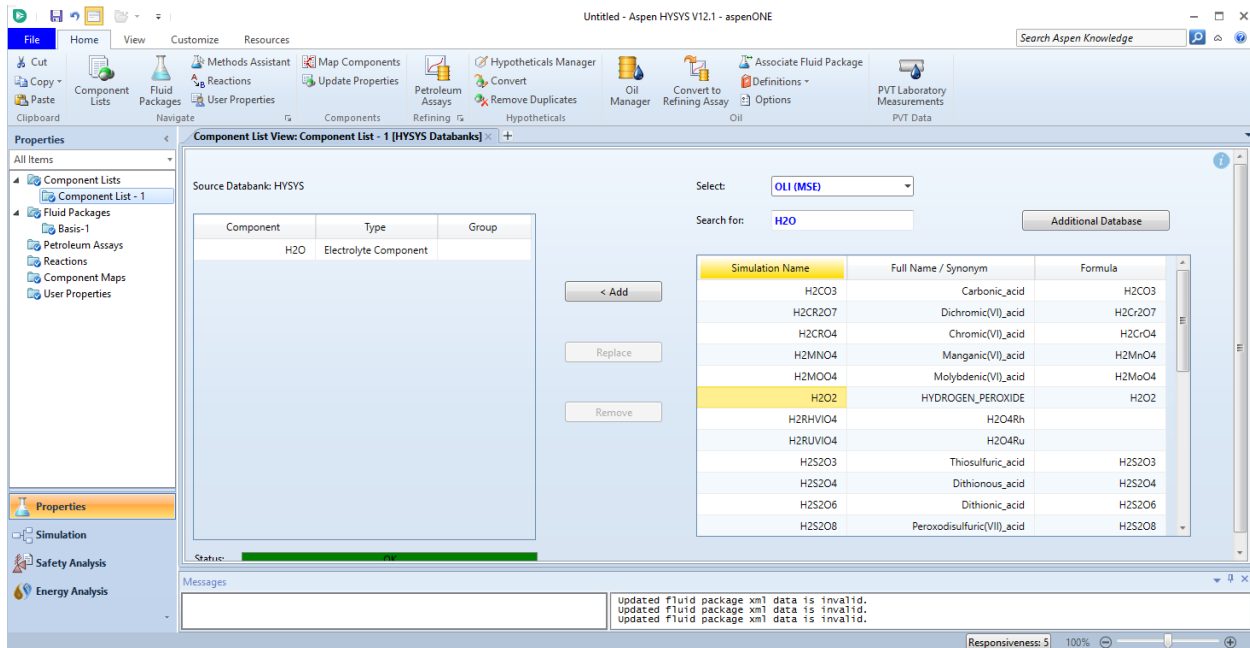
Enter the species **H2O** into the **Search For:** box.

You can see the components list scrolls to the species. If the species highlighted is the correct species, click the **Add** button.



As you type, the component list changes to search for the species. As you can see the species H₂O is highlighted. Also, there is the species H₂O₂ (peroxide) which has a similar formula. Select the species you need.

You will notice that the component list no longer displays H₂O in the available box. Rather it now appears in the Selected components.



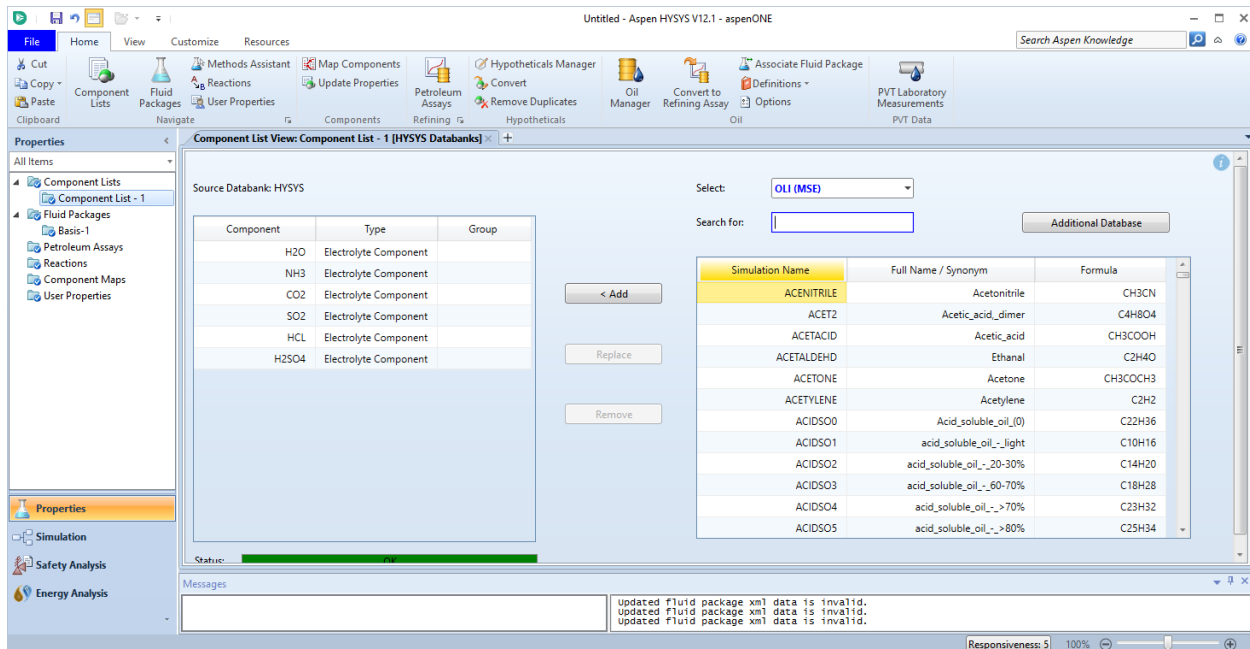
If you wish to remove a component from the selected list, highlight it and use the **Replace** button.

Using the same procedure, add the following components¹.

- NH₃
- CO₂
- SO₂
- HCL
- H₂SO₄

The input should look like this:

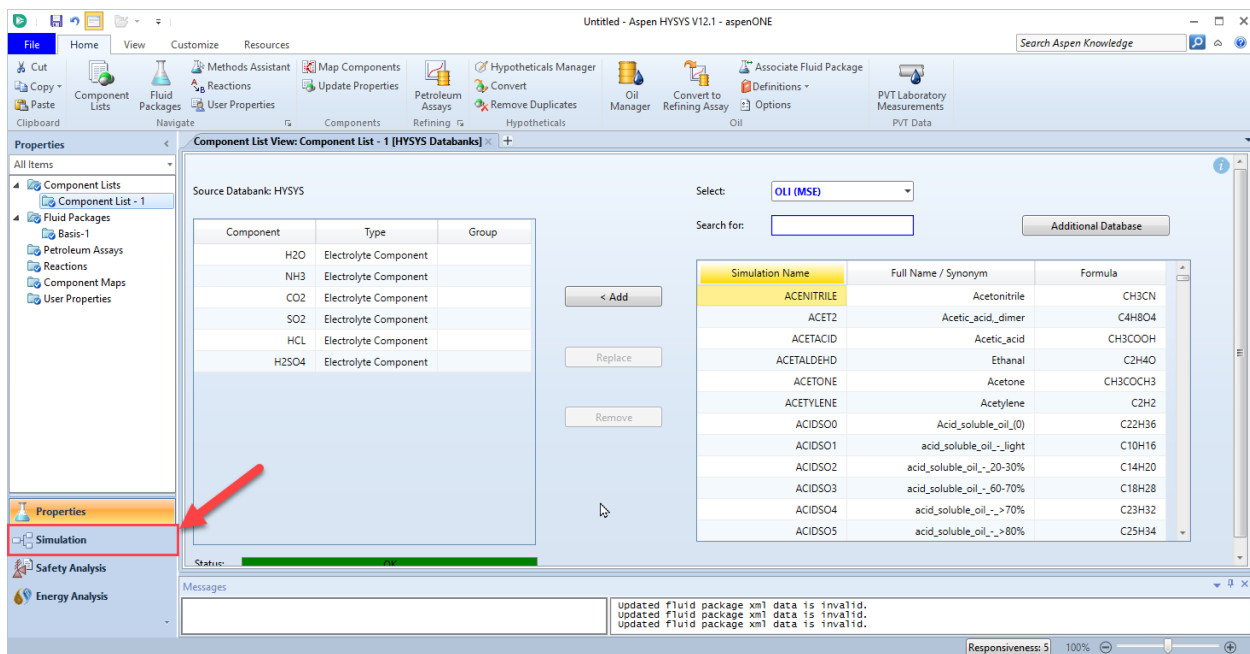
¹ You can also just enter the name in the search box, if you are sure, it is the right name, and then press the Enter key to automatically select it. This saves some time.



The component selection has been completed. We are now ready to start building our process.

Creating the Simulation

Click on the **Simulation** section



As you click this button, Aspen HYSYS temporarily passes control to the OLI software to create the electrolyte model. Progress messages can be seen in the status line at the bottom of the window as well as in the summary box. After a few moments, the standard ASPEN HYSYS development window is displayed.

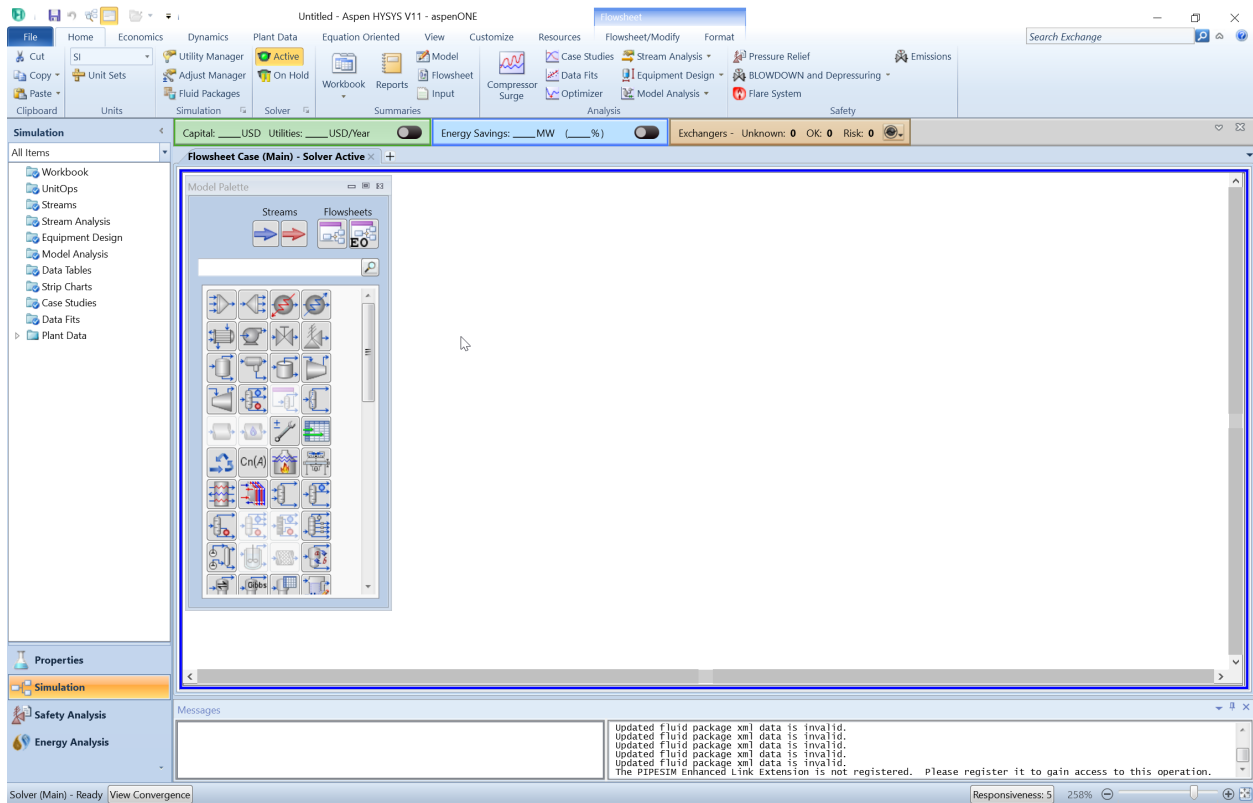


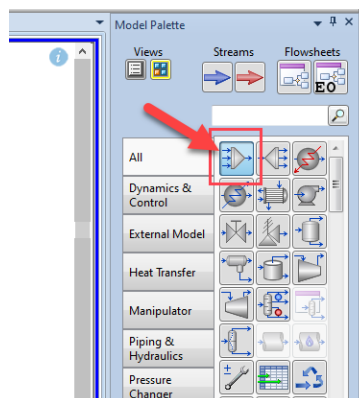
Figure 1. Simulation window (move the palate if it is obscuring the window)

We will now create a small process using a mixer with two inlet streams. The user is expected to know how to create the process. Please do not enter any conditions for the inlet streams at this time.

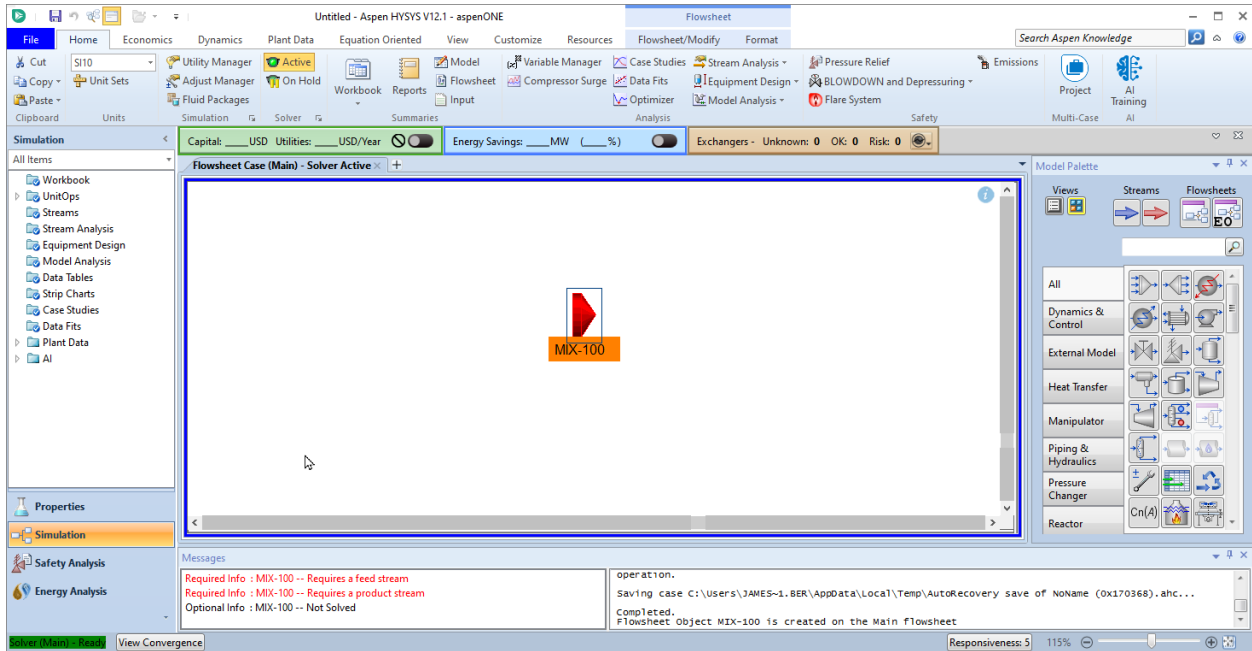
In this example, we will “Dock” the palette to the right side of the environment.

Selecting the mixer

From the tools pallet we will Click on the **mixer** and then click on the workspace.



The workspace now looks like this:



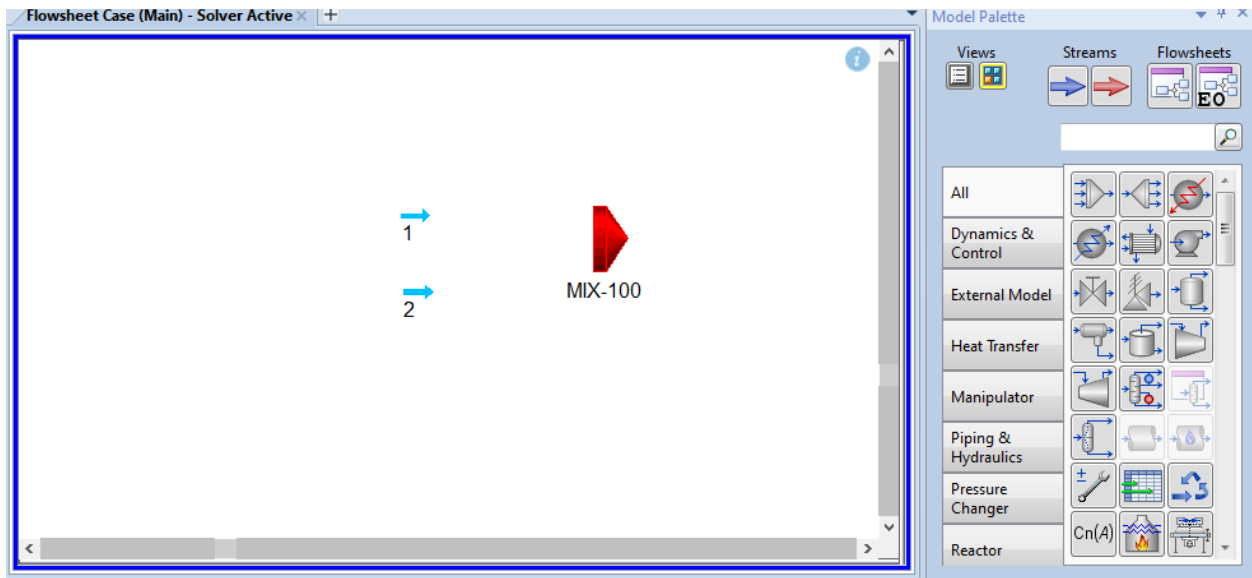
The mixer is given a default name of MIX-100. You can change it later if you wish. The block is also colored RED. This indicates that the block does not have sufficient information to calculate.

We need to create two inlet streams.

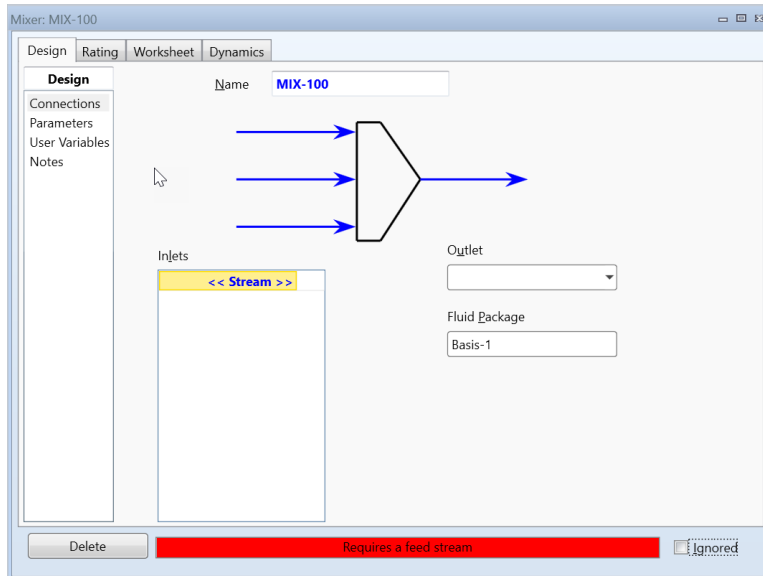
Click on the **Material Streams** arrows and place them on the workspace.



The material streams arrows are colored blue. Place two (2) material streams arrows on the workspace.



Double-Click the Mixer Block. This will open another window.



Locate the *Inlets* area and click in the first cell. Select stream "1". Repeat for stream "2".

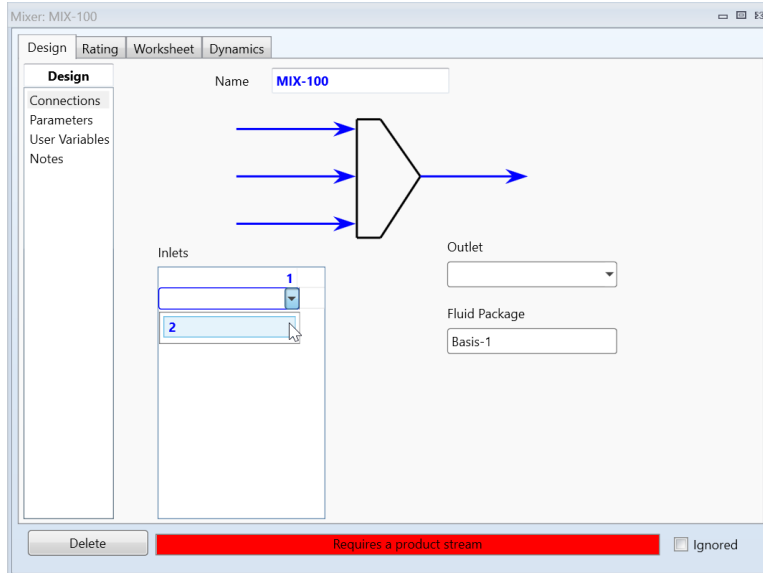
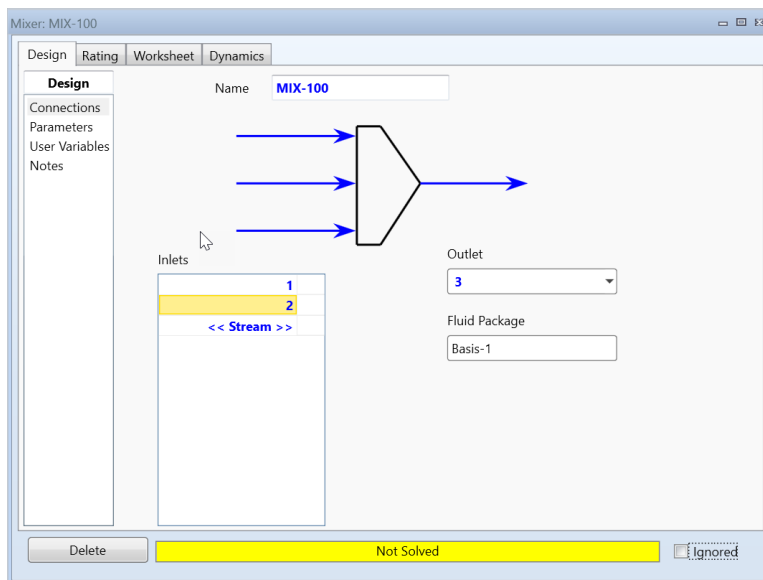


Figure 2. Selecting stream "2". Stream "1" has already been selected.

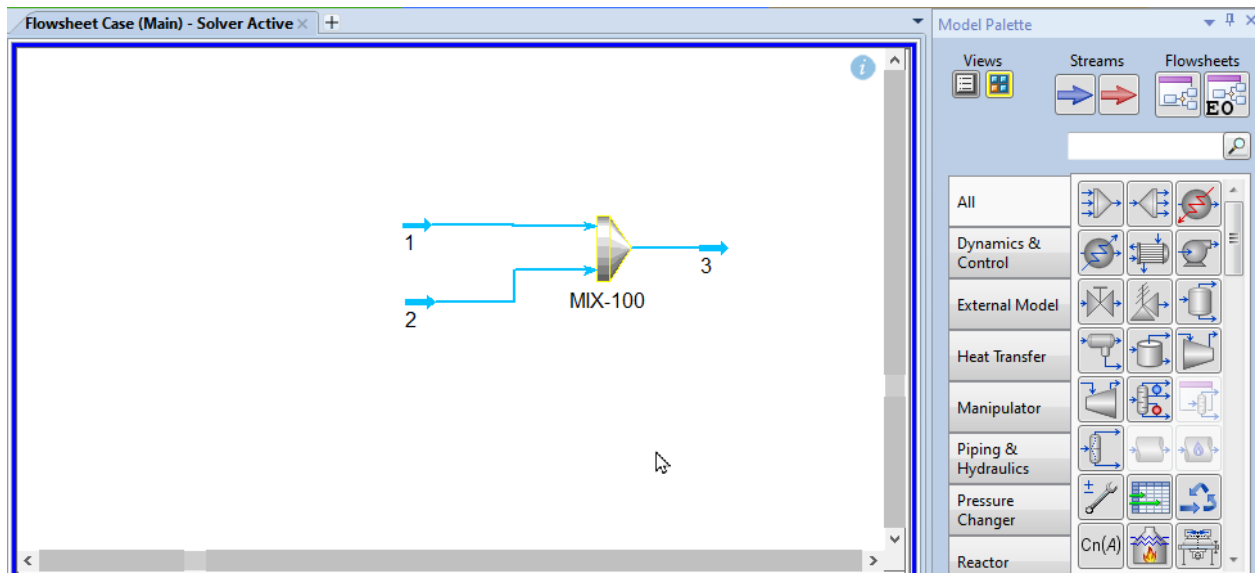
Locate the **Outlet** box and enter the number "3". This completes this block.



The status bar should be yellow. This indicates that the block has not been calculated.

Click the **x** in the upper right-hand corner to close this dialog.

This is the partially completed process. The streams are light-blue to indicate that they have not been calculated.



Entering Stream Composition Data

Double-click stream “1”. This will open a new window.

Material Stream: 1

Worksheet Attachments Dynamics

Worksheet	Stream Name	1	1_Elec
Conditions	Vapour / Phase Fraction	<empty>	<empty>
Properties	Temperature [C]	<empty>	<empty>
Composition	Pressure [kPa]	<empty>	<empty>
Oil & Gas Feed	Molar Flow [kgmole/h]	<empty>	<empty>
Petroleum Assay	Mass Flow [kg/h]	<empty>	<empty>
K Value	Std Ideal Liq Vol Flow [m3/h]	<empty>	<empty>
Electrolytes	Molar Enthalpy [kJ/kgmole]	<empty>	<empty>
User Variables	Molar Entropy [kJ/kgmole-C]	<empty>	<empty>
Notes	Heat Flow [kJ/h]	<empty>	<empty>
Cost Parameters	Liq Vol Flow @Std Cond [m3/h]	<empty>	<empty>
Normalized Yields	Fluid Package	Basis-1	
Emissions	Utility Type		

Unknown Compositions

Delete Define from Stream... View Assay

This is the standard input window for a stream. We will now add our conditions.

- Locate the cell for Temperature (C) and enter 40
- Locate the cell for Pressure (kPa) and enter 101.3

Material Stream: 1

Worksheet Attachments Dynamics

Worksheet	Stream Name	1	1_Elec
Conditions	Vapour / Phase Fraction	<empty>	<empty>
Properties	Temperature [C]	40.00	40.00
Composition	Pressure [kPa]	101.3	101.3
Oil & Gas Feed	Molar Flow [kgmole/h]	<empty>	<empty>
Petroleum Assay	Mass Flow [kg/h]	<empty>	<empty>
K Value	Std Ideal Liq Vol Flow [m3/h]	<empty>	<empty>
Electrolytes	Molar Enthalpy [kJ/kgmole]	<empty>	<empty>
User Variables	Molar Entropy [kJ/kgmole-C]	<empty>	<empty>
Notes	Heat Flow [kJ/h]	<empty>	<empty>
Cost Parameters	Liq Vol Flow @Std Cond [m3/h]	<empty>	<empty>
Normalized Yields	Fluid Package	Basis-1	
Emissions	Utility Type		

Unknown Compositions

Delete Define from Stream... View Assay

Now click the **Composition** line

Material Stream: 1

Worksheet Attachments Dynamics

Worksheet		Mole Fractions	Mole Fractions_Elec
Conditions	H2O	<empty>	<empty>
Properties	NH3	<empty>	<empty>
Composition	CO2	<empty>	<empty>
Oil & Gas Feed	SO2	<empty>	<empty>
Petroleum Assay	HCL	<empty>	<empty>
K Value	H2SO4	<empty>	<empty>
Electrolytes	H2CO3	<empty>	<empty>
User Variables	H2SO3	<empty>	<empty>
Notes	HNH2CO2	<empty>	<empty>
Cost Parameters	NH42CO3	<empty>	<empty>
Normalized Yields	NH42SO3	<empty>	<empty>
Emissions	NH42SO3.1H2O	<empty>	<empty>
	NH42SO4	<empty>	<empty>
	NH43HSO42	<empty>	<empty>
	NH44H2CO33	<empty>	<empty>
	NH4CL	<empty>	<empty>
	NH4CLB	<empty>	<empty>
	NH4CO2NH2	<empty>	<empty>
	NH4H3SO42	<empty>	<empty>
	NH4HCO3	<empty>	<empty>
	NH4HSO3	<empty>	<empty>
	NH4HSO4	<empty>	<empty>
	NH4OH	<empty>	<empty>

Total 0.00000

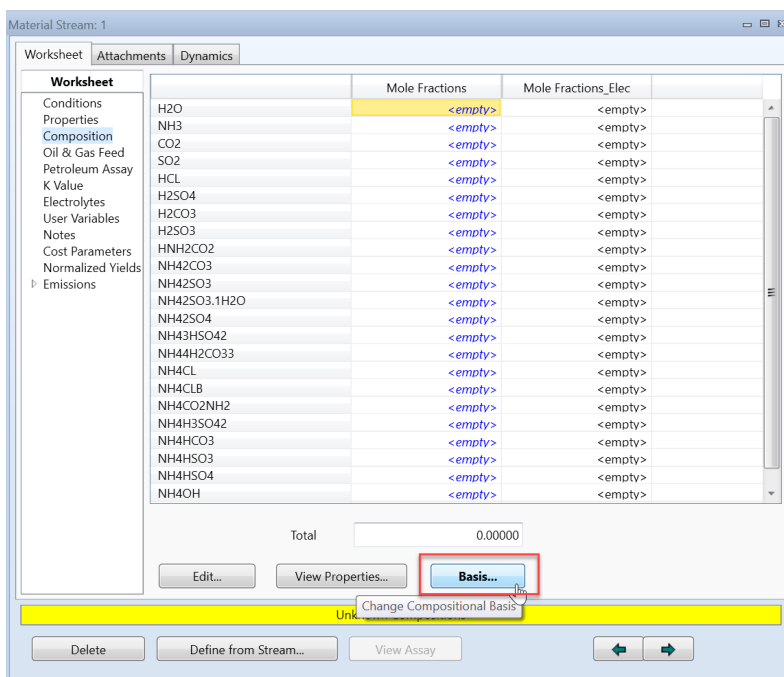
Edit... View Properties... Basis...

Unknown Compositions

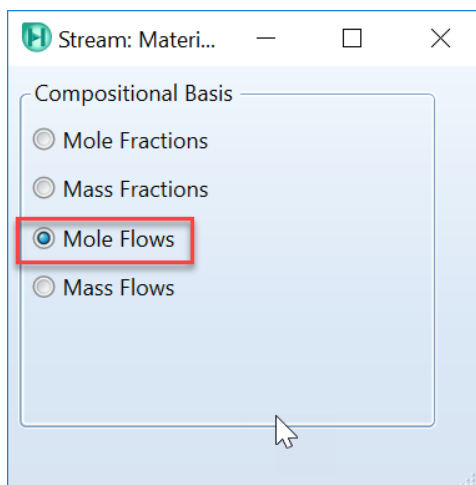
Delete Define from Stream... View Assay

We can now enter our composition for our components. In this case, we want to use mole flow rather than mole fractions.

Click the **Basis...** button



This will open a new window



Select the *Mole Flows* radio button. Click the **x** when done.

Now begin entering the value for **H2O** of 55.51

	Molar Flows	Molar Flows_Elec
H2O	55.51	<empty>
NH3	<empty>	<empty>
CO2	<empty>	<empty>
SO2	<empty>	<empty>
HCL	<empty>	<empty>
H2SO4	<empty>	<empty>
H2CO3	<empty>	<empty>
H2SO3	<empty>	<empty>
HNH2CO2	<empty>	<empty>
NH42CO3	<empty>	<empty>
NH42SO3	<empty>	<empty>
NH42SO3.1H2O	<empty>	<empty>
NH42SO4	<empty>	<empty>
NH43HSO42	<empty>	<empty>
NH44H2CO33	<empty>	<empty>
NH4CL	<empty>	<empty>
NH4CLB	<empty>	<empty>
NH4CO2NH2	<empty>	<empty>
NH4H3SO42	<empty>	<empty>
NH4HCO3	<empty>	<empty>

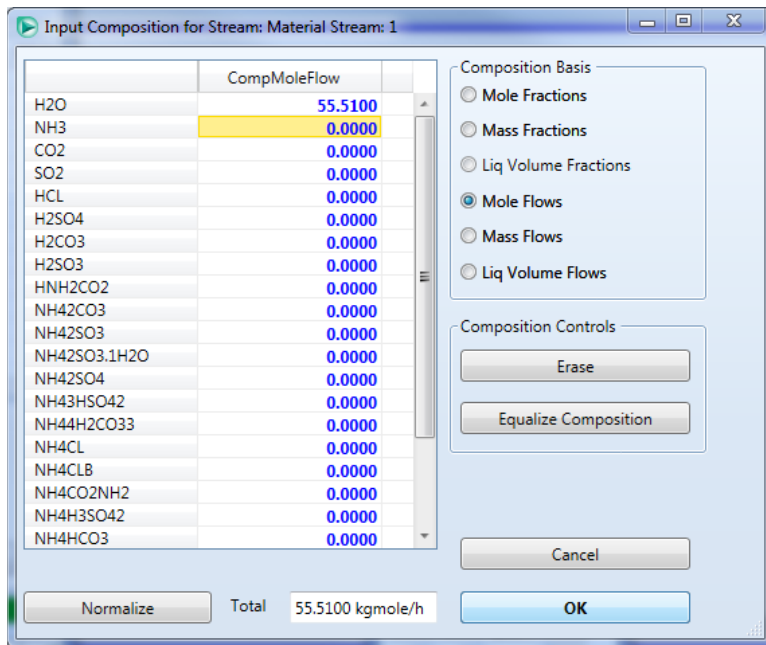
Total: 0.00000 kgmole/h

Once you hit enter it will prompt you to a new window to finish entering the composition of the stream. A fly-out unit selection box appears near the composition. Use the defaults at this time.

Comp	Mole Flow
H2O	55.51
NH3	<empty>
CO2	<empty>
SO2	<empty>
HCL	<empty>
H2SO4	<empty>
H2CO3	<empty>
H2SO3	<empty>
HNH2CO2	<empty>
NH42CO3	<empty>
NH42SO3	<empty>
NH42SO3.1H2O	<empty>
NH42SO4	<empty>
NH43HSO42	<empty>
NH44H2CO33	<empty>
NH4CL	<empty>
NH4CLB	<empty>
NH4CO2NH2	<empty>
NH4H3SO42	<empty>
NH4HCO3	<empty>

Total: 55.5100 kgmole/h

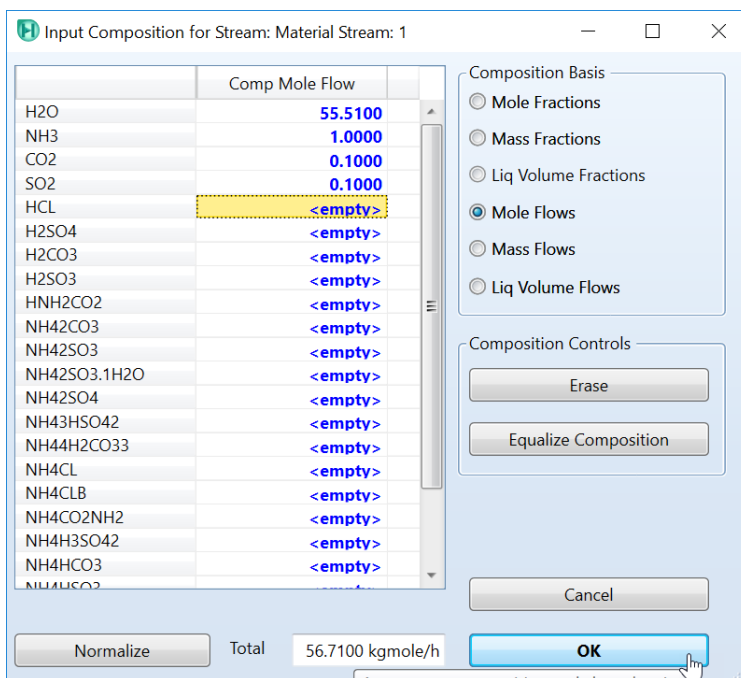
Press the **<Enter>** key to continue.



This will display the composition data entry dialog. Complete the following data entry in mole flow units:

- H2O 55.51
- NH3 1.0
- CO2 0.1
- SO2 0.1

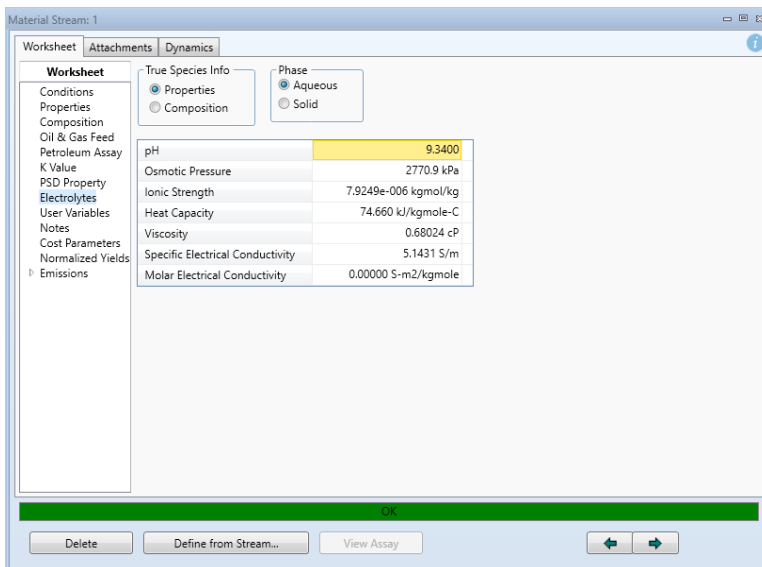
The remaining values can be zero.



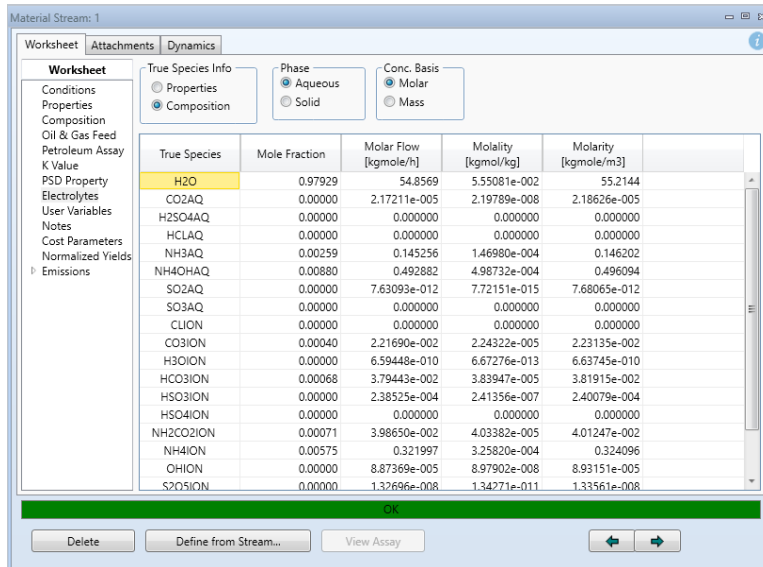
Click the **OK** button.

The status bar should turn green. This indicates that the program has already converged the stream. We can see some useful information at this time.

Click on the **Electrolytes** line.



The pH of this solution is approximately 9.3. We also provide additional information. You can also explore other buttons such as composition, to see more information about our report.

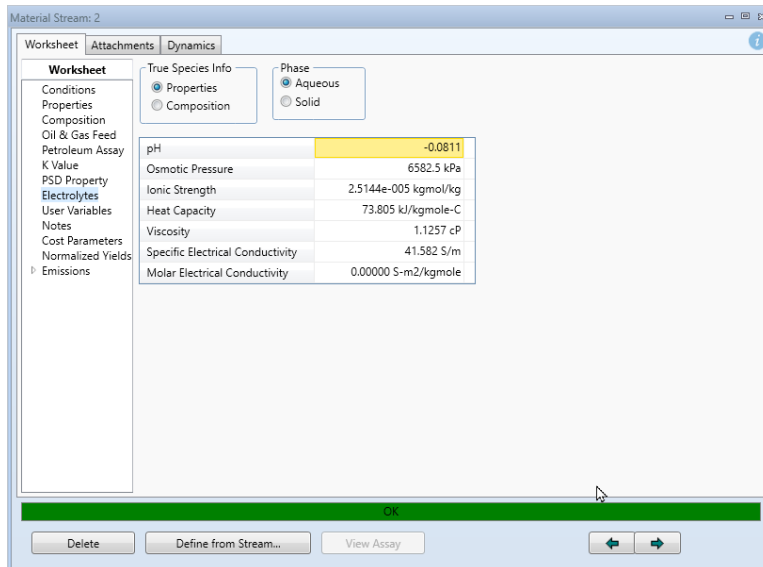


Click on the **x** to close this dialog.

We will now repeat the steps for stream "2" but with different compositions. Please enter the following composition for stream "2" in mole flow.

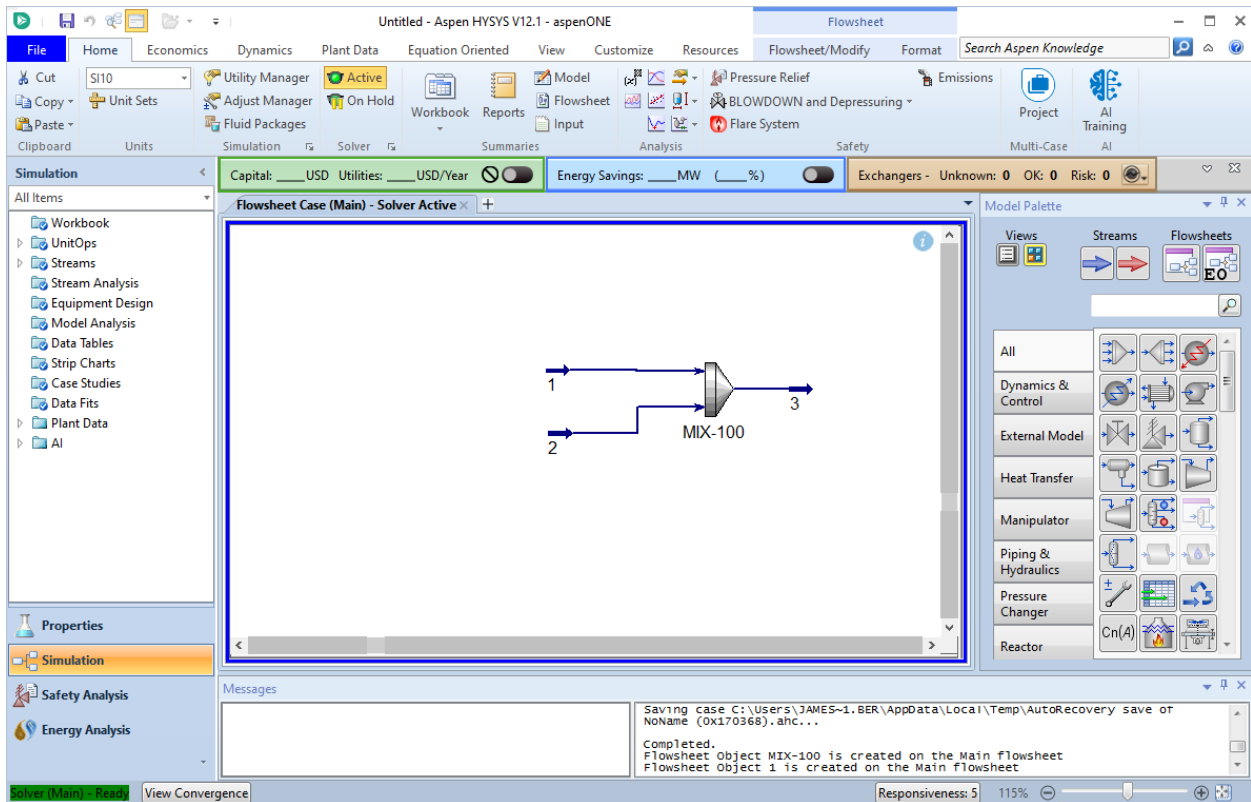
Temperature 25 C
 Pressure 101.3 kPa
 H2O 55.51
 HCl 0.1
 H2SO4 1.0

Click the **Electrolytes** line to see the pH.



Click the **x** to close the dialog.

Hysys will attempt to converge the process as you create it. As you close the final dialog box for data entry you will see that the output stream “3” is “Blue” which means it has converged.



Reviewing the output

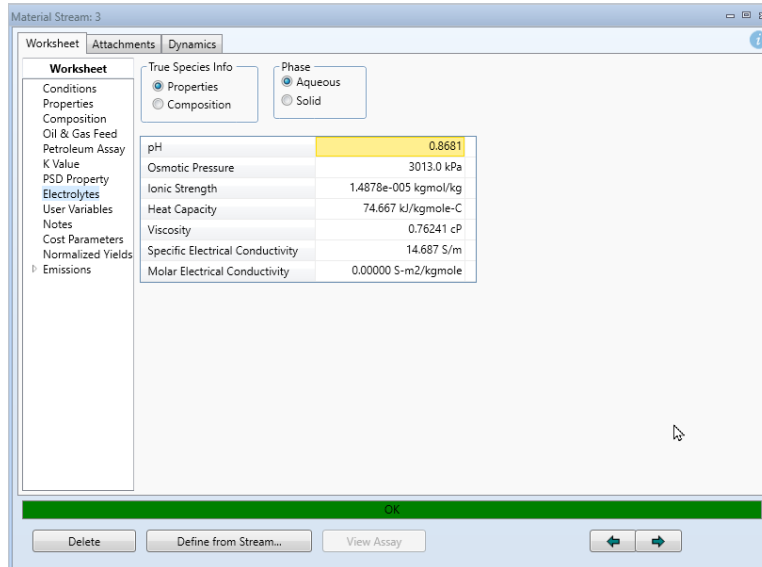
Double-Click stream “3”

The screenshot shows the "Material Stream: 3" dialog box. The "Worksheet" tab is active, displaying a table of simulation results for stream 3. The table has columns for "Stream Name", "3", "3_Elec", and "Vapour Phase". The "Temperature [C]" row is highlighted in red, showing a value of 36.99. The "Vapour / Phase Fraction" row is also highlighted in red, showing a value of 0.0006. The "OK" button is highlighted in green at the bottom of the dialog.

Worksheet	Stream Name	3	3_Elec	Vapour Phase
Conditions	Vapour / Phase Fraction	0.0006	0.0006	0.0006
Properties	Temperature [C]	36.99	36.99	36.99
Composition	Pressure [kPa]	101.3	101.3	101.3
Oil & Gas Feed	Molar Flow [kgmole/h]	114.3	114.3	6.574e-002
Petroleum Assay	Mass Flow [kg/h]	2130	2130	<empty>
K Value	Std Ideal Liq Vol Flow [m3/h]	<empty>	<empty>	<empty>
PSD Property	Molar Enthalpy [kJ/kgmole]	-2.865e+005	-2.865e+005	-3.787e+005
Electrolytes	Molar Entropy [kJ/kgmole-C]	72.66	72.66	215.4
User Variables	Heat Flow [kJ/h]	-3.275e+007	-3.275e+007	-2.490e+004
Notes	Liq Vol Flow @Std Cond [m3/h]	<empty>	<empty>	<empty>
Cost Parameters	Fluid Package	Basis-1	<empty>	<empty>
Normalized Yields	Utility Type			
Emissions				

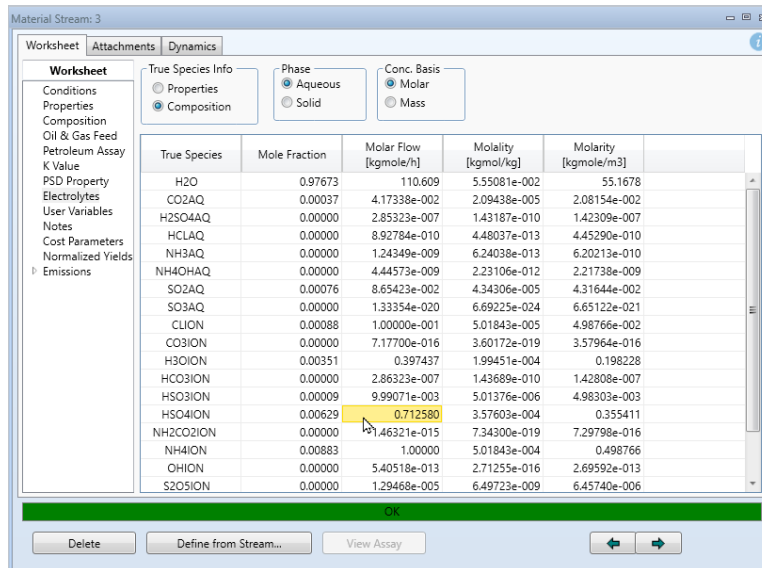
The converged process temperature is approximately 37.0 °C.

Click on the **Electrolytes** line.



The converged pH is 0.87 indicating that some acid/base chemistry has taken place. What about the equilibrium compositions that have been calculated?

Click the **Composition** radio button at the top of the dialog. This creates a scrollable area where you can see the actual true-species composition.



Click on the **Composition** line at the left.

Material Stream: 3

Worksheet Attachments Dynamics

Worksheet		Mole Fractions	Mole Fractions_Elec	Vapour Phase	Aqueous Phase
Conditions	H2O	0.9799	0.9799	0.0613	0.9804
Properties	NH3	0.0087	0.0087	0.0000	0.0088
Composition	CO2	0.0009	0.0009	0.8863	0.0004
Oil & Gas Feed	SO2	0.0009	0.0009	0.0523	0.0008
Petroleum Assay	HCL	0.0009	0.0009	0.0000	0.0009
K Value	H2SO4	0.0000	0.0000	0.0000	0.0000
PSD Property	H2CO3	0.0000	0.0000	0.0000	0.0000
Electrolytes	H2SO3	0.0000	0.0000	0.0000	0.0000
User Variables	HCL.1H2O	0.0000	0.0000	0.0000	0.0000
Notes	HCL.2H2O	0.0000	0.0000	0.0000	0.0000
Cost Parameters	HCL.3H2O	0.0000	0.0000	0.0000	0.0000
Normalized Yields	NH42CO3	0.0000	0.0000	0.0000	0.0000
Emissions	NH42CO3.1H2O	0.0000	0.0000	0.0000	0.0000
	NH42S2O5	0.0000	0.0000	0.0000	0.0000
	NH42SO3	0.0000	0.0000	0.0000	0.0000
	NH42SO3.1H2O	0.0000	0.0000	0.0000	0.0000
	NH42SO4	0.0000	0.0000	0.0000	0.0000
	NH43CO32	0.0000	0.0000	0.0000	0.0000
	NH43HSO42	0.0000	0.0000	0.0000	0.0000
	NH44HCO3.1H2O	0.0000	0.0000	0.0000	0.0000
	Total	1.00000			

Buttons: Edit... View Properties... Basis...

Buttons: Delete Define from Stream... View Assay

This displays the composition on an apparent-species basis. However, the true-species vapor composition is also reported in this section. Use the scroll bars to scroll to the right to see the vapor composition (we have dragged the window to the right to see more information)

Here we see the mole fraction basis for the vapor phase composition. You can change the basis by clicking the **Basis...** button and looking at mole flow for example.

The actual mole flows are reported as well as the total mole flow for the phase.

Material Stream: 3

Worksheet Attachments Dynamics

Worksheet		Molar Flows	Molar Flows_Elec	Vapour Phase	Aqueous Phase
Conditions	H2O	112.0200	112.0200	0.0040	112.0160
Properties	NH3	1.0000	1.0000	0.0000	1.0000
Composition	CO2	0.1000	0.1000	0.0583	0.0417
Oil & Gas Feed	SO2	0.1000	0.1000	0.0034	0.0966
Petroleum Assay	HCL	0.1000	0.1000	0.0000	0.1000
K Value	H2SO4	0.0000	0.0000	0.0000	0.0000
PSD Property	H2CO3	0.0000	0.0000	0.0000	0.0000
Electrolytes	H2SO3	0.0000	0.0000	0.0000	0.0000
User Variables	HCL.1H2O	0.0000	0.0000	0.0000	0.0000
Notes	HCL.2H2O	0.0000	0.0000	0.0000	0.0000
Cost Parameters	HCL.3H2O	0.0000	0.0000	0.0000	0.0000
Normalized Yields	NH42CO3	0.0000	0.0000	0.0000	0.0000
Emissions	NH42CO3.1H2O	0.0000	0.0000	0.0000	0.0000
	NH42S2O5	0.0000	0.0000	0.0000	0.0000
	NH42SO3	0.0000	0.0000	0.0000	0.0000
	NH42SO3.1H2O	0.0000	0.0000	0.0000	0.0000
	NH42SO4	0.0000	0.0000	0.0000	0.0000
	Total	114.32000 kgmole/h			

Buttons: Edit... View Properties... Basis...

Buttons: Delete Define from Stream... View Assay

This now completes the getting started guide. It is strongly recommended that you save your file at this time.

