



# OLI Engine for Aspen HYSYS V8.4

## Getting Started Guide

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### Overview

The OLI Engine for Aspen HYSYS interface greatly enhances AspenHYSYS' 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 are 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 V8.4 is being used.
6. The user is expected to know how to run Aspen HYSYS.

## Application

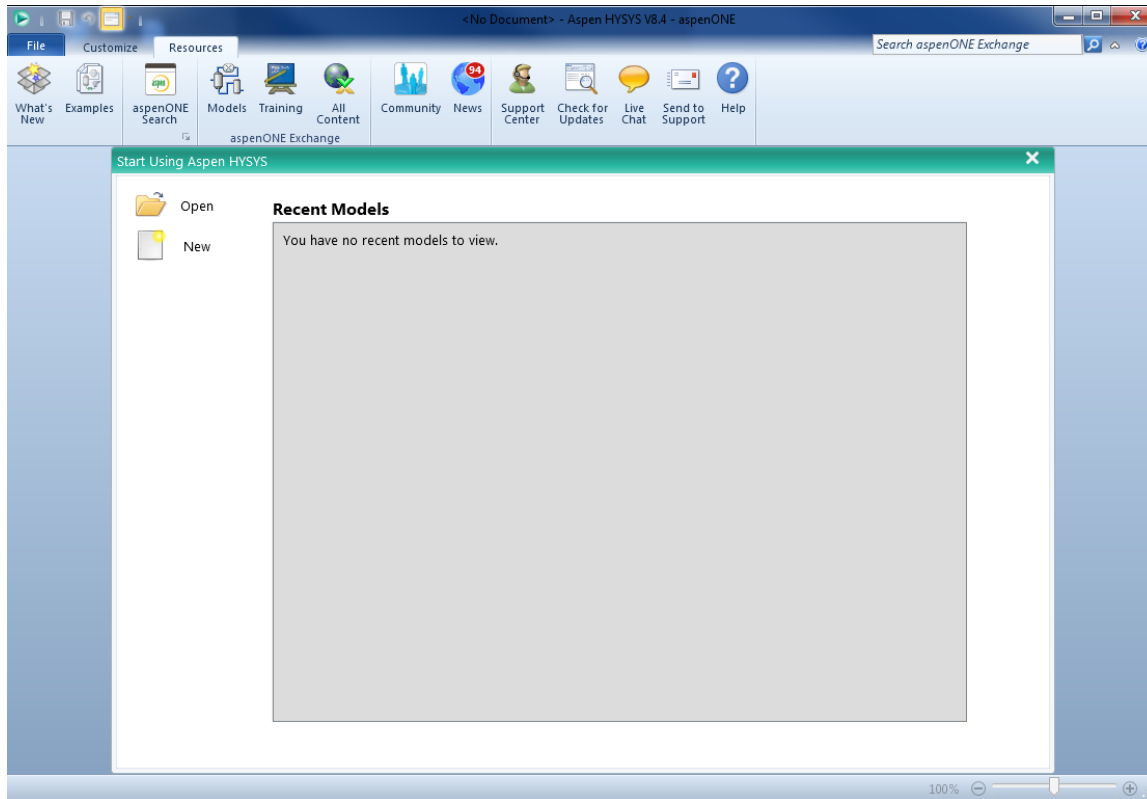
This application will take an acid stream and titrate it against a basic stream to see the resultant pH changes. Some heat and vapor are expected to be evolved.

## Using the OLI Engine for Aspen HYSYS

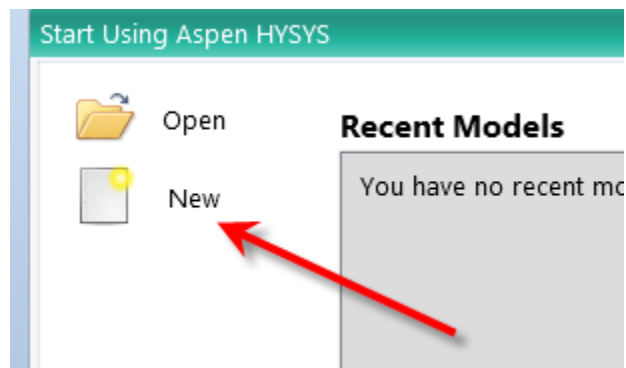
Start Hysys in the normal manner. A splash screen will display and then disappear.



This will now display the Aspen HYSYS development environment.

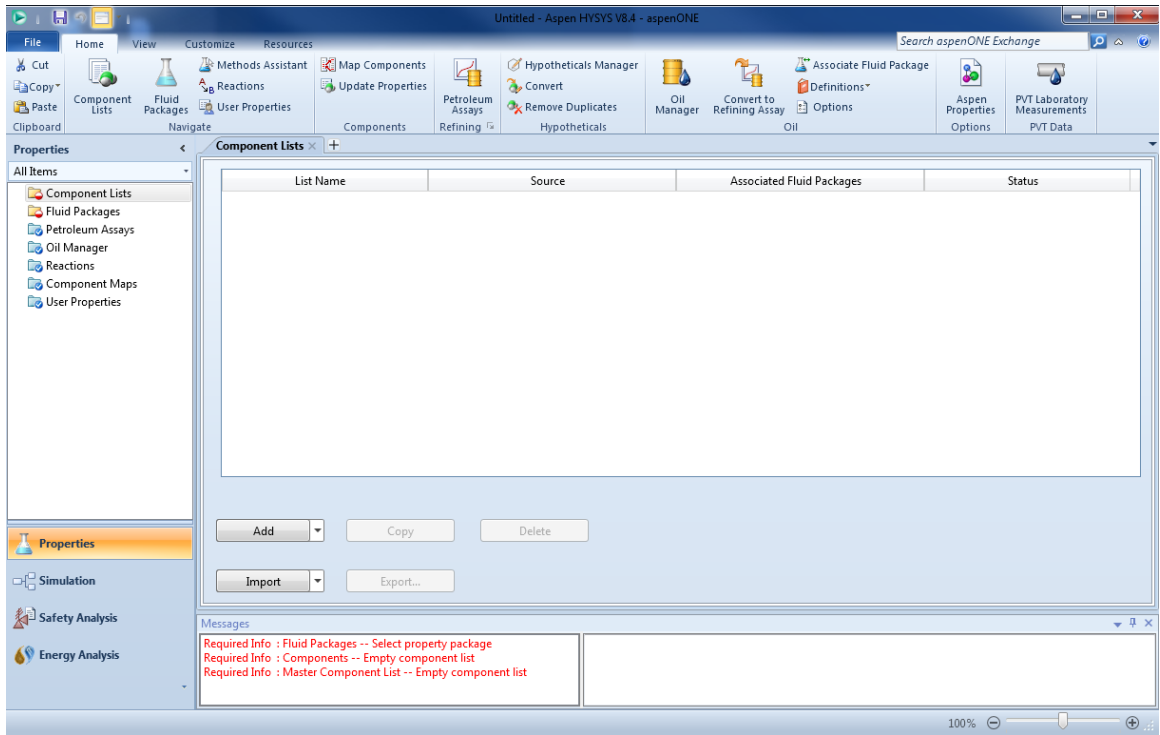


## Entering the Chemistry and fluid packages



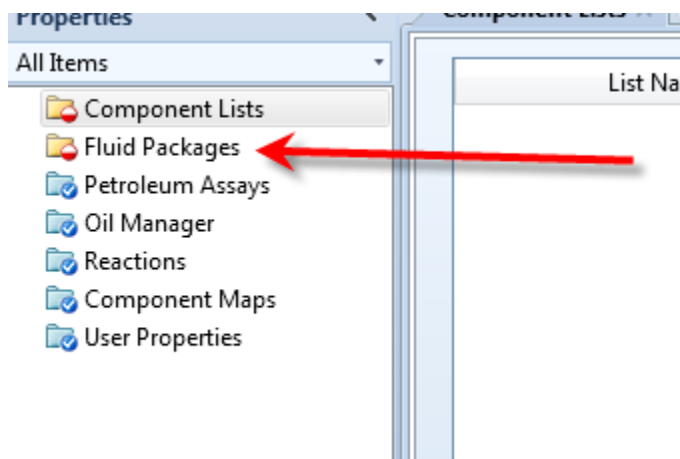
Select *New*

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

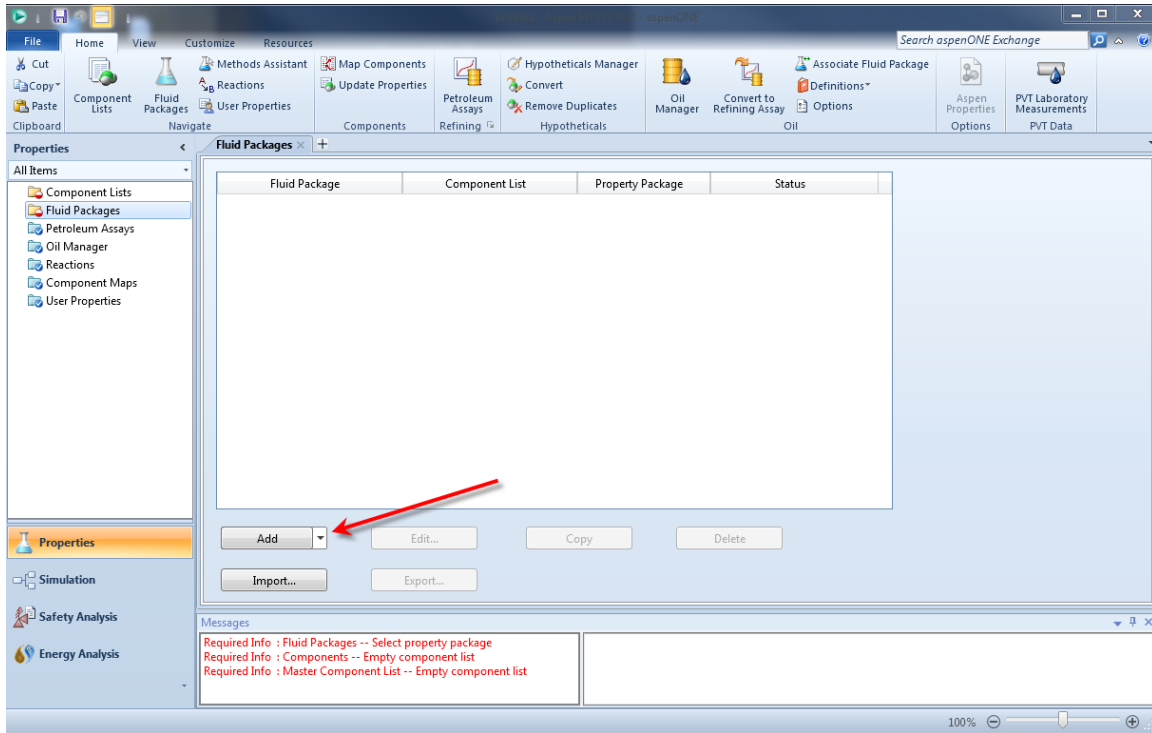


## Selecting Fluid Packages

### Select *Fluid Packages*



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

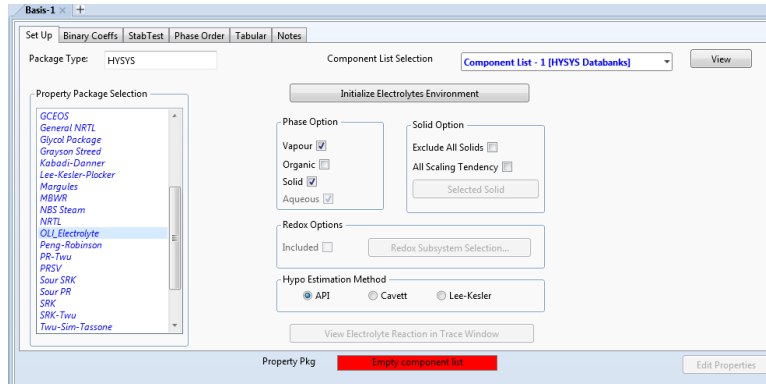


Click the **Add** button



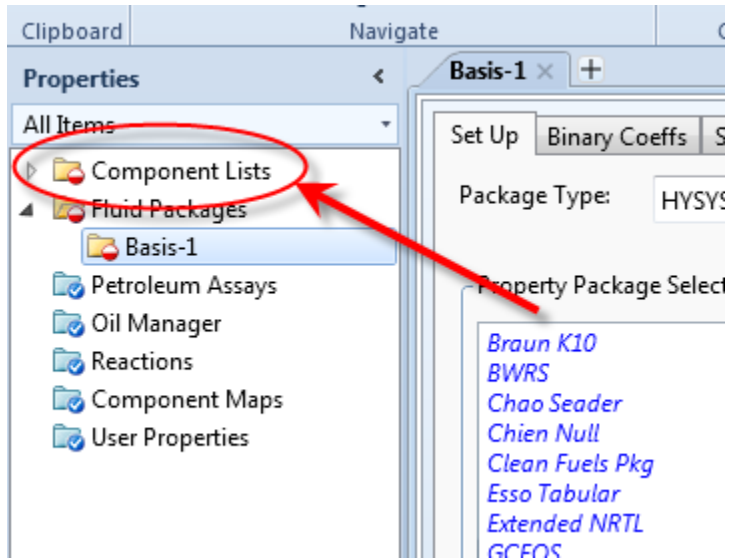
Scroll down the window to find **OLI\_Electrolyte**.

Highlight the object.

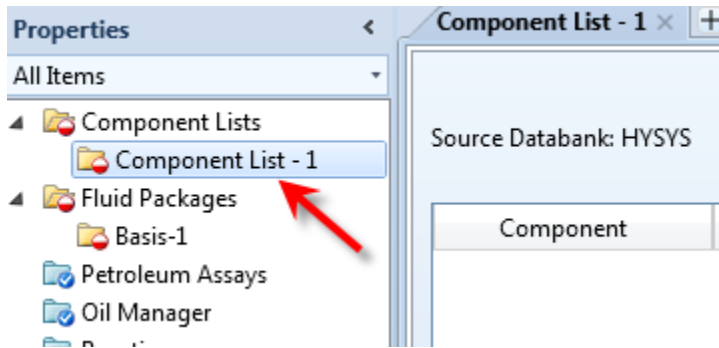


The window changes to display some OLI specific options. It is beyond the scope of this document to explain those options at this time. Notice that the name of the component list is **Component List -1** .

In the tree-view, click on **Component Lists**.



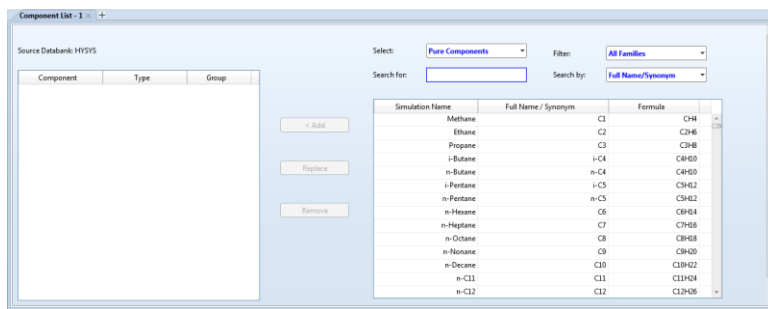
Click the small arrow to expand the list. This will expand the list to display all the component lists.



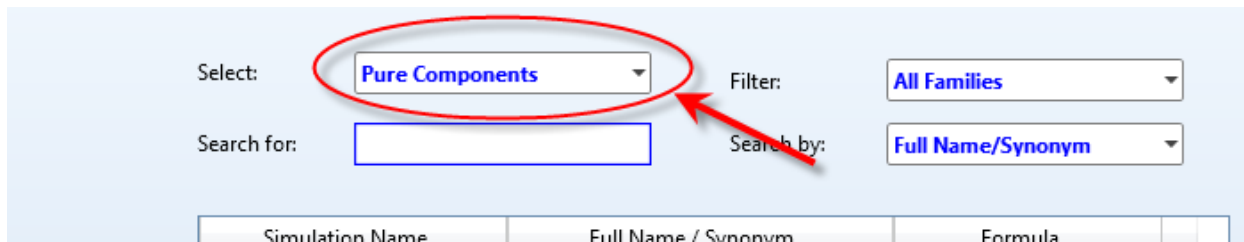
Select **Component List -1**

### Entering Components

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

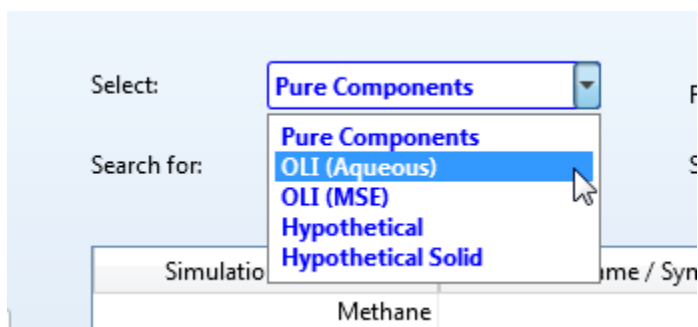


Aspen HYSYS categorizes the components according to function and type. OLI Components are no different. Expand the drop-down list from the **Select** box.



This will display several options:

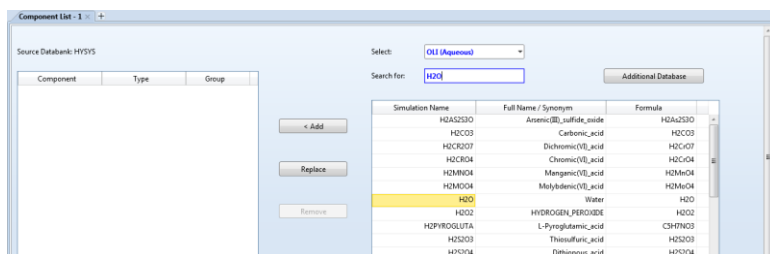




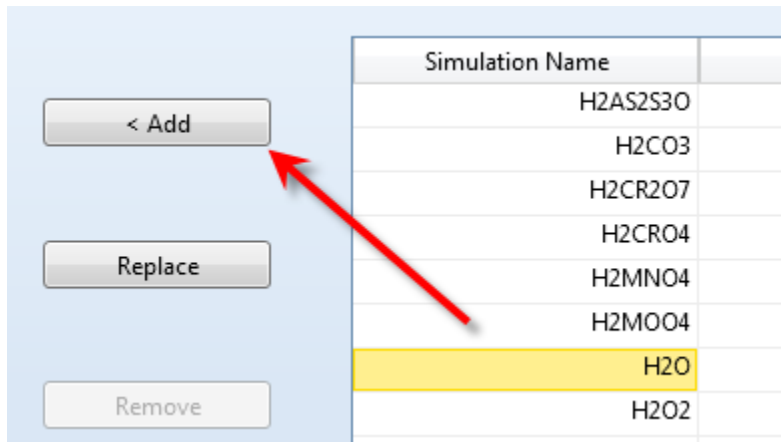
For this example we will use **OLI (Aqueous)**

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.

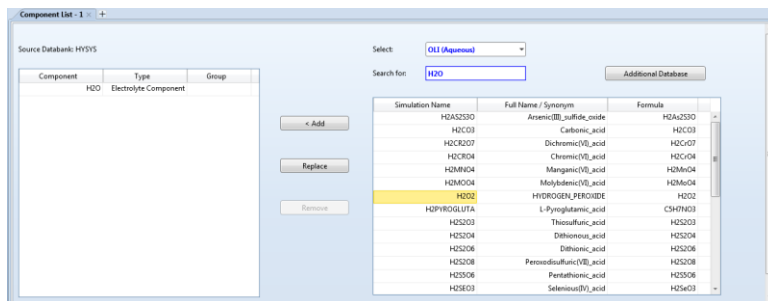
Enter the species **H2O** into the **Search For:** box.



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.



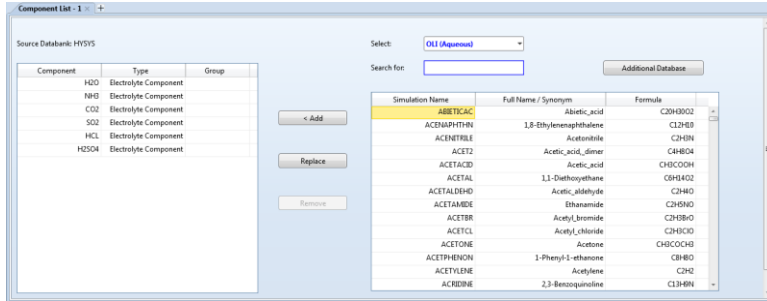
You will notice that the component list no longer displays H2O in the available box. Rather it now appears in the Selected components. If you wish to remove a component from the selected list, highlight it and use the **Replace** button.

Using the same procedure, add the following components.

**NH3**  
**CO2**  
**SO2**

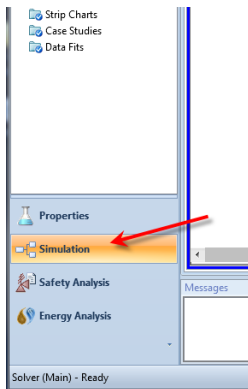
HCL  
H2SO4

The input should look like this:

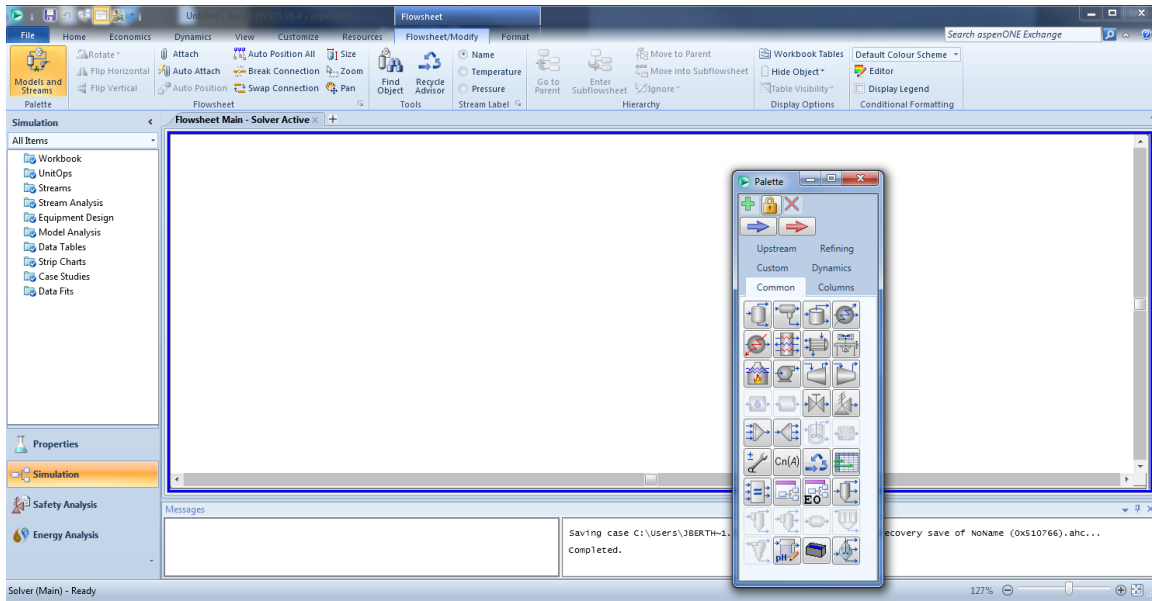


The component selection has been completed. We are now ready to start building our process.

## Creating the Simulation



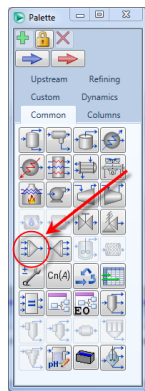
As you click this button Aspen HYSYS temporarily passes control to the OLI software to create the electrolyte model. Progress messages can be seen in the status line at the bottom of the window as well as in the summary box. After a few moments, the standard ASPEN HYSYS development window is displayed.



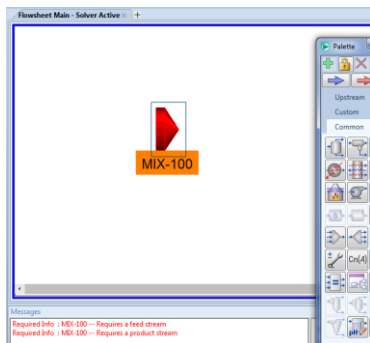
**the Simulation window (move the palate if it is obscuring the window)**

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.

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



The workspace now looks like this:



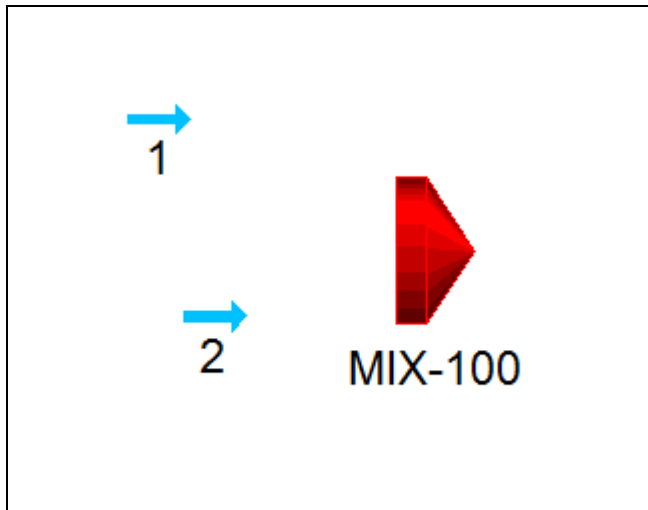
The mixer is given a default name of MIX-100. You can change it later if you wish. The block is also colored RED. This indicates that the block does not have sufficient information to calculate.

We need to create two inlet streams.

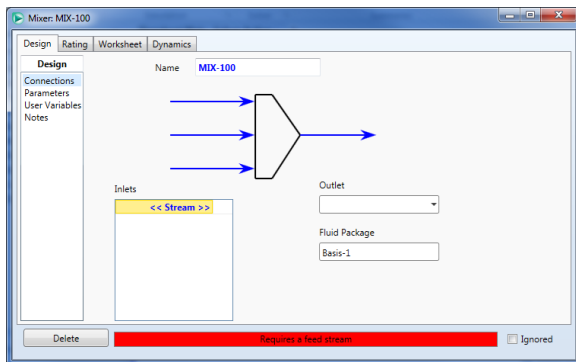
Click on the **Material Streams** arrows and place them on the workspace.



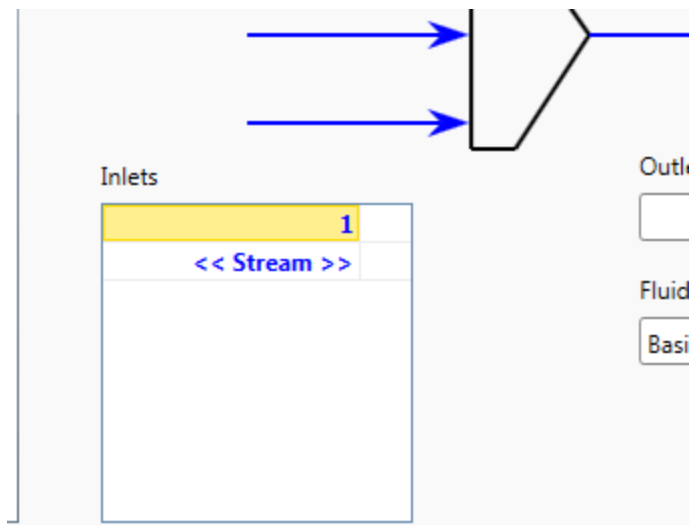
The material streams arrows are colored blue. Place two (2) material streams arrows on the workspace.



**Double-Click the Mixer Block.**

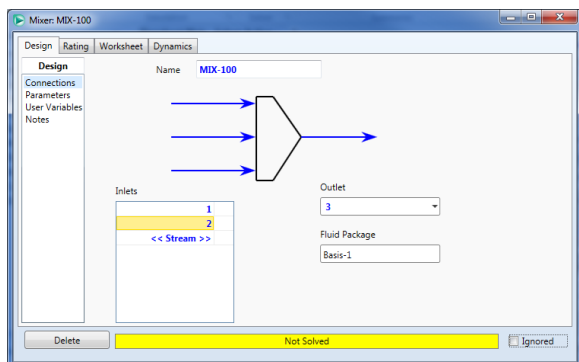


**Locate the *Inlets* area on this dialog and click in the first cell. Select stream “1”. Repeat for stream “2”.**



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

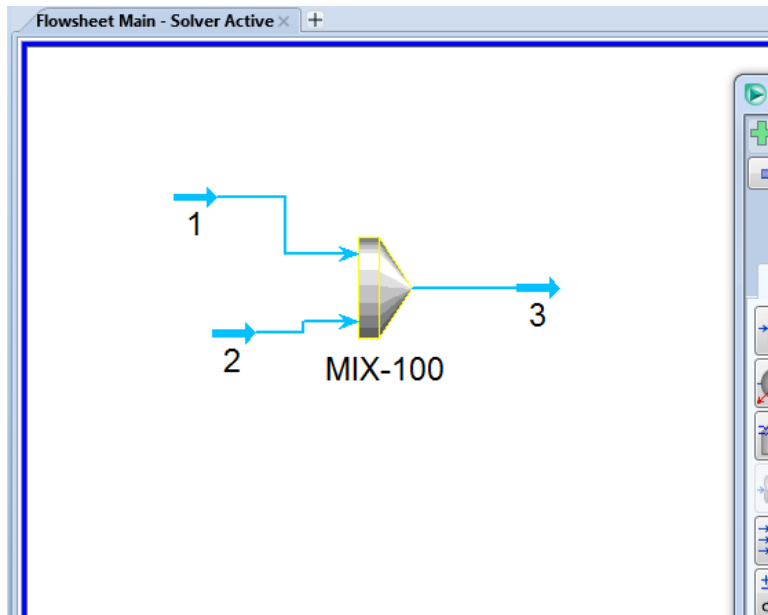
Locate the **Outlet** box and enter the number "3". This completes this block.



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"

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

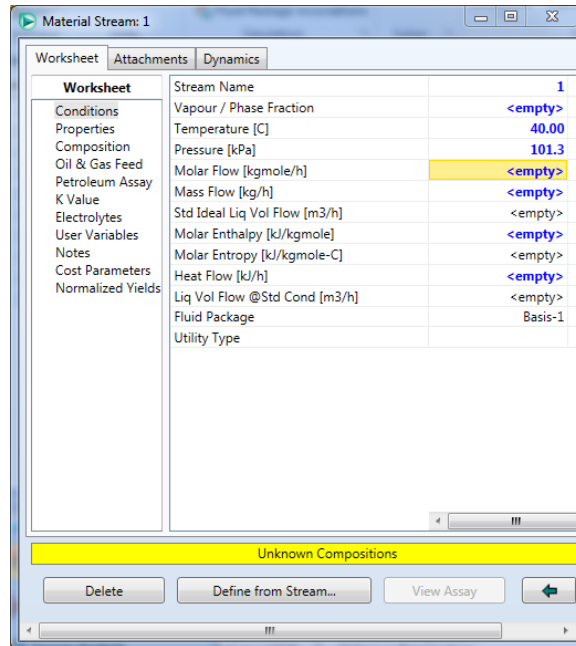
Unknown Compositions

Buttons: Delete, Define from Stream..., View Assay, Back Arrow

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

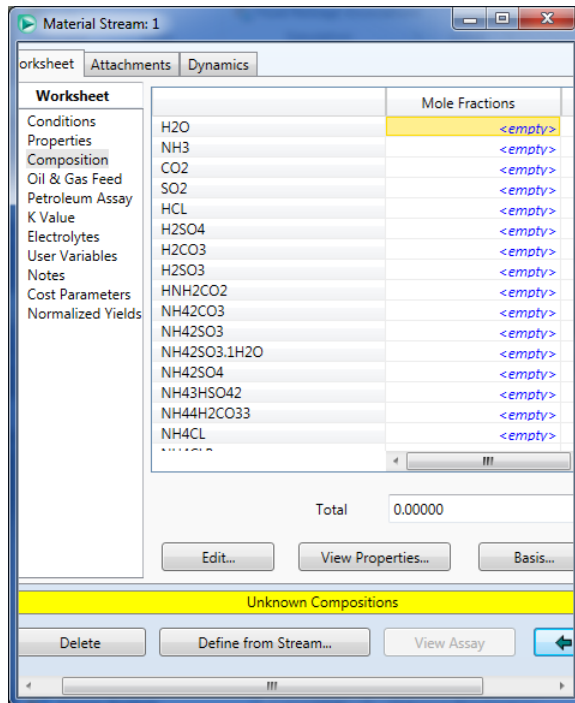
Locate the cell for Temperature ( C) and enter 40

Locate the cell for Pressure (kPa) and enter 101.3



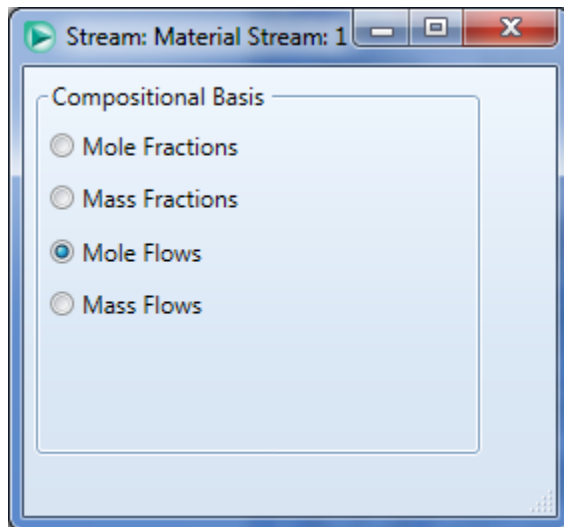
Now click the *Composition* line



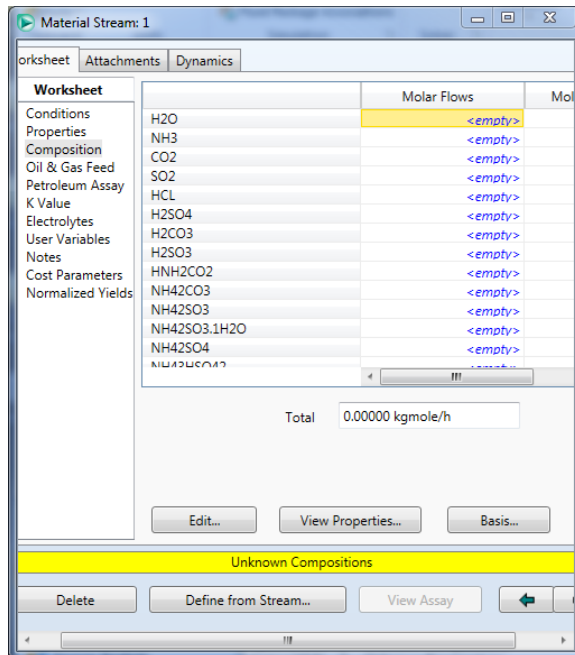


We can now enter our composition for our components. In this case, we desire to use mole flow rather than mole fractions.

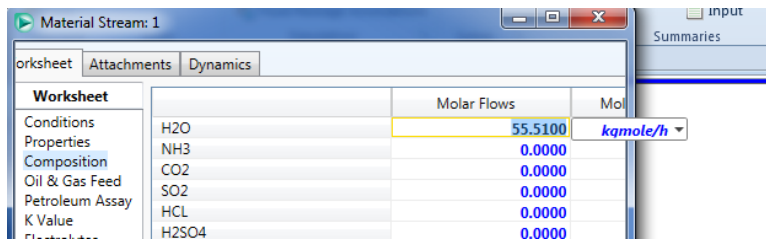
Click the ***Basis...*** button



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

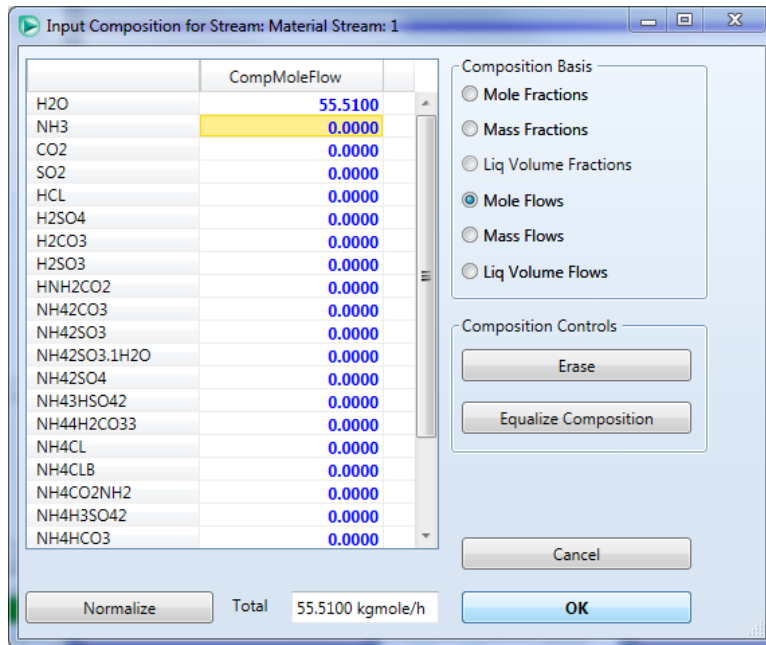


Now begin to enter a value for **H2O** of **55.51**



This time we get a fly-out unit selection box. Use the defaults at this time.

**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

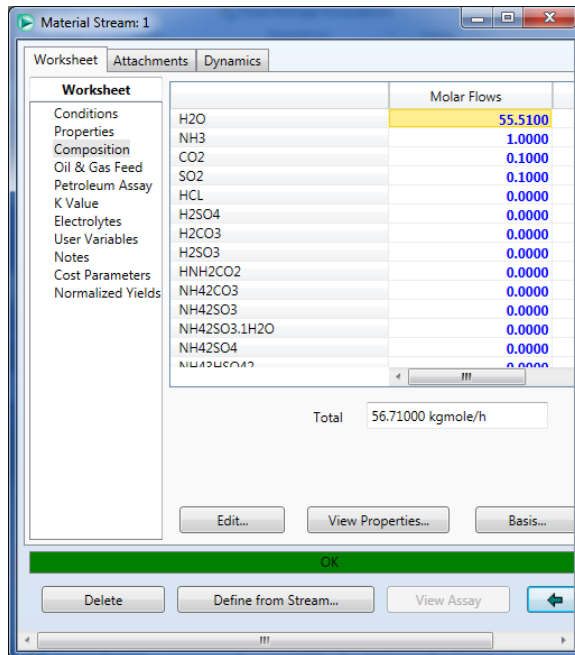
NH3            1.0

CO2            0.1

SO2            0.1

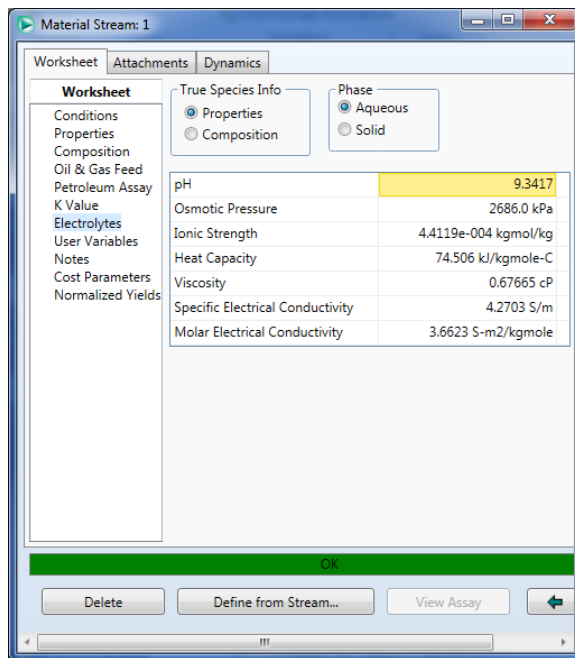
The remaining values can be zero.

**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. Click on the other buttons to see what we 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**

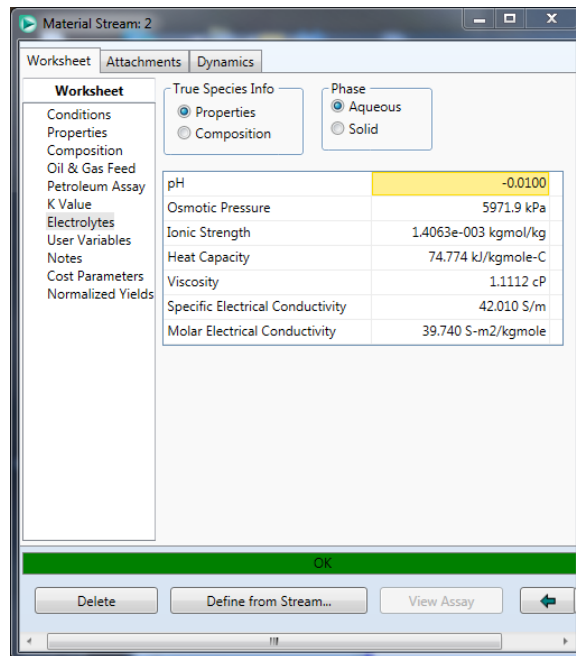
**Pressure                101.3   kPa**

**H2O                        55.51**

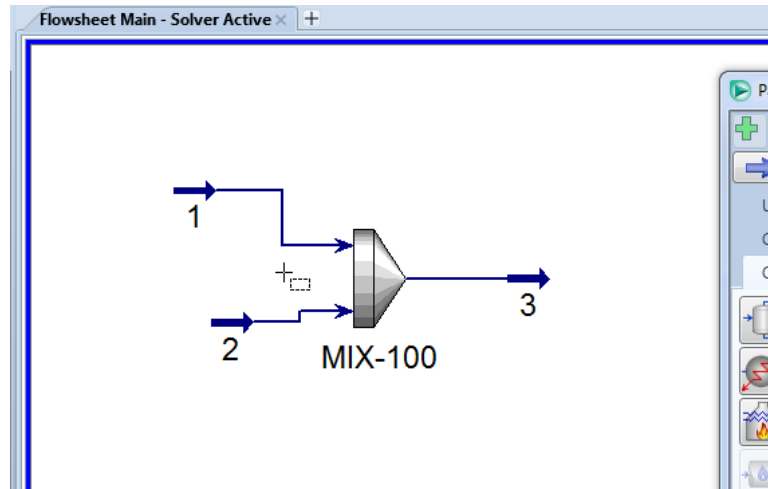
**HCl                        0.1**

**H2SO4                    1.0**

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



**Click the X to close the dialog.**



### Reviewing the output

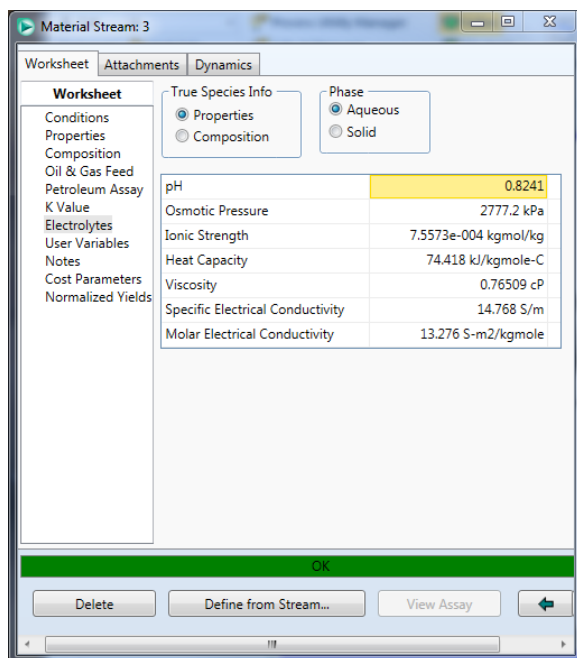
Hysys will attempt to converge the process as you create it. As you close the final dialog box for data entry you will see that the output stream “3” is “Blue” which means it has converged.

### Double-Click stream “3”

Worksheet	Stream Name	3
Conditions	Vapour / Phase Fraction	0.0006
Properties	Temperature [C]	36.85
Composition	Pressure [kPa]	101.3
Oil & Gas Feed	Molar Flow [kgmole/h]	114.3
Petroleum Assay	Mass Flow [kg/h]	2130
K Value	Std Ideal Liq Vol Flow [m3/h]	<empty>
Electrolytes	Molar Enthalpy [kJ/kgmole]	-2.865e+005
User Variables	Molar Entropy [kJ/kgmole-C]	72.55
Notes	Heat Flow [kJ/h]	<empty>
Cost Parameters	Liq Vol Flow @Std Cond [m3/h]	<empty>
Normalized Yields	Fluid Package	Basis-1
	Utility Type	

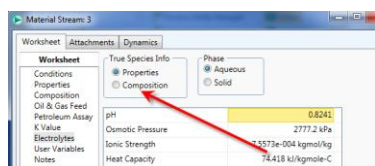
The converged process temperature is approximately 36.8 °C.

Click on the Electrolytes line.

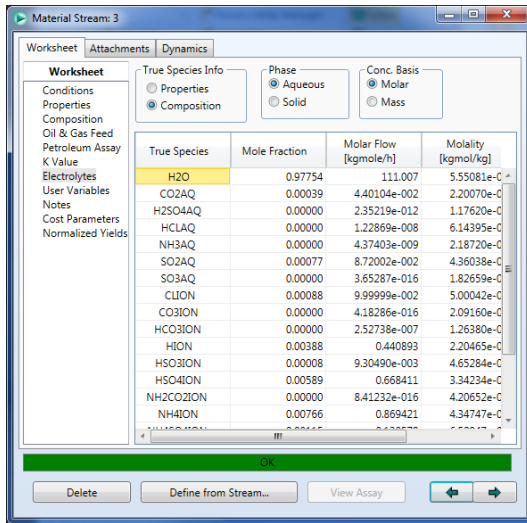


The converged pH is 0.8 indicating that some acid/base chemistry has taken place. What about the equilibrium compositions that have been calculated?

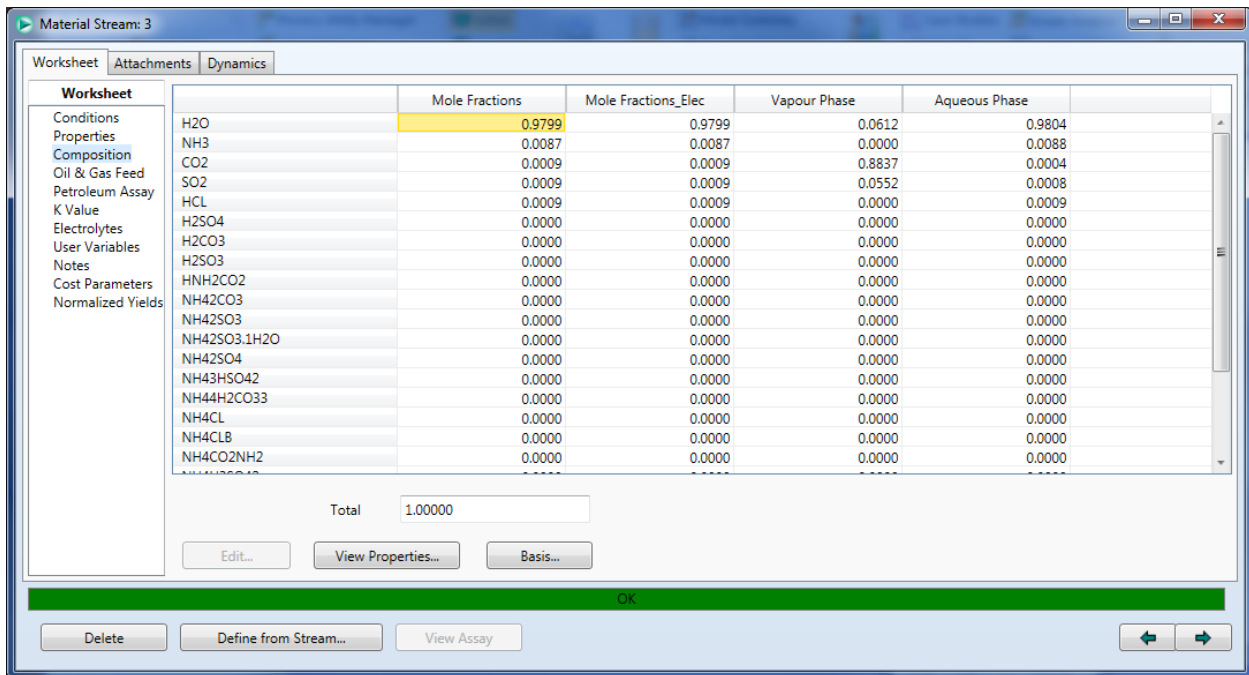
Click the *Composition* radio button at the top of the dialog.



This creates a scrollable area where you can see the actual true-species composition (we have dragged the window to the right to see more information)



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



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 screenshot shows the 'Material Streams 3' window with a 'Worksheet' tab selected. The table displays molar flows for various chemical species across four phases: Molar Flows, Molar Flows\_Elec, Vapour Phase, and Aqueous Phase. The total molar flow is reported as 114.31993 kgmole/h.

Species	Molar Flows	Molar Flows_Elec	Vapour Phase	Aqueous Phase
H2O	112.02000	112.01999	0.00399	112.01611
NH3	1.00000	1.00000	0.00000	1.00000
CO2	0.10000	0.10000	0.05600	0.04400
SO2	0.10000	0.10000	0.00350	0.09650
HCl	0.10000	0.10000	0.00000	0.10000
H2SO4	0.00000	0.00000	0.00000	0.00000
H2CO3	0.00000	0.00000	0.00000	0.00000
H2SO3	0.00000	0.00000	0.00000	0.00000
HNH2CO2	0.00000	0.00000	0.00000	0.00000
NH4CO3	0.00000	0.00000	0.00000	0.00000
NH4SO3	0.00000	0.00000	0.00000	0.00000
NH4SO3.1H2O	0.00000	0.00000	0.00000	0.00000
NH4SO4	0.00000	0.00000	0.00000	0.00000
NH4HSO4	0.00000	0.00000	0.00000	0.00000
NH4H2CO3	0.00000	0.00000	0.00000	0.00000
NH4HSO3	0.00000	0.00000	0.00000	0.00000
<b>Total</b>	<b>114.31993</b>	<b>114.31993</b>	<b>0.00399</b>	<b>114.31594</b>

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

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

## **Disclaimer**

This tutorial was created with Aspen HYSYS V8.4 and the OLI Engine version 9.0.14. As time progresses, updates to the OLI databanks and engine may result in changes to the results displayed here. It is not guaranteed that later versions of either Aspen HYSYS or OLI will yield the same results.

## **Trademarks**

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OLI, OLI Systems and the “OLI Engine for Aspen HYSYS” are trademarks of OLI Systems, Inc. Cedar Knolls, New Jersey.