OLI systems, inc.

INTRODUCTION TO

OLI Engine for Aspen Hysys

think simulation

getting the
chemistry right

Introduction to OLI Engine for Aspen Hysys

OLI Engine for Aspen Hysys

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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.

Trademarks

Table of Contents

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.

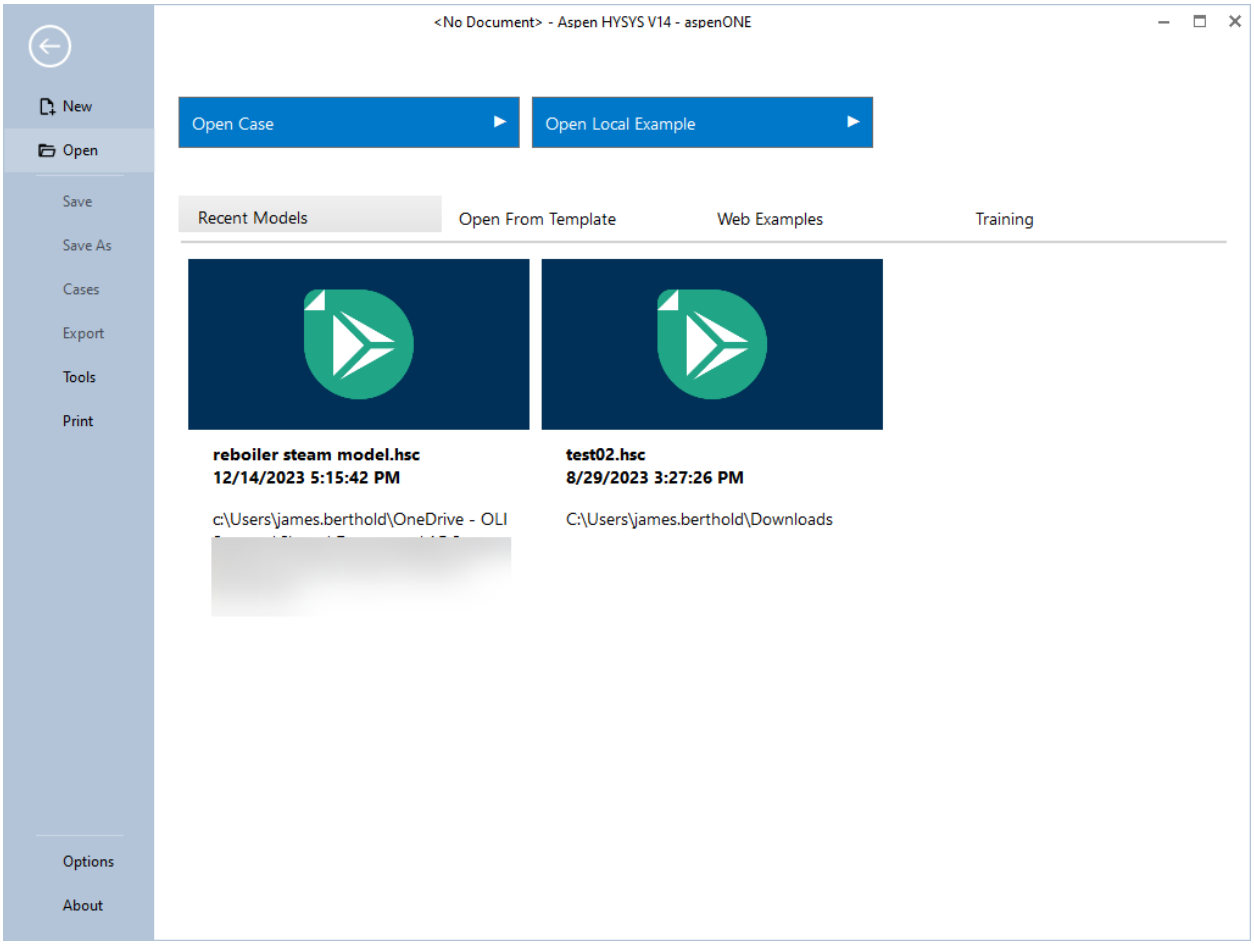
Application

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

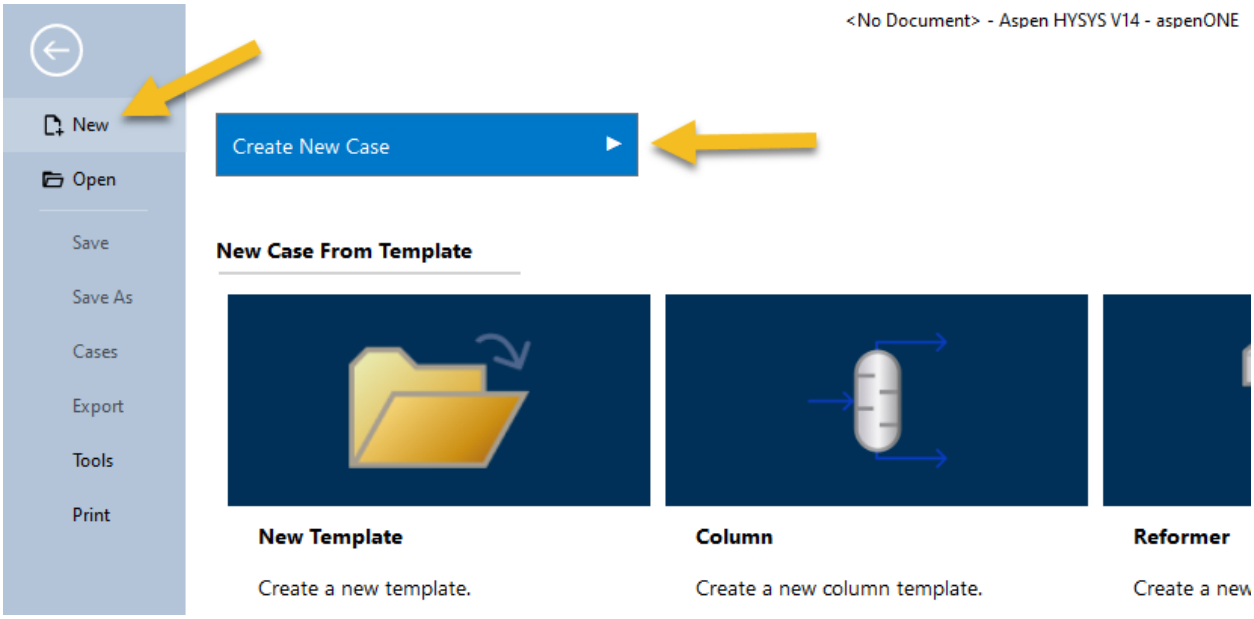
Start Aspen Hysys in the normal manner. A splash screen will display and then disappear.

This will now display the Aspen HYSYS development environment.

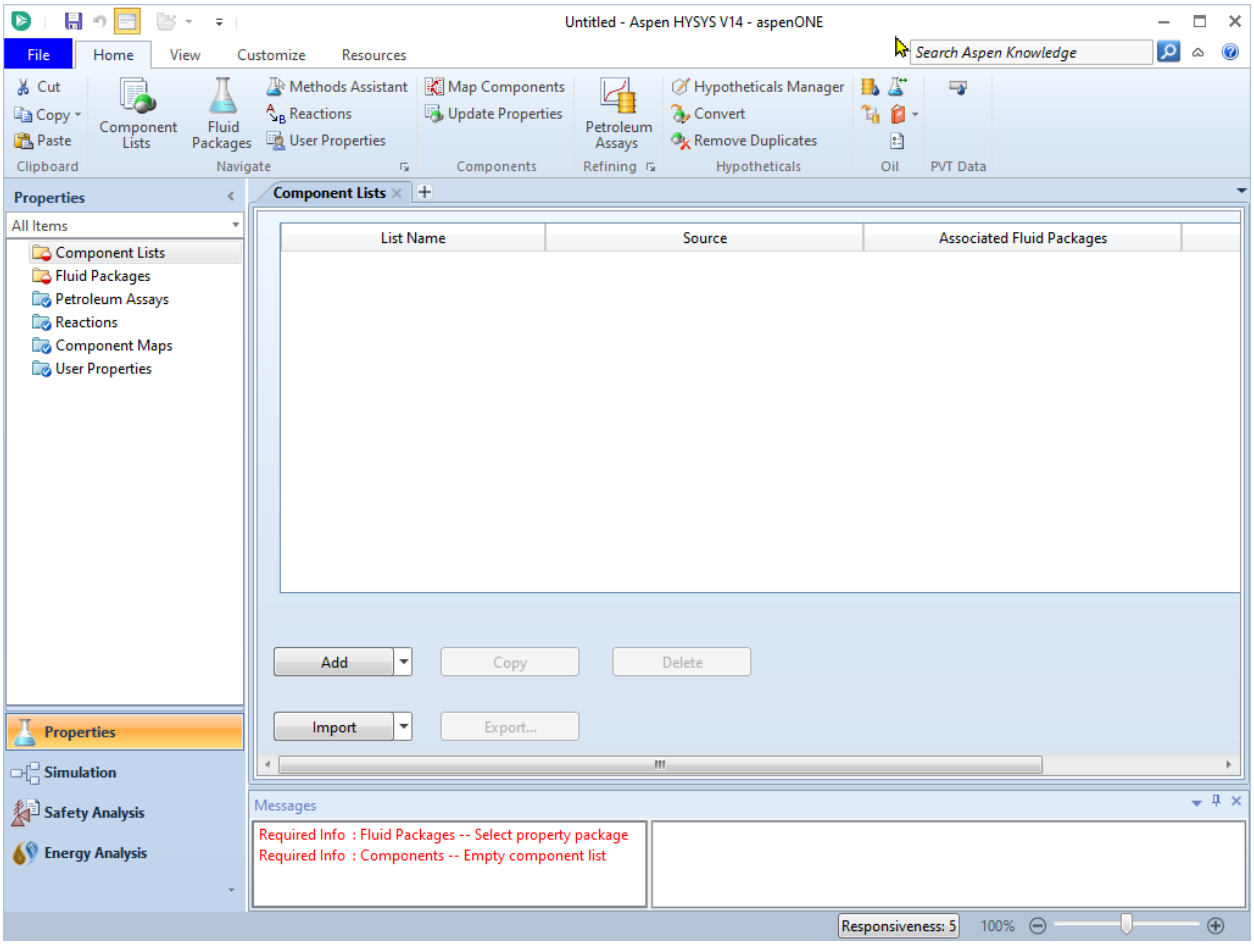


Entering the Chemistry and fluid packages

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


<No Document> - Aspen HYSYS V14 - aspenONE
New
Open
Save
Save As
Cases
Export
Tools
Print
Create New Case
New Case From Template
New Template
Create a new template.
Column
Create a new column template.
Reformer
Create a new

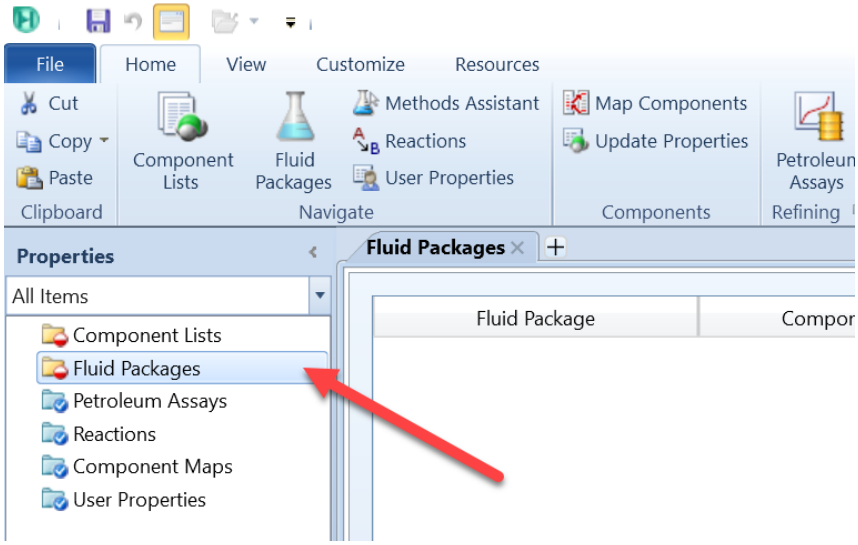
This will bring up the **Simulation Environment**.



Selecting Fluid Packages

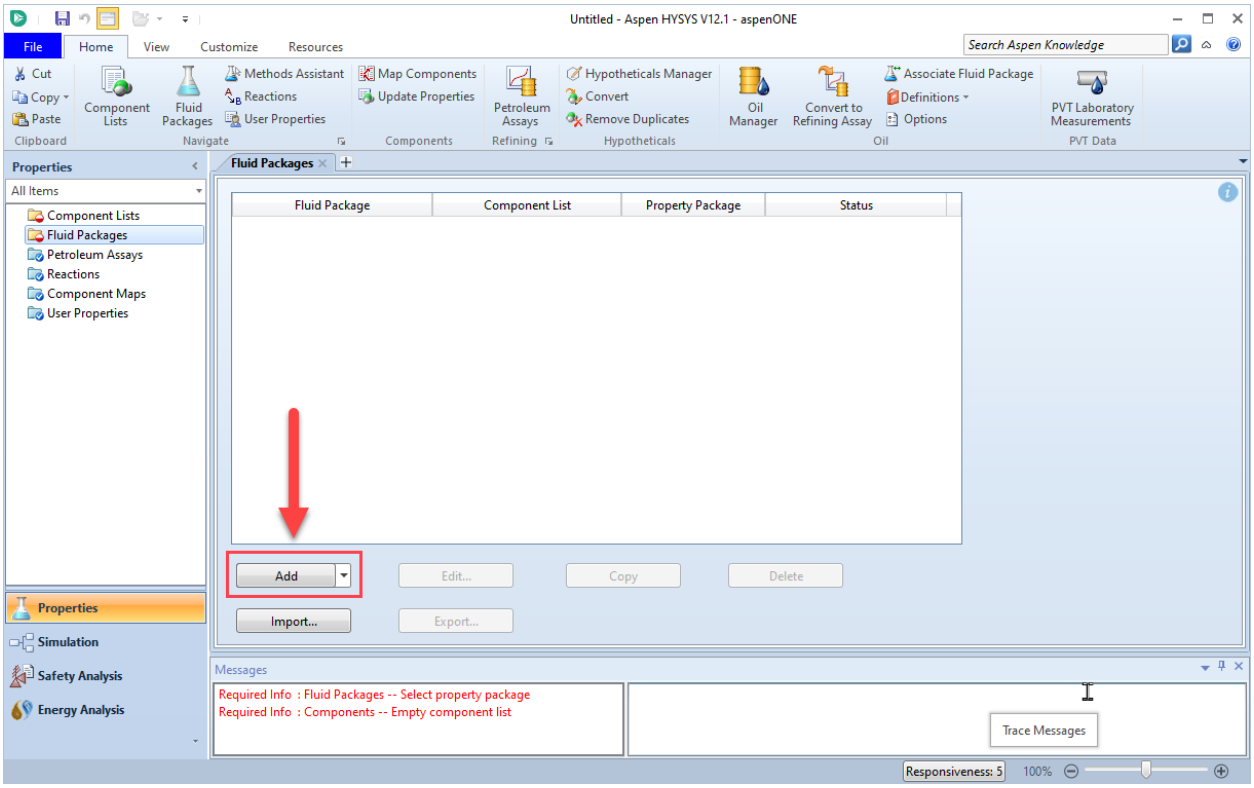
OLI recommends starting with adding a fluid package.

Select *Fluid Packages*

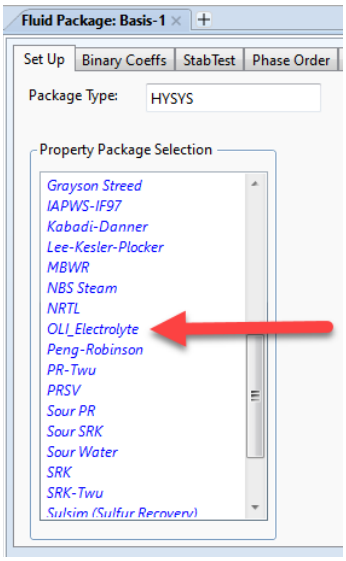


There are no fluid packages currently defined for this simulation. We need to add a package.

Click the ***Add*** button

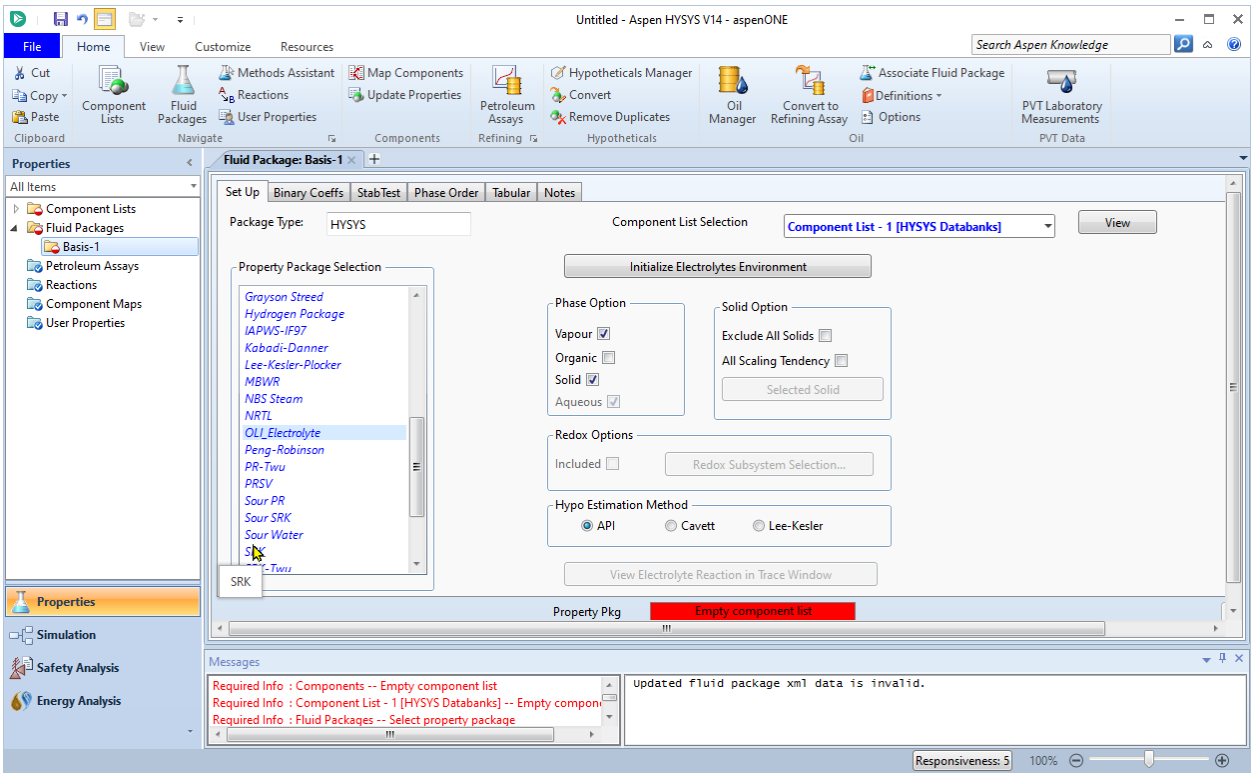


Scroll down the window to find ***OLI_Electrolyte***



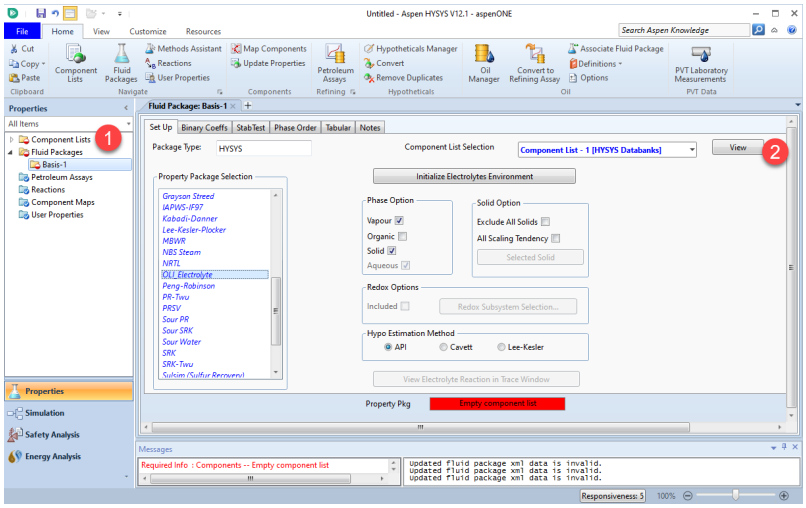
Highlight the object ***OLI_Electrolyte.***

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

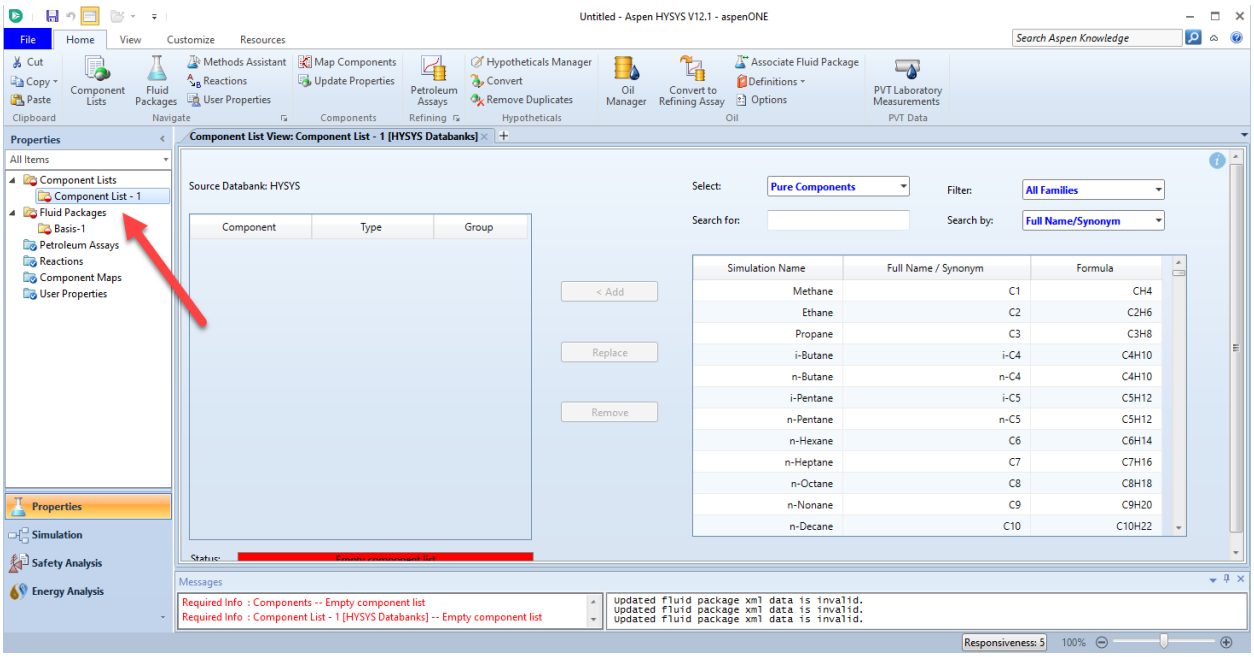
(options 1) or click the View Button next to the list (option 2)



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.

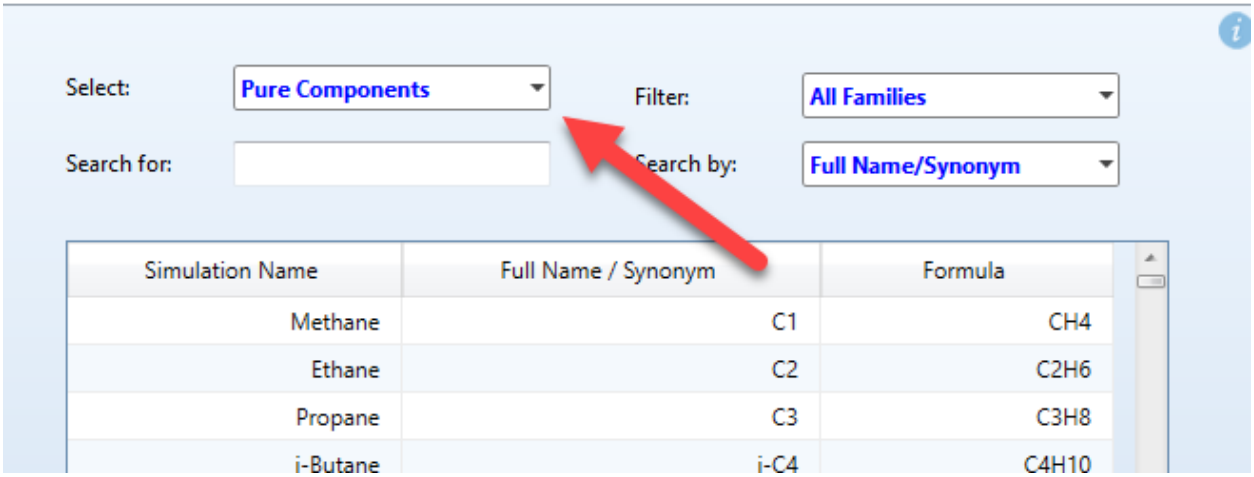
Select **Component List -1**



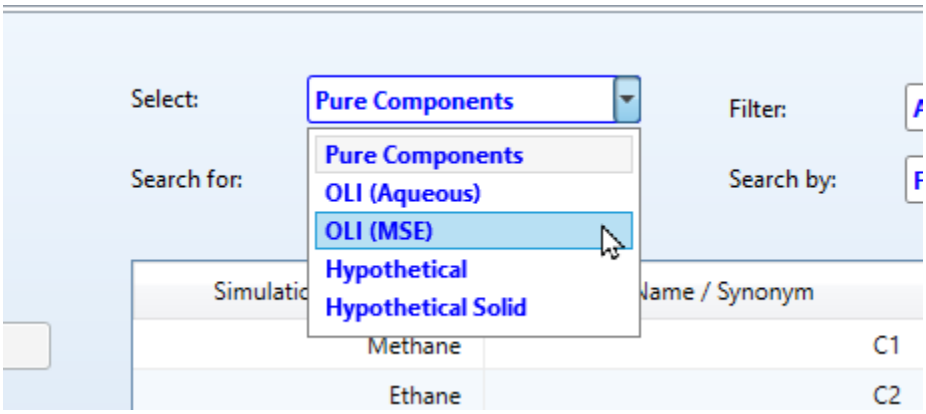
Entering Components

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

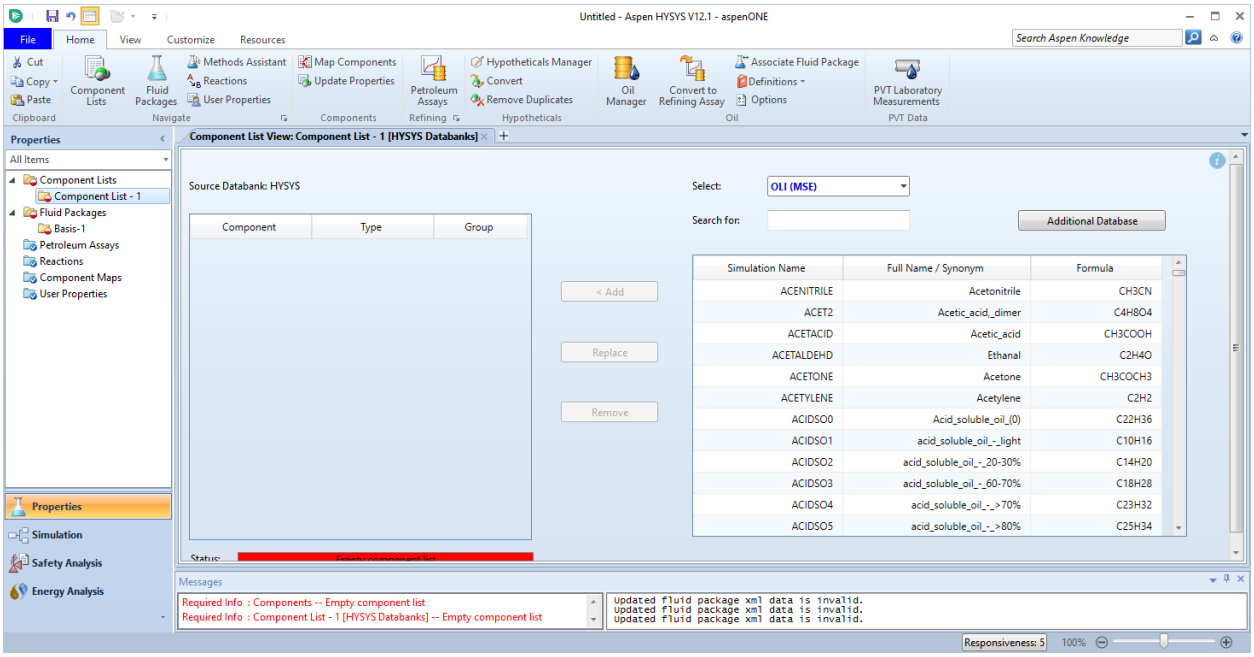
Aspen HYSYS categorizes the components according to function and type. OLI Components are no different. Expand the drop-down list from the ***Select*** box.



This will display several options:



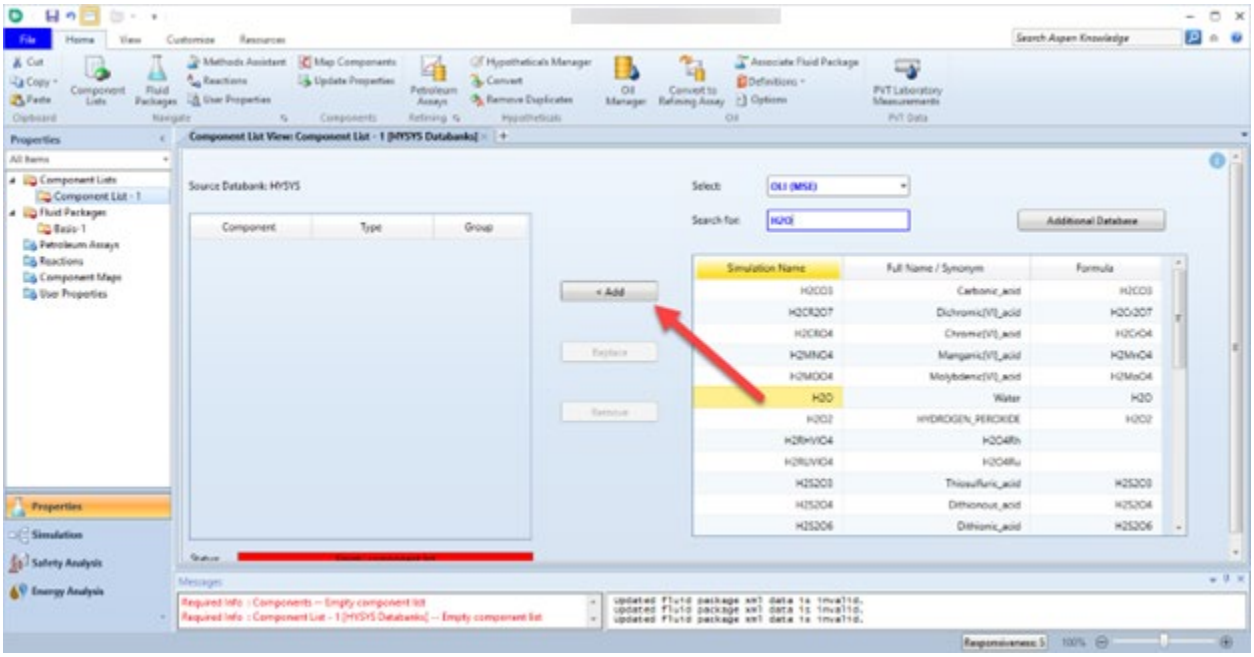
For this example, we will use ***OLI (MSE)***



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.

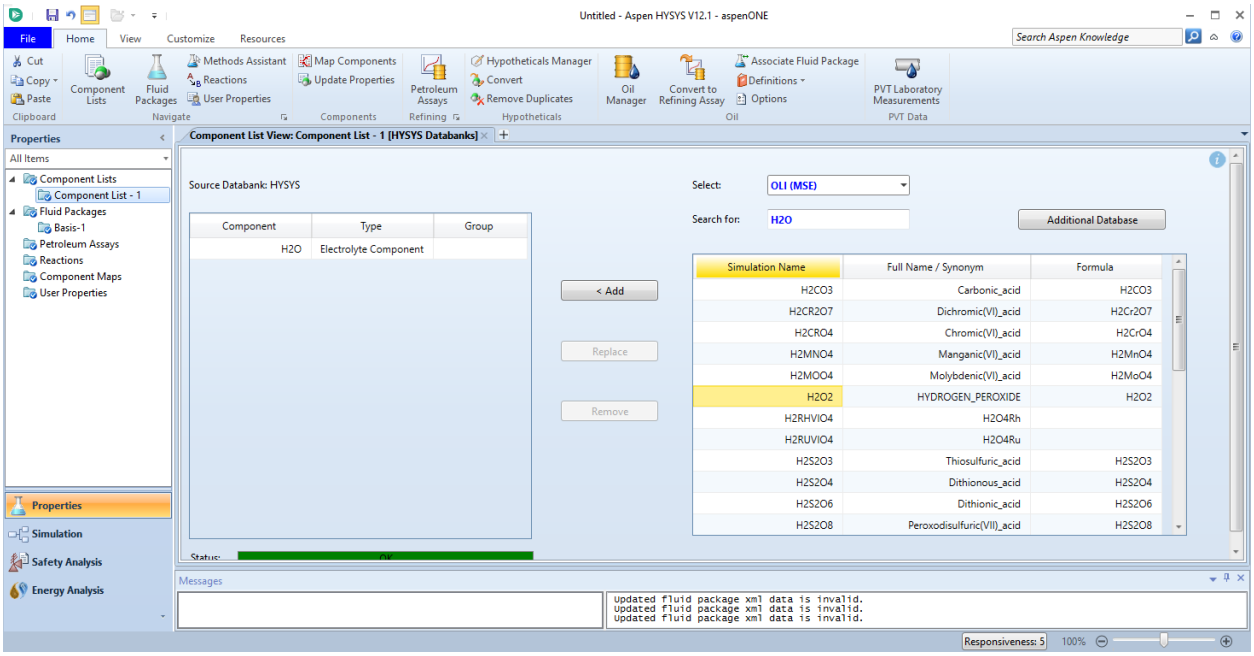
Enter the species **H2O** into the ***Search For:*** box.

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.



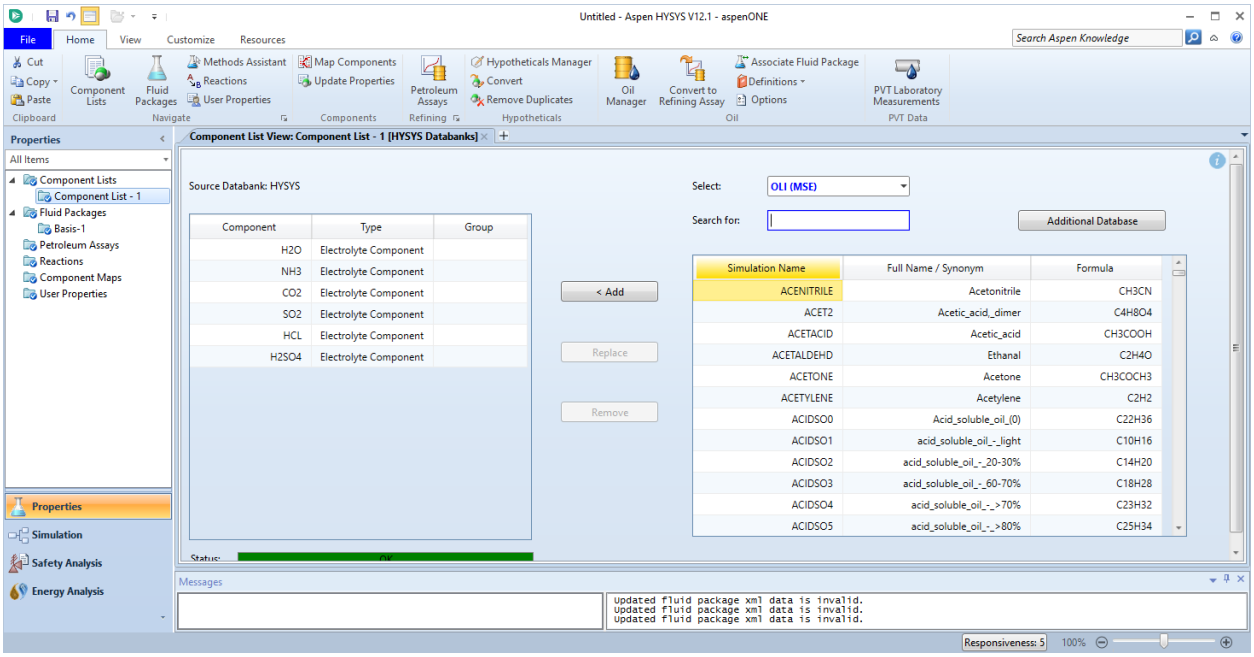
If you wish to remove a component from the selected list, highlight it and use the ***Replace*** button.

Using the same procedure, add the following components[1].

- **NH3**
- **CO2**
- **SO2**
- **HCL**
- **H2SO4**

The input should look like this:

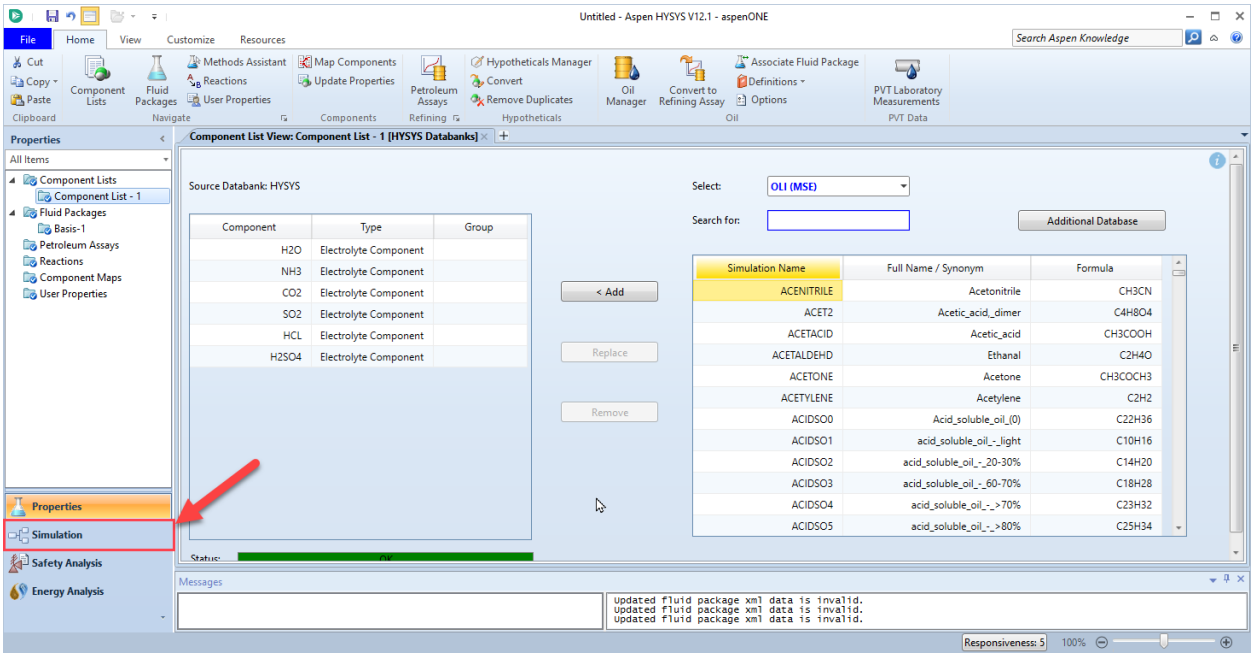
[1] You can also just enter the name in the search box, if you are sure, it is the right name, and then press the Enter key to automatically select it. This saves some time.



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.

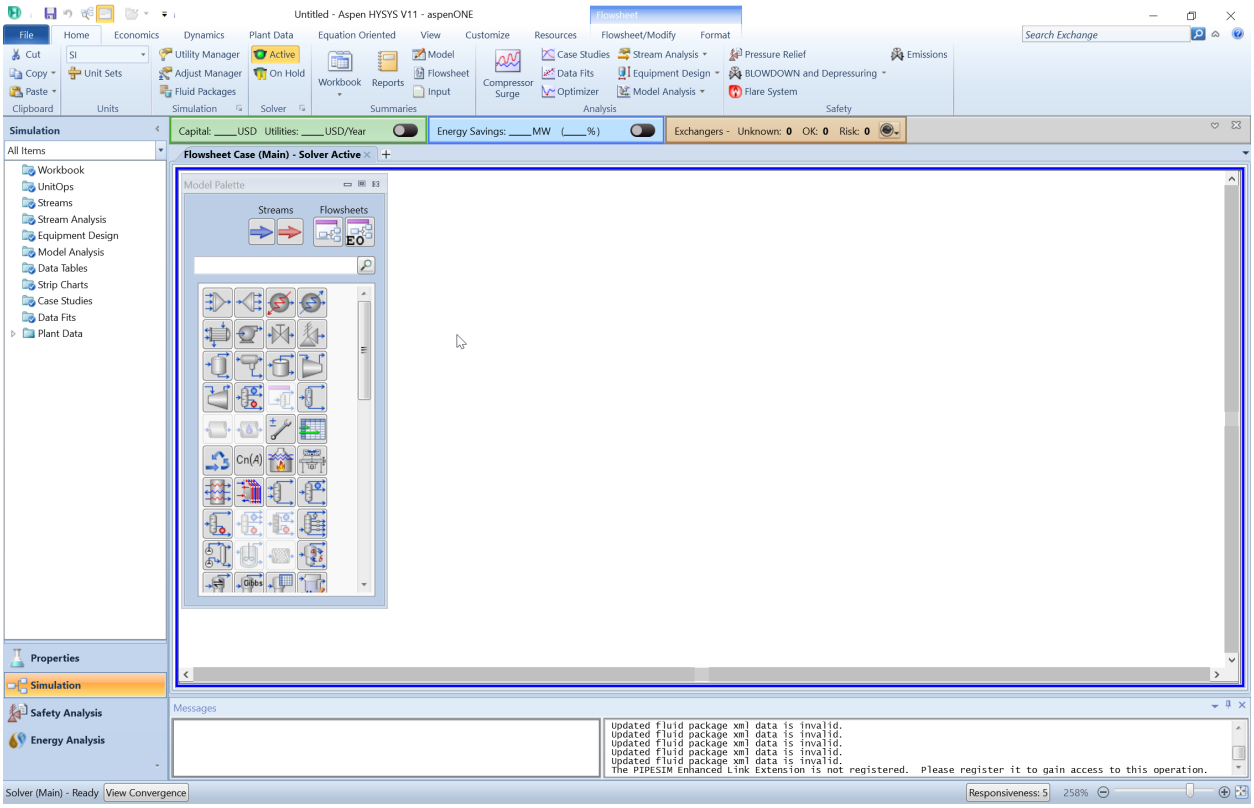


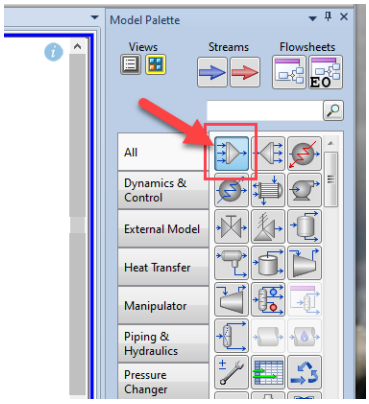
Figure 1. Simulation window (move the palate if it is obscuring the window)

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.

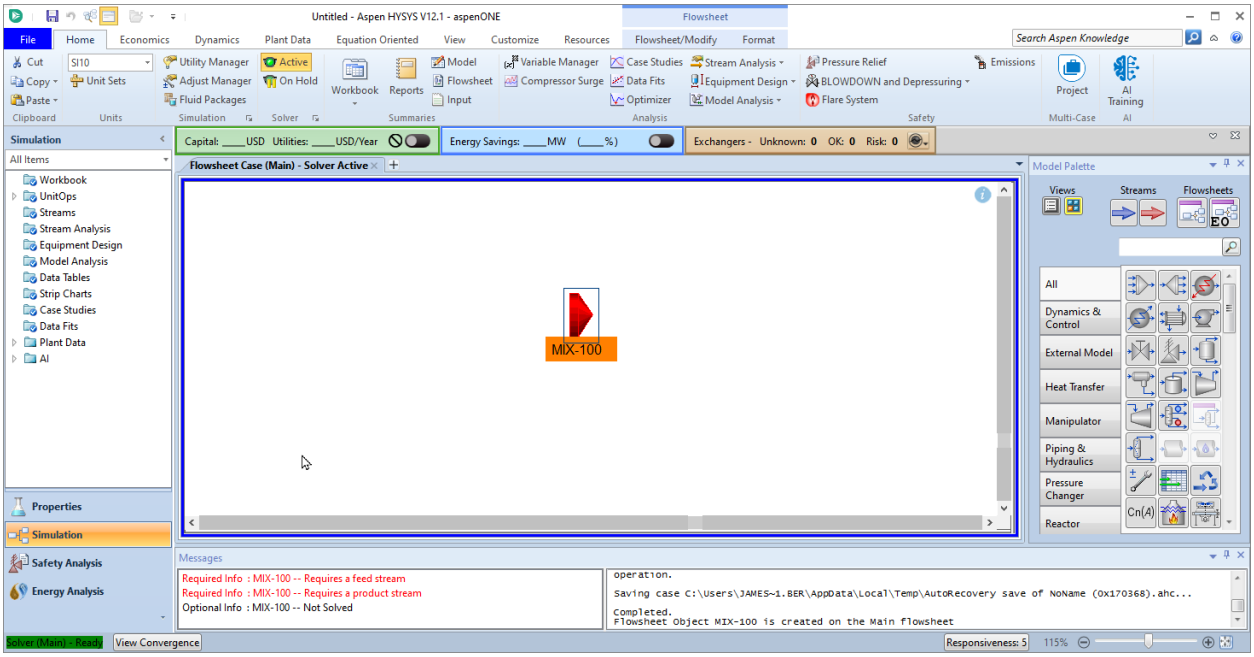
In this example, we will “Dock” the palate to the right side of the environment.

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:

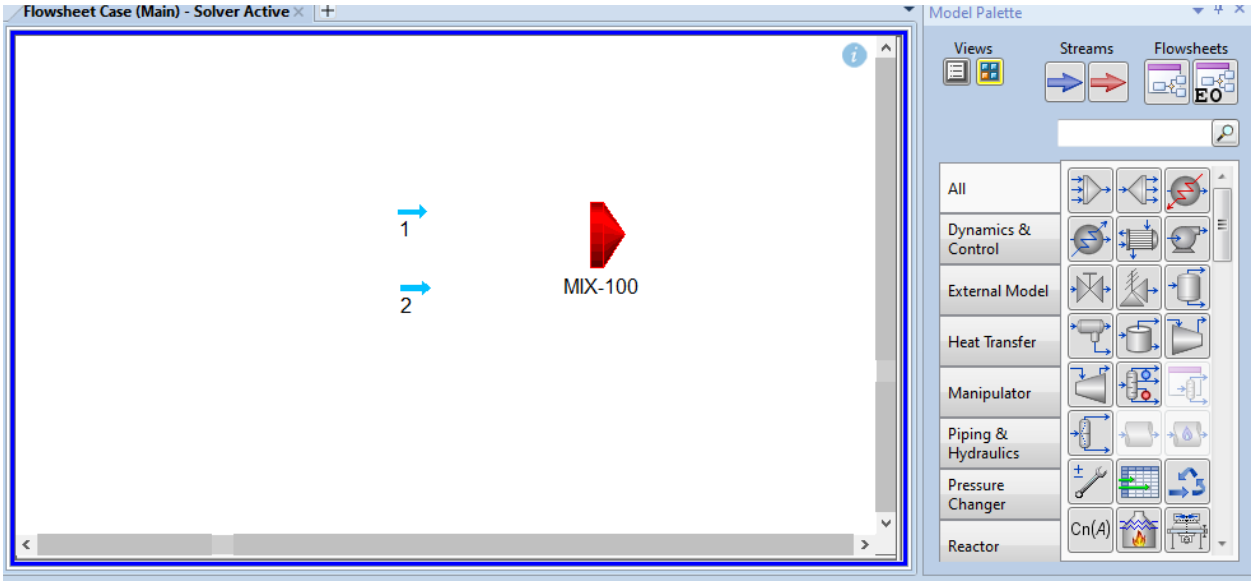


The mixer is given a default name of MIX-100. You can change it later if you wish. The block is also colored RED. This indicates that the block does not have sufficient information to calculate.

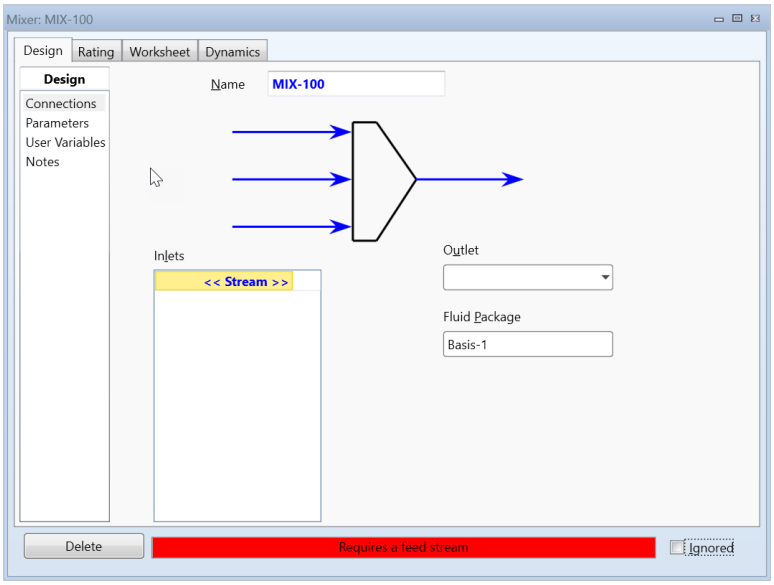
We need to create two inlet streams.

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”.

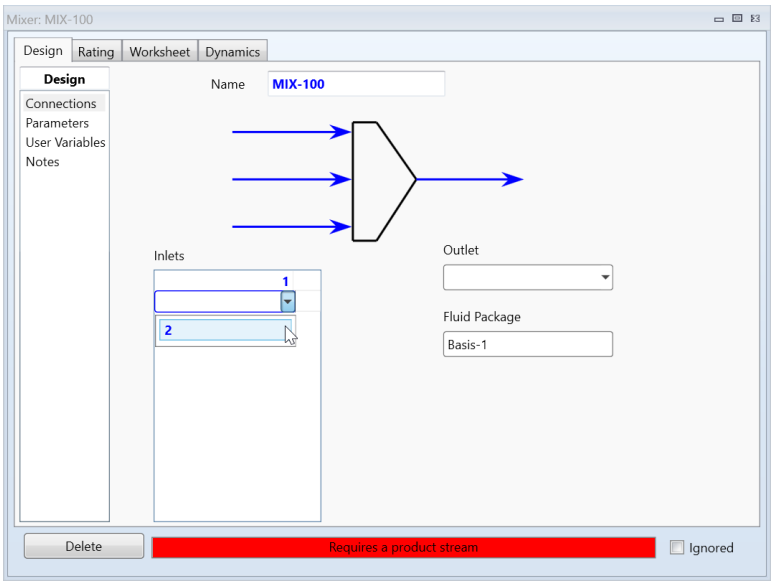
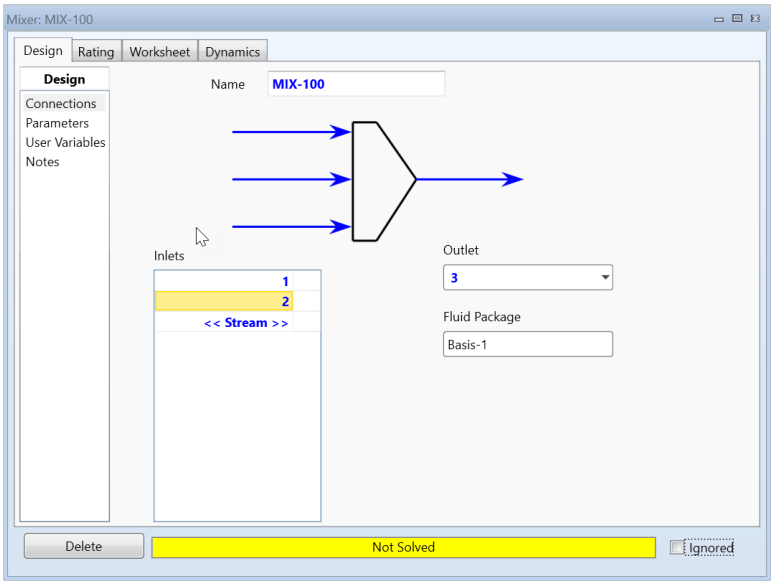


Figure 2. Selecting stream "2". Stream "1" has already been selected.

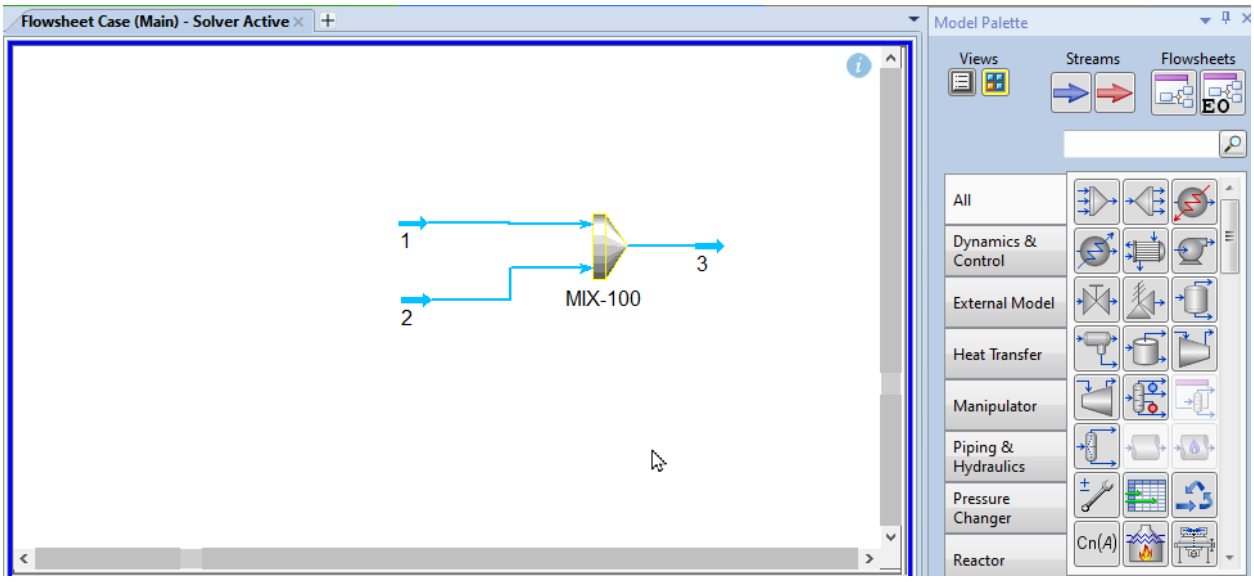
Locate the ***Outlet*** box and enter the number "**3**". This completes this block.



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

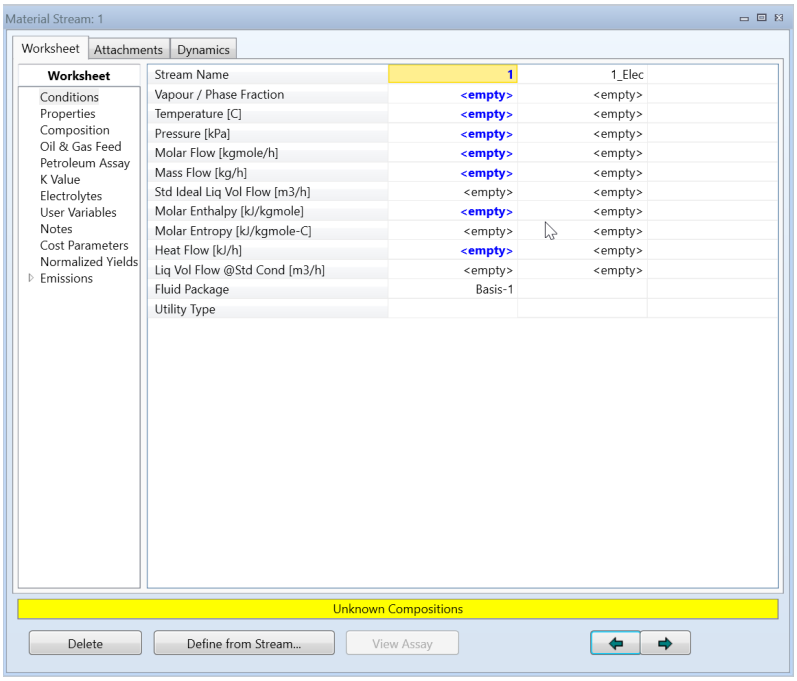
Click the ***x*** in the upper right-hand corner to close this dialog.

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



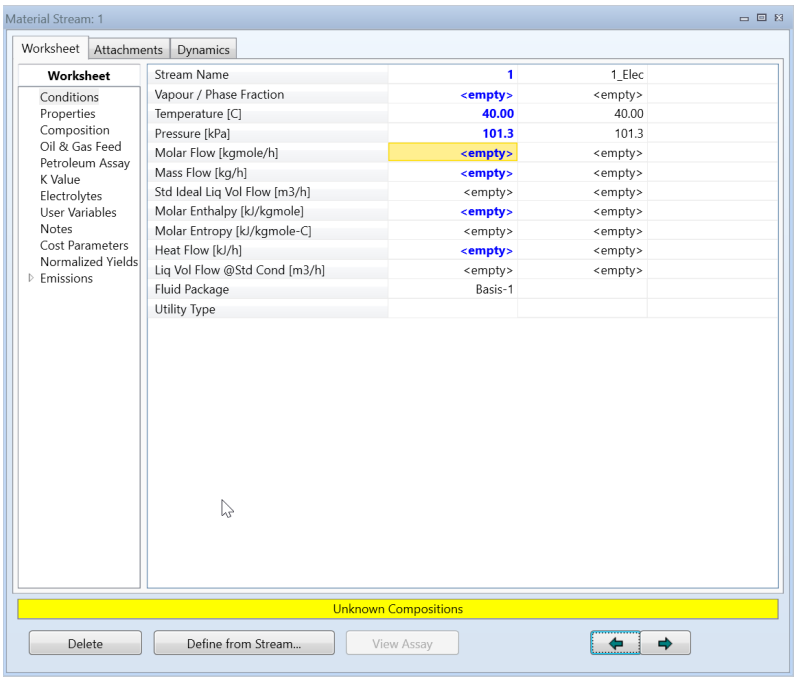
Entering Stream Composition Data

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

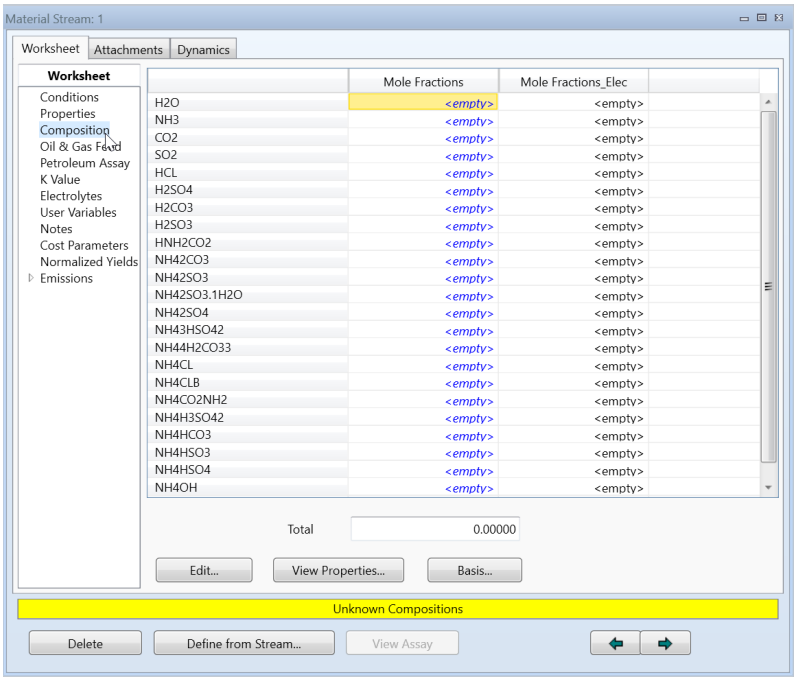


This is the standard input window for a stream. We will now add our conditions.

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

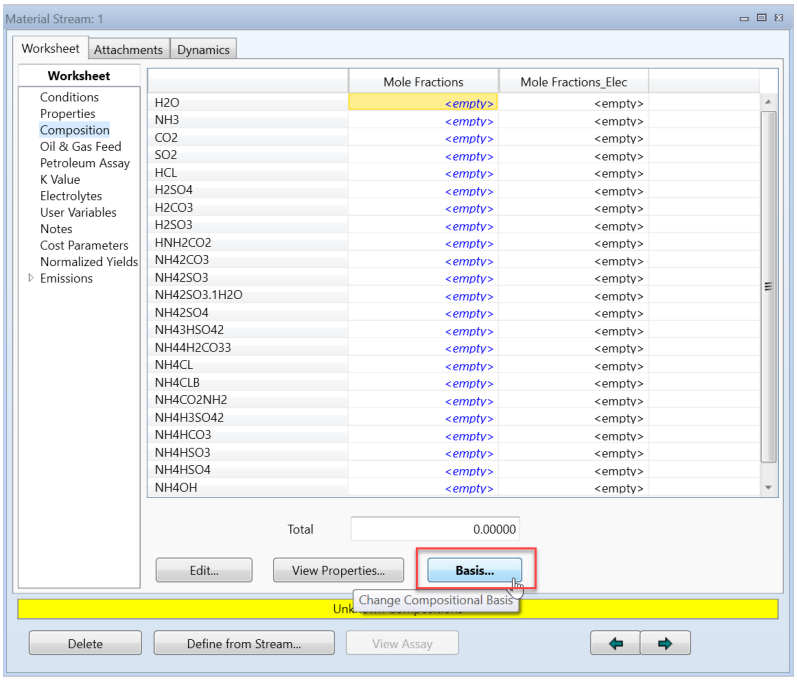


Now click the ***Composition*** line

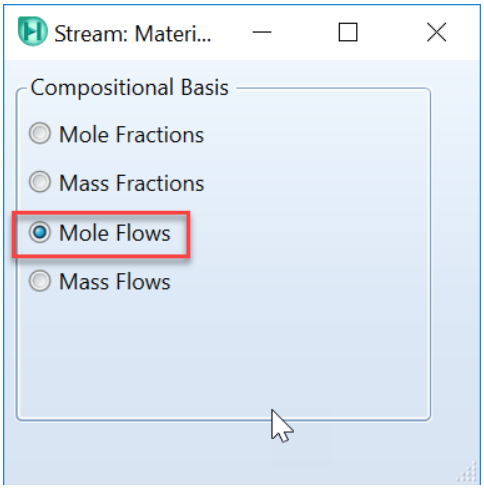


We can now enter our composition for our components. In this case, we want to use mole flow rather than mole fractions.

Click the ***Basis***… button

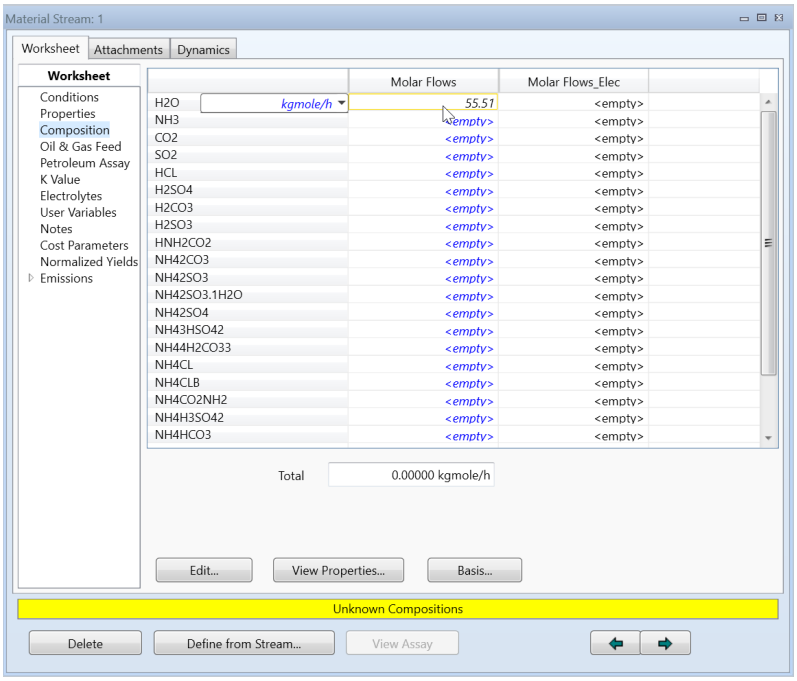


This will open a new window

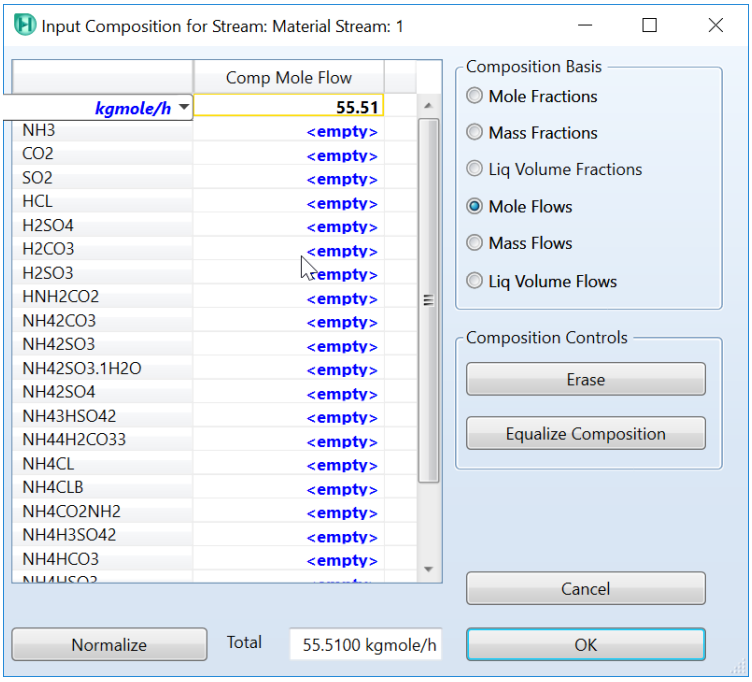


Select the *Mole Flows* radio button. Click the ***x*** when done.

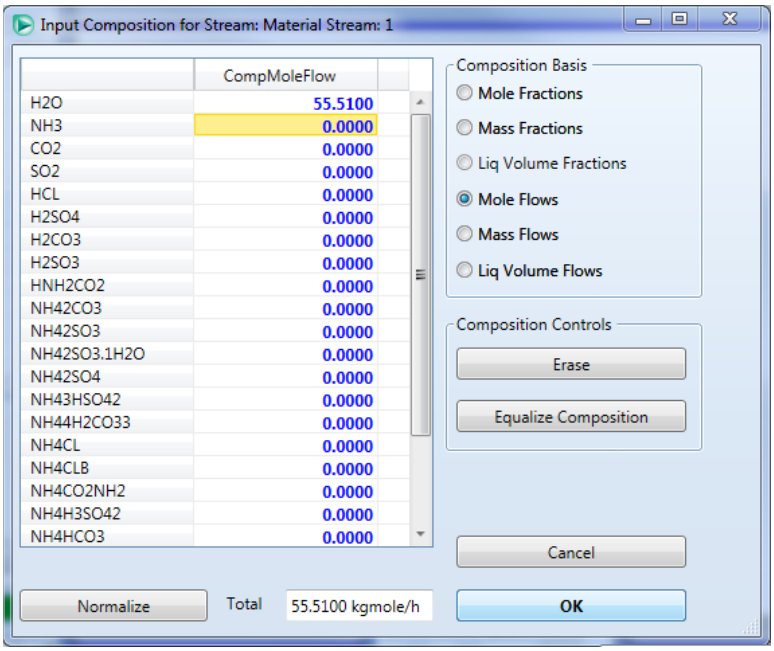
Now begin entering the value for **H2O** of 55.51



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.



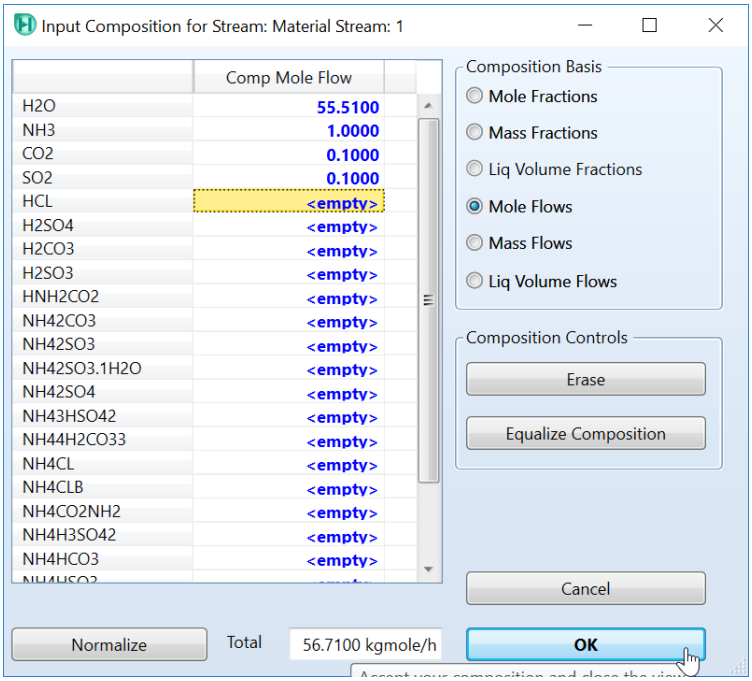
Press the **<Enter>** key to continue.



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

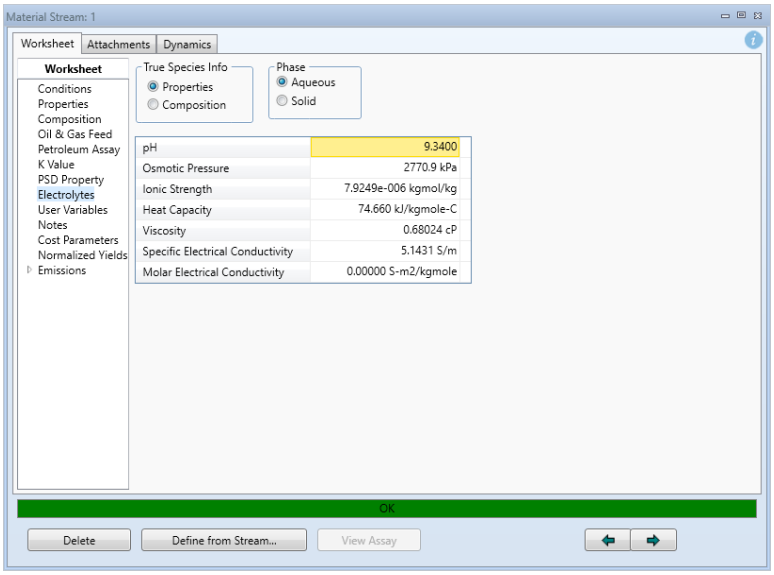
The remaining values can be zero.



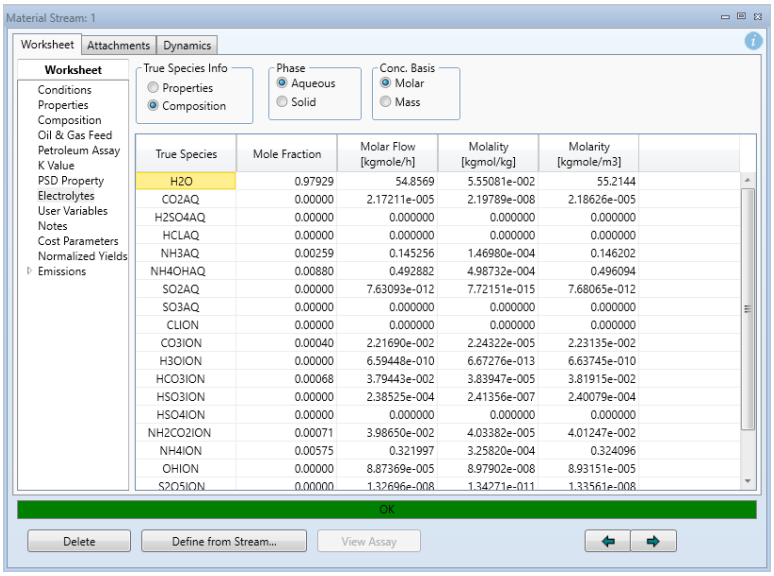
Click the ***OK*** button.

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.

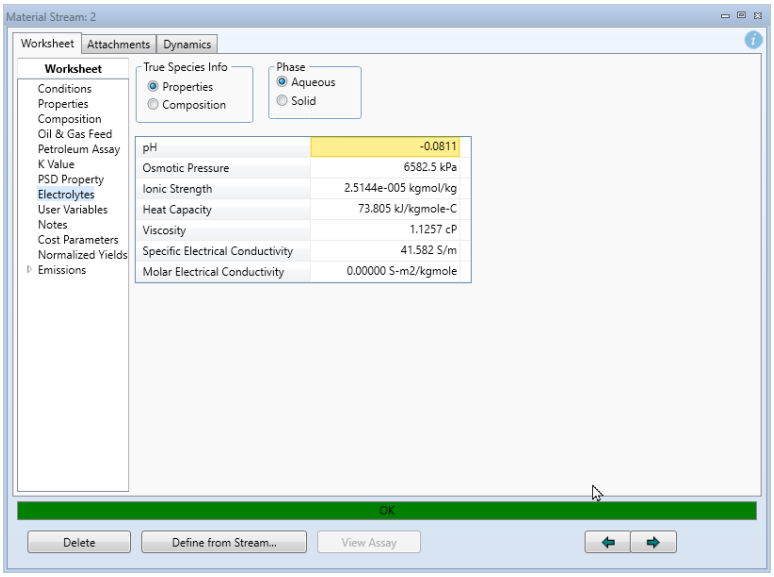


Click on the ***x*** to close this dialog.

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

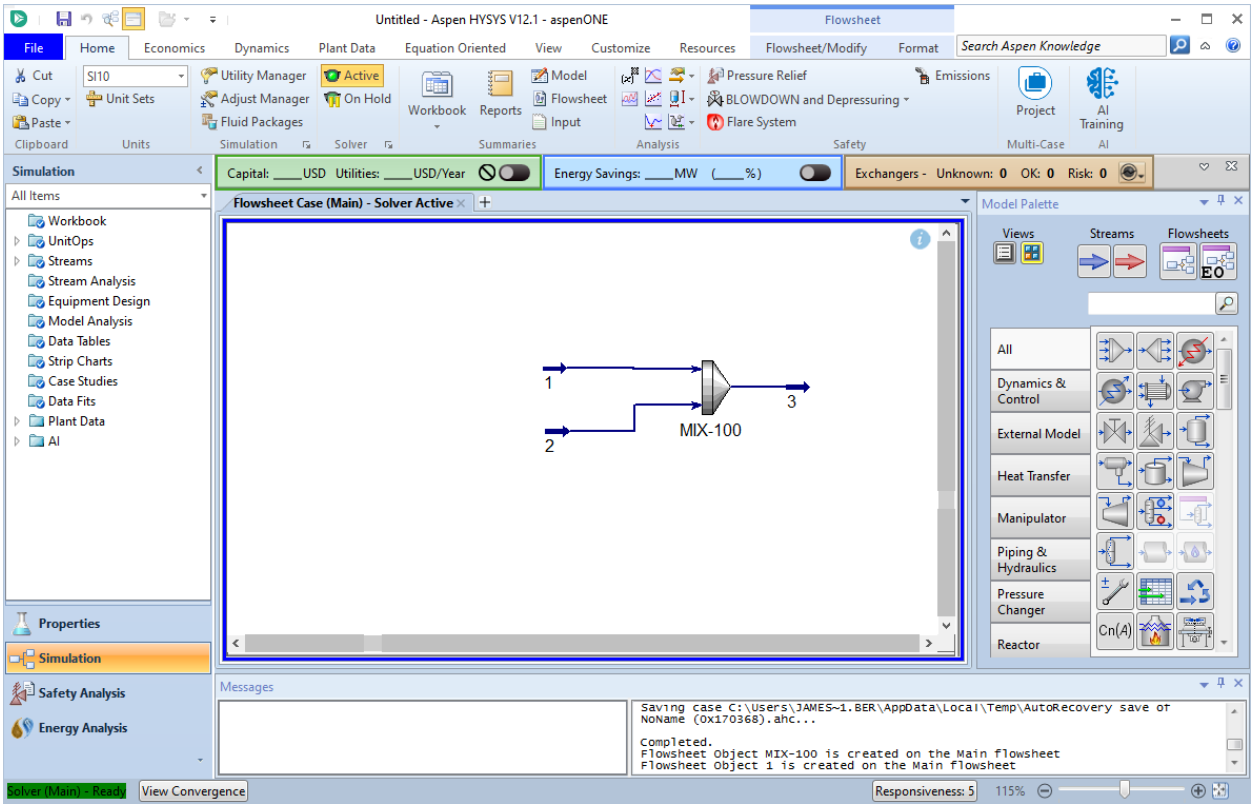
Temperature	25	C
Pressure	101.3	kPa
H2O	55.51	
HCl	0.1	
H2SO4	1.0	

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



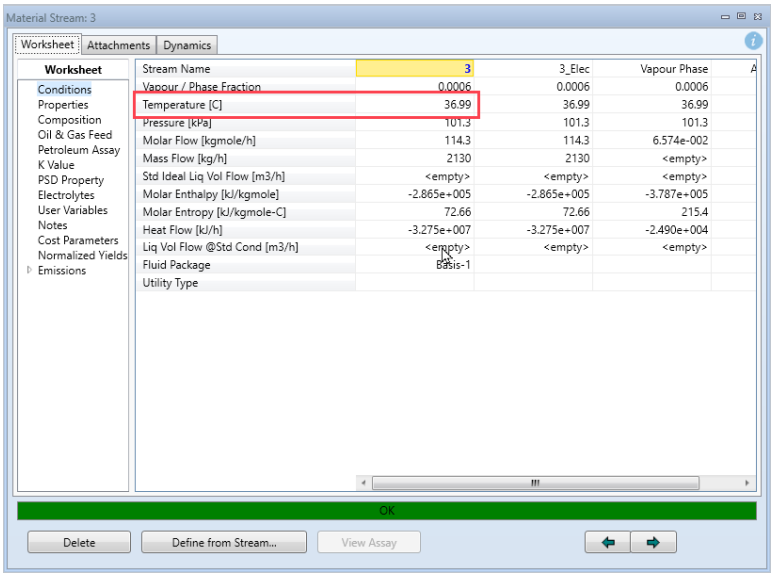
Click the ***x*** to close the dialog.

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.



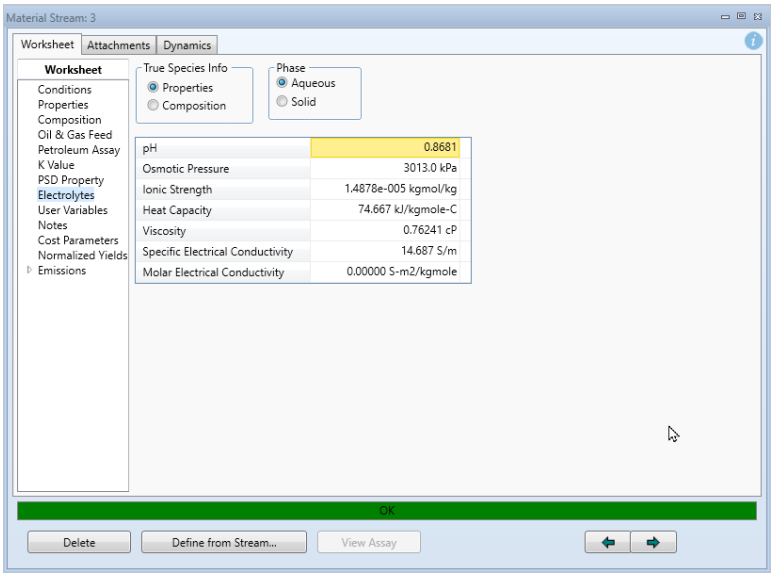
Reviewing the output

Double-Click stream “3”



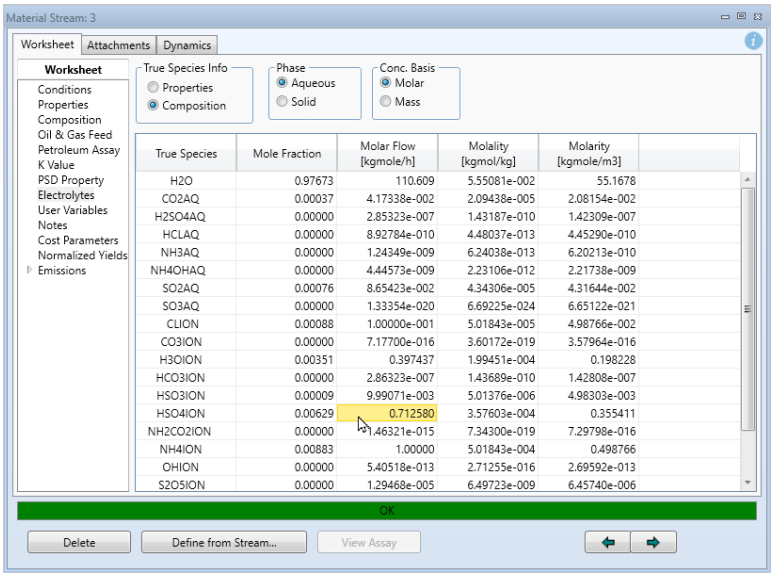
The converged process temperature is approximately 37.0 °C.

Click on the ***Electrolytes*** line.

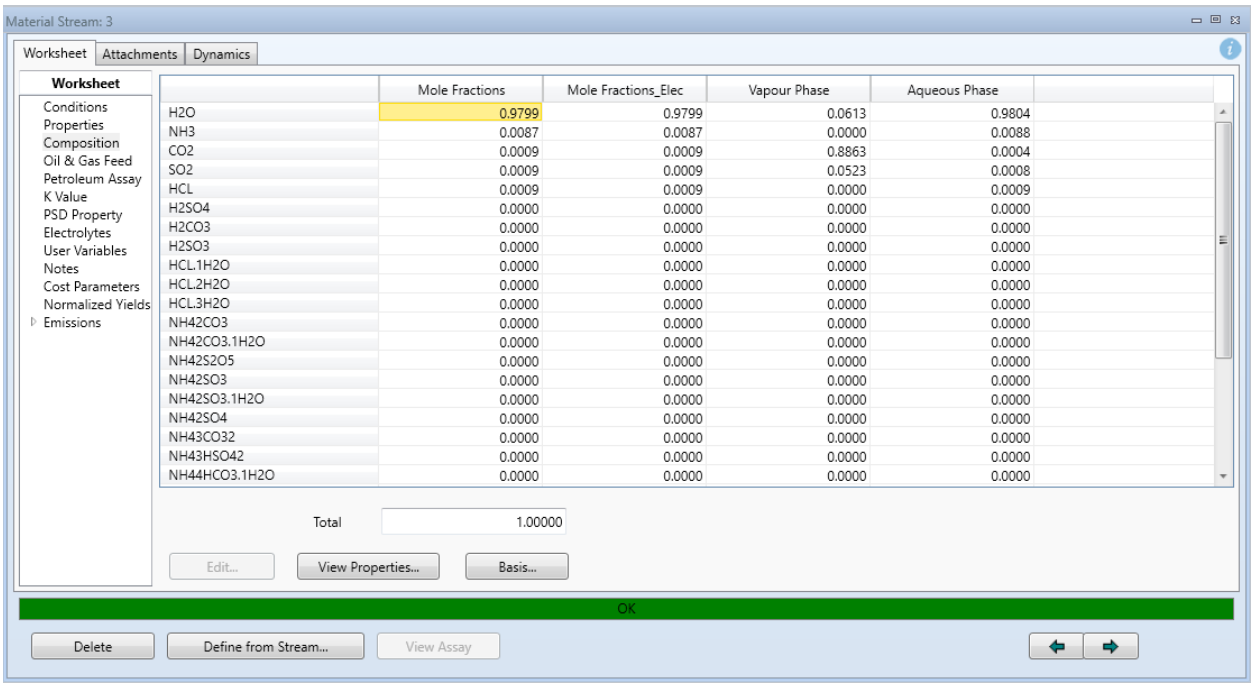


The converged pH is 0.87 indicating that some acid/base chemistry has taken place. What about the equilibrium compositions that have been calculated?

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.



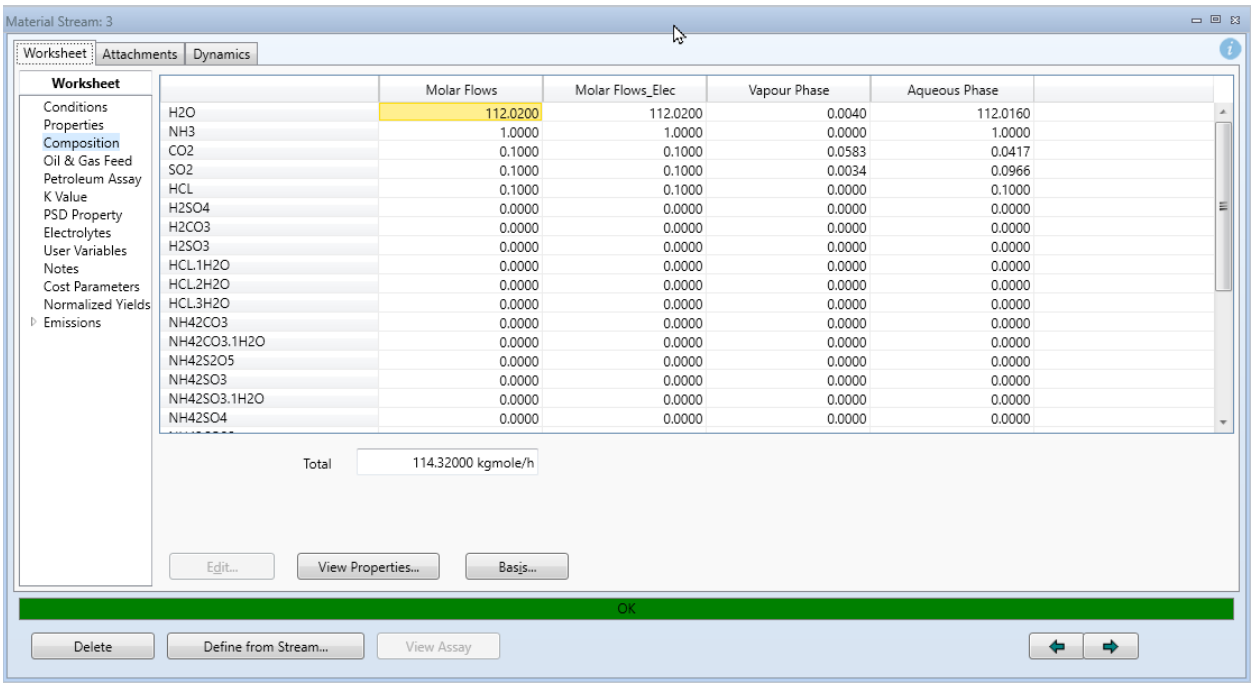
Click on the ***Composition*** line at the left.



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.



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