OLI systems, inc.

INTRODUCTION TO

OLI Engine 12.x for Unisim Design

think simulatio

getting the
chemistry right

Introduction to OLI Engine 12.x for Unisim Design

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OLI Engine 12.x for Unisim Design

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Disclaimer

This manual was produced using the OLI Engine 12.0.0.6 for Unisim Design R500

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 Unisim Design interface greatly enhances Unisim Design's 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 fluid package within Unisim Design This "Getting Started" guide will show you how to create the electrolyte chemistry for a simple case and then create a simple flowsheet in Unisim Design

Assumptions

The following assumptions are made for this guide:

1. Unisim Design is currently installed and running on your computer.
2. The license manager for Unisim Design is currently set up.
3. The OLI Engine for Unisim Design product has been installed.
4. The OLI security model is running.
5. Unisim Design R500 (or later) is being used.
6. The user is expected to know how to use Unisim Design

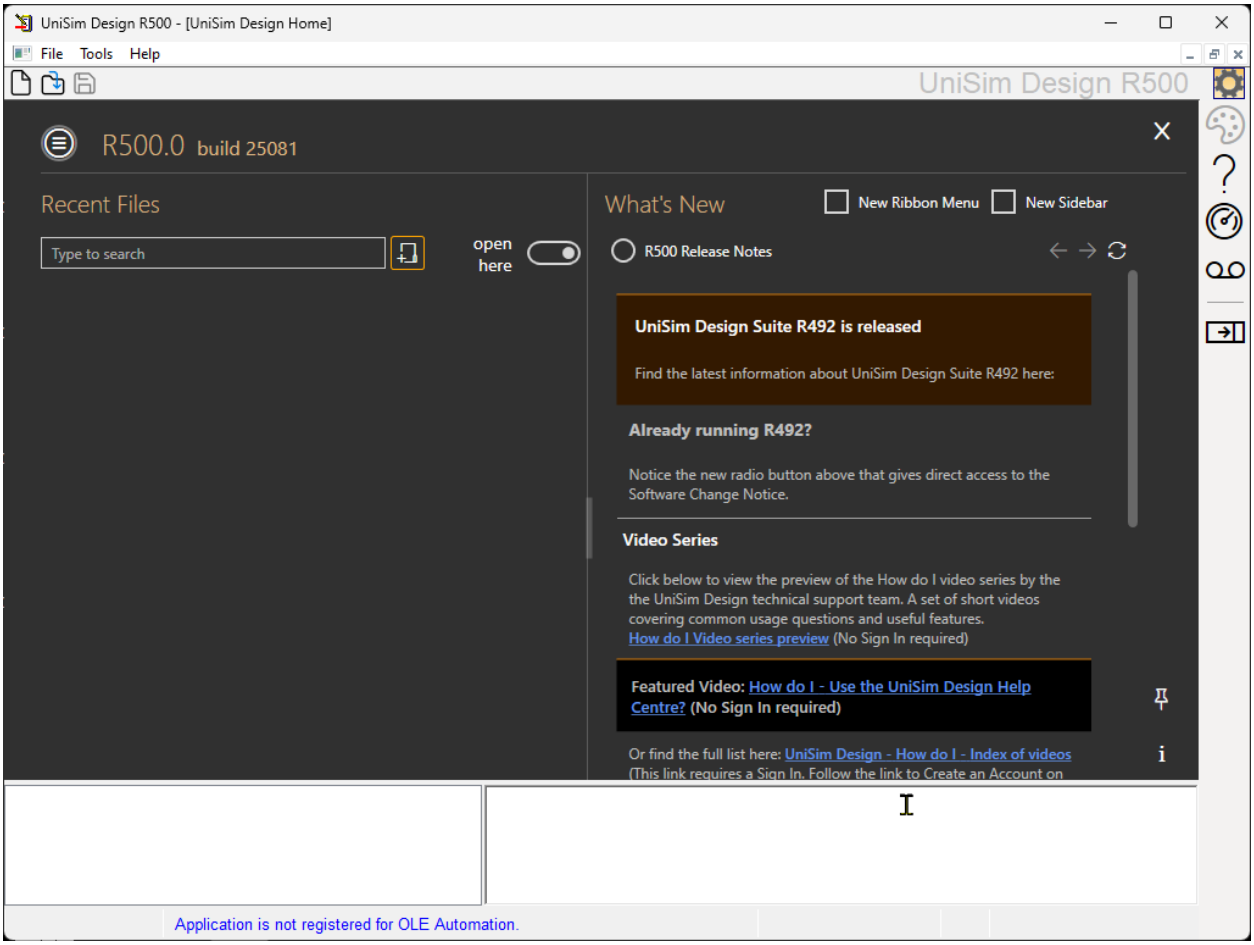
Application

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 Unisim Design

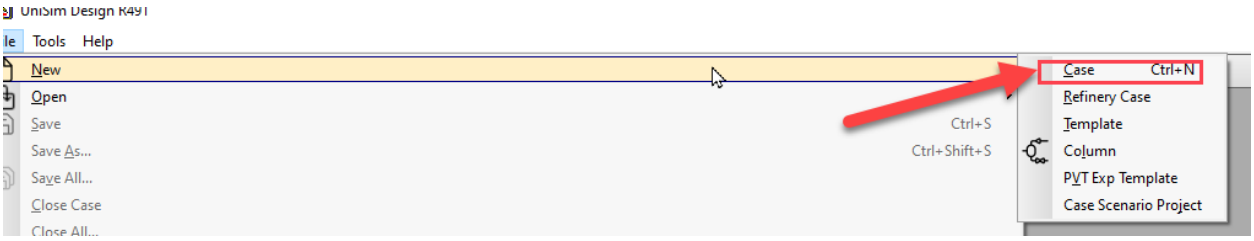
Start Unisim Design in the normal manner. A splash screen will display and then disappear.

This will now display the Unisim Design development environment.

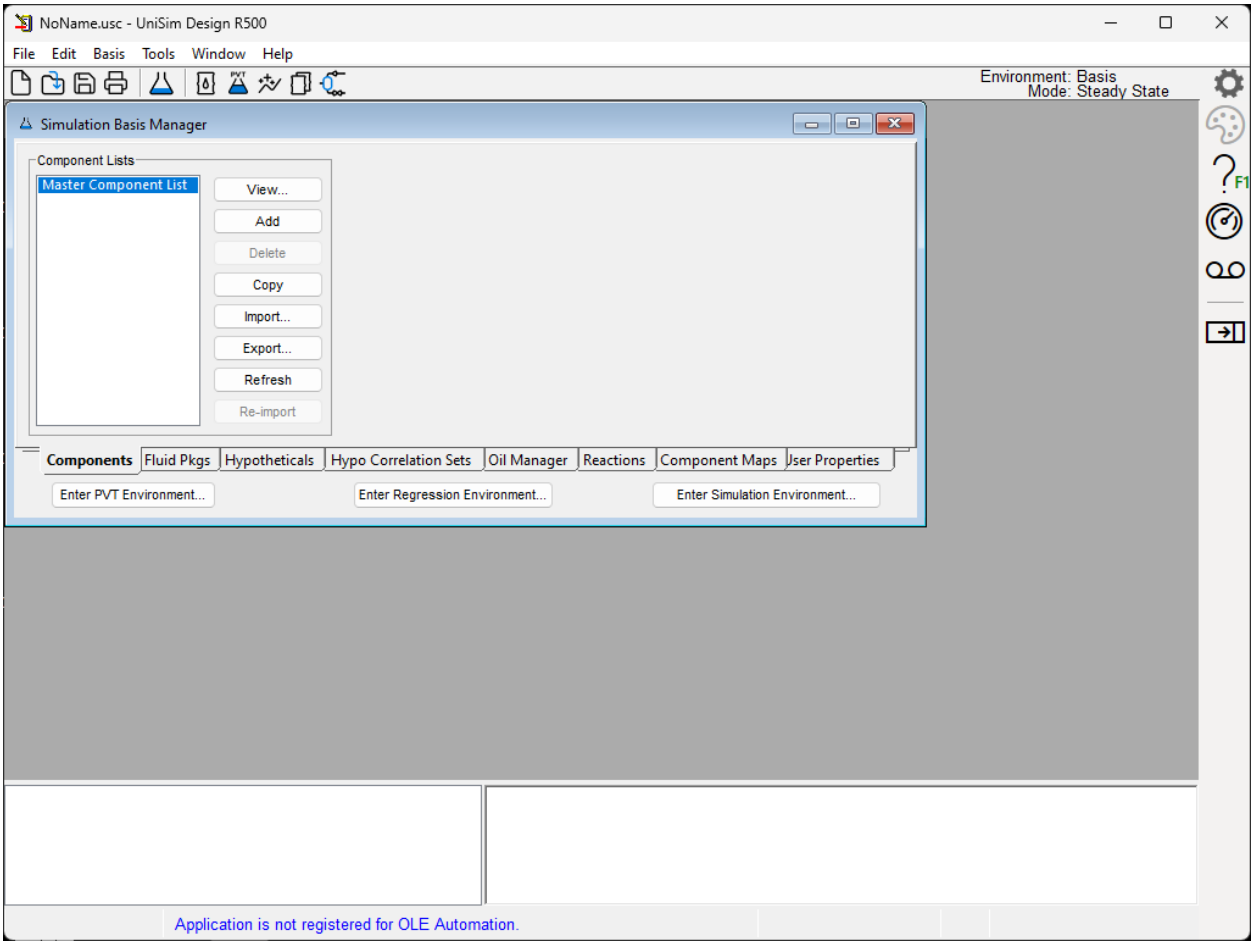


Entering the Chemistry and fluid packages

Select ***File*** | ***New*** | ***Case***



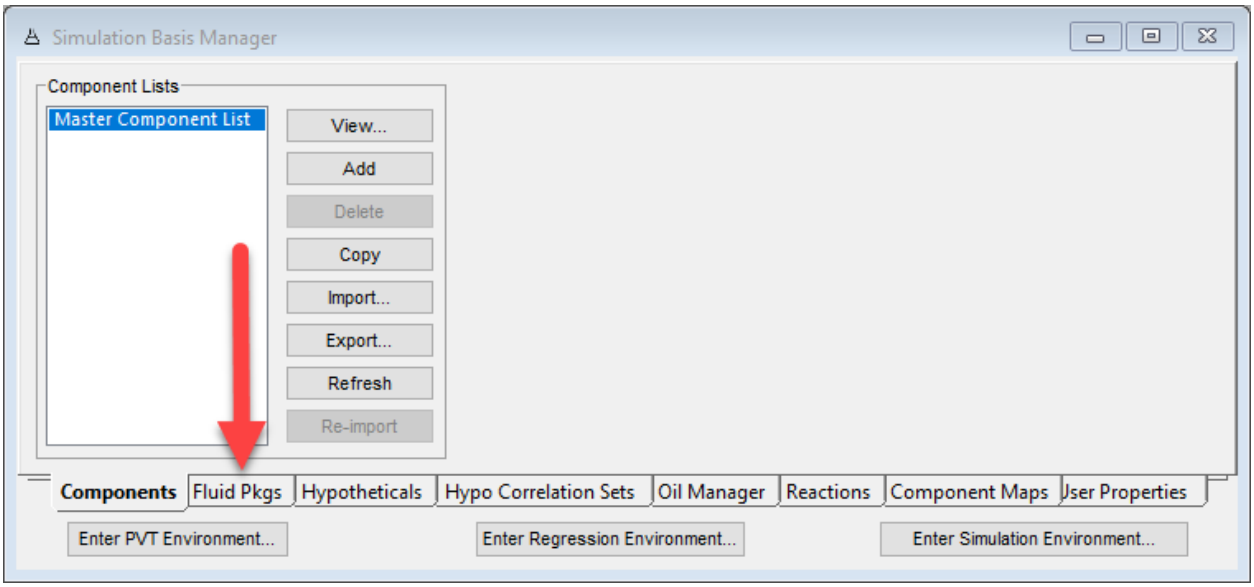
This will bring up the **Simulation Environment**.



Selecting Fluid Packages

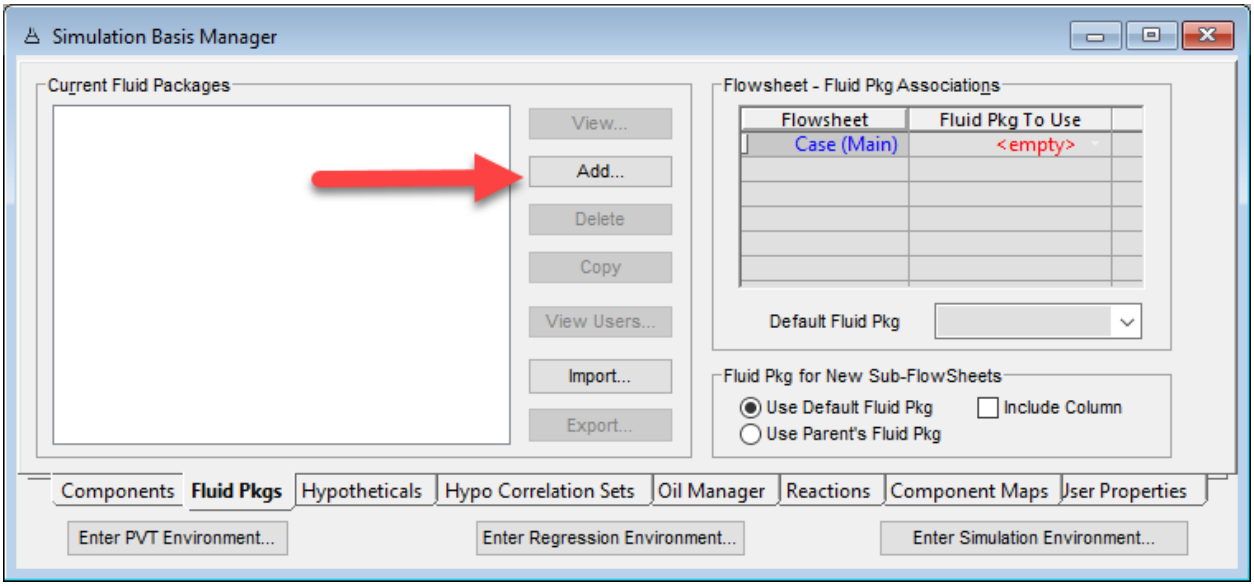
OLI recommends starting with adding a fluid package.

Select *Fluid Packages*

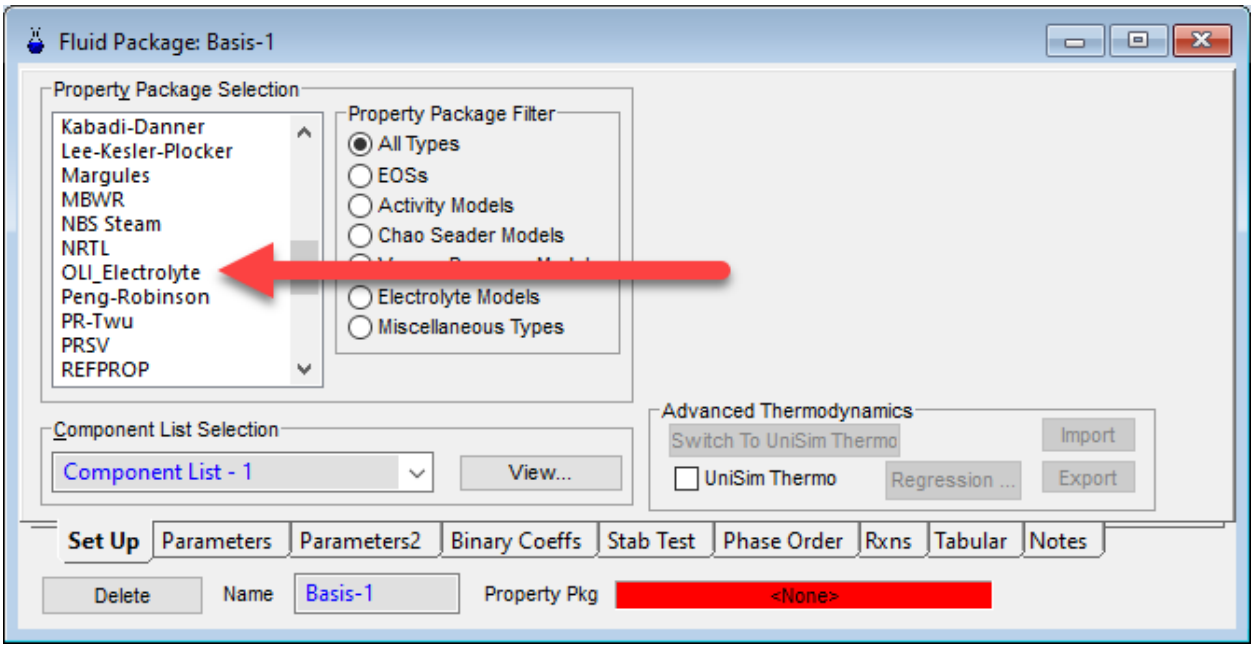


There are no fluid packages currently defined for this simulation. We need to add a package.

Click the ***Add*** button

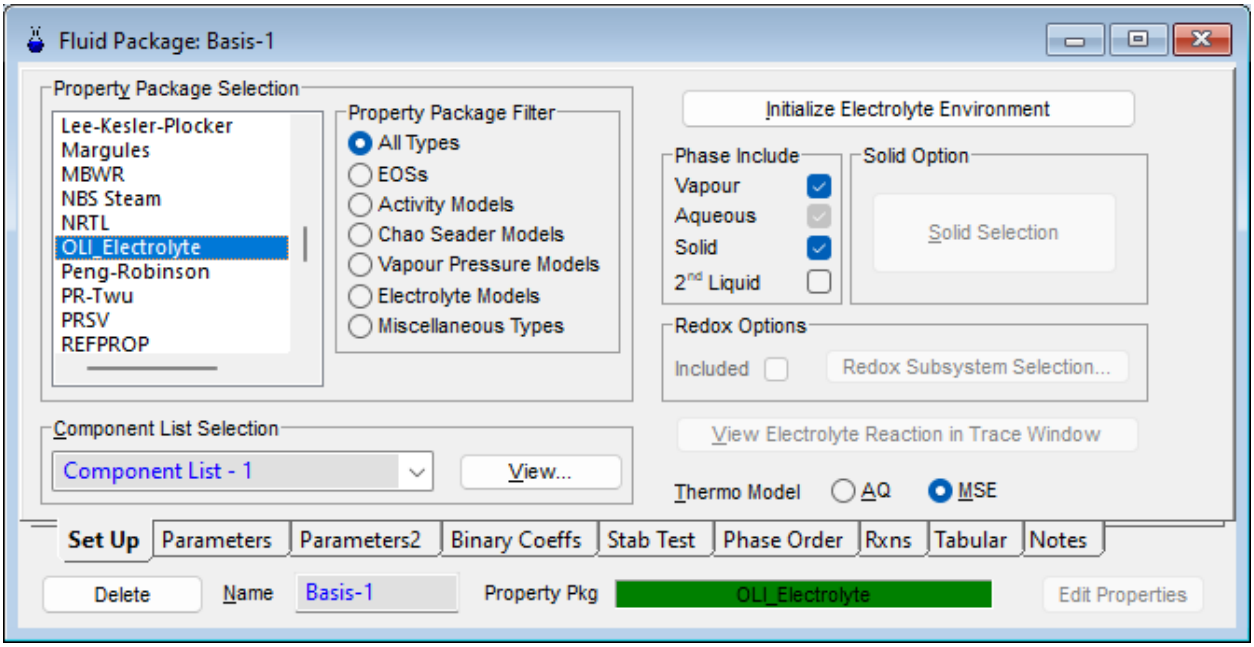


Scroll down the window to find ***OLI_Electrolyte***



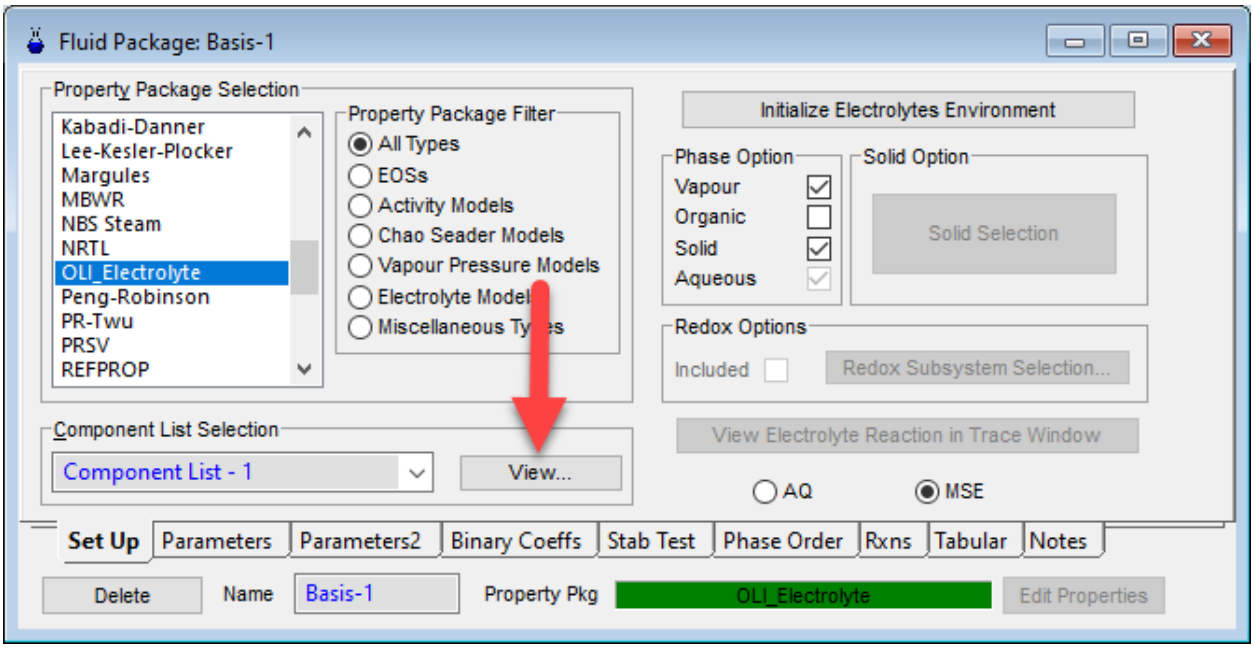
Highlight the object ***OLI_Electrolyte.***

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.**

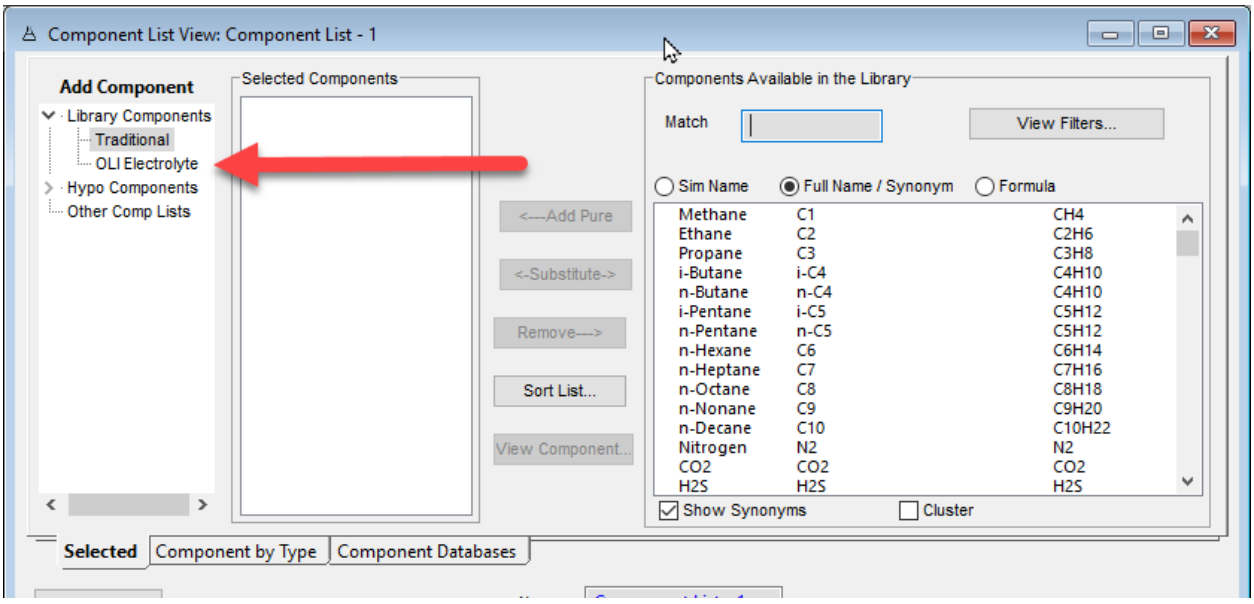


For this example, we will use the MSE thermodynamic framework.

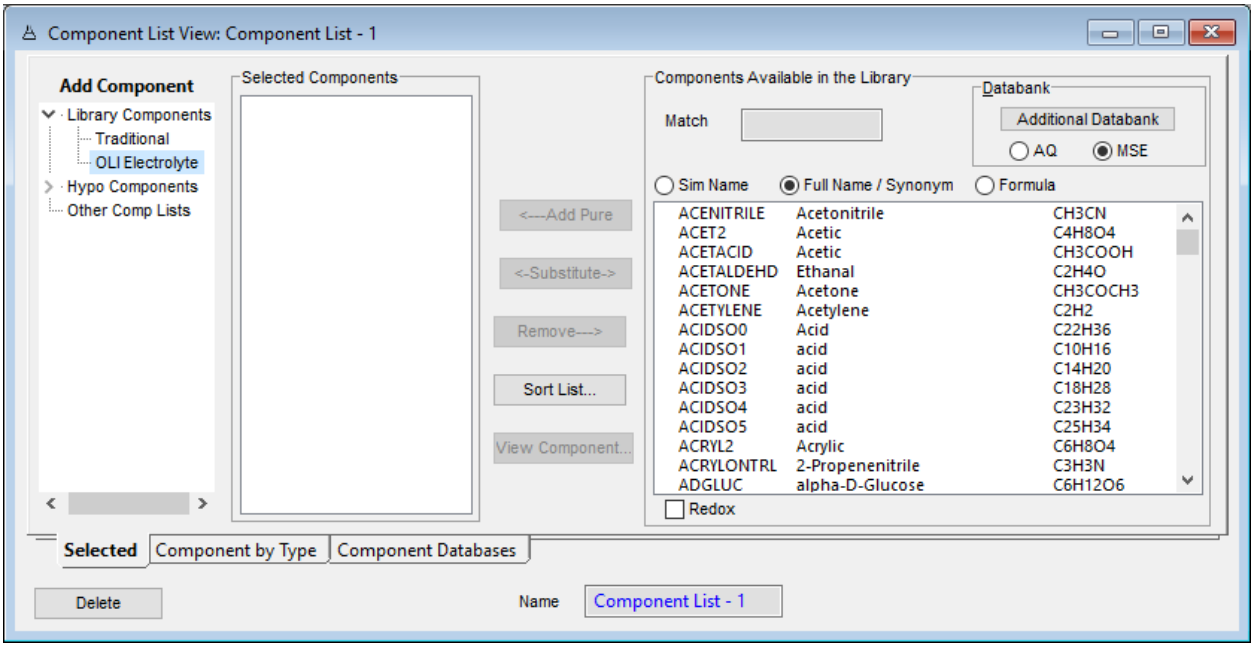
There are numerous methods to enter components for the simulation. For OLI, we recommend clicking the **View** button.



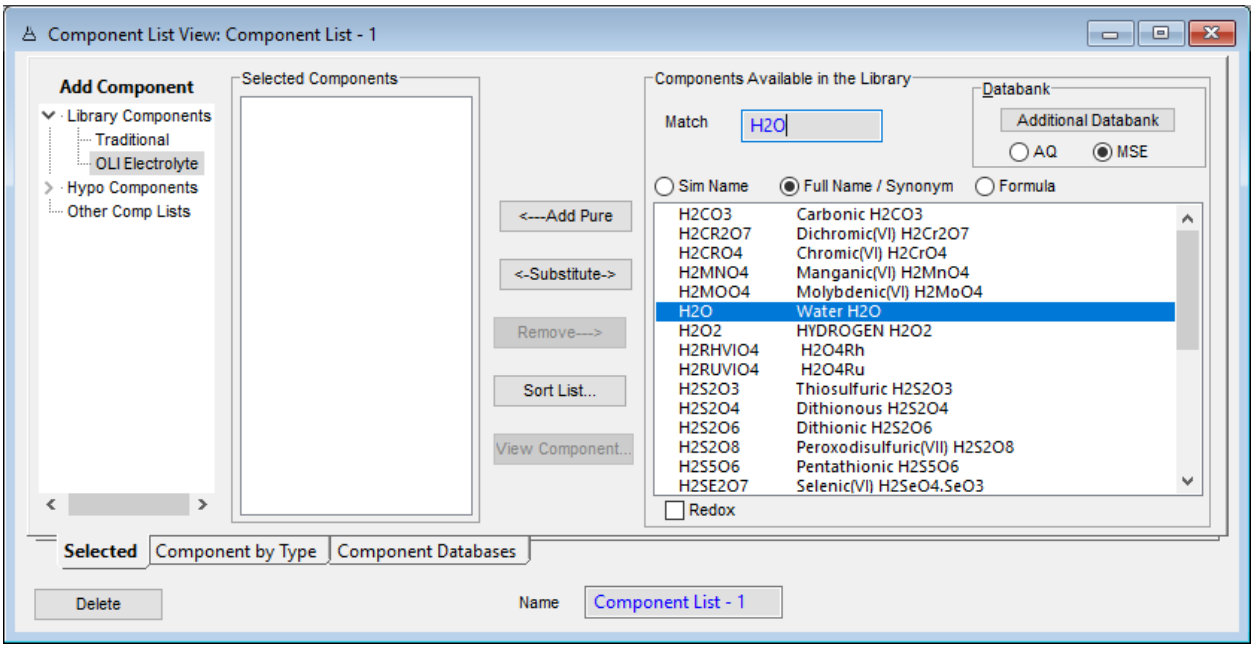
This will bring up the component list.



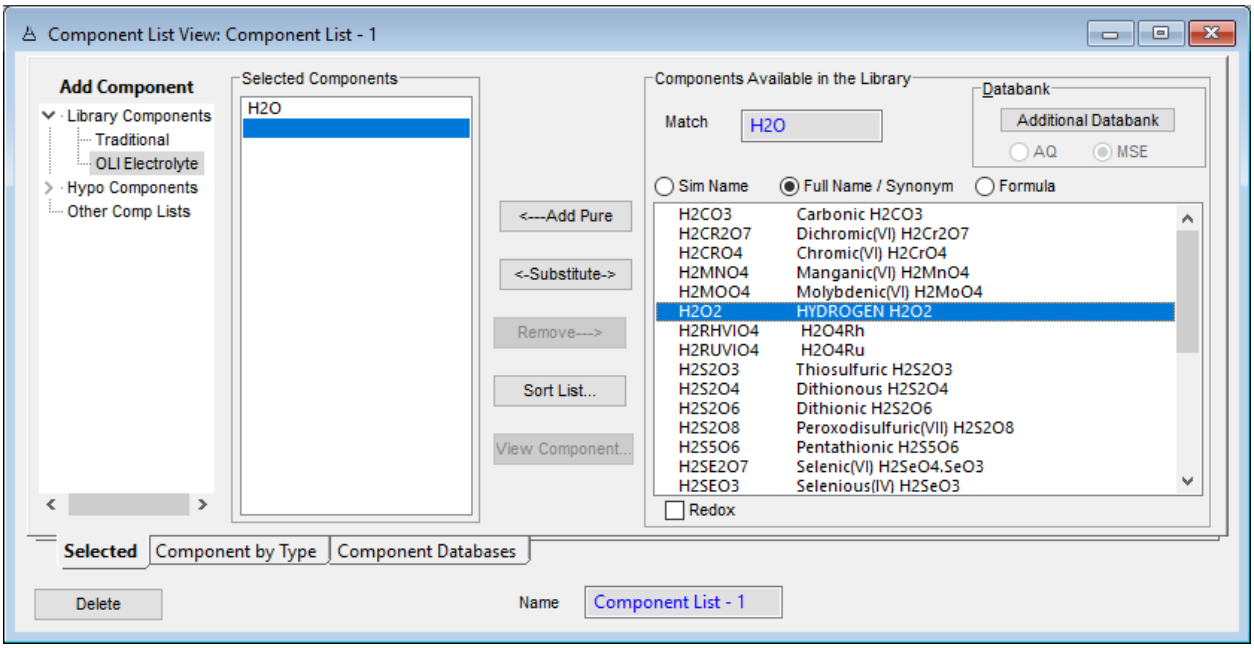
You have two types of components to choose from. The default is the ***Traditional*** Unisim Design components. However, these components are not suitable for electrolyte calculations. Please select ***OLI Electrolyte***.



For OLI electrolyte calculations, OLI recommends that the first component you enter is H2O (water). Note, that the names in this list are often referred to as the OLI Tag name.



You can either double-click the highlighted name or use the **Add Pure** button.



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

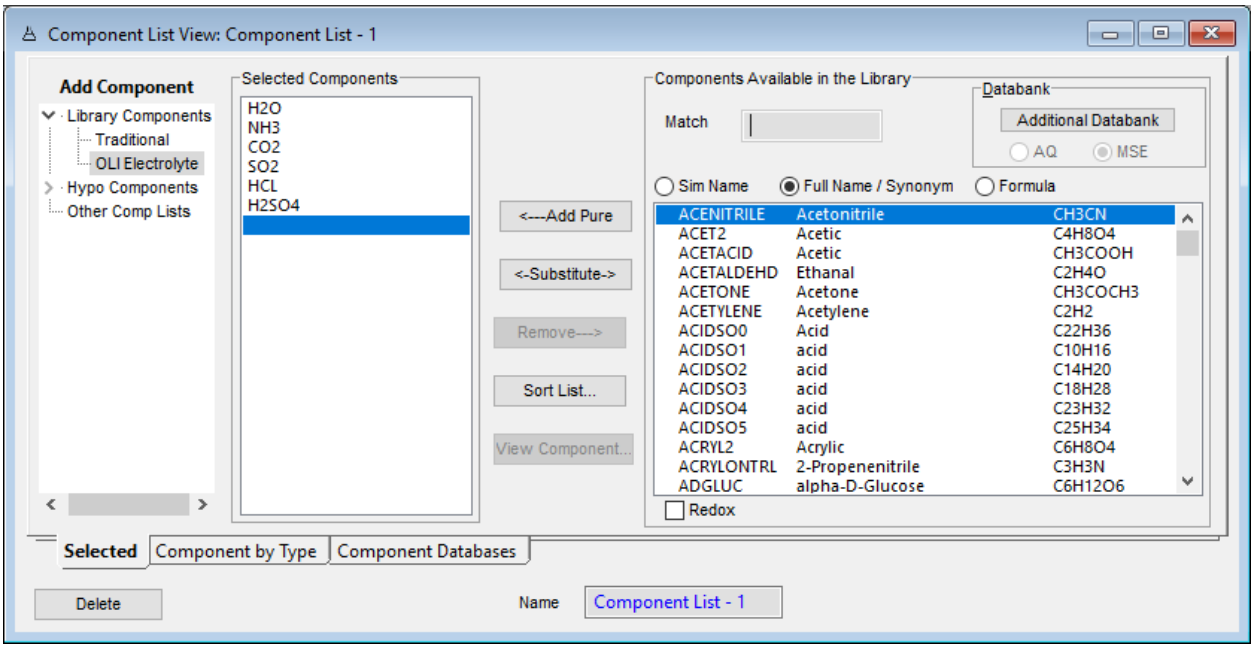
Entering Components

We will now add the remaining components for this example

Using the same procedure, add the following components.

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

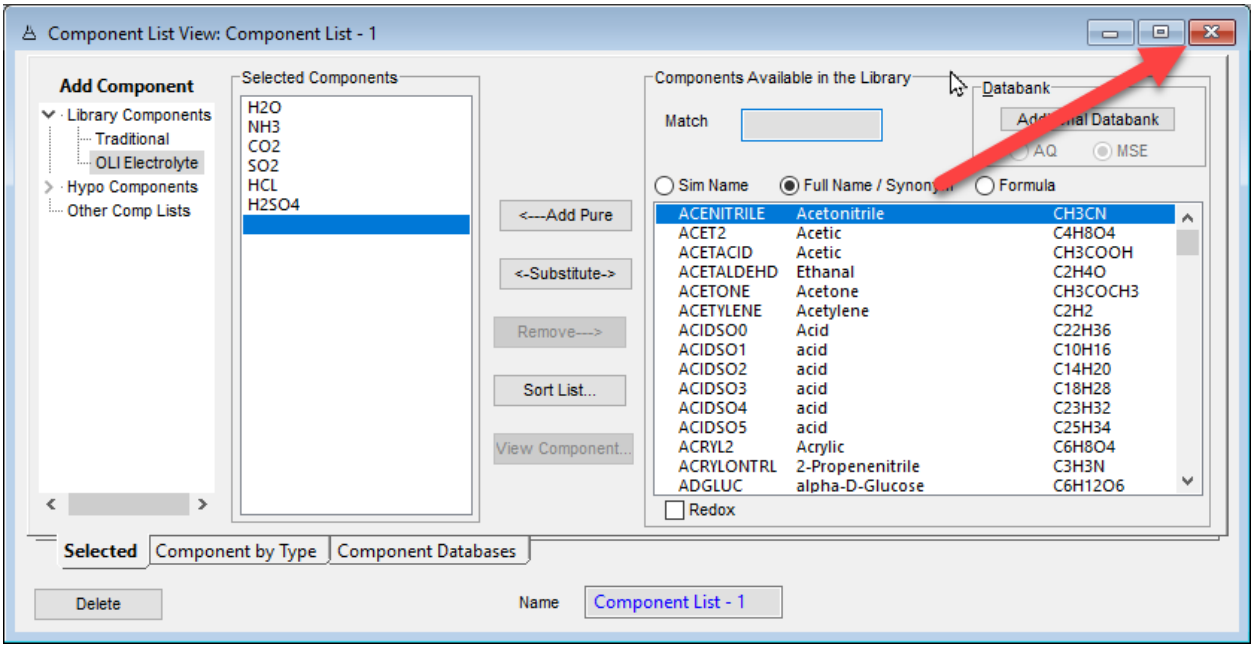
The input should look like this:



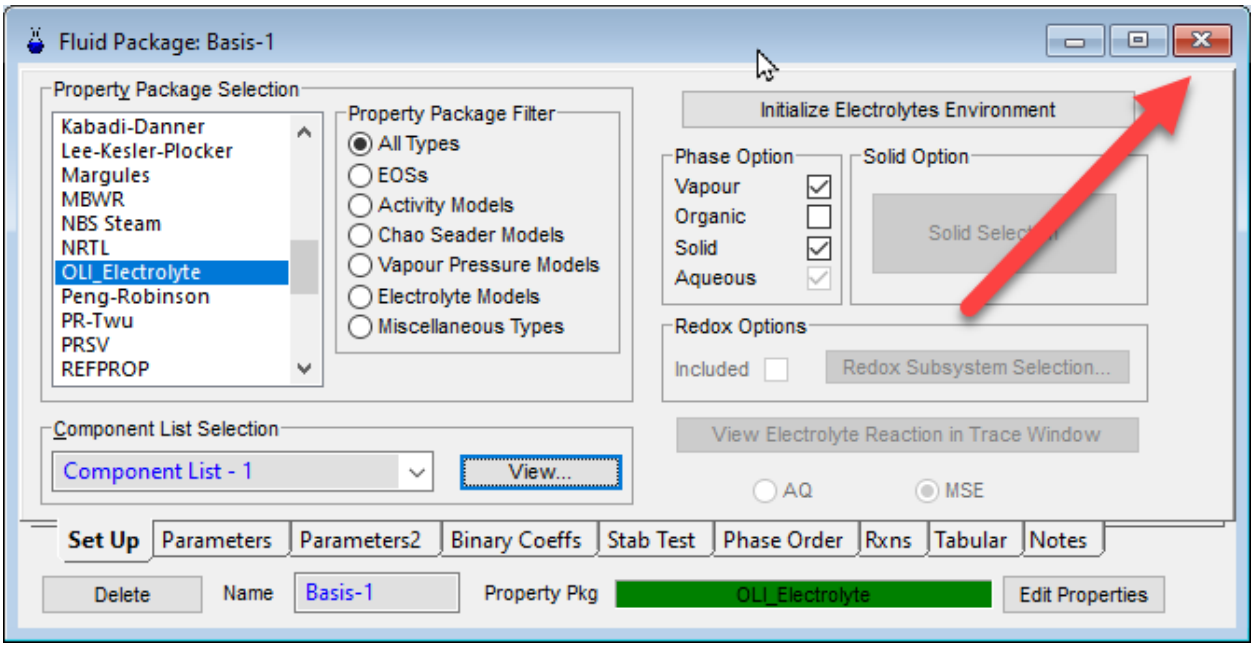
The component selection has been completed. We are now ready to start building our process.

Creating the Simulation

Click the “X” to close the component selection.

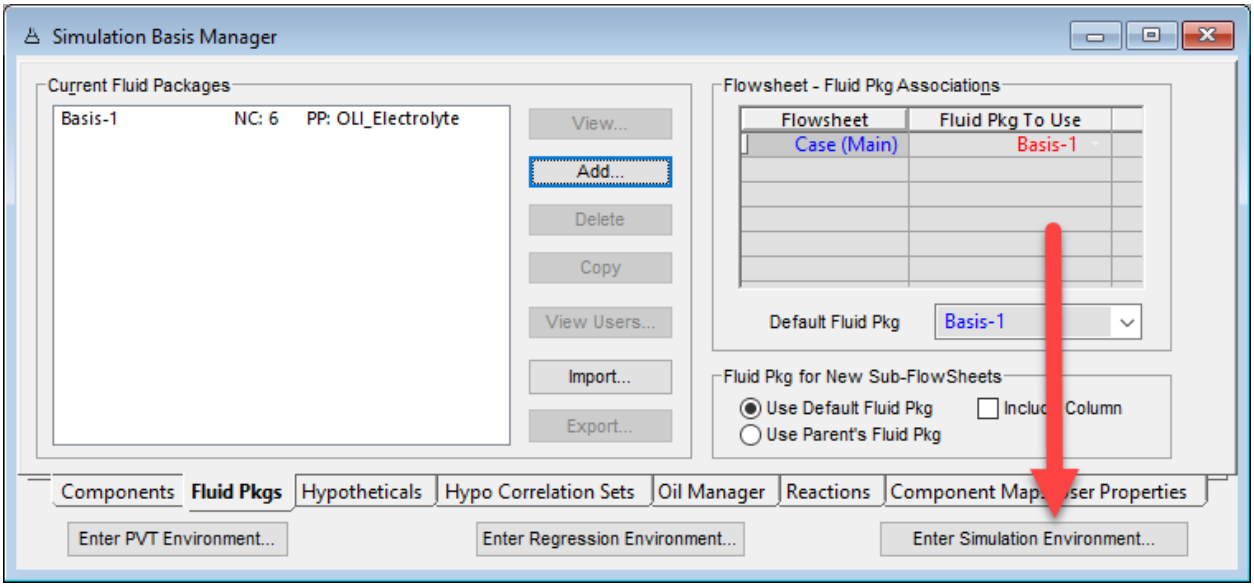


This brings you back to the fluid package page.



If you need to modify the chemistry, particularly solid phase selections, you will need to click the

Initialize Electrolytes Environment button. For this example, we do not need to do this. Once again, click the "X" in the upper right-hand corner.



This brings us back to the Simulation Basis Manager dialog. For this example, please click the

Enter Simulation Environment button

Several things will occur. The most important action is that the internal OLI Chemistry Model is created in memory and can now be used.

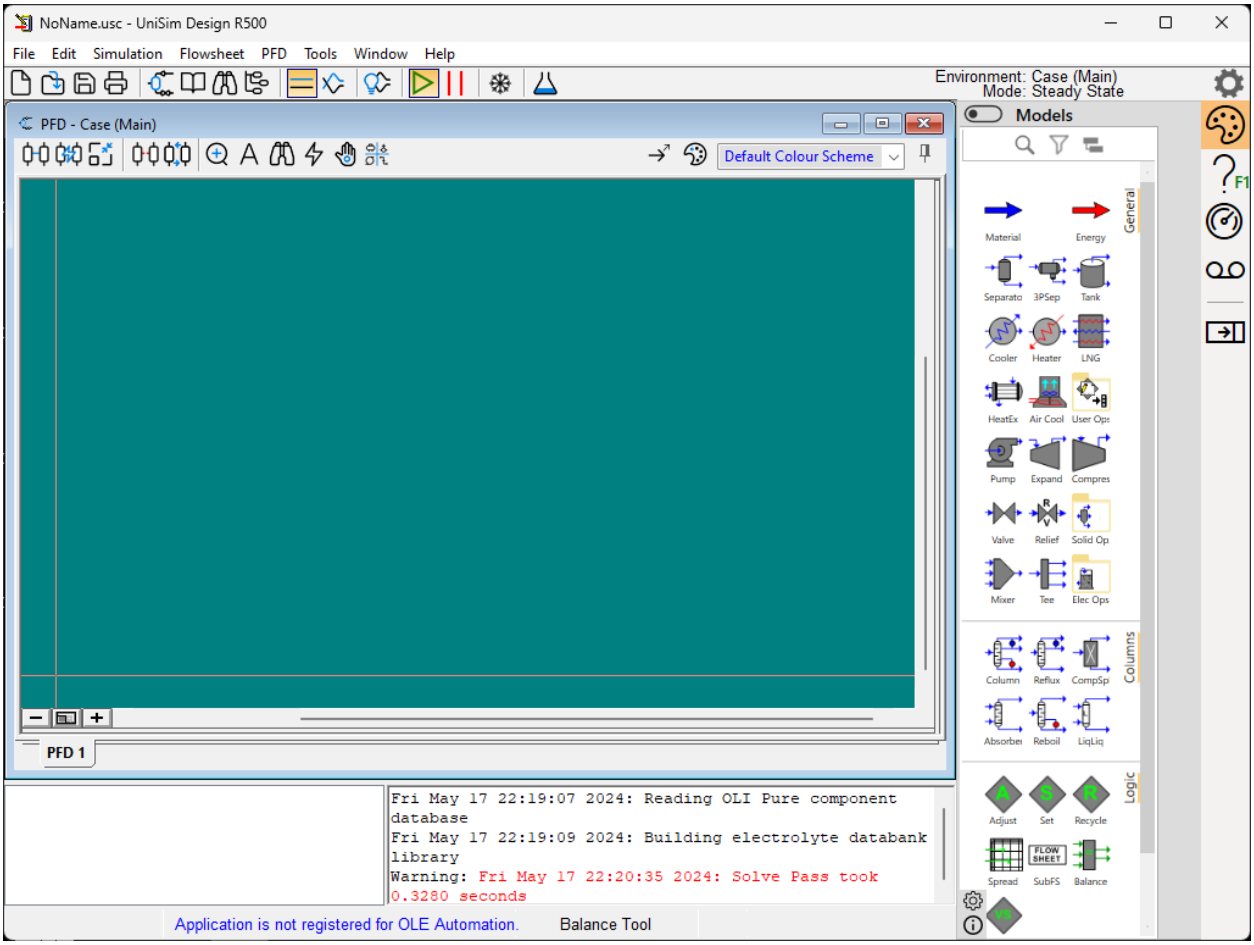
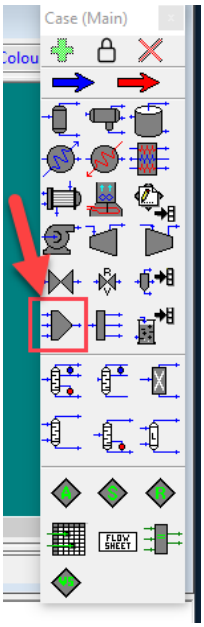


Figure 1. Simulation window (move the palate if it is obscuring the window)

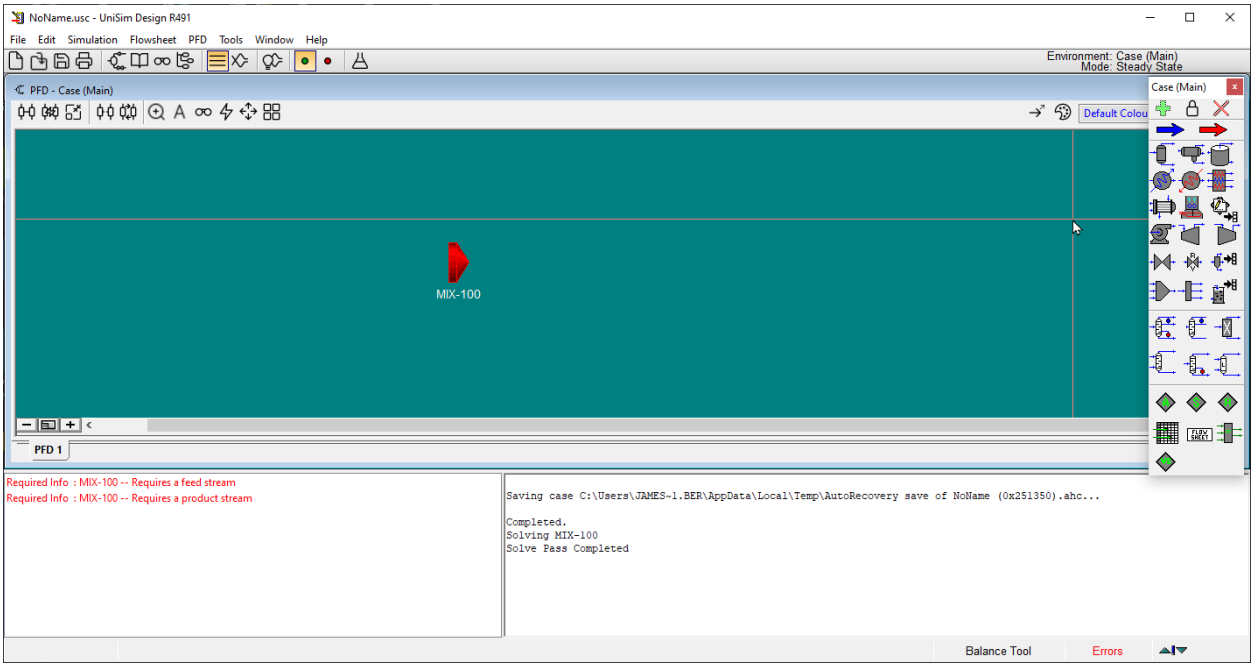
We will now create a small process using a mixer with two inlet streams. The user is expected to know how to create the process. Please do not enter any conditions for the inlet streams currently.

Selecting the mixer

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


Case (Main)
FLOW SHEET

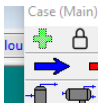
The workspace now looks like this:



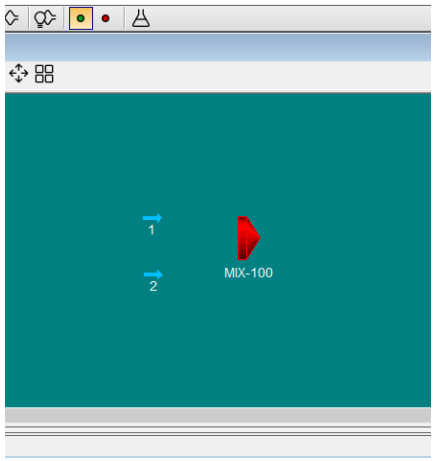
The mixer is given a default name of MIX-100. You can change it later if you wish. The block is also colored RED. This indicates that the block does not have sufficient information to calculate.

We need to create two inlet streams.

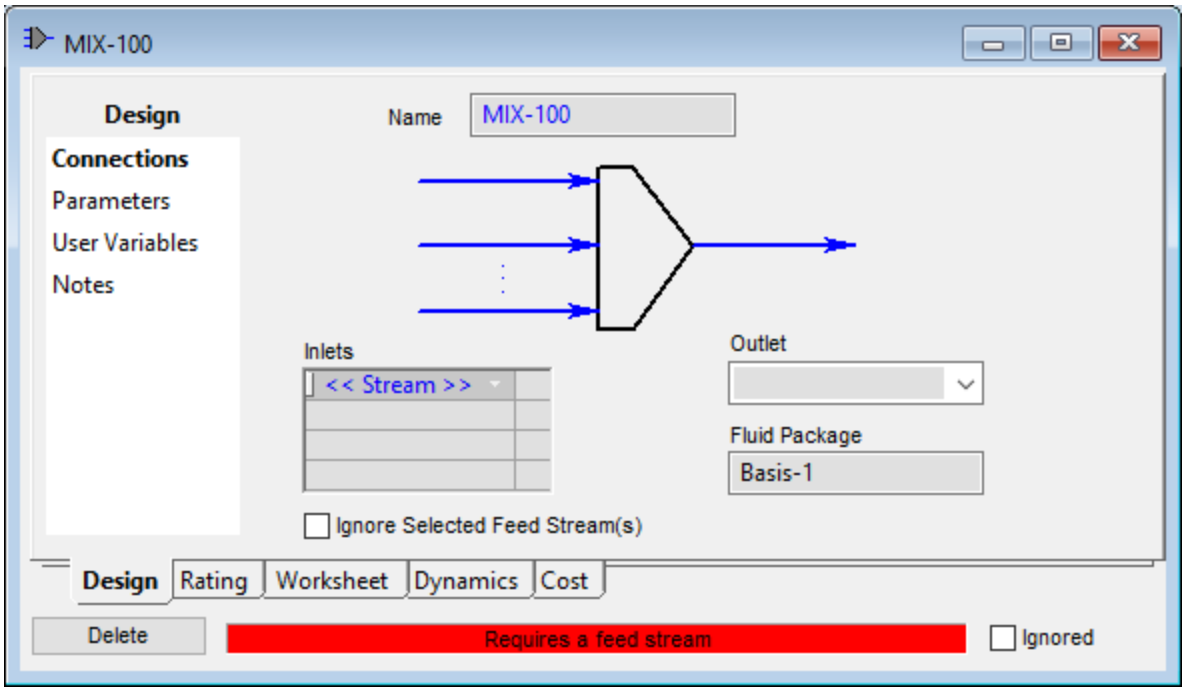
Click on the **Material Streams** arrows and place them on the workspace.



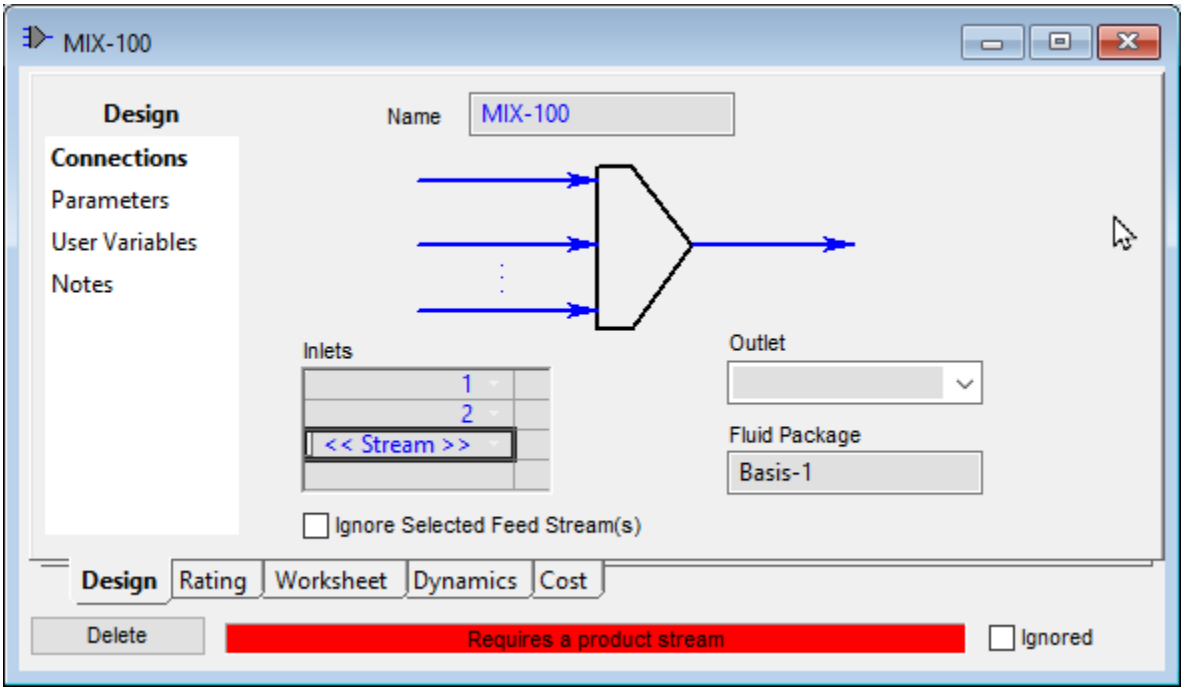
The material streams arrows are colored blue. Place two (2) material streams arrows on the workspace.



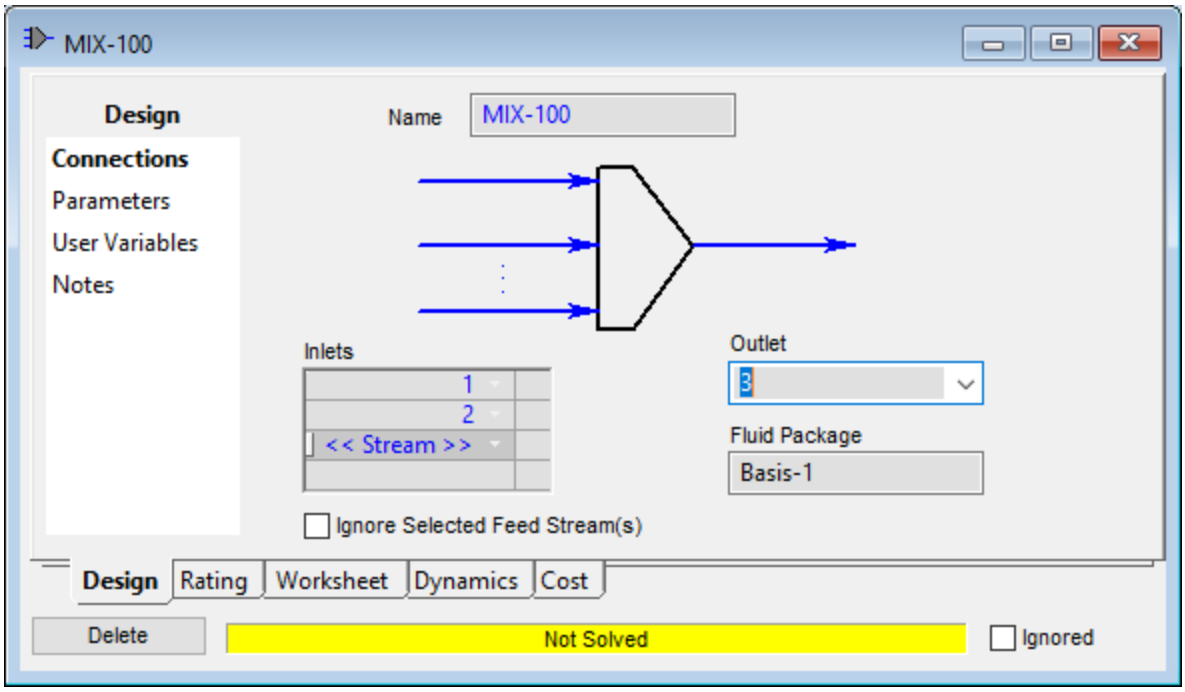
Double-Click the Mixer Block. This will open another window.



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



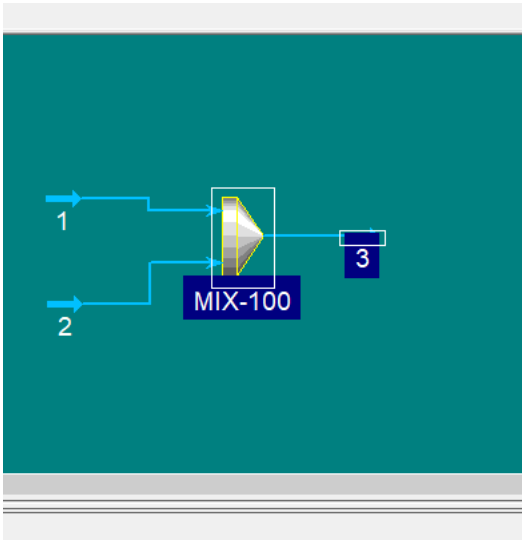
Locate the ***Outlet*** box and enter the number “**3**”. This completes this block.



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

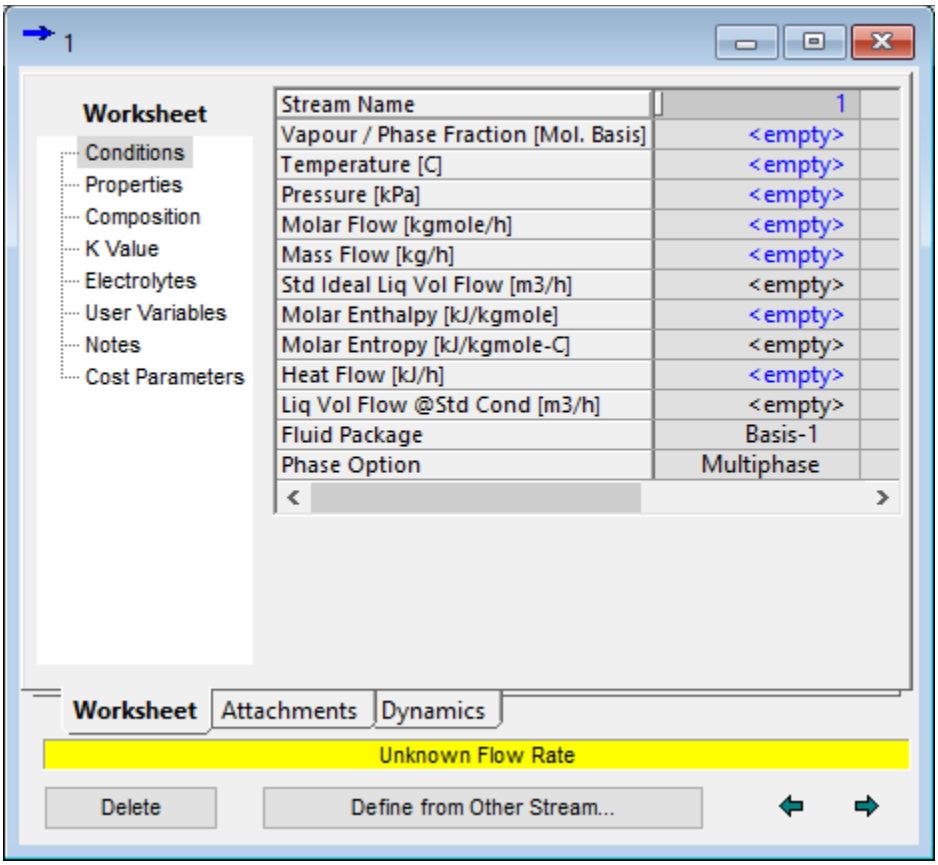
Click the ***x*** in the upper right-hand corner to close this dialog.

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



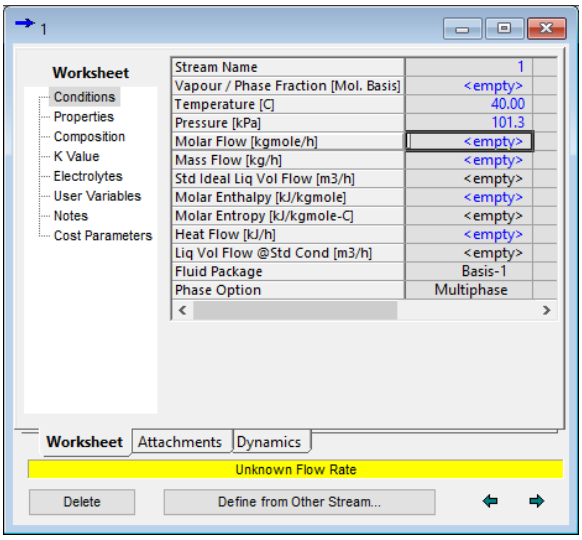
Entering Stream Composition Data

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

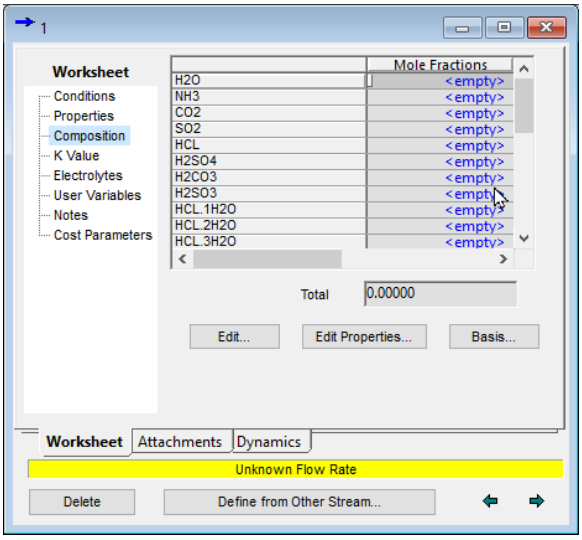


This is the standard input window for a stream. We will now add our conditions.

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



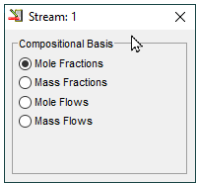
Now click the ***Composition*** line



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

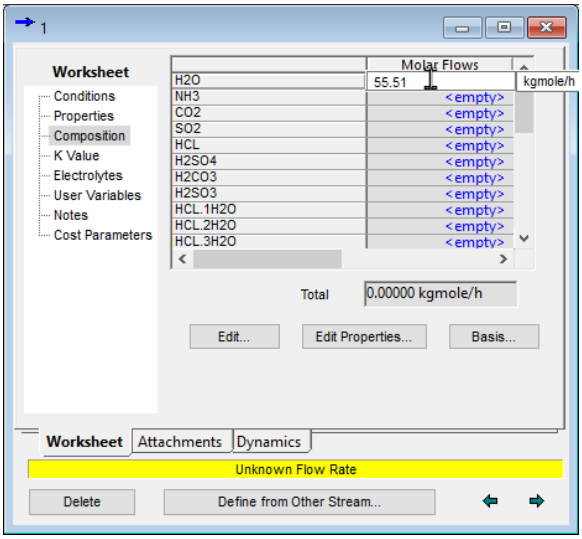
Click the ***Basis…*** button

This will open a new window

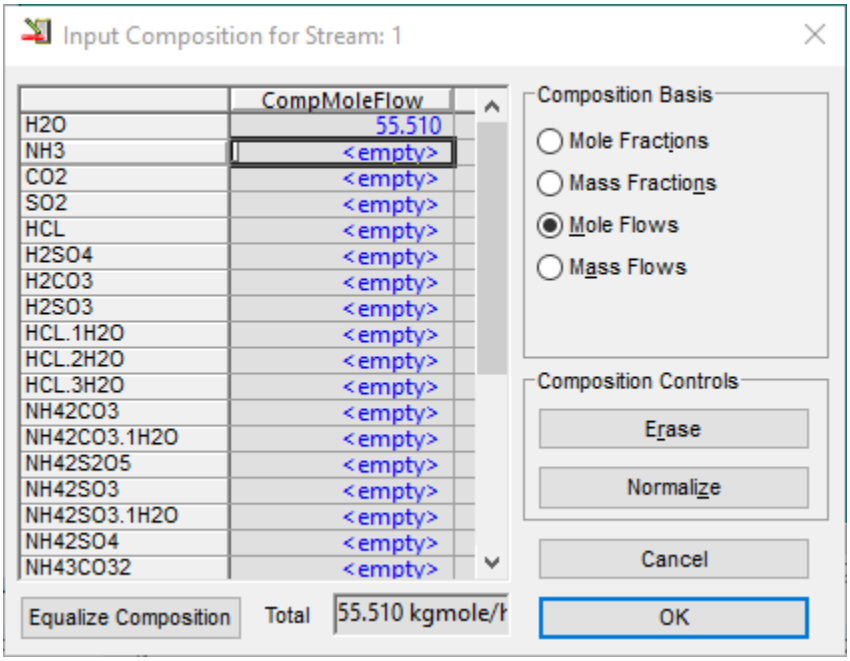


Select the *Mole Flows* radio button. Click the ***x*** when done.

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



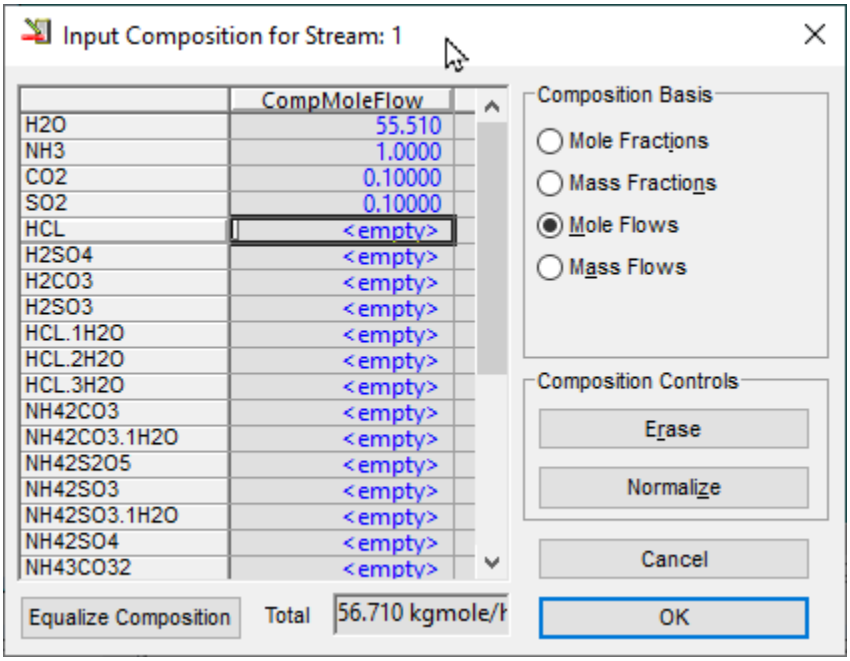
Once you hit enter it will prompt you to a new window to finish entering the composition of the stream.



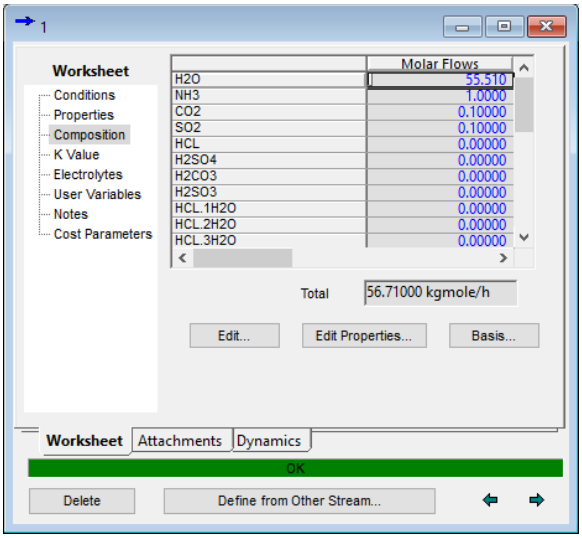
This will display the composition data entry dialog. Complete the following data entry in mole flow units:

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

The remaining values can be zero.

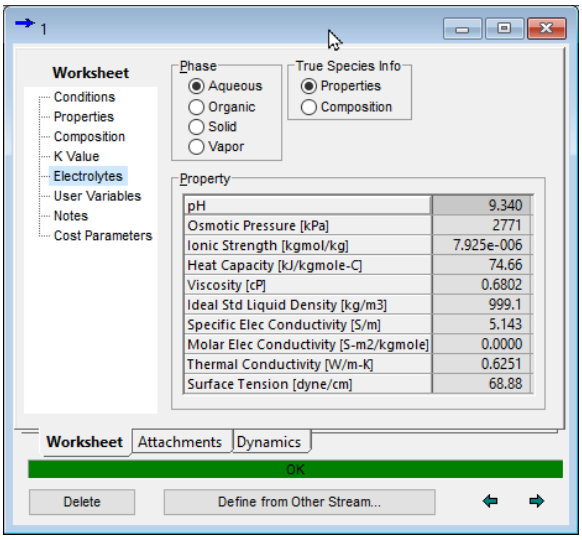


Click the ***OK*** button.



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.

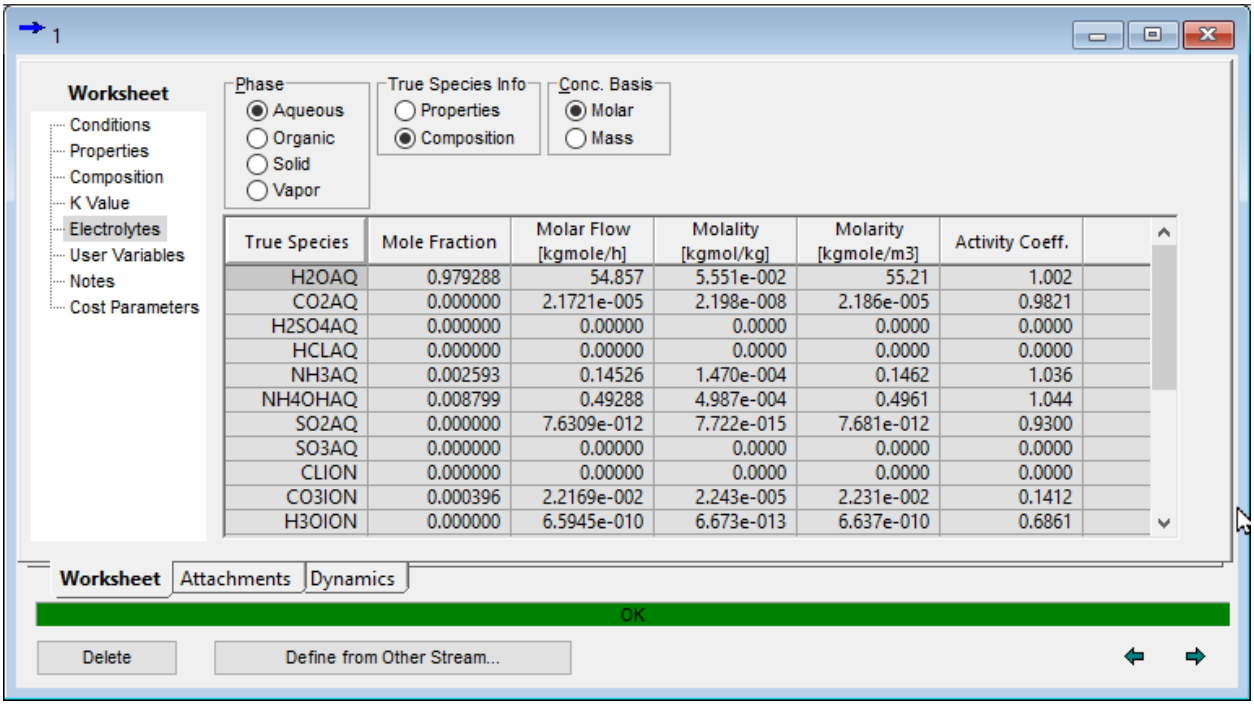


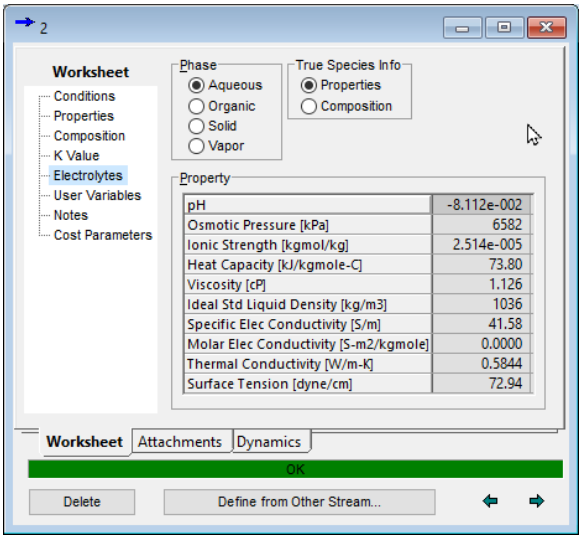
Figure 2 Notice that we have dragged the width of the dialog to the right.

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.

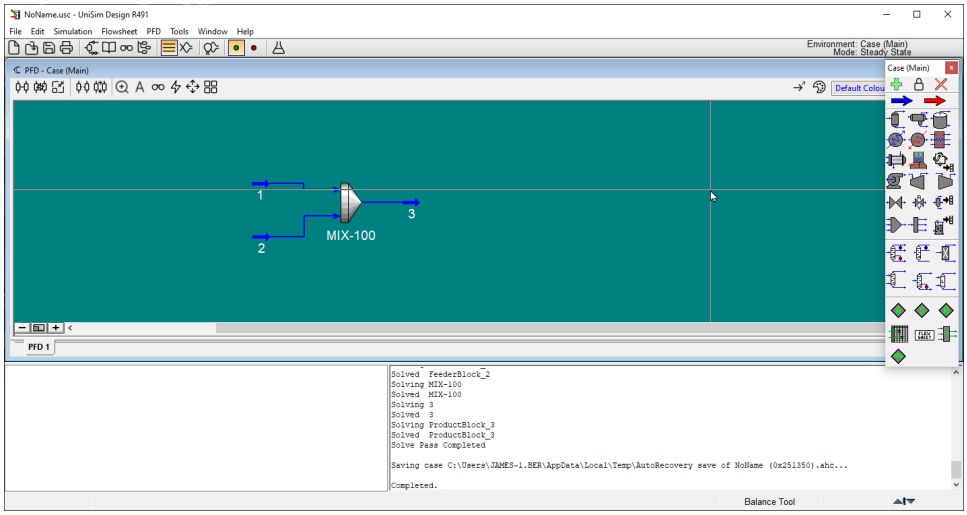
Temperature	25	C
Pressure	101.3	kPa
H2O	55.51	
HCl	0.1	
H2SO4	1.0	

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



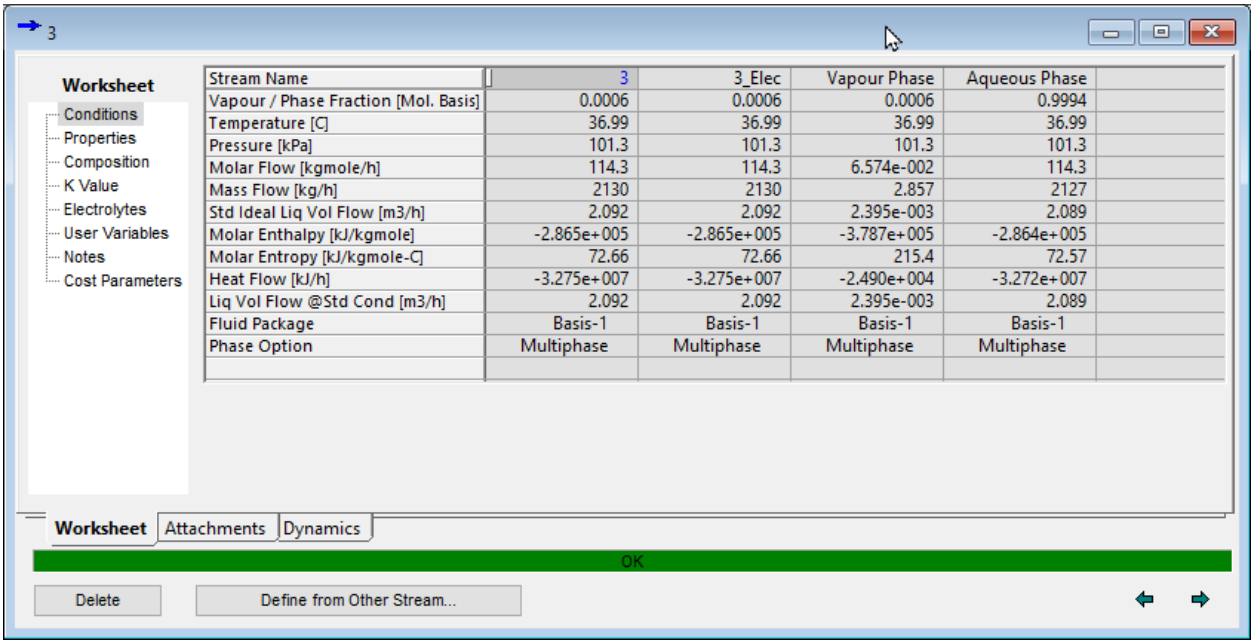
Click the ***x*** to close the dialog.

Unisim Design 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

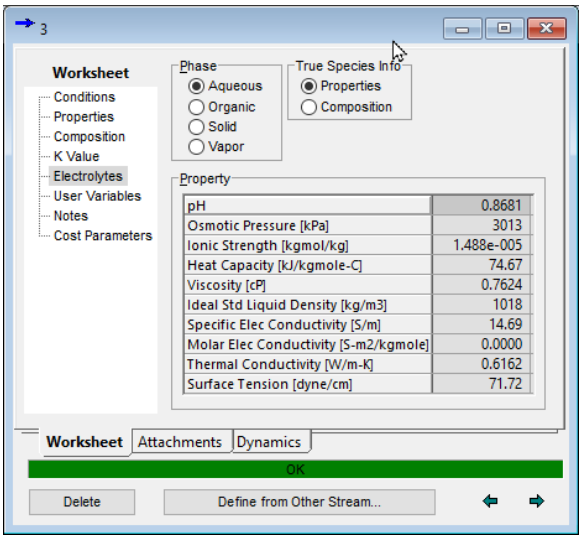
Double-Click stream “3”



Stream Name	3	3_Elec	Vapour Phase	Aqueous Phase
Vapour / Phase Fraction [Mol. Basis]	0.0006	0.0006	0.0006	0.9994
Temperature [C]	36.99	36.99	36.99	36.99
Pressure [kPa]	101.3	101.3	101.3	101.3
Molar Flow [kgmole/h]	114.3	114.3	6.574e-002	114.3
Mass Flow [kg/h]	2130	2130	2.857	2127
Std Ideal Liq Vol Flow [m3/h]	2.092	2.092	2.395e-003	2.089
Molar Enthalpy [kJ/kgmole]	-2.865e+005	-2.865e+005	-3.787e+005	-2.864e+005
Molar Entropy [kJ/kgmole-C]	72.66	72.66	215.4	72.57
Heat Flow [kJ/h]	-3.275e+007	-3.275e+007	-2.490e+004	-3.272e+007
Liq Vol Flow @Std Cond [m3/h]	2.092	2.092	2.395e-003	2.089
Fluid Package	Basis-1	Basis-1	Basis-1	Basis-1
Phase Option	Multiphase	Multiphase	Multiphase	Multiphase

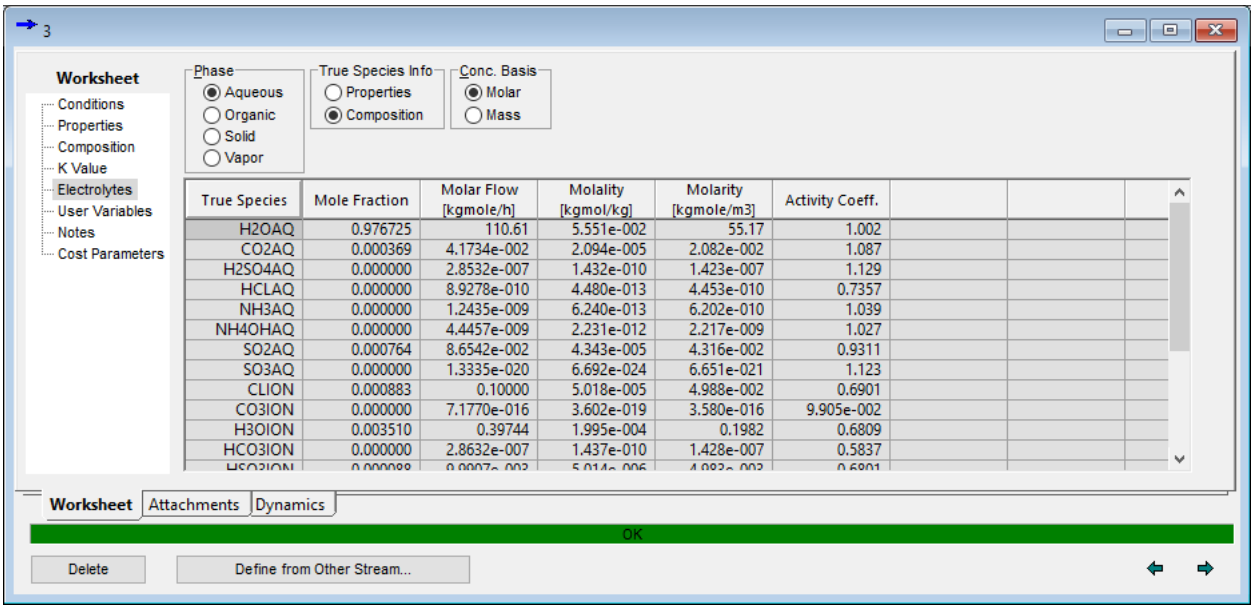
The converged process temperature is approximately 37.0 ºC.

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

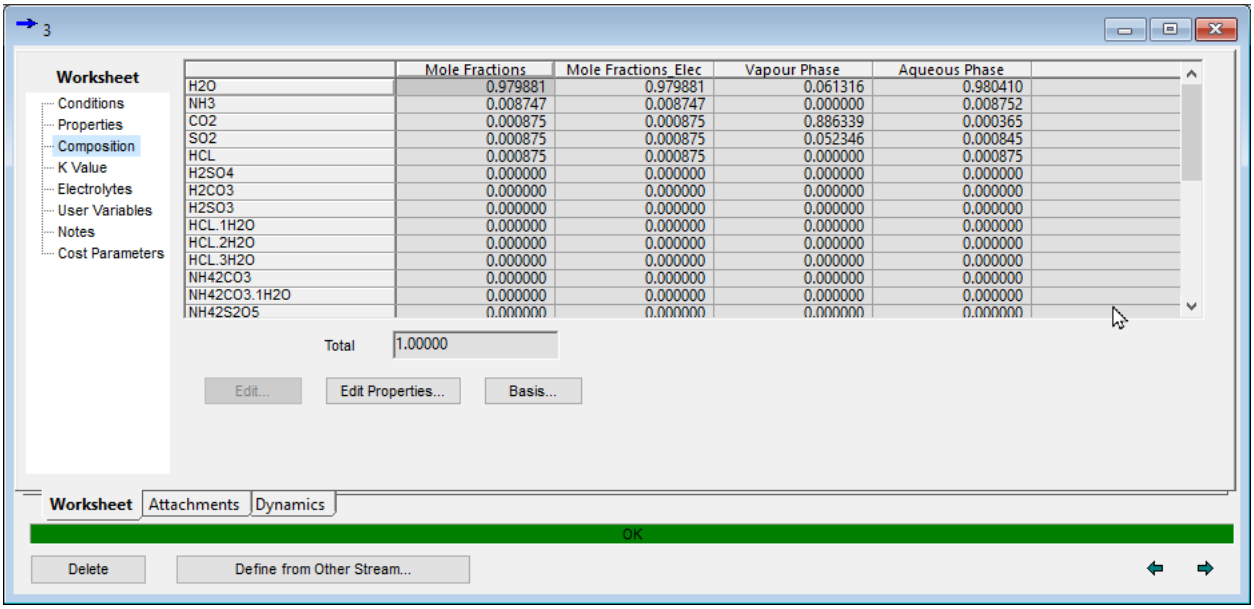


The converged pH is 0.87 indicating that some acid/base chemistry has taken place. What about the equilibrium compositions that have been calculated?

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.



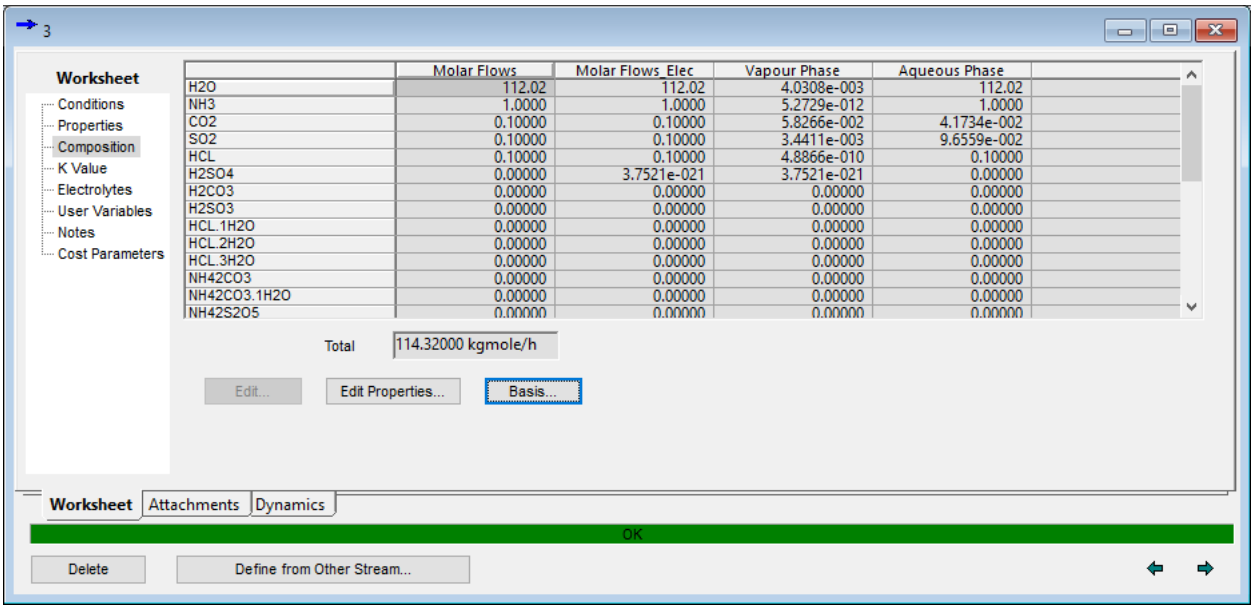
Click on the ***Composition*** line at the left.



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.