Using two fluid packages in Aspen HYSYS 7.3 using OLI

Overview

There are many times when a user wishes to use a traditional fluid package (such and Peng-Robinson) in one part of the HYSYS flowsheet and then to use the OLI fluid package in another part of the flowsheet. The user may not care to use the rigorous electrolytes (and the potentially large computational overhead) in all of the flowsheet but needs the rigor in only a portion. There are two major issues when attempting to do this in HYSYS.

The first issue is that HYSYS permits only one fluid package per flowsheet section. If you need to use a second fluid package, you must create a sub-flowsheet. The second issue is that the component names between fluid packages may not be the same.

In this example we are going to use the Peng-Robinson fluid package in the main flowsheet and the OLI Fluid package in a sub-flowsheet. The following table illustrates the component name differences between the Peng-Robinson (hereafter referred to as "PR") and the OLI fluid package that we are using in our example.

Component	Peng Robinson Name	OLI Name
Hydrogen	Hydrogen	H2
Nitrogen	Nitrogen	N2
Carbon Monoxide	CO	CO
Argon	Argon	Ar
Oxygen	Oxygen	O2
Methane	Methane	CH4
Carbon Dioxide	CO2	CO2
Carbonyl Sulfide	COS	COS
Ammonia	Ammonia	NH3
Hydrogen Cyanide	HCN	HCN
Water	H2O	H2O

As you can see the naming system is not consistent between the two fluid packages. In fact, HYSYS considers the species to be completely different even if the names are the same (e.g., H2O).

Assumptions

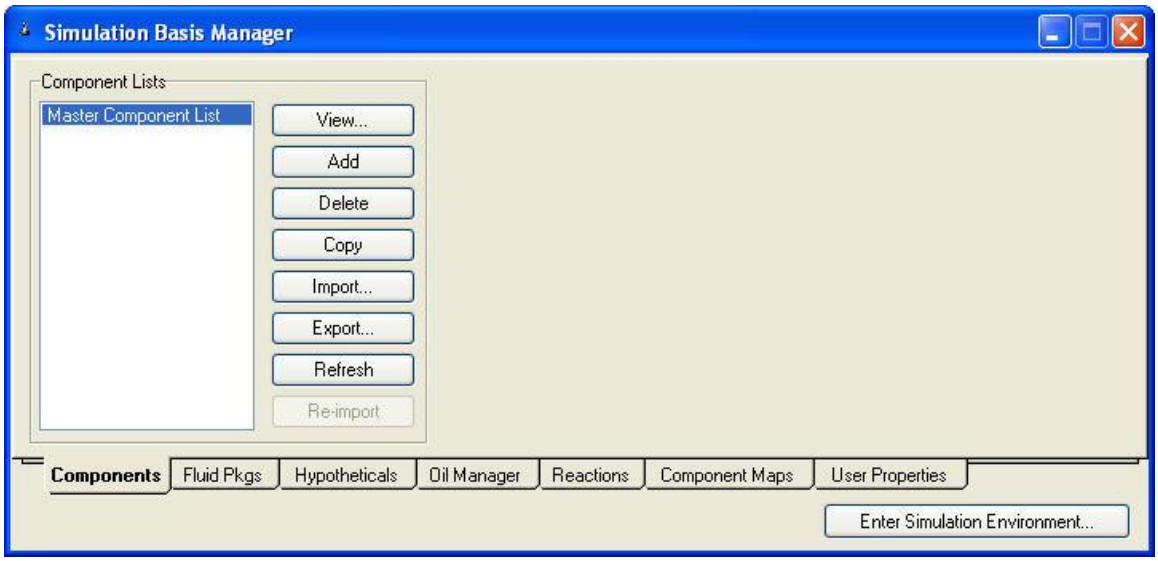
We make the following assumptions:

1. The user knows how to start and operate HYSYS 2006 or later. This example was created in 7.3 but should be applicable to all versions since 2006.
2. The user has OLI properly installed
3. The user has a familiarity with aqueous chemistry

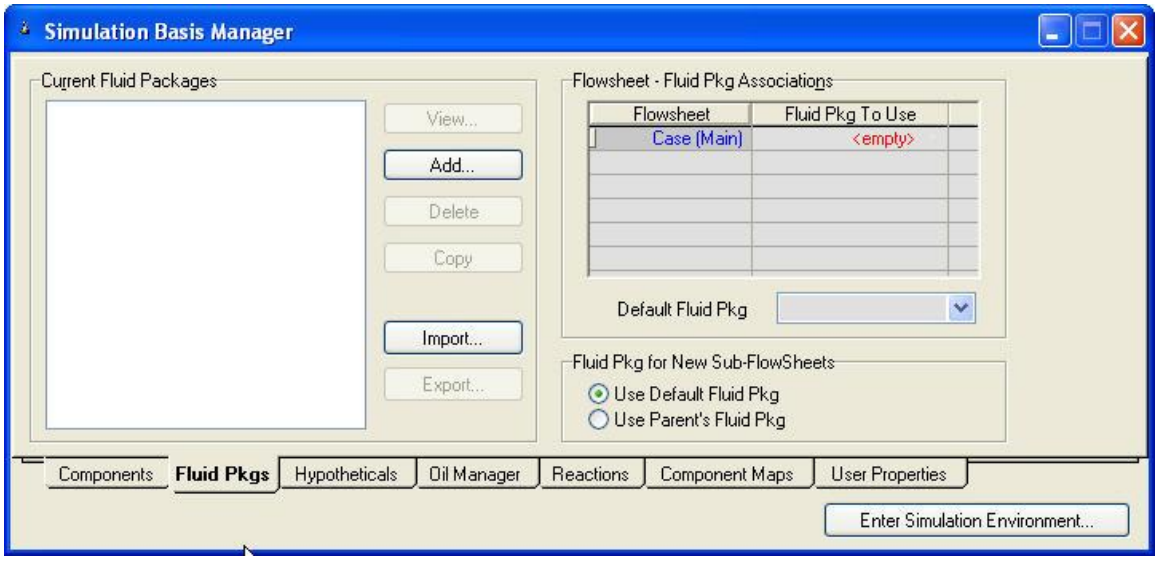
The Example

Simulation Basis Manager: Peng-Robinson Basis-1

Start Aspen HYSYS 7.3. This should display the ***Simulation Basis Manager***

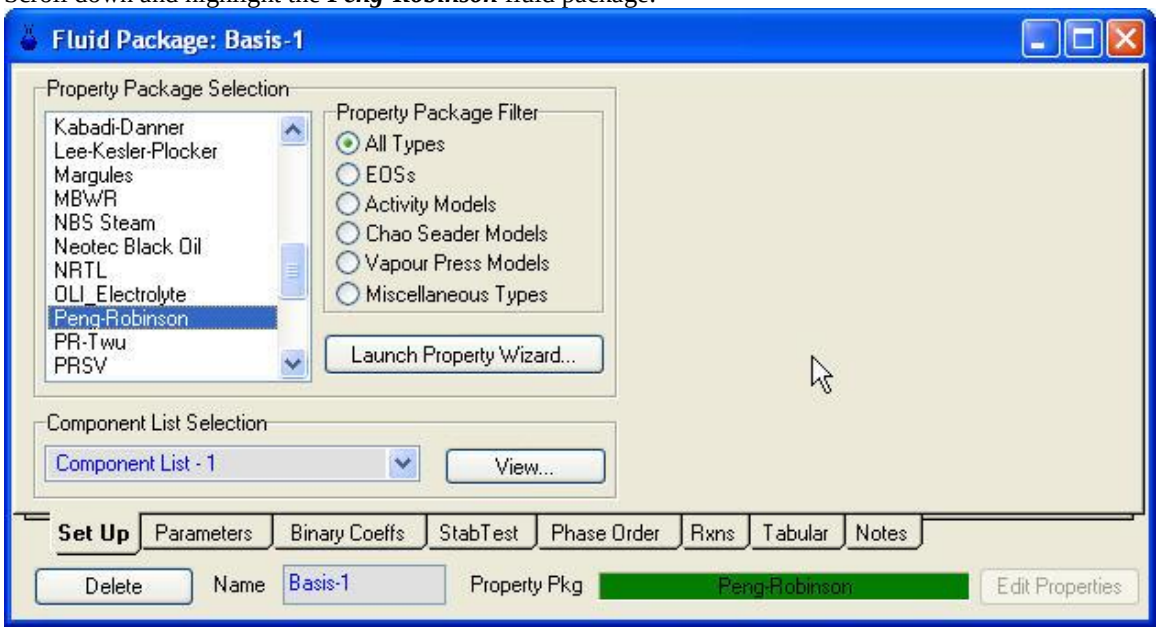


OLI finds it easier to start on the ***Fluid Pkgs*** tab. Click that tab

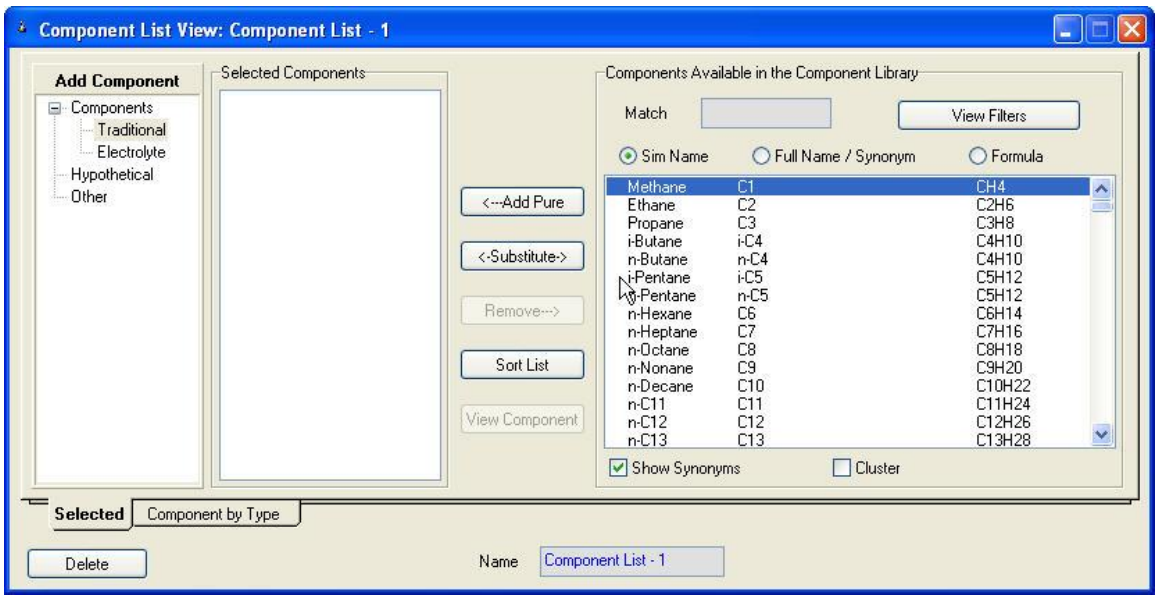


We need to add a fluid package. We will start with the PR fluid package. Click the ***Add…*** button.

Scroll down and highlight the ***Peng-Robinson*** fluid package.

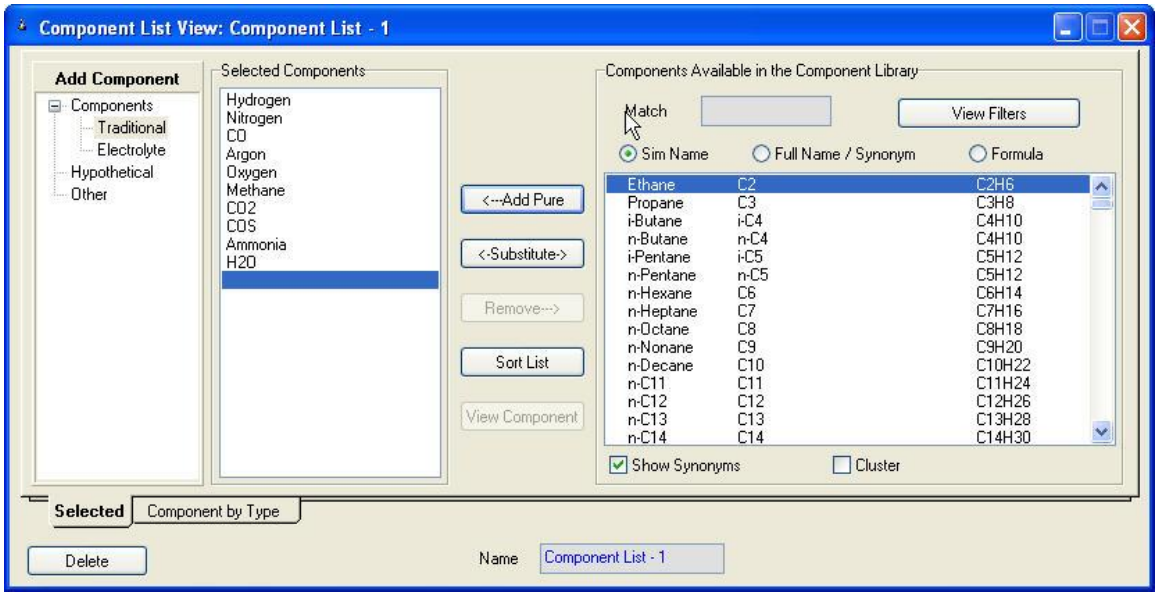


By-default the name of the component list is ***Component List – 1*** we will use the default name. Click the ***View*** button next to ***Component List – 1***

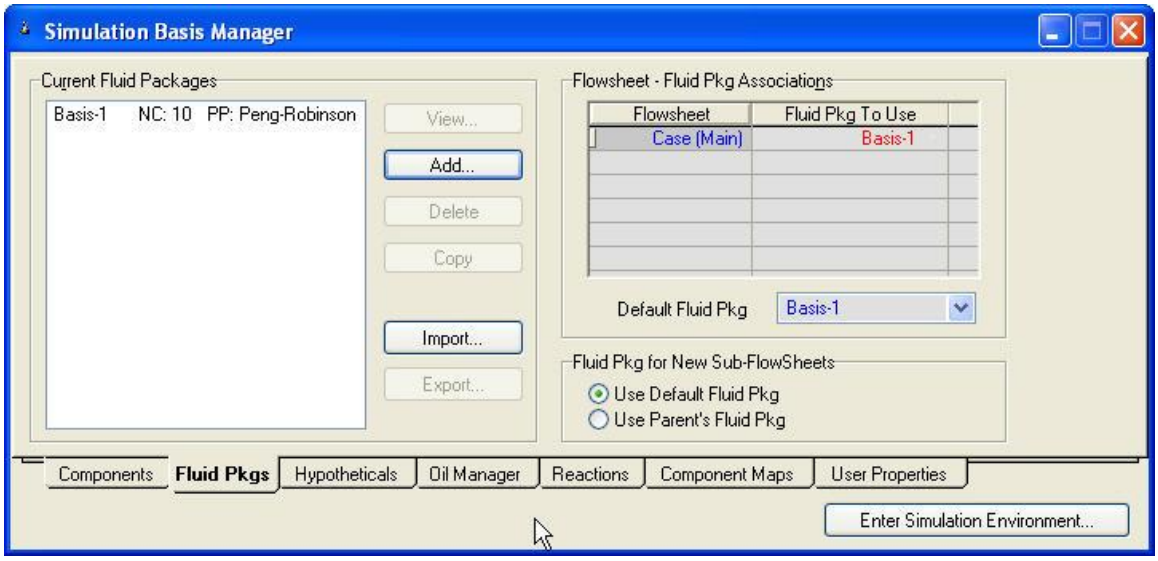


There are several types of components. For the PR fluid package we will select the ***Traditional*** components. We have also selected the ***Sim Name*** radio button.

Add the components displayed in the list below.



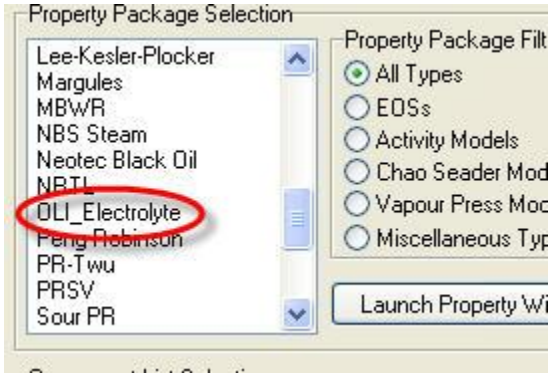
Click on the "X" in the upper right-hand corner to close this dialog.



We now have our first fluid package defined. By default this is named ***Basis-1***.

Simulation Basis Manager: OLI Electrolytes Basis-2

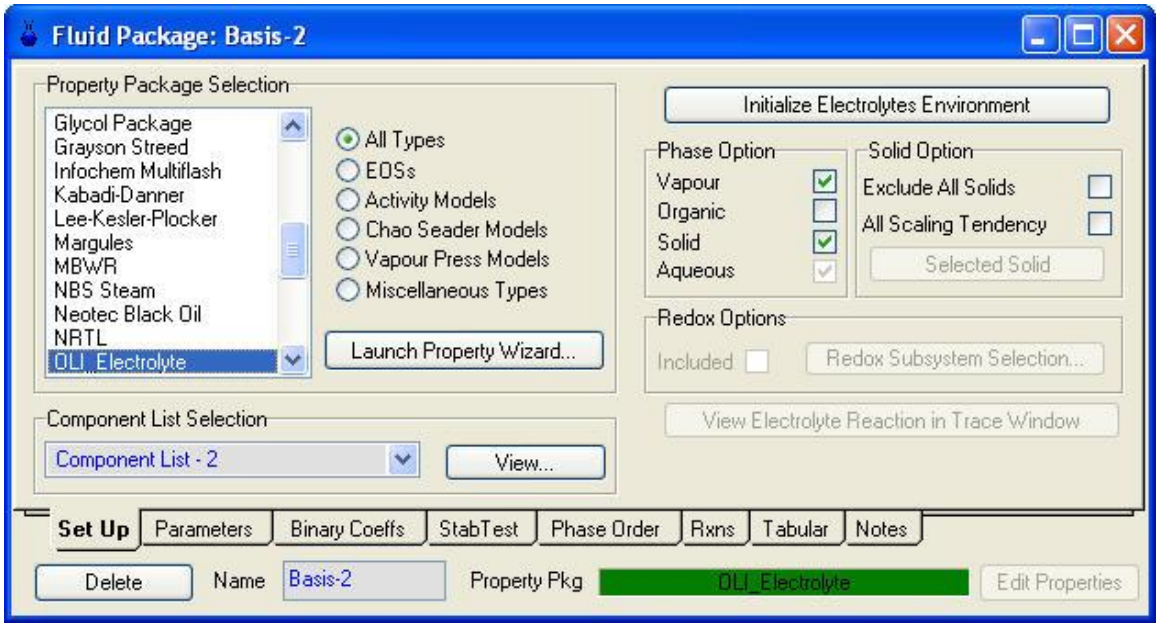
We now need to add the OLI fluid package. Click the ***Add…*** button.
Scroll down to find the ***OLI_Electrolyte*** package.



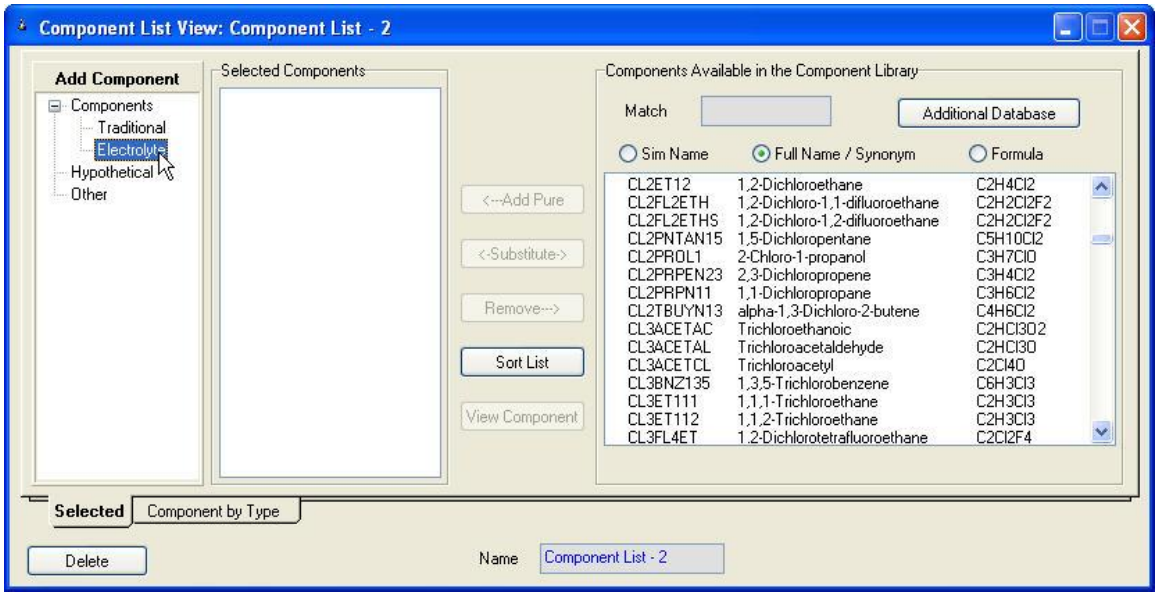
Immediately after selecting the fluid package, a warning about incompatible components will be displayed.

This message seems strange. Essentially the PR fluid package does not understand about the OLI fluid package and thinks that all of the species listed above do not exist in the OLI fluid package. From a computational point of view this is correct although thermodynamically this is not correct. Since this is a computer program we need to resolve this limitation. We will accept the action ***"If you continue, I will delete the listed components."*** This sounds a bit dramatic and somewhat personal. It is ok to accept this action.

Click the ***OK*** button.

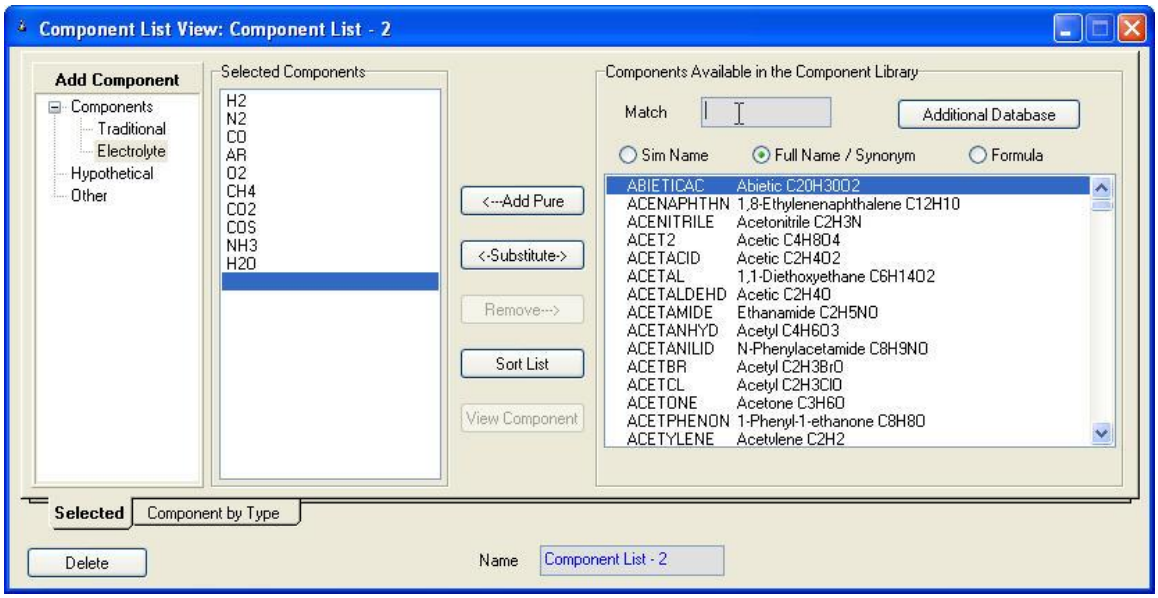


A new basis is created (***Basis-2***) and a new component list is created (***Component List – 2***). As before, click the ***View…*** button next to ***Component List – 2***.

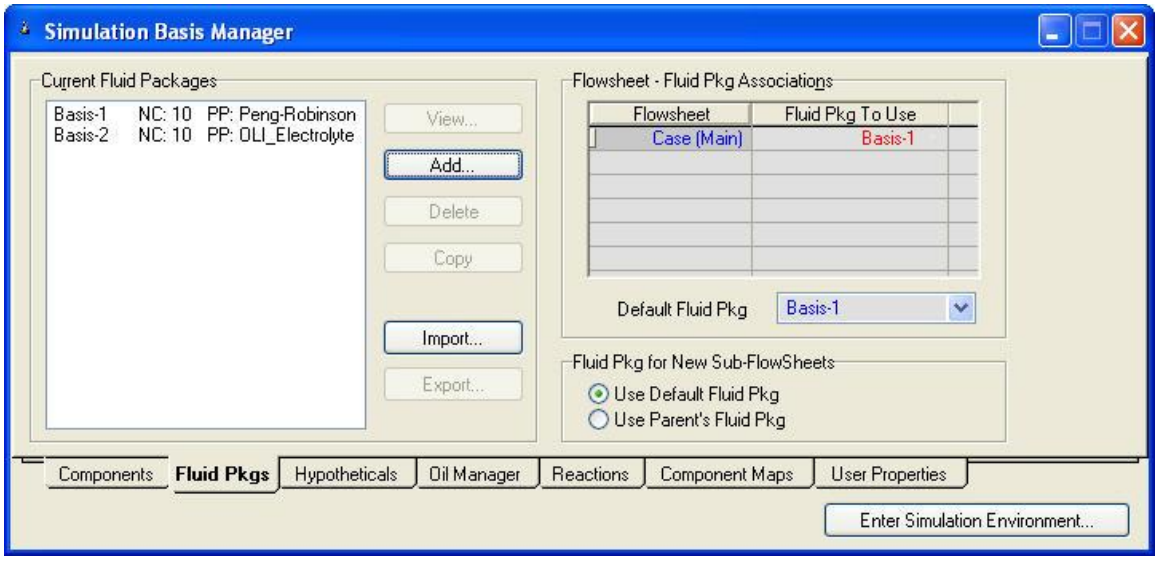


The OLI property package requires the use of ***Electrolyte*** components and you can see it highlighted above.

By default the ***Full Name / Synonym*** radio button is selected. It is recommended that you leave this button on. Enter the components below as displayed.



Click the "***X***" in the upper right-hand corner to close this dialog



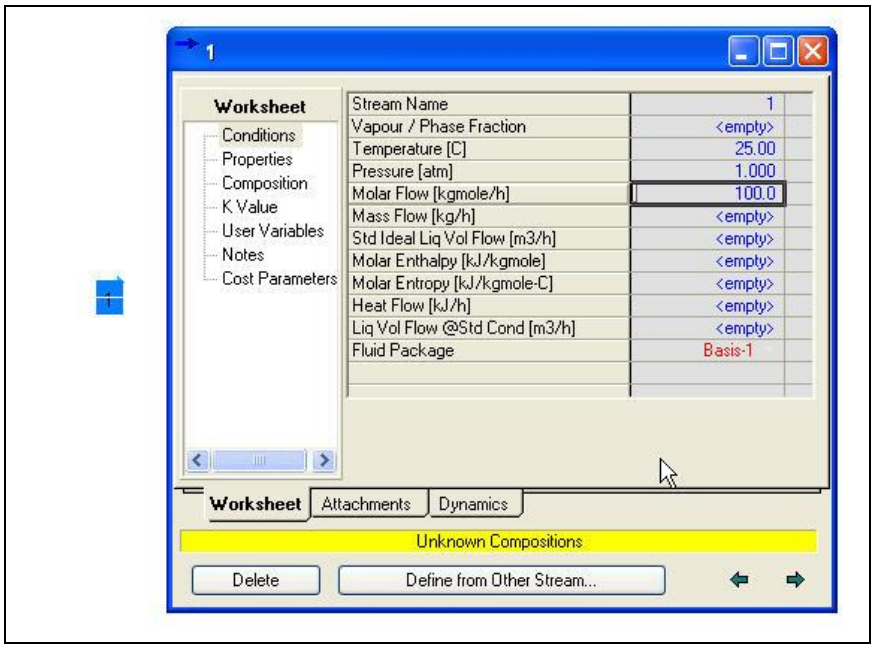
We now have two basis's entered. Notice that in the ***Flowsheet – Fluid Pkg Associations*** we only have on association. We will leave this alone for the moment.

Click the ***Enter Simulation Environment…*** button.

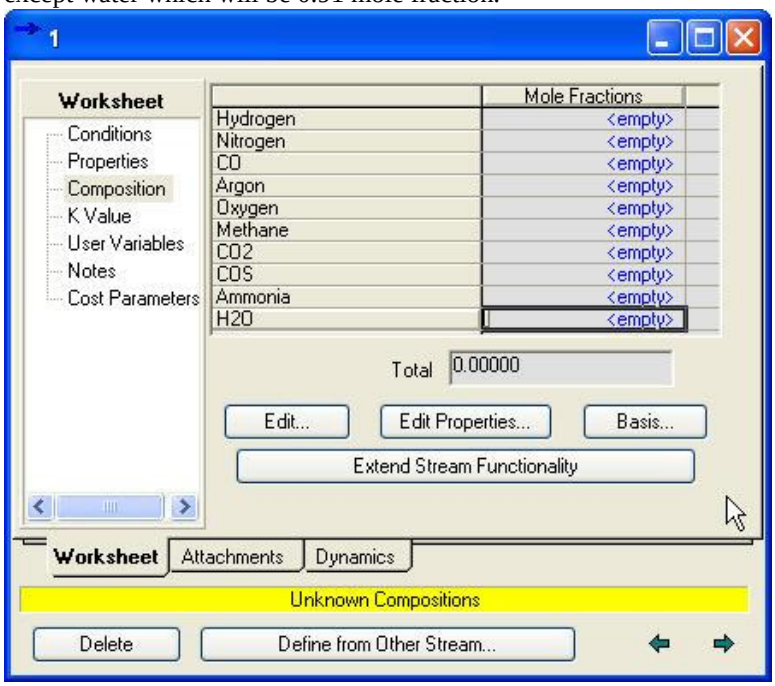
Main-flowsheet

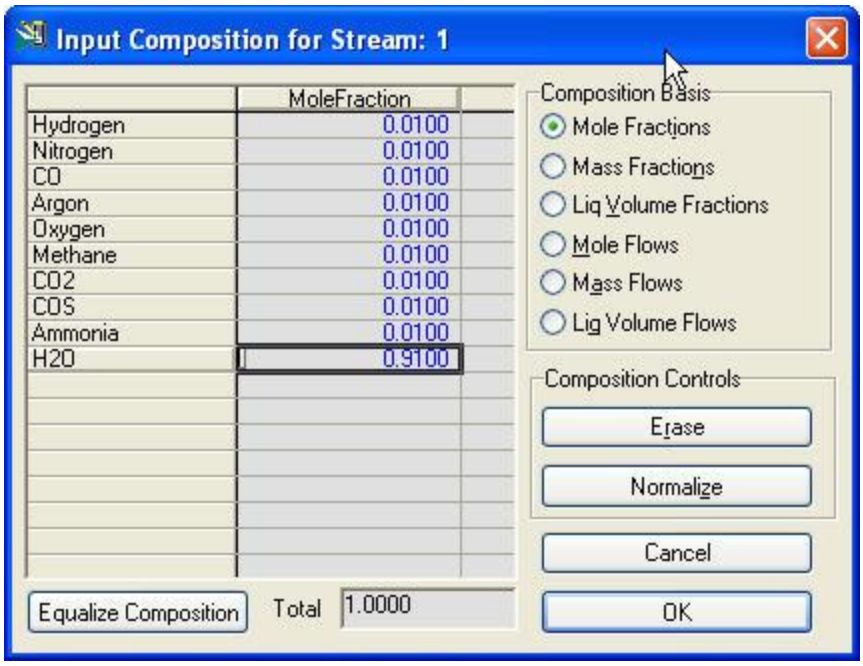
Here we have simply added a stream using the palate. The stream conditions are at 25 C and 1 atmosphere pressure. We are using 100 kgmole/hr as the molar flow. Notice that the stream is set to ***Basis-1***.

Click the ***Composition*** category.

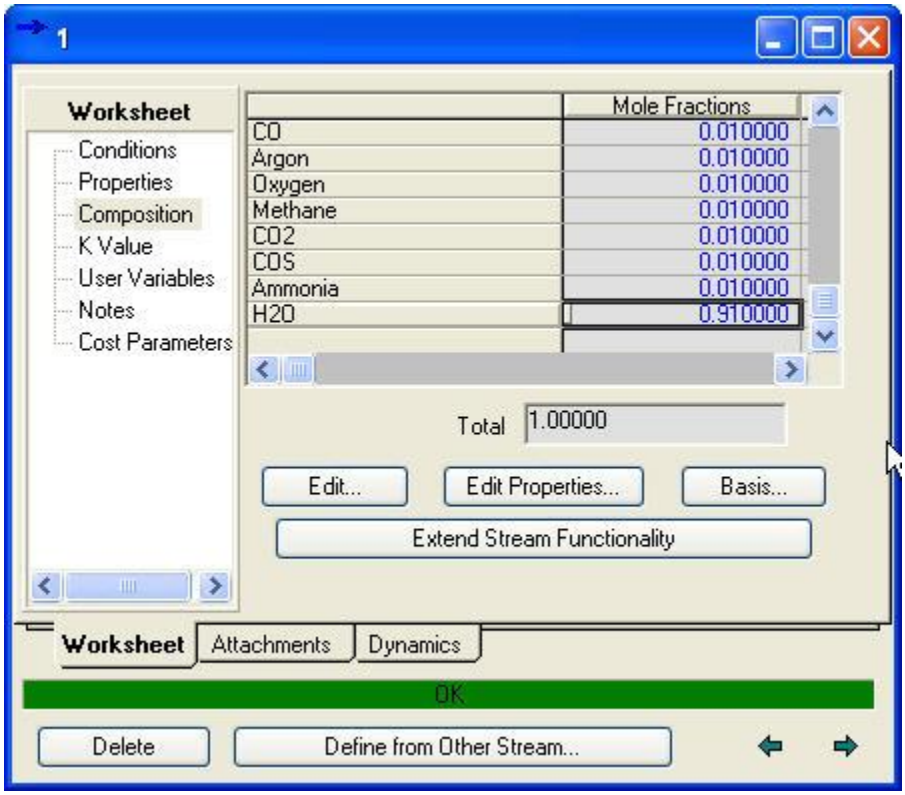


Now we will enter the composition of the stream. We will enter 0.01 mole fraction for each component except water which will be 0.91 mole fraction.





Click on ***OK*** to close this dialog

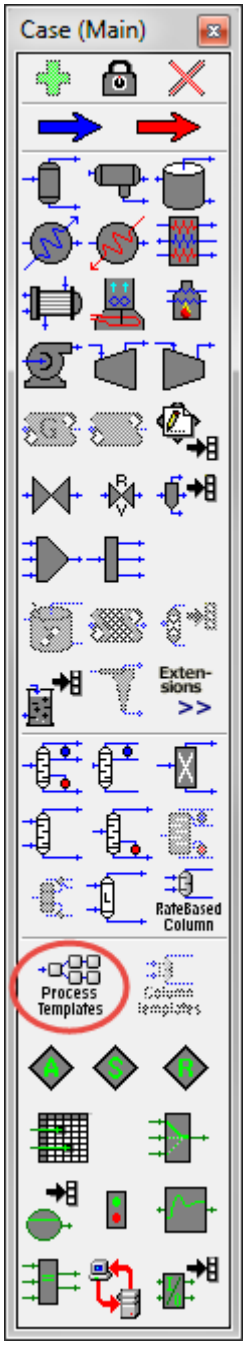


The status bar has turned green indicating that the stream has converged.

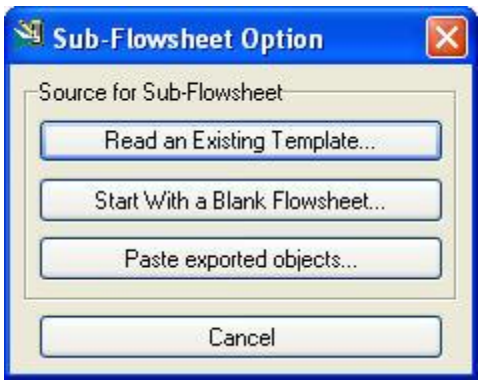
Click on the "***X"*** in the upper right-hand corner to close the dialog.

Sub-flowsheet

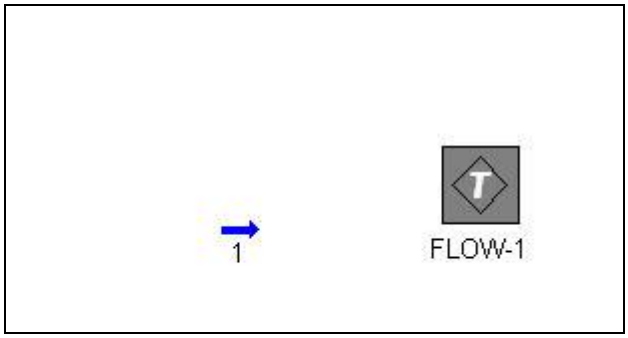
Next select the ***Flowsheet*** icon from the palate.



A Sub-flowsheet option dialog will appear.



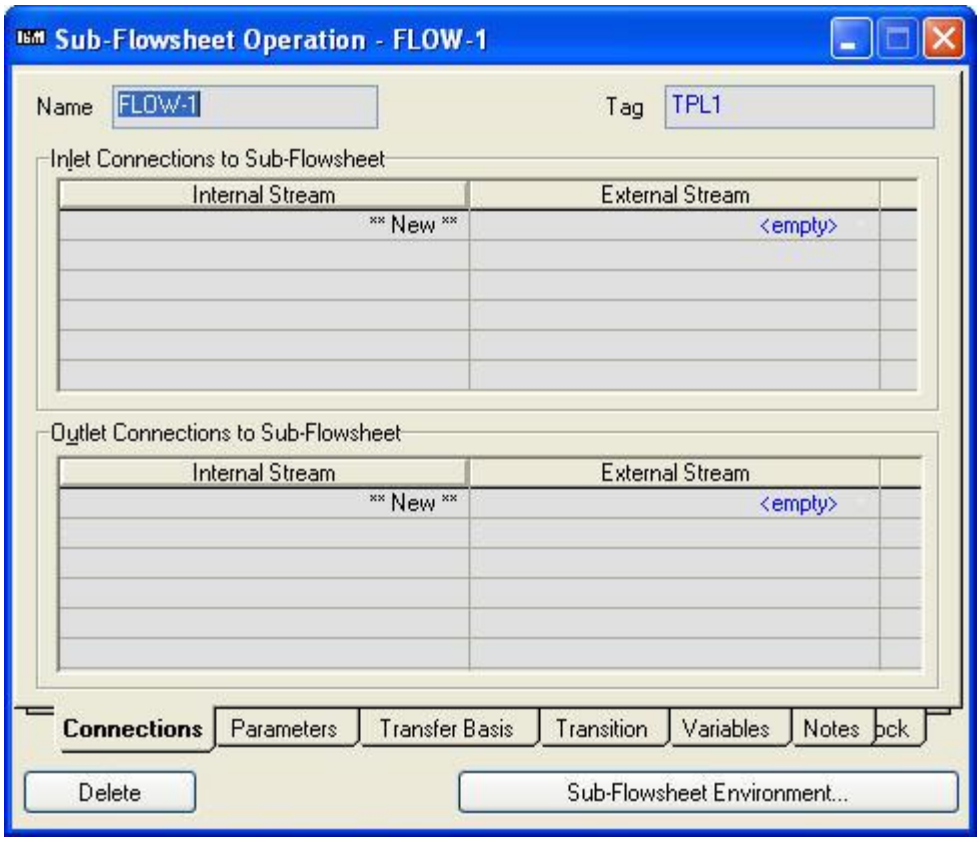
For this example click the ***Start With a Blank Flowsheet…*** button



This will place the sub-flowsheet ***FLOW-1*** on the PFD.

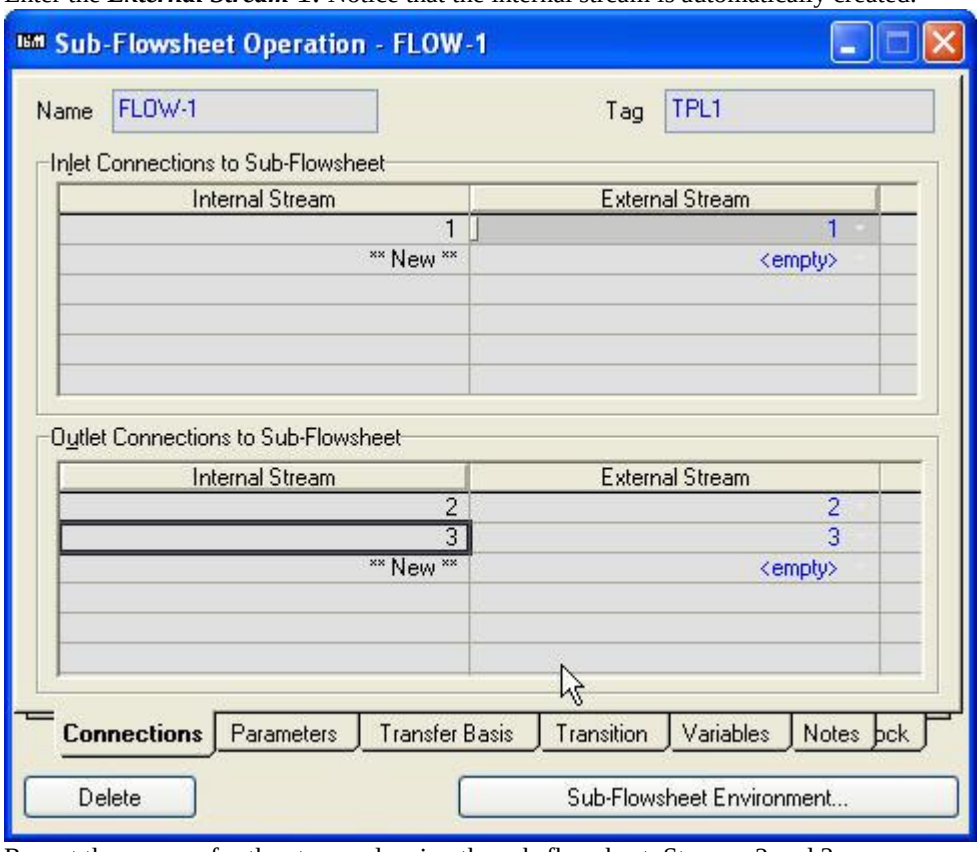
Double-Click ***FLOW-1***

This will display several options for the sub-flowsheet. The first option is to connect the streams going to and from the flowsheet (referred to as external streams) to the streams inside the flowsheet (referred to as internal streams).



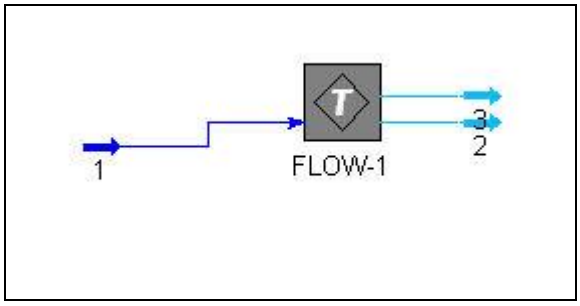
We will make life easy for ourselves and use the same numbers on the main-flowsheet as the sub-flowsheet. In small flowsheets this is ok but for large flowsheets you may get confused.

Enter the ***External Stream*** 1. Notice that the internal stream is automatically created.



Repeat the process for the streams leaving the sub-flowsheet, Streams 2 and 3.

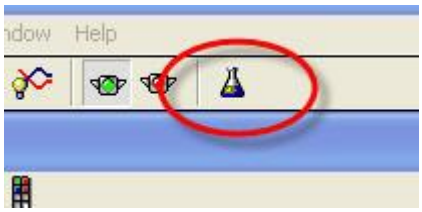
Click the "***X***" in the upper right-hand corner to close the dialog.



The main flowsheet now has the converged inlet stream "1" to the FLOW-1 sub-flowsheet and two unconverged outlet streams "2" and "3".

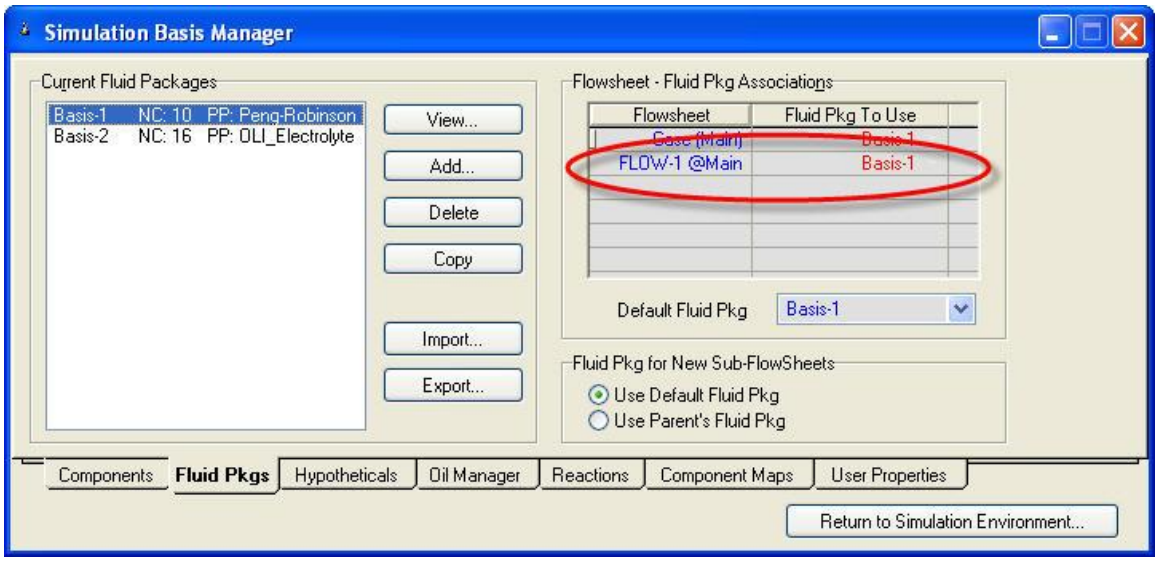
Changing the basis of the sub-flowsheet

By default the sub-flowsheet will have the same basis as the main-flowsheet. We need to change the basis of the sub-flowsheet.

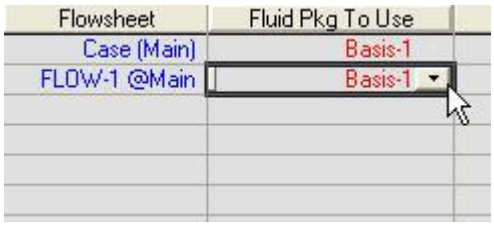


Click the small flask in the button bar at the top of the PFD. It is usually located at the right-most position.

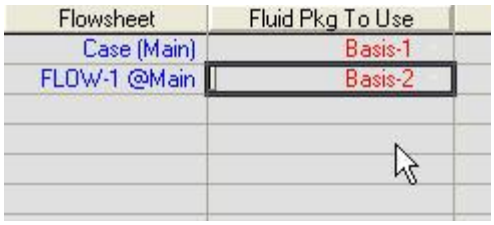
This will return you to the ***Simulation Basis Manger.*** Notice that under the ***Flowsheet – Fluid Pkg Associations*** that we have the name of the sub-flowsheet. Currently the fluid package assigned to the sub-flowsheet is ***Basis-1***.

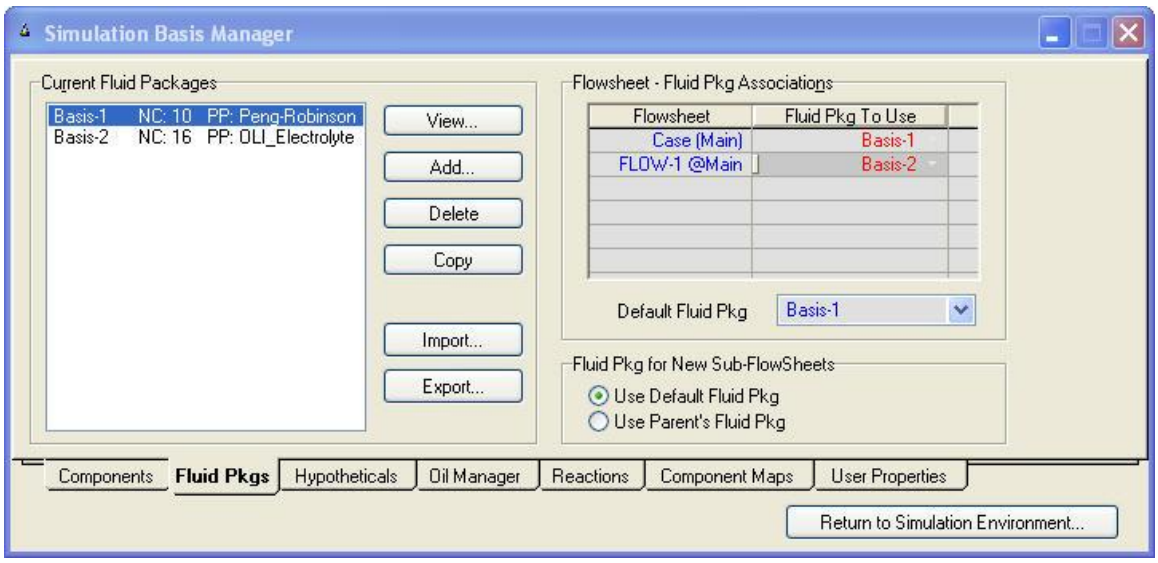


Hold your mouse over the box containing the word ***Basis-1*** and you will see that it becomes a drop-down arrow.

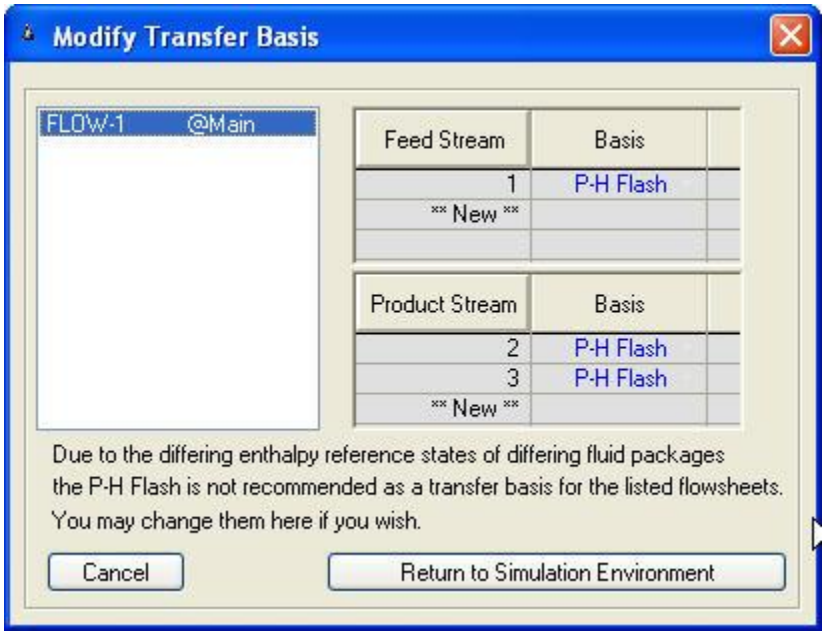


Select ***Basis-2*** from the list. Remember that Basis-2 is the OLI Electrolyte fluid package.





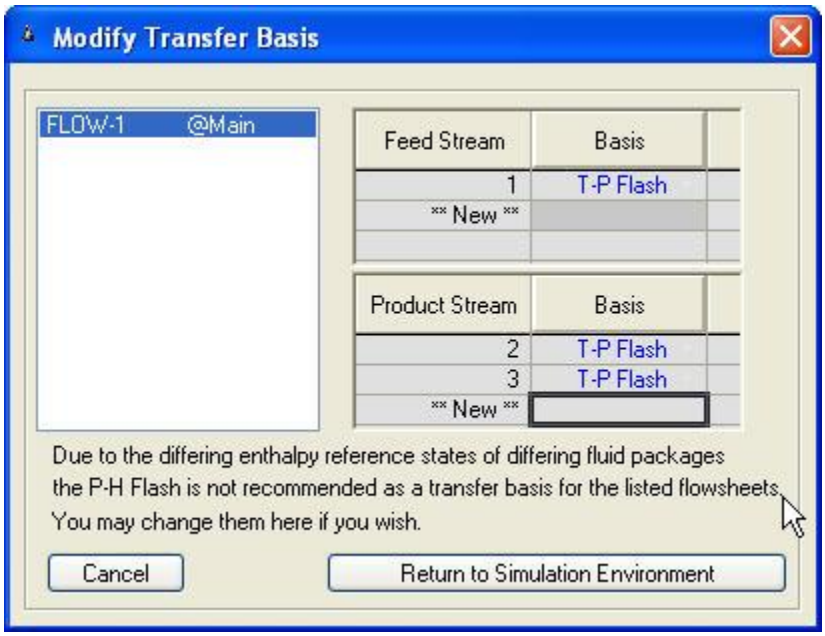
We have now updated the fluid package for the sub-flowsheet. This may display a warning dialog.



The major problem with using multiple fluid packages (OLI or some other package) is the reference point for enthalpy may be different. These differences in enthalpy can cause a temperature creep to occur between flowsheets. The default transfer basis is a P-H (pressure-enthalpy) calculation. In this we set the enthalpy to be constant and a new temperature is determined.

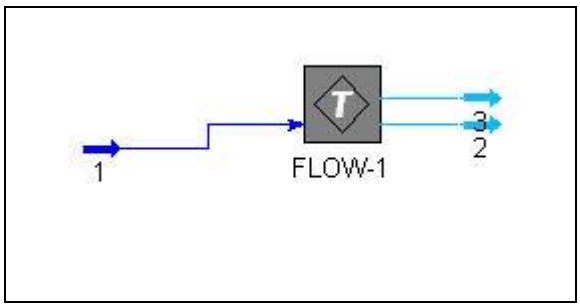
OLI recommends that the temperature be held constant (something that is easily measured) and so we select a T-P flash.

Position your mouse in each box and change the drop-down box to T-P flash.



When done, click the ***Return to Simulation Environment***.

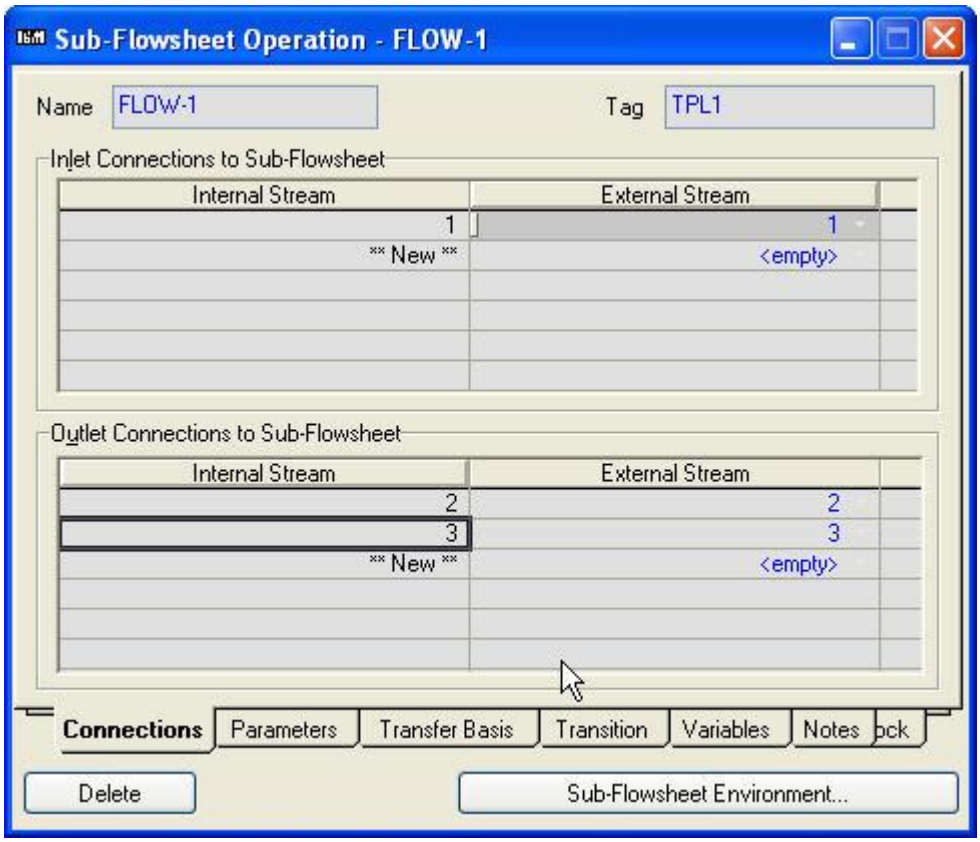
Mapping components from one basis to another



We can see that the diagram has not changed except for repositioning of the lines.

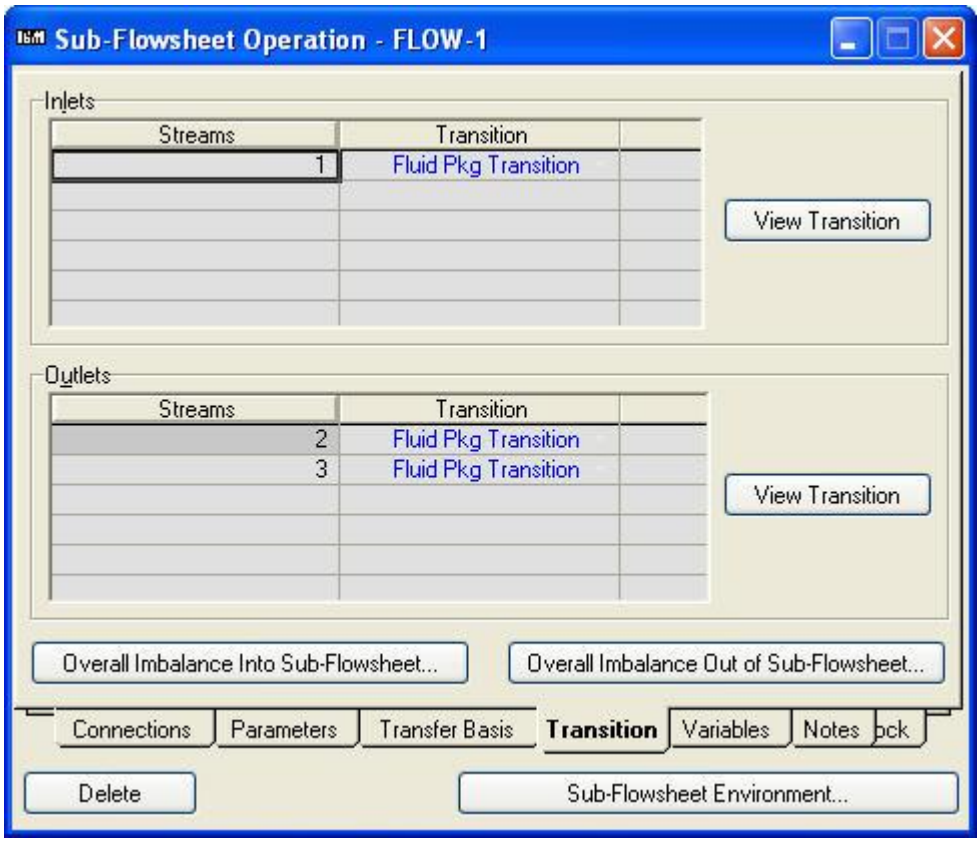
Double-click the ***FLOW-1*** sub-flowsheet.

Once again we are returned to the sub-flowsheet options. We now need a method of transferring the data for our components from the main flowsheet to the sub-flowsheet. For example, the species Argon in the main-flowsheet is AR in the sub-flowsheet. This is called a ***Transition***.



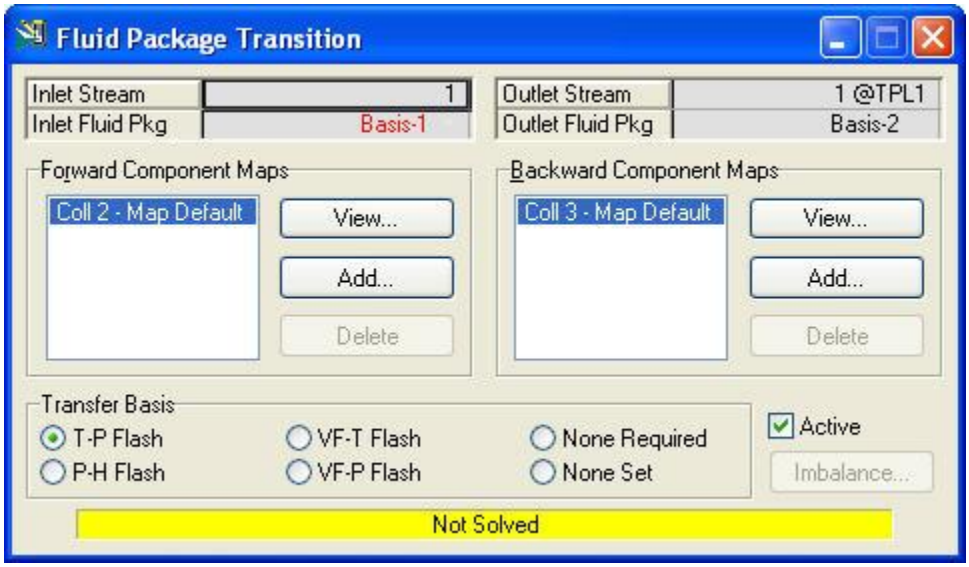
Click the ***Transition*** tab

We now need to create the transition of components for the inlet to the sub-flowsheet and do the same for the outlet of the sub-flowsheet. We wills start with the inlet stream (from the main-flowsheet) "1".



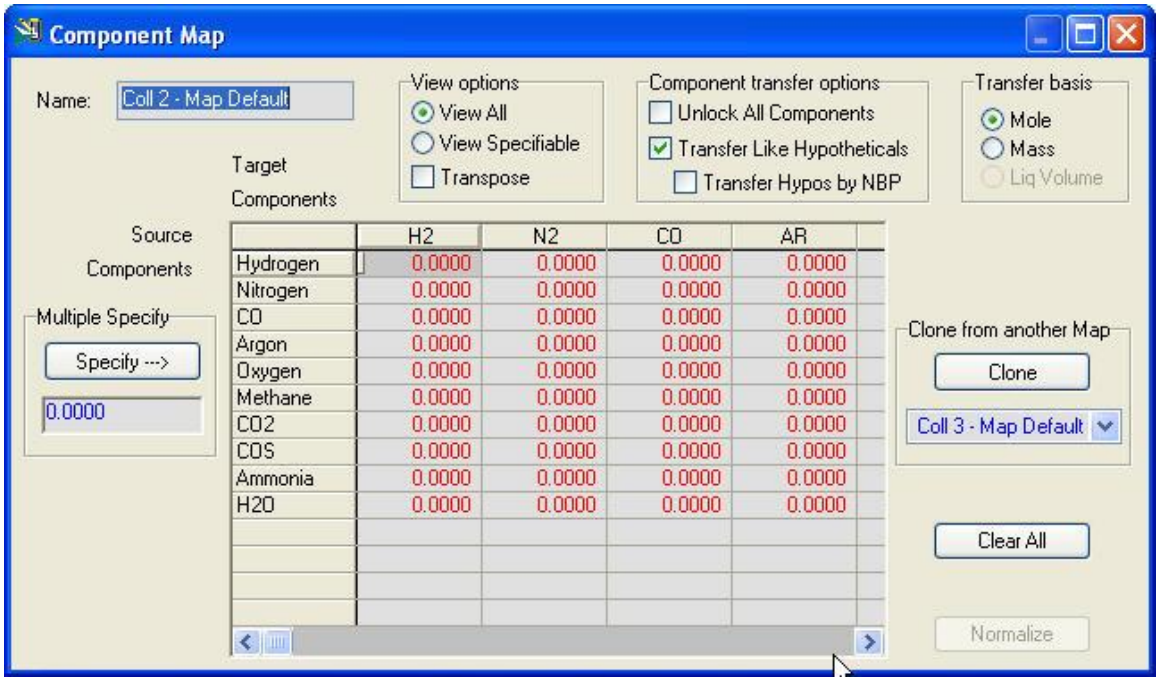
Position your mouse on "1" and then click the ***View Transition*** in the upper box.

This dialog has a lot of options. We can see that the inlet stream "1" has Basis-1 as its fluid package. Stream "1" in the sub-flowsheet is represented as "1@TPL1" and has Basis-2. We need a mapping of components from Basis-1 to Basis-2.

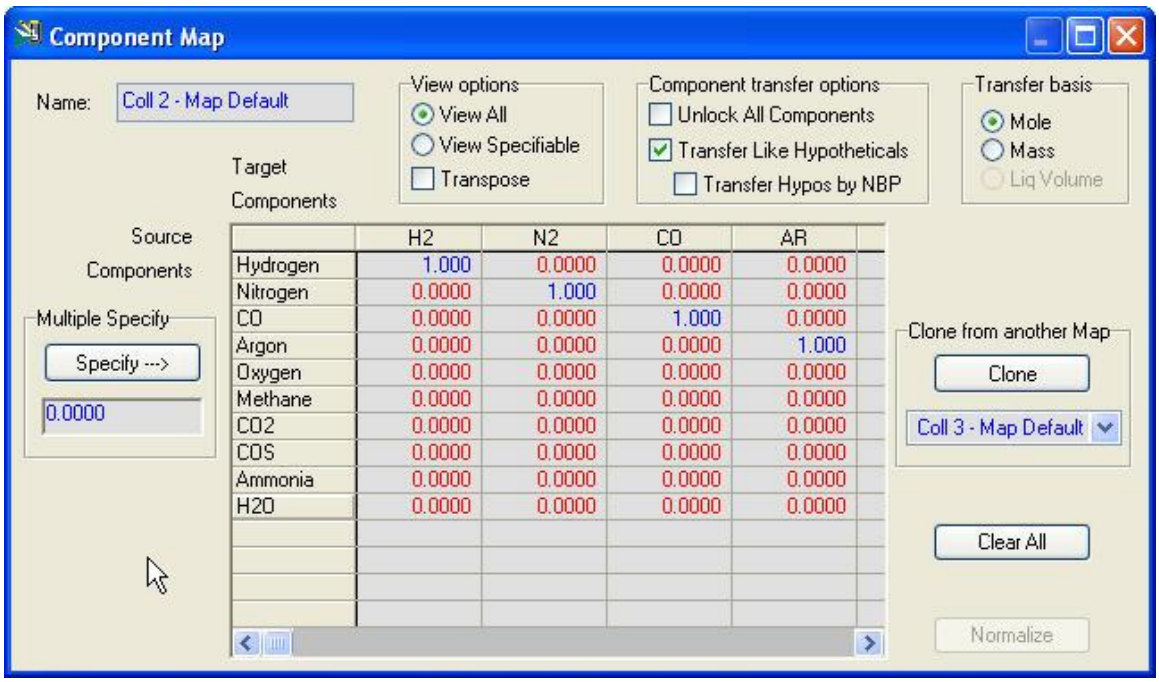


Click the ***View…*** button in the ***Forward Component Maps*** box.

This displays a very busy box. The components listed going down the column are the Basis-1 (Peng-Robinson) components. The components listed across the columns are for Basis-2 (OLI). At the moment there are no mappings.



Find each cross-reference (e.g., Hydrogen – H2) and enter a 1.0. This maps every mole of the component Hydrogen in Basis-1 (Peng-Robinson) to a single mole of H2 in Basis-2 (OLI).

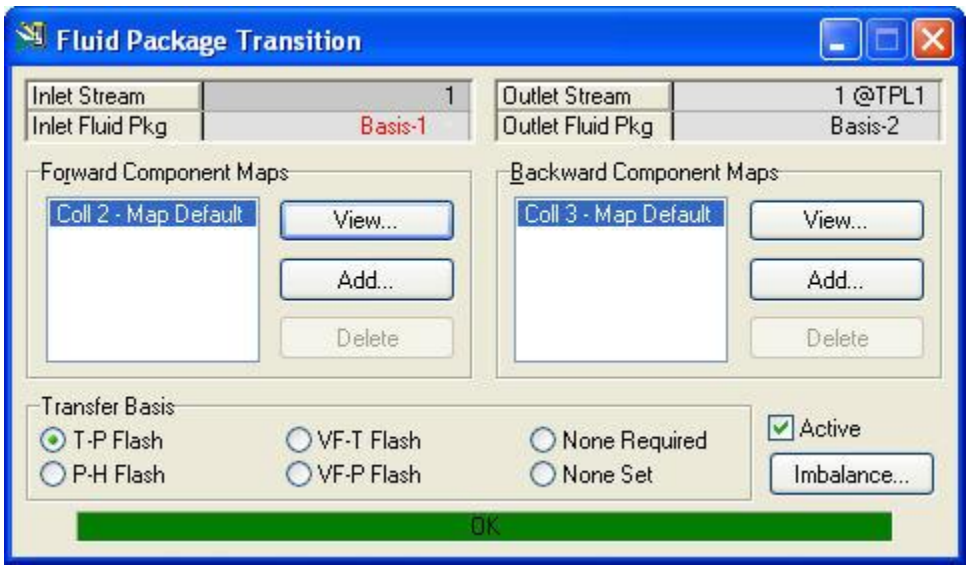


Here we cans see that we have a partially completed list. Scroll to the right to finish the list.

	COS	NH3	H2O	H2CO3	HN
Hydrogen	0.0000	0.0000	0.0000	0.0000	
Nitrogen	0.0000	0.0000	0.0000	0.0000	
CO	0.0000	0.0000	0.0000	0.0000	
Argon	0.0000	0.0000	0.0000	0.0000	
Oxygen	0.0000	0.0000	0.0000	0.0000	
Methane	0.0000	0.0000	0.0000	0.0000	
CO2	0.0000	0.0000	0.0000	0.0000	
COS	1.000	0.0000	0.0000	0.0000	
Ammonia	0.0000	1.000	0.0000	0.0000	
H2O	0.0000	0.0000	1.000	0.0000	

Here the Peng-Robinson components (Basis-1) have been mapped to the corresponding OLI (Basis-2) components. Notice that there are no mapped components to a species such as H2CO3 (OLI, Basis-2). This component will be determined by the OLI solvers.

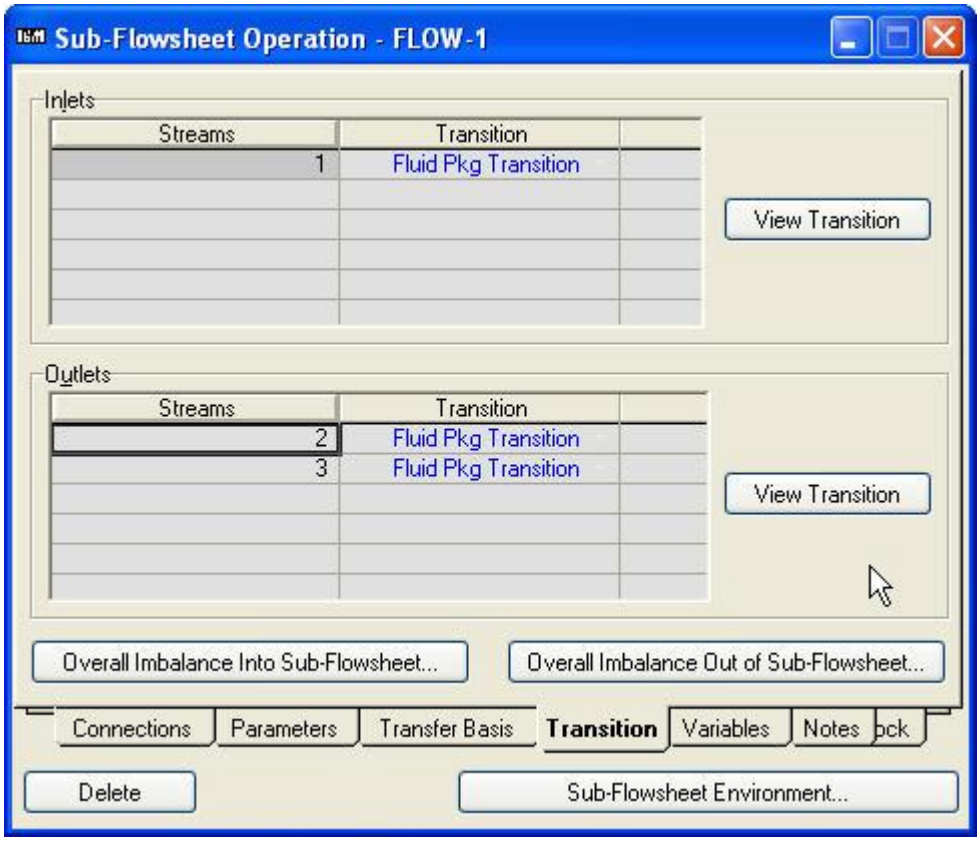
Click the "***X***" in the upper right-hand corner to close the dialog.



We can see that the status bar has turned green. This indicates that the transition was complete and the OLI solvers converged.

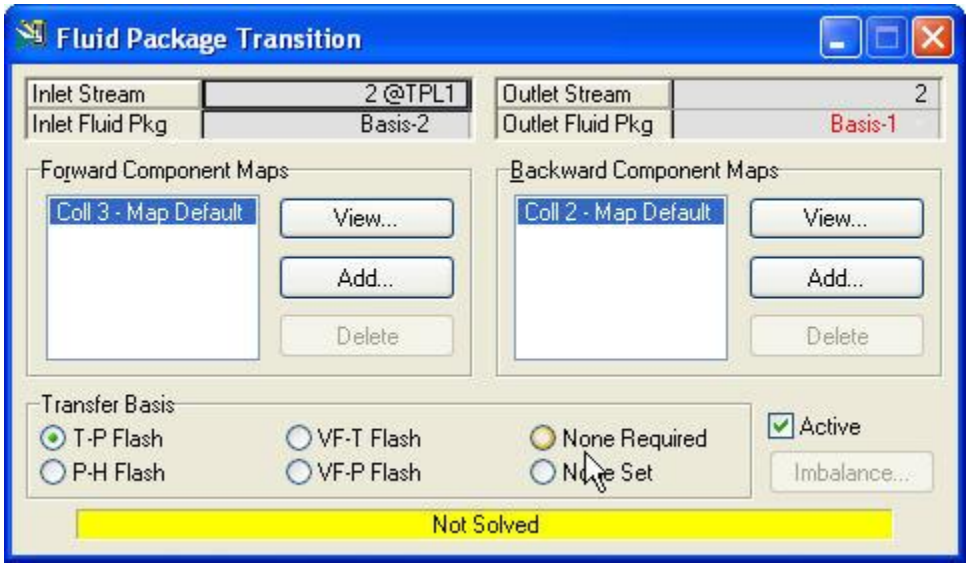
Click on the "X" in the upper right-hand corner to close the dialog.

We now have to map the OLI (Basis-2) components back to the PR (Basis-1) components).



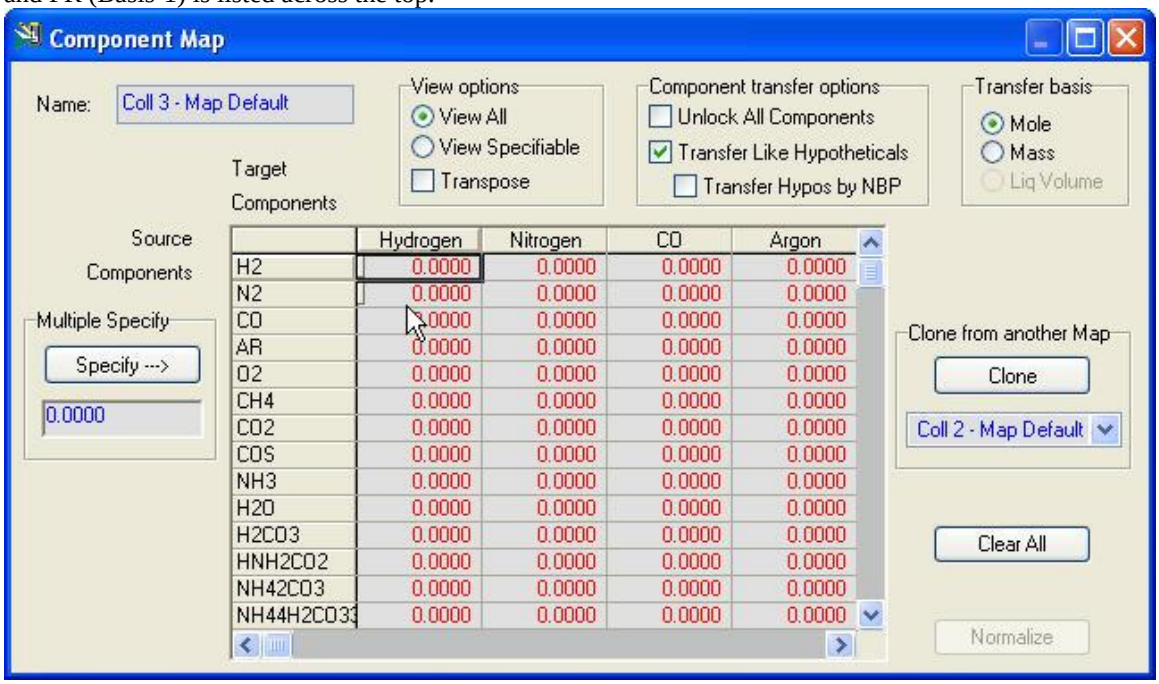
Click on stream "2" and then click on ***View Transition*** in the lower box.

This dialog is similar to the inlet dialog. You can see that the internal stream "2" is actually referred to as 2@TPL1) and is set to Basis-2 (OLI). The outlet stream on the main-flowsheet is "2 and is set to Basis-1 (PR).

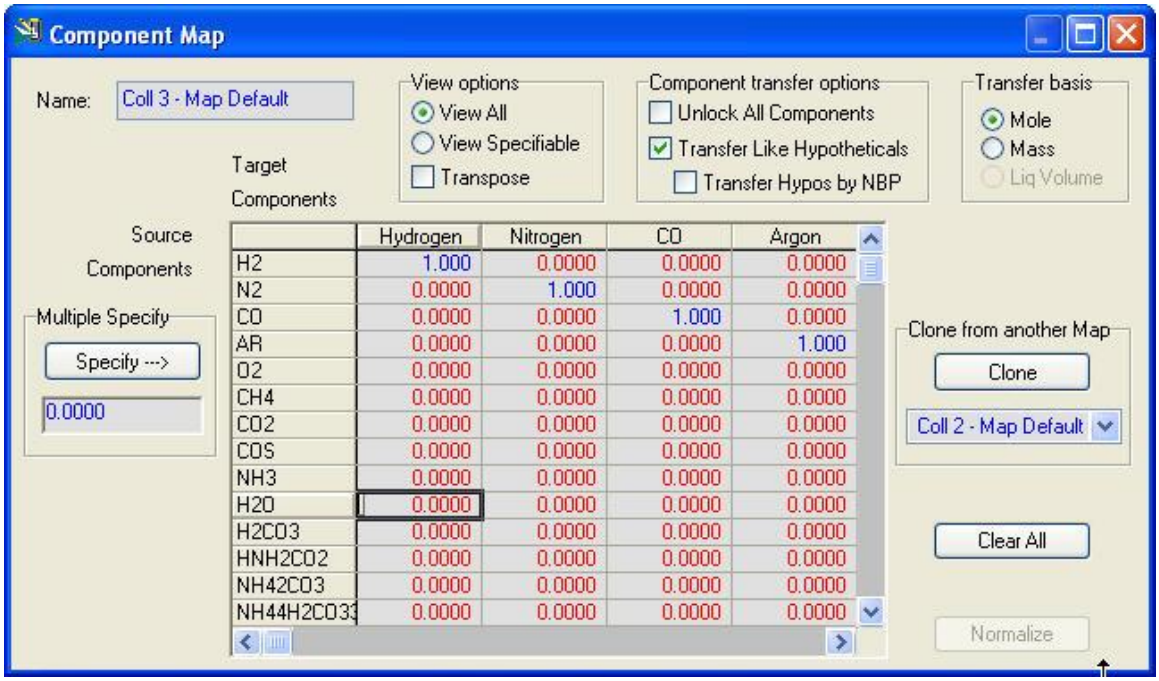


Click the ***View…*** button in the ***Forward Component Maps*** box.

This brings up a similar dialog as before except this time OLI (Basis-2) is listed going down the column and PR (Basis-1) is listed across the top.



As before, enter a 1.0 to map the OLI component to the PR component. Do not map OLI species that do not appear as PR species.



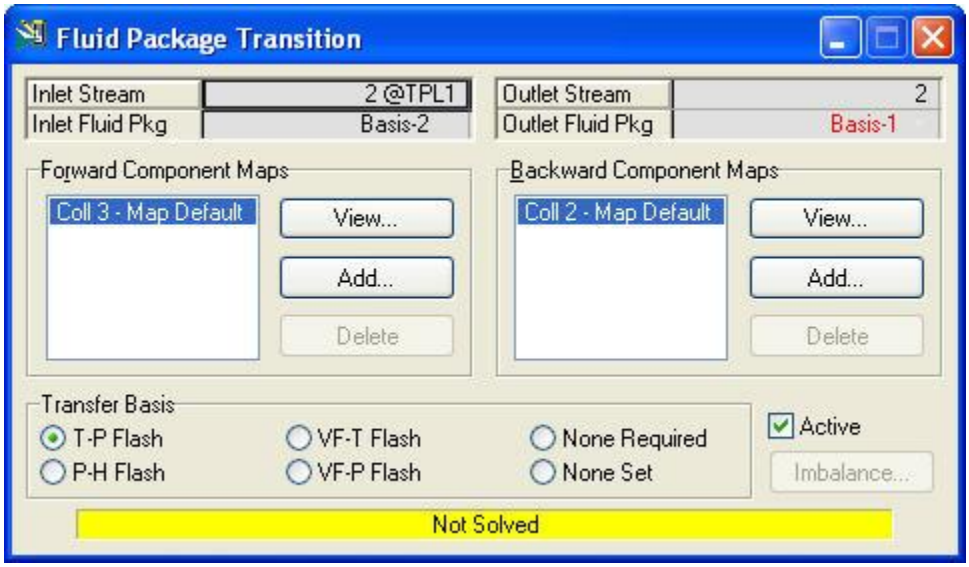
Why not map OLI species such as “H2CO3” to PR species? You may be tempted to make the following conversion:

H2CO3 = CO2 + H2O

This means in the mapping columns under both CO2 and H2O there will be two entries with a 1.0, lined up with the component H2CO3.

When OLI and HYSYS were originally developed (back in version 3.2 of HYSYS) a convention was made that the OLI solvers will automatically map the moles of the electrolyte species (such as the ions) back to the same species originally entered (the Basis-2 components). If you do this same conversion here you will be double-accounting for the species and may introduce a mass imbalance. Let OLI manage the conversion and you should only map the components you actually entered in the ***Simulation Basis Manager***.

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

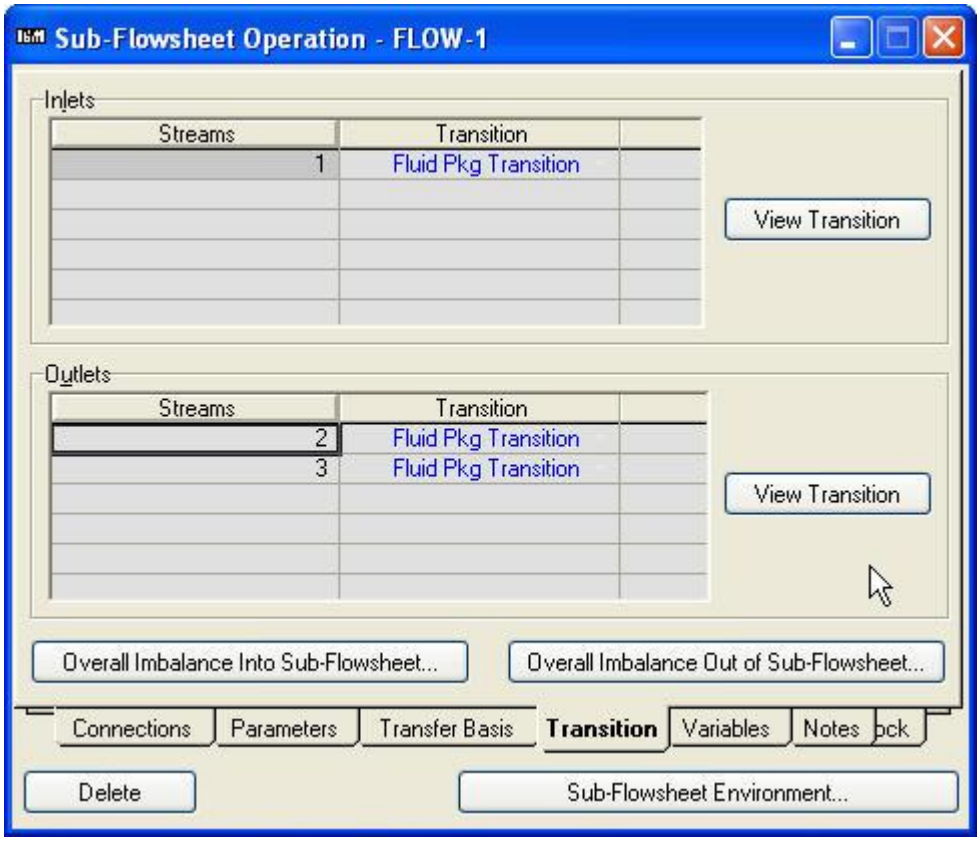


You are returned to this dialog. Notice that the status bar is yellow (not solved). This is because we have not yet made a connection to the outlet streams inside the sub-flowsheet.

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

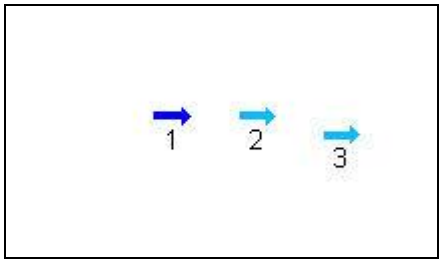
This returns you to the sub-flowsheet operation dialog.

Finishing the sub-flowsheet

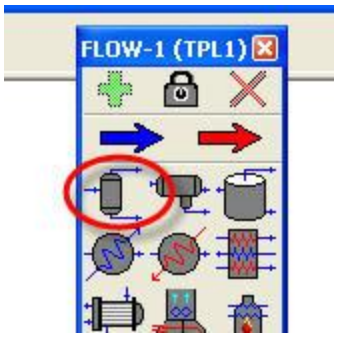


We are now ready to go.

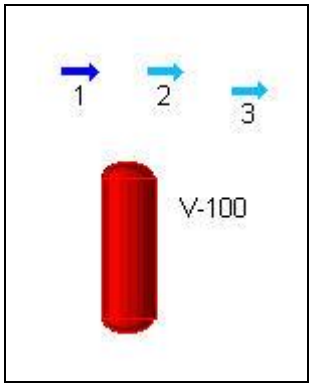
Click the ***Sub-Flowsheet Environment…***Button.



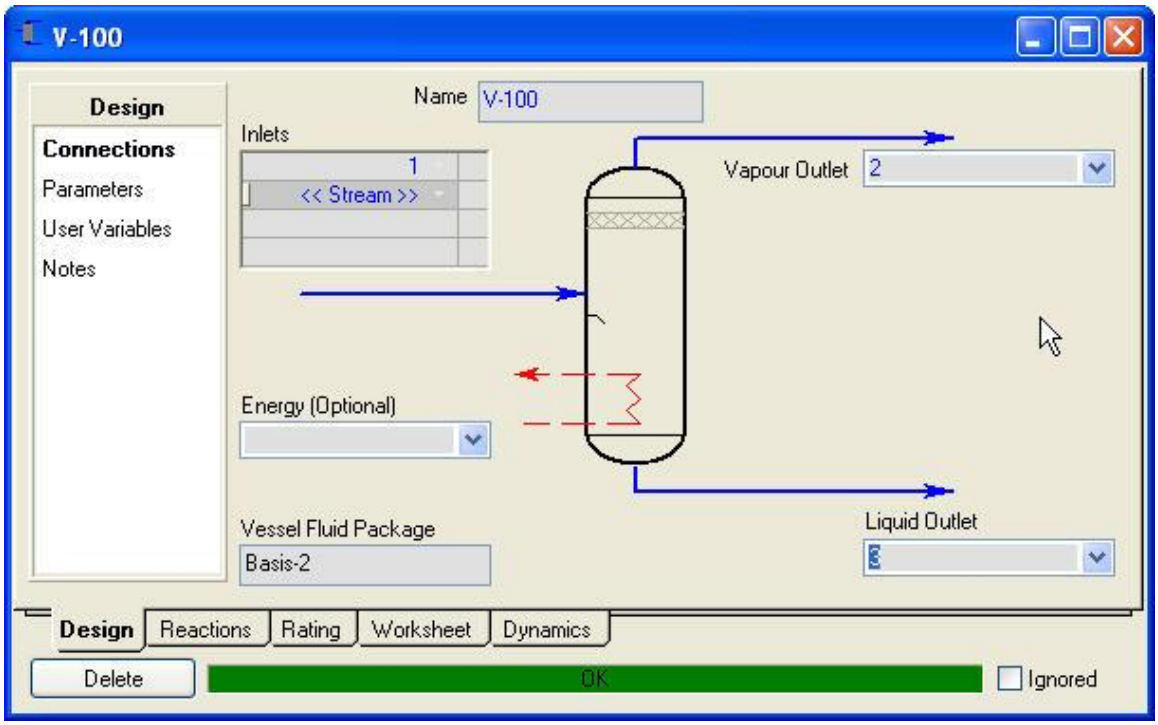
You can see that the sub-flowsheet has disconnected streams. For this example we will introduce a 2-phase separator.



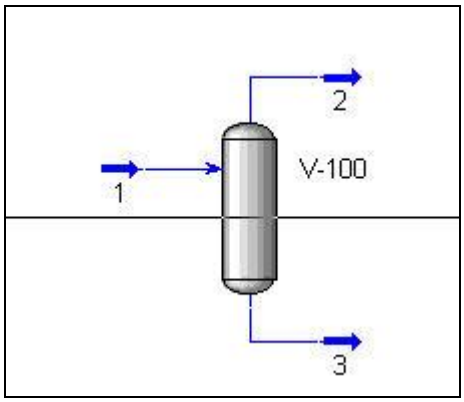
Select the 2-phase separator from the palate and place it on the sub-flowsheet PFD.



Double-click the V-100 unit operation to make the connections or use the connection tool.

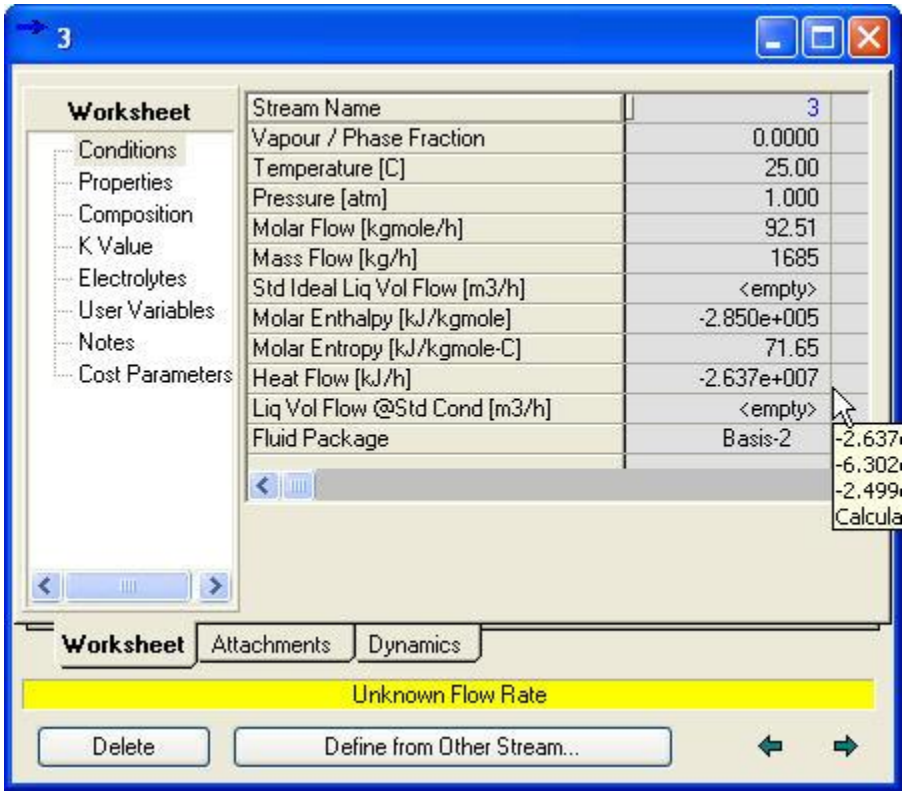


Once the connections are made the unit operation is converged.
Click on the ***"X"*** to close the dialog.



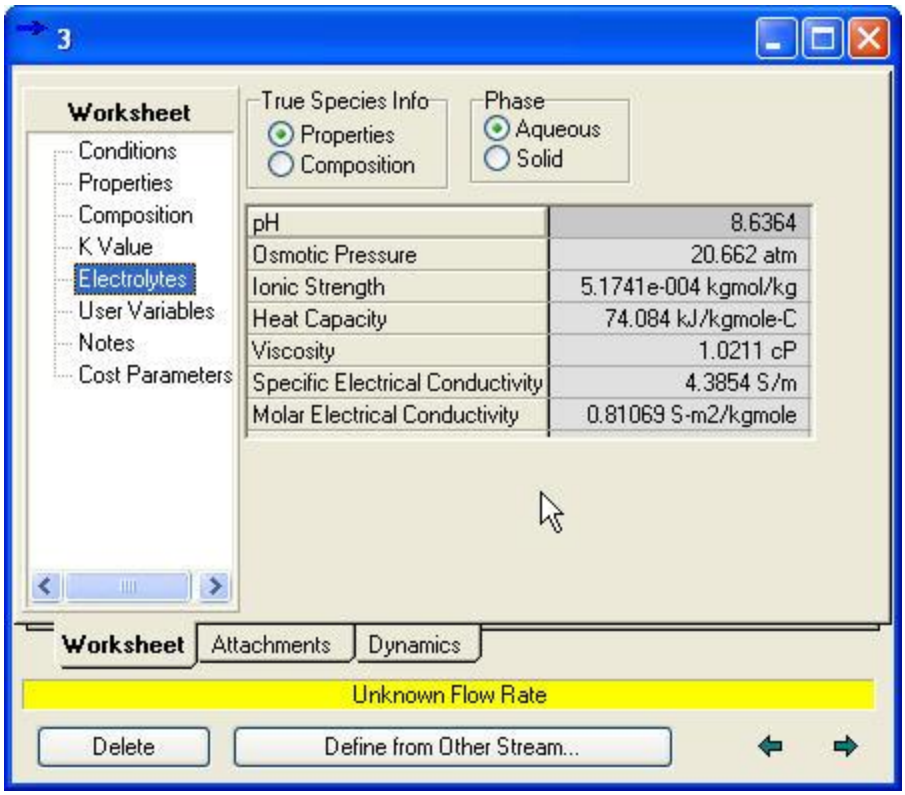
We can see that the unit has converged. The vapor is leaving stream "2" and the aqueous liquid is leaving stream "3"

Click on Stream "3"



You can see that there is molar flow of 92.51 kgmole/hr. The stream is "Yellow" because there is no "**Std Ideal Liq Vol Flow"** value. These values are not returned by the OLI solver and the error checking sub-routines have identified a flash-failure. The stream is actually converged.

Click on the ***Electrolytes*** category.

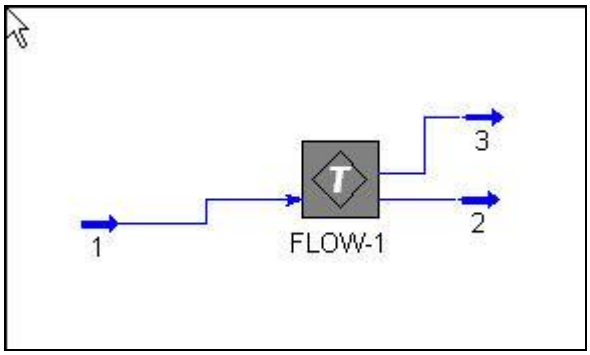


Here we can see that there is a pH of 8.6 which is a value returned by the OLI solvers.

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

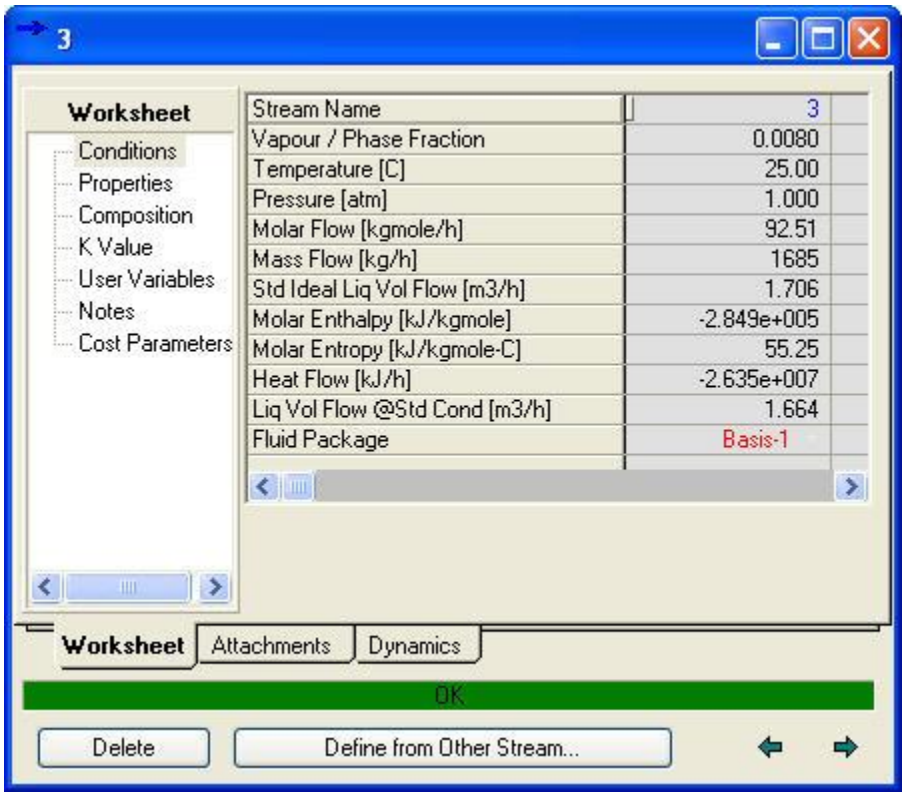
Once back on the sub-flowsheet we can return to the main flowsheet by locating the "UP Arrow". This is usually the right-most button on the button toolbar.

Click the ***UP Arrow***



We are now returned to the main flowsheet. Notice that the streams "2" and "3" are reversed on the PFD. Please remember that one stream is a vapor and the other liquid as determined by the sub-flowsheet. Stream "3" was the liquid stream.

Click ***Stream "3"***.



Notice that the basis is now Basis-1 (PR). The molar flow is the same but the other flow rates have been calculated. Also notice that the category ***Electrolytes*** is not present. This is because the PR fluid package does not support electrolyte components. The aqueous electrolyte information is only contained in the sub-flowsheet.