OLI Engine for Petro-SIM V7.x

Getting Started Guide

Contents

Overview

The OLI Engine for Petro-SIM interface greatly enhances Petro-SIM'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 property set within Petro-SIM. This "Getting Started" guide will show you how to create the electrolyte chemistry for a simple case and then create a simple flowsheet in Petro-SIM.

Assumptions

The following assumptions are made for this guide:

1. Petro-SIM is currently installed and running on your computer.
2. The license manager for Petro-SIM is currently set up.
3. The OLI Engine for the Petro-SIM product has been installed.
4. The OLI security model is running.
5. Petro-SIM V7.4 is being used.
6. The user is expected to know how to run Petro-SIM.

Application

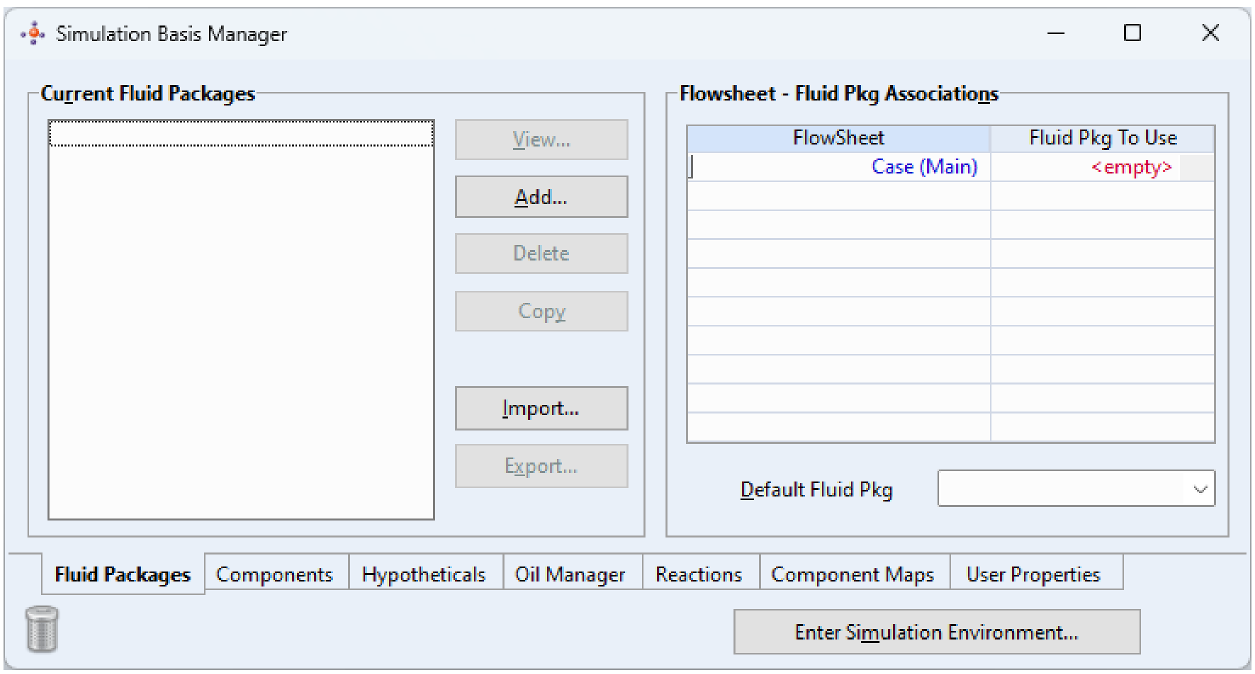
This application will take an acid stream and titrate it against a basic stream to see the resultant pH changes. Some heat and vapor are expected to be evolved.

Here we will provide a few steps to get you started.

In this application, we will mix a nominally basic stream of H_2O, CO_2, NH_3, and SO_2 with an acidic stream of H_2O, H_2SO_4, and HCl.

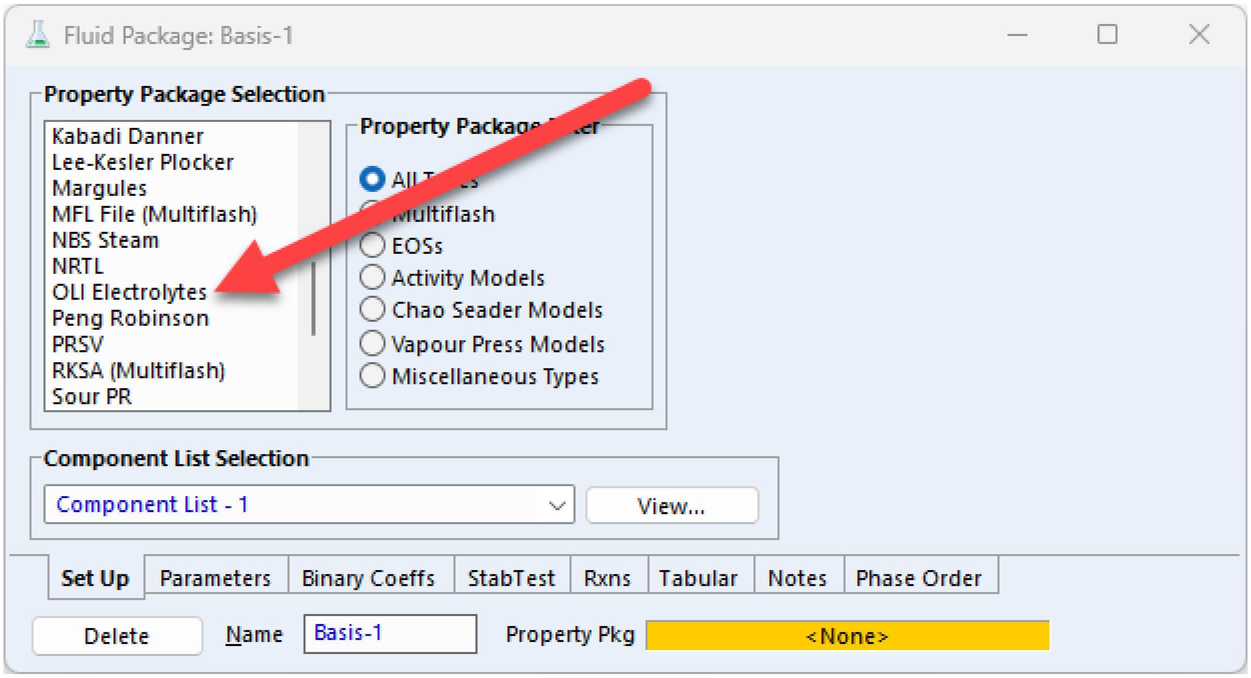
Using the OLI Engine for Petro-SIM

Start Petro-SIM in the normal manner. Create a New **Case from Scratch** **(File > New > Case from scratch)**. The Simulation Basis Manager will be displayed.

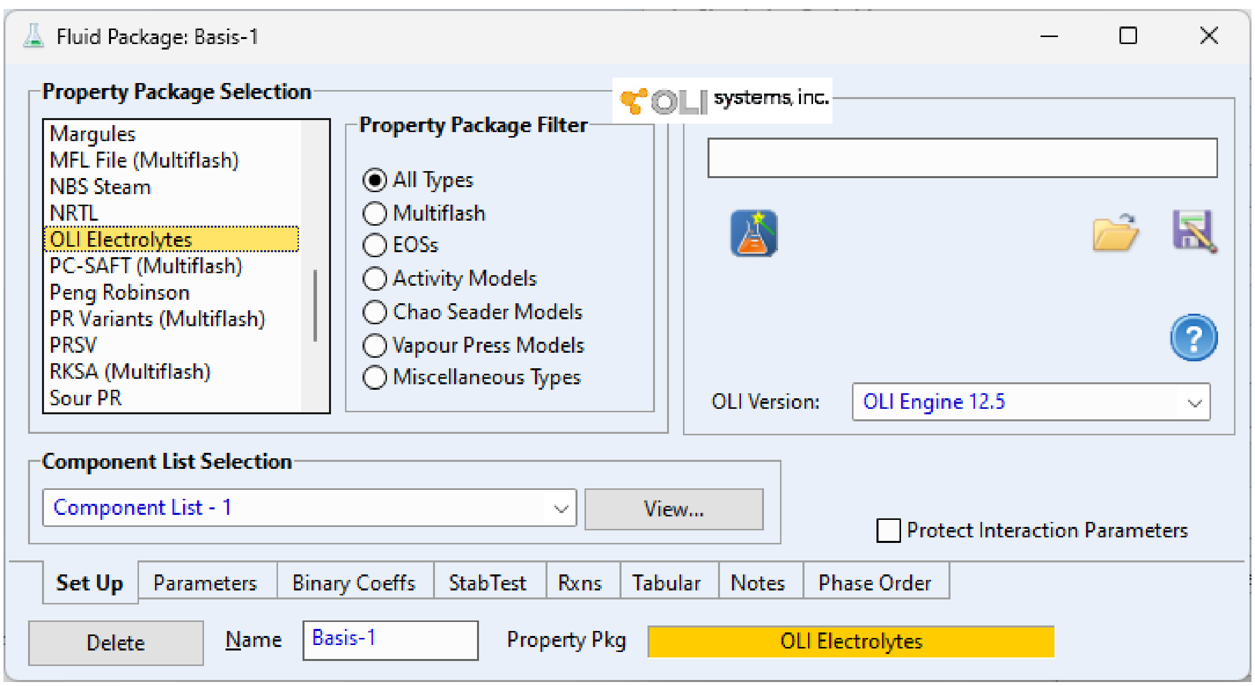


Click the **Add...** button.

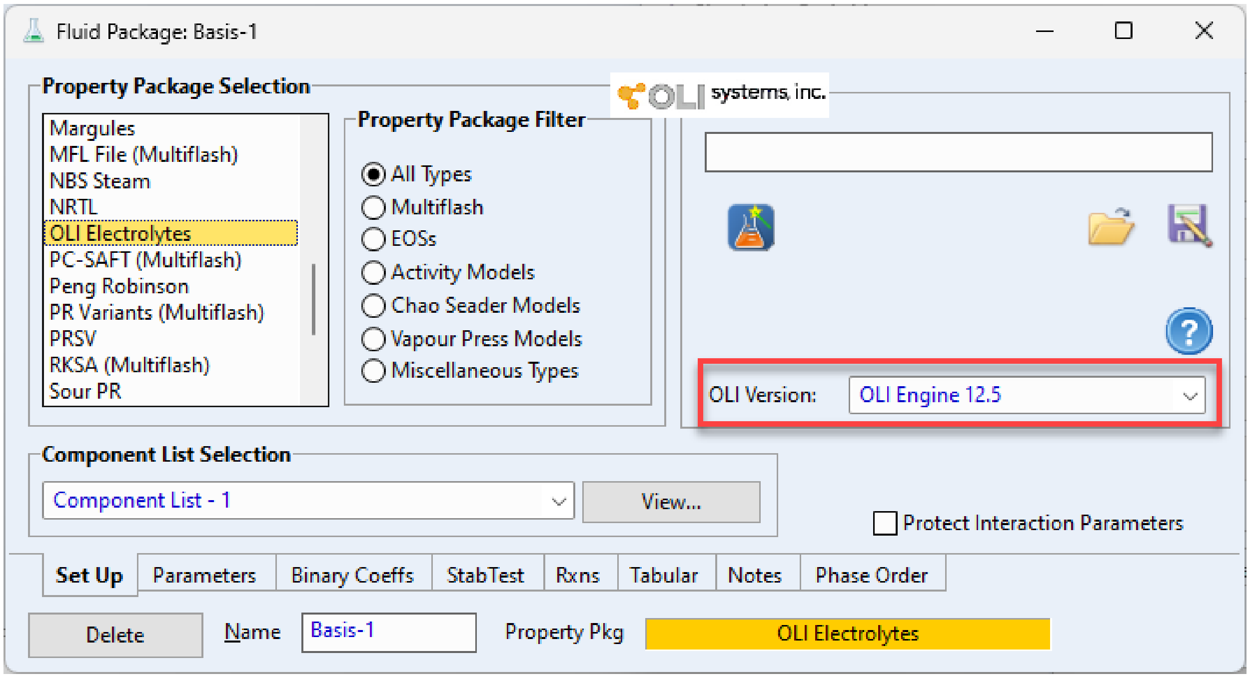
The Fluid Package: Basis-1 screen will appear. OLI recommends that you now select the ***OLI Electrolytes fluid package***.



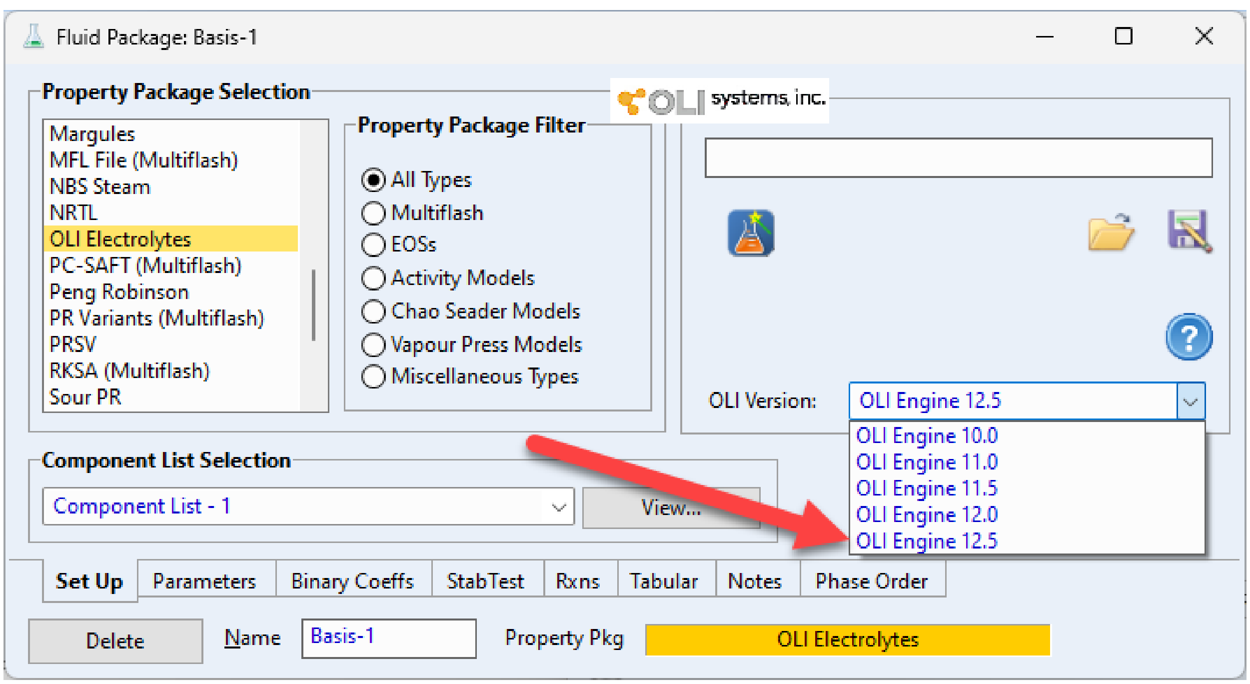
This will display a new panel:



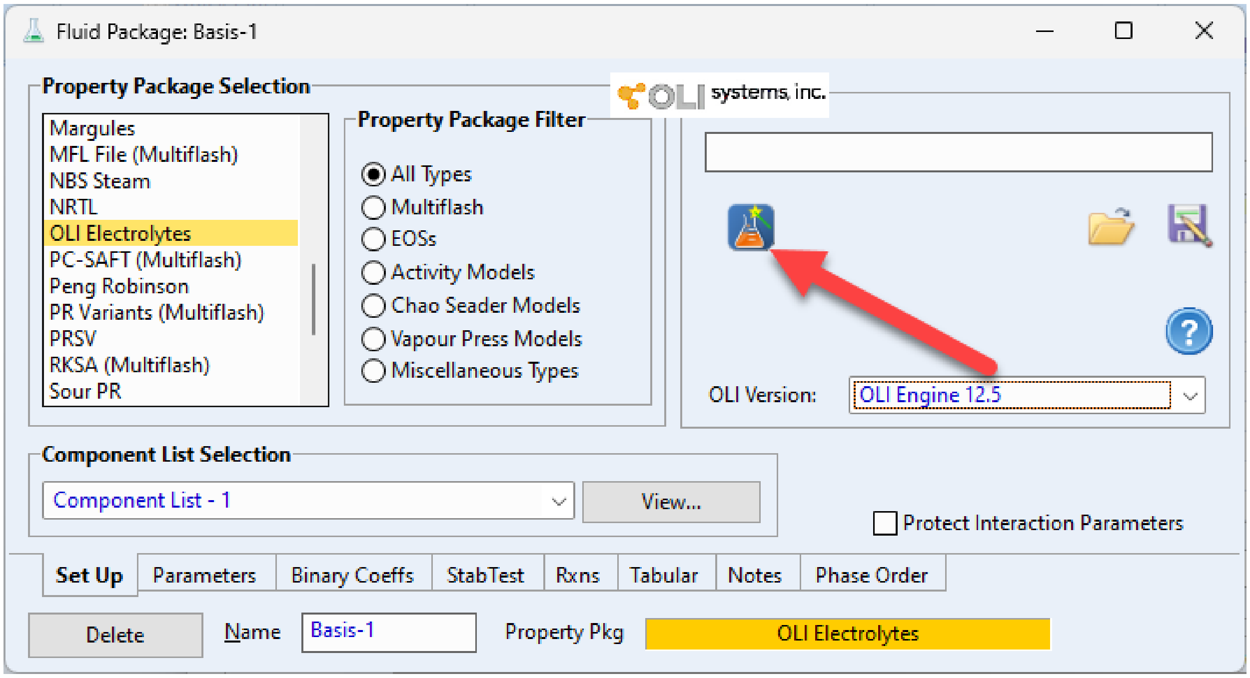
You can use multiple versions of the OLI Engine. Currently displayed is OLI Engine 12.5. If you have more than one OLI Engine, you can select from an older version. Click the drop-down button:



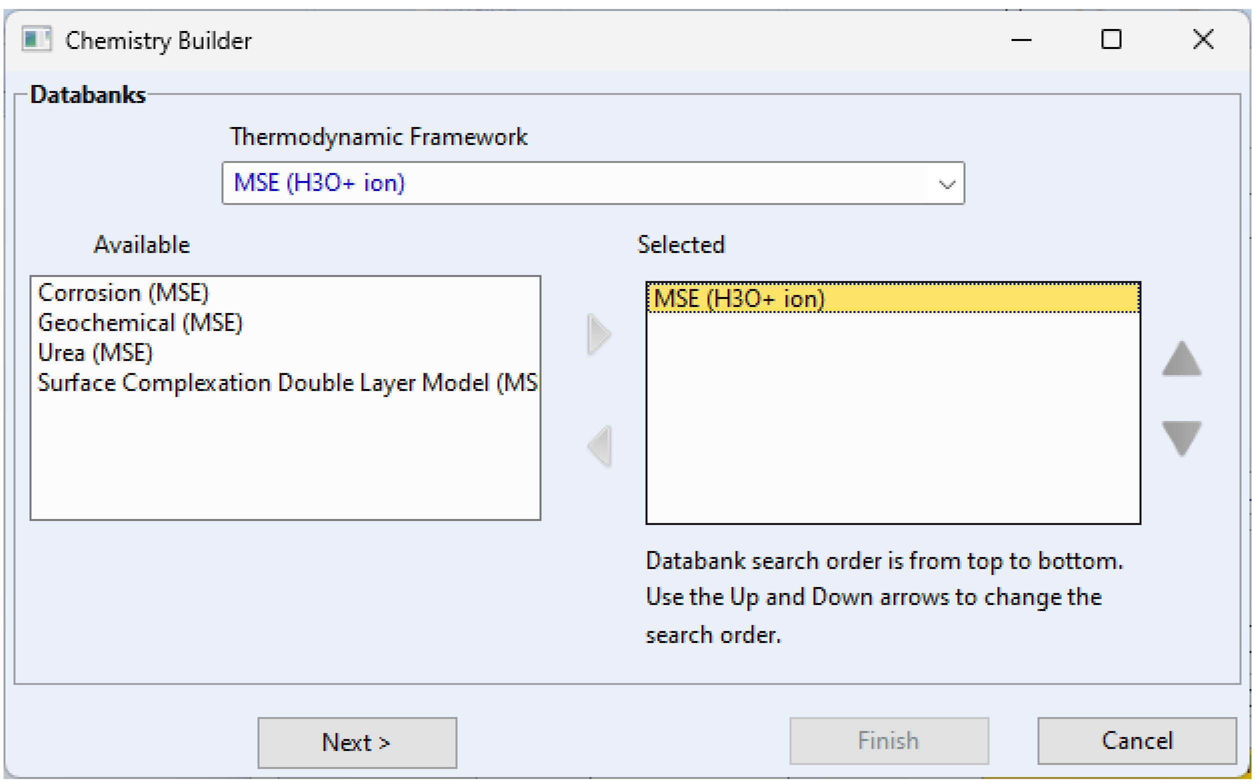
This will show the OLI Engines for Petro-SIM that are installed. Be careful to choose the engine you require (OLI recommends the most recent version).



You can import a previously built OLI model (called a .dbs file) or, preferentially, use the internal OLI Chemistry Wizard.



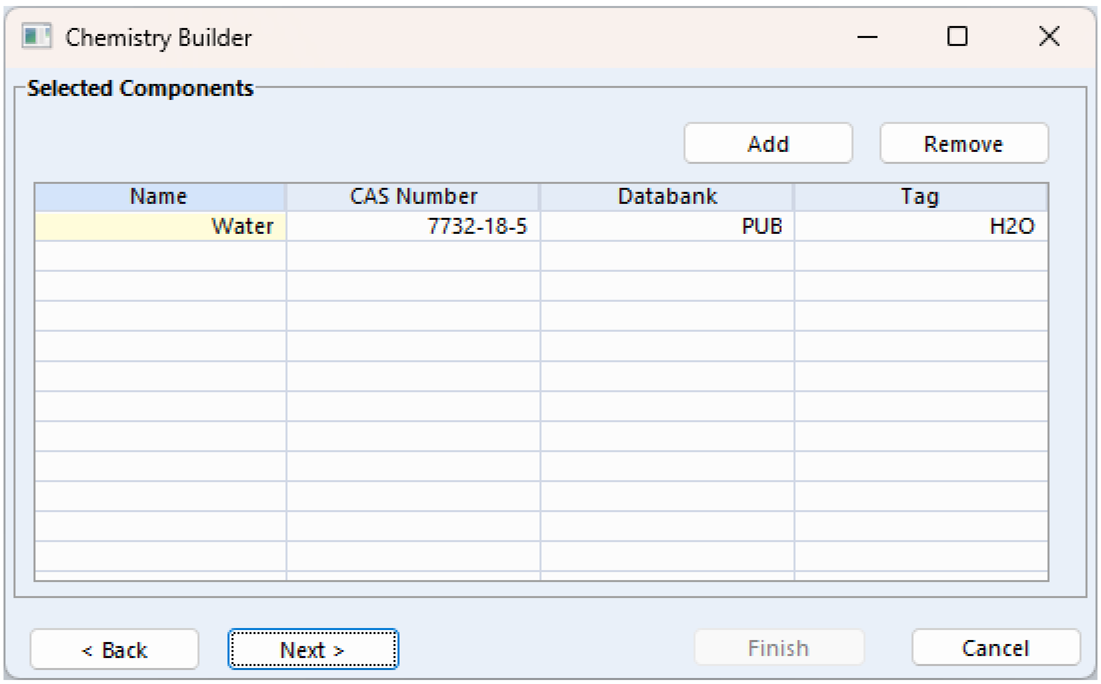
Click the indicated icon.



You can change the thermodynamic framework on this screen as well as select private databases. We'll use the Mixed-Solved Electrolyte (MSE) thermodynamic framework. You can read more on this topic from the following links:

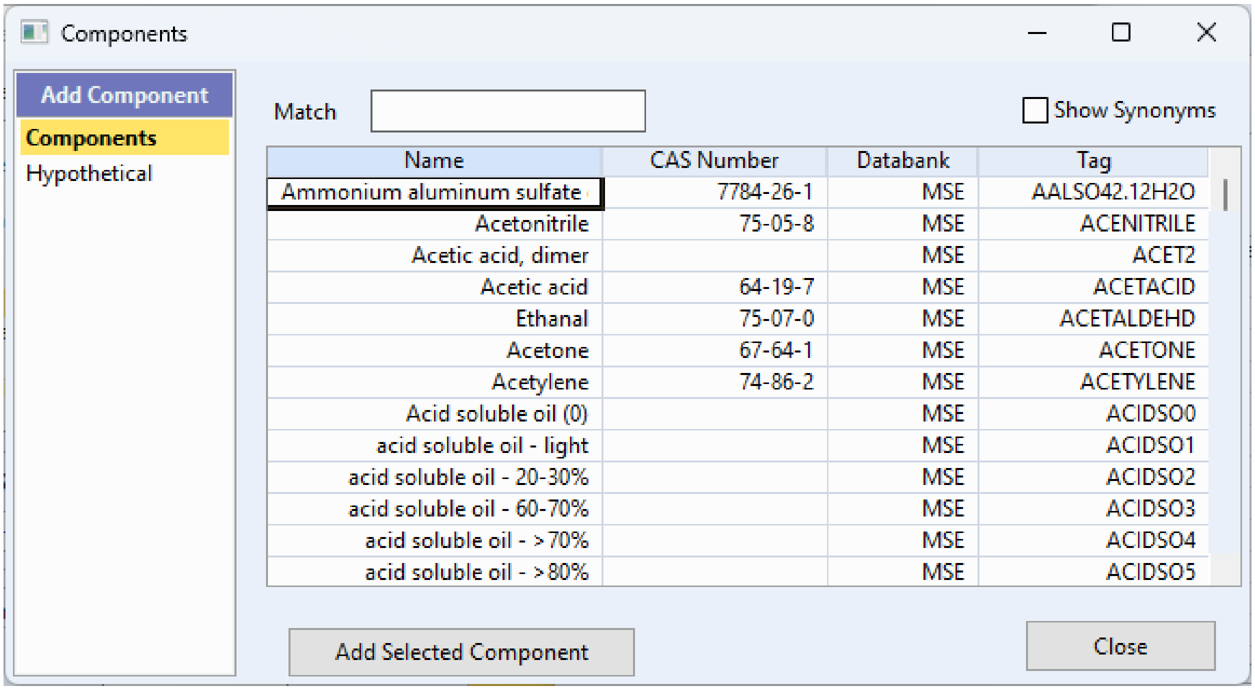
- **When to use the MSE thermodynamic framework instead of the AQ thermodynamic framework**: https://support.olisystems.com/hc/en-us/articles/28774537885331-When-to-use-the-MSE-thermodynamic-framework-instead-of-the-AQ-thermodynamic-framework
- **Thermodynamic Frameworks**: https://support.olisystems.com/hc/en-us/sections/24116537677843-Thermodynamic-Frameworks

Click the **Next>** button.

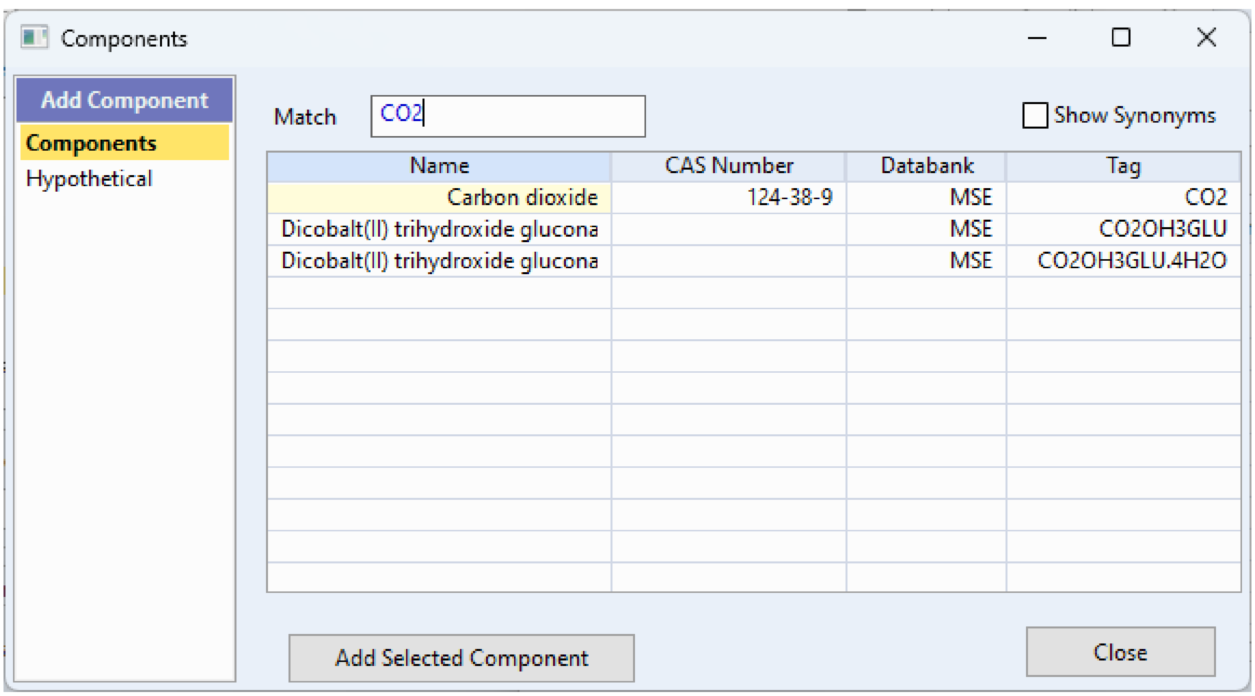


On this dialog, we will enter our components. H_2O is required for all models regardless if there is no flowrate for the component. You cannot remove this species. It will show its databank as PUB (AQ); however, it will actually be using the thermodynamic framework selected in the previous screen (MSE).

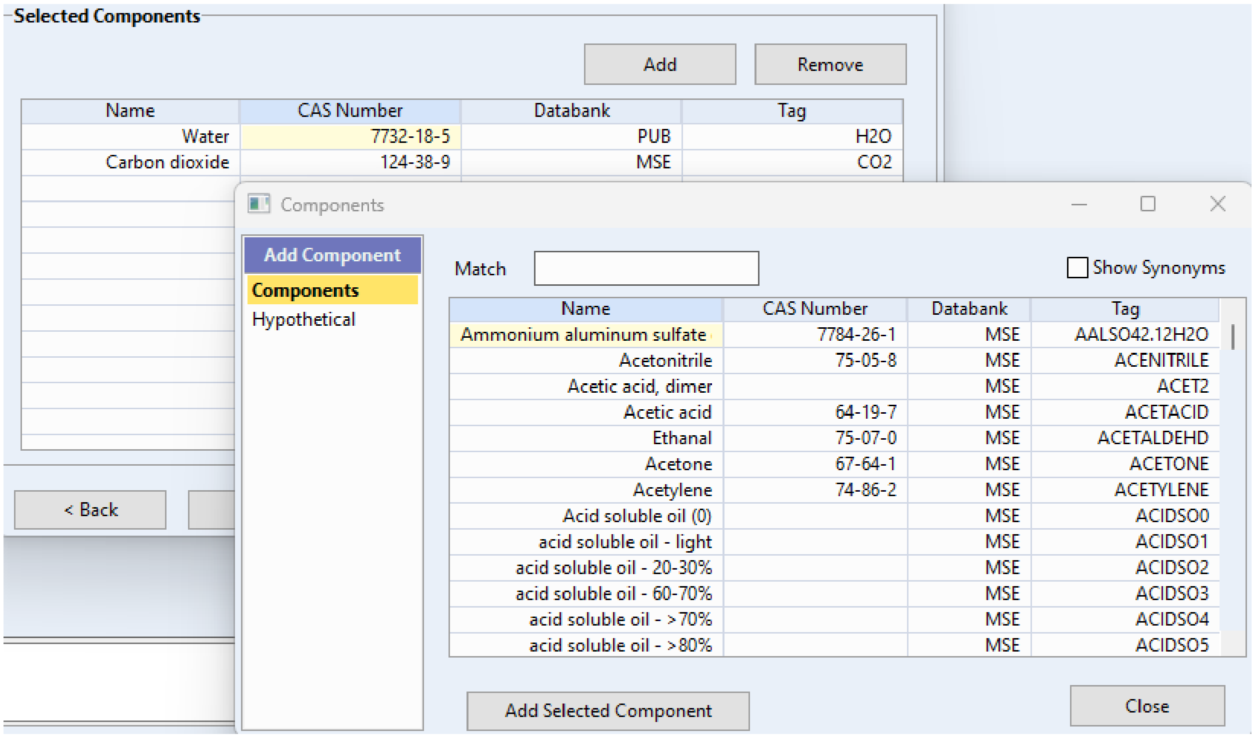
Click the **Add** button.



In the **Match** box, enter the first component which is CO_2. You can also scroll down to find the component, but the Match Box is faster.



Click the **Add Selected Component** button.



We have moved the dialog to the side to show that carbon dioxide has been added. Repeat these steps to add the following components:

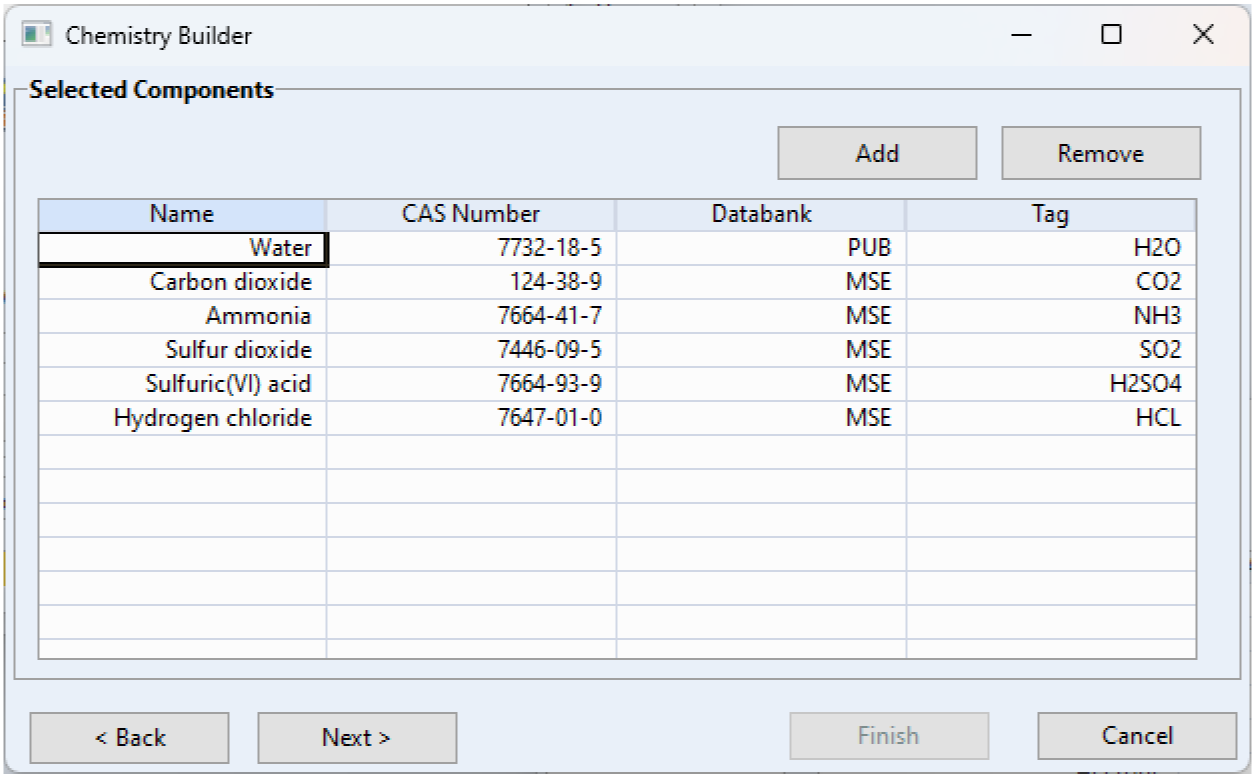
NH_3

SO_2

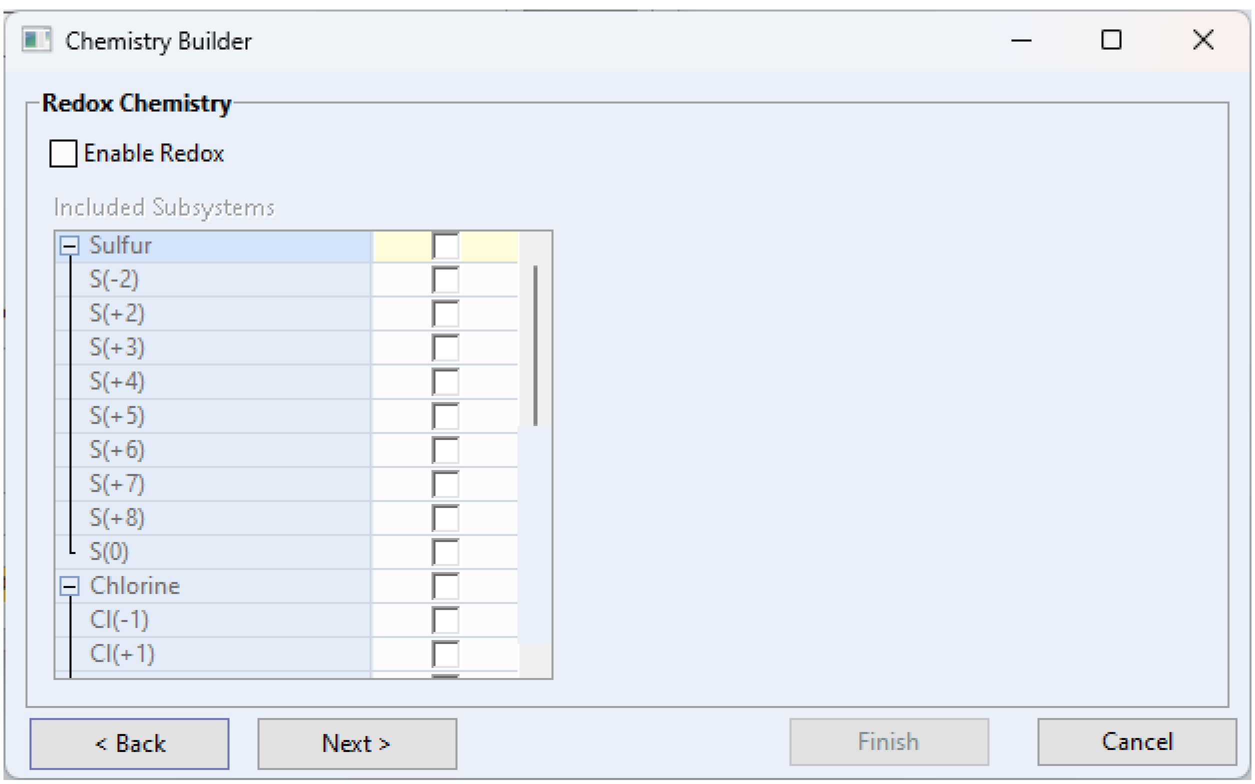
H_2SO_4

HCl

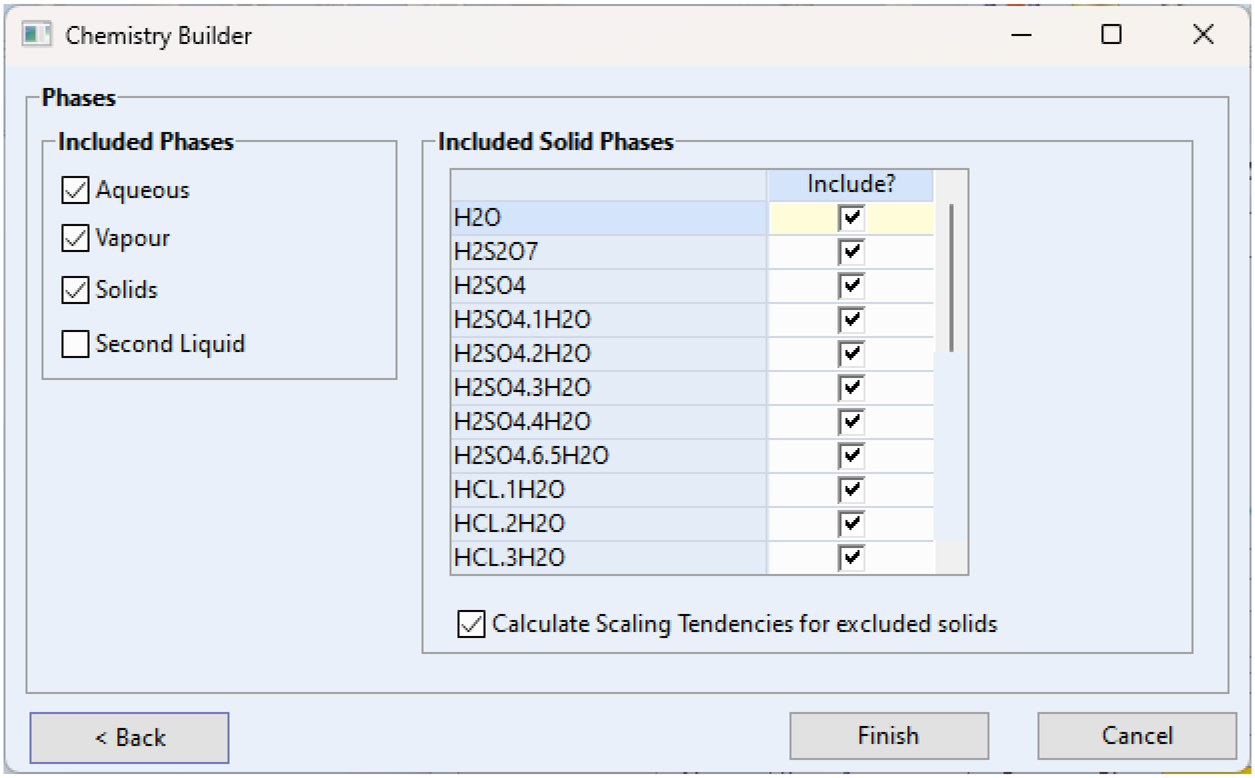
Click the **Close** button when finished.


Chemistry Builder
Selected Components
Add
Remove
Name
CAS Number
Databank
Tag
Water 7732-18-5 PUB H2O
Carbon dioxide 124-38-9 MSE CO2
Ammonia 7664-41-7 MSE NH3
Sulfur dioxide 7446-09-5 MSE SO2
Sulfuric(VI) acid 7664-93-9 MSE H2SO4
Hydrogen chloride 7647-01-0 MSE HCL
< Back
Next >
Finish
Cancel

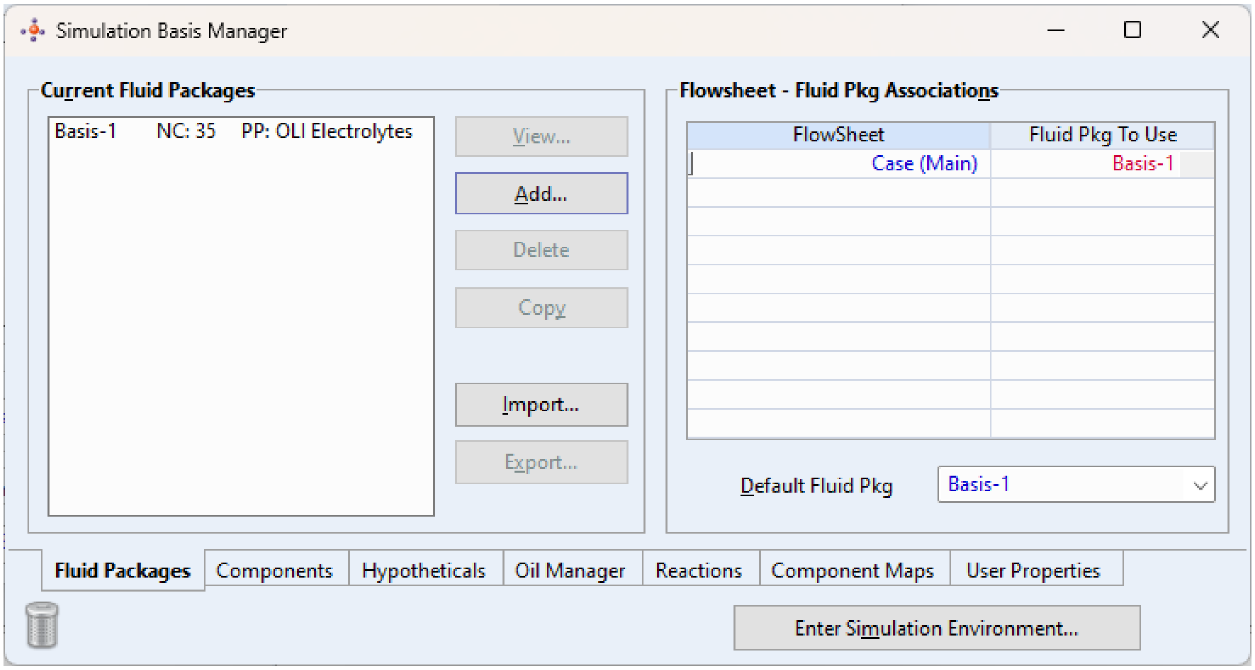
Click **Next>**


Chemistry Builder
Redox Chemistry
Enable Redox
Included Subsystems
Sulfur
S(-2)
S(+2)
S(+3)
S(+4)
S(+5)
S(+6)
S(+7)
S(+8)
S(0)
Chlorine
Cl(-1)
Cl(+1)
< Back
Next >
Finish
Cancel

The OLI Chemistry property package allows for oxidation and reduction chemistry. For this example, we will not be adding any of these features. Click the **Next>** button.



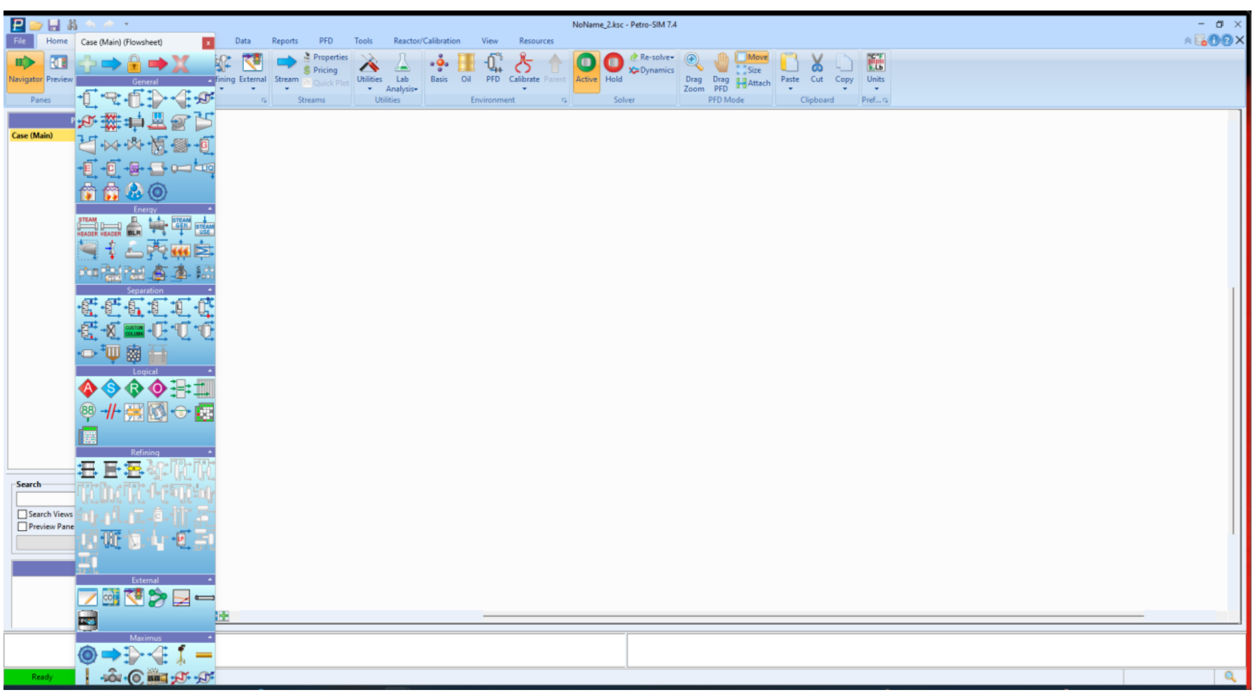
You can modify the phases in the model as well as select individual solid phases to remove. This can speed up the execution of the model by orders of magnitude but should be used with caution and experience. We will not make any modifications here. Click the **Finish>** button.



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

Creating the Simulation

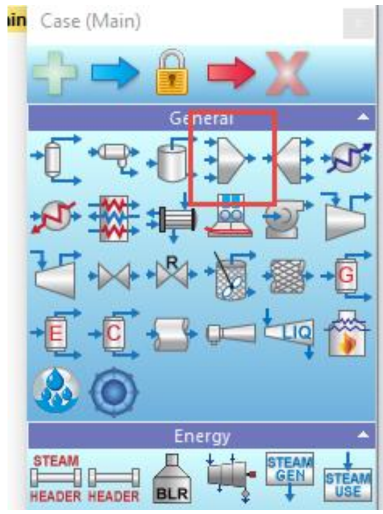
At this point, everything you know about creating simulations in Petro-SIM is still true.



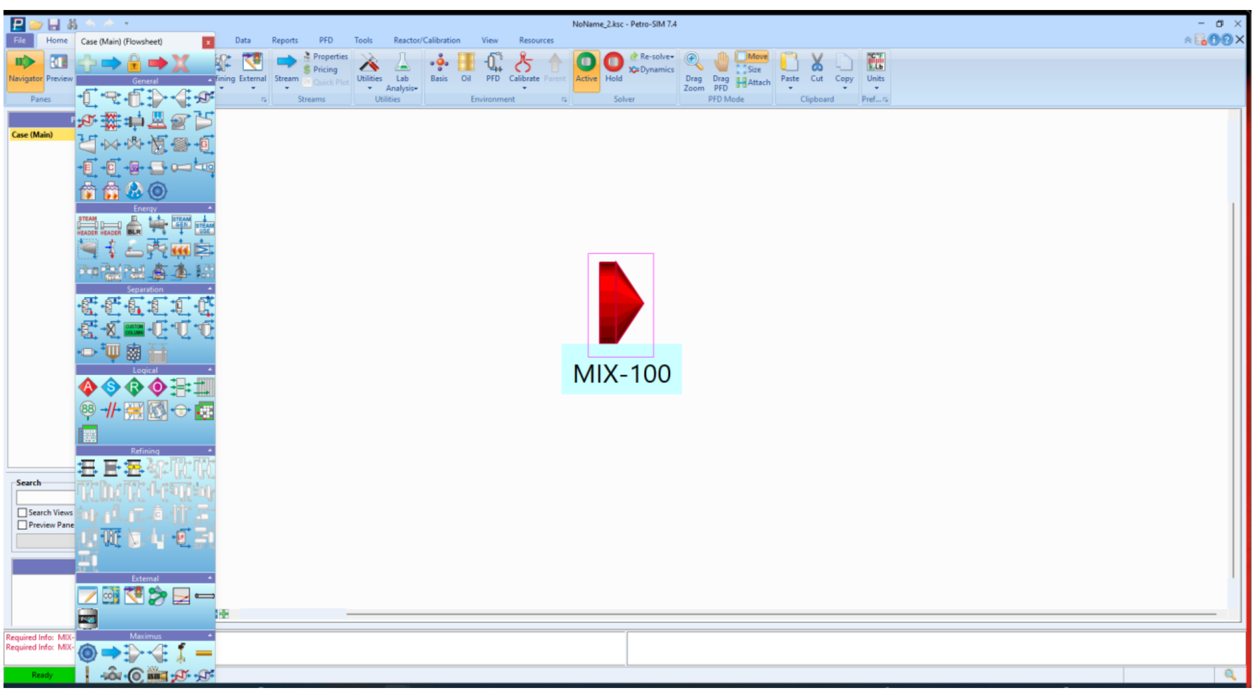
We will now create a small process using a mixer with two inlet streams. The user is expected to know how to create the process. Please do not enter any conditions for the inlet streams at this time.

Selecting the mixer

From the tools palette, we will click on the **mixer** (in General) and then drag it to the workspace.



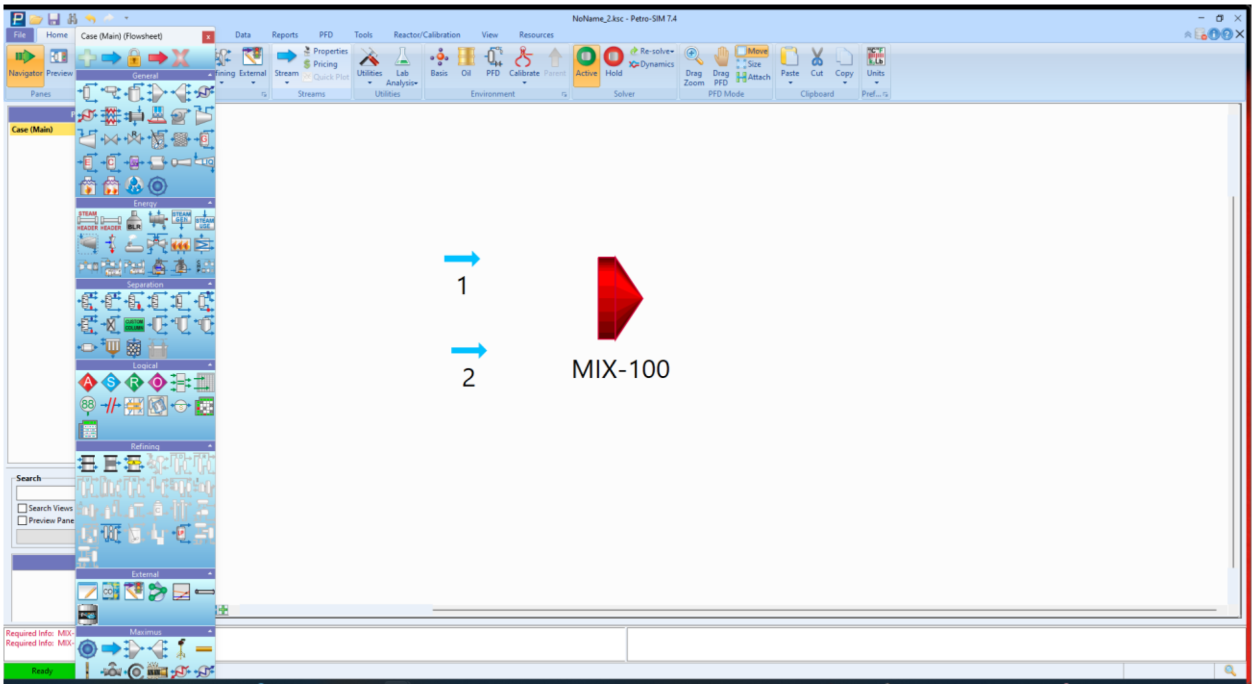
The workspace now looks like this:



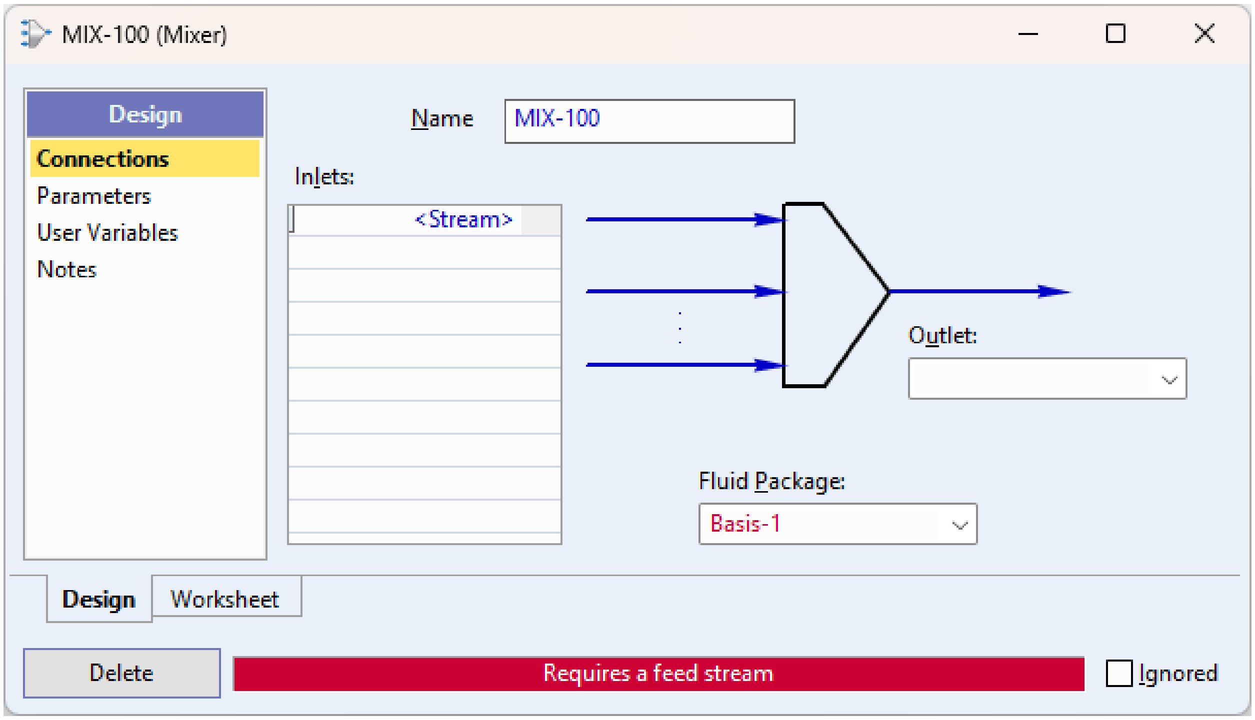
The mixer is given a default name of MIX-100. You can change it later if you wish. The block is also colored RED. This indicates that the block does not have sufficient information to calculate.

We need to create two inlet streams.

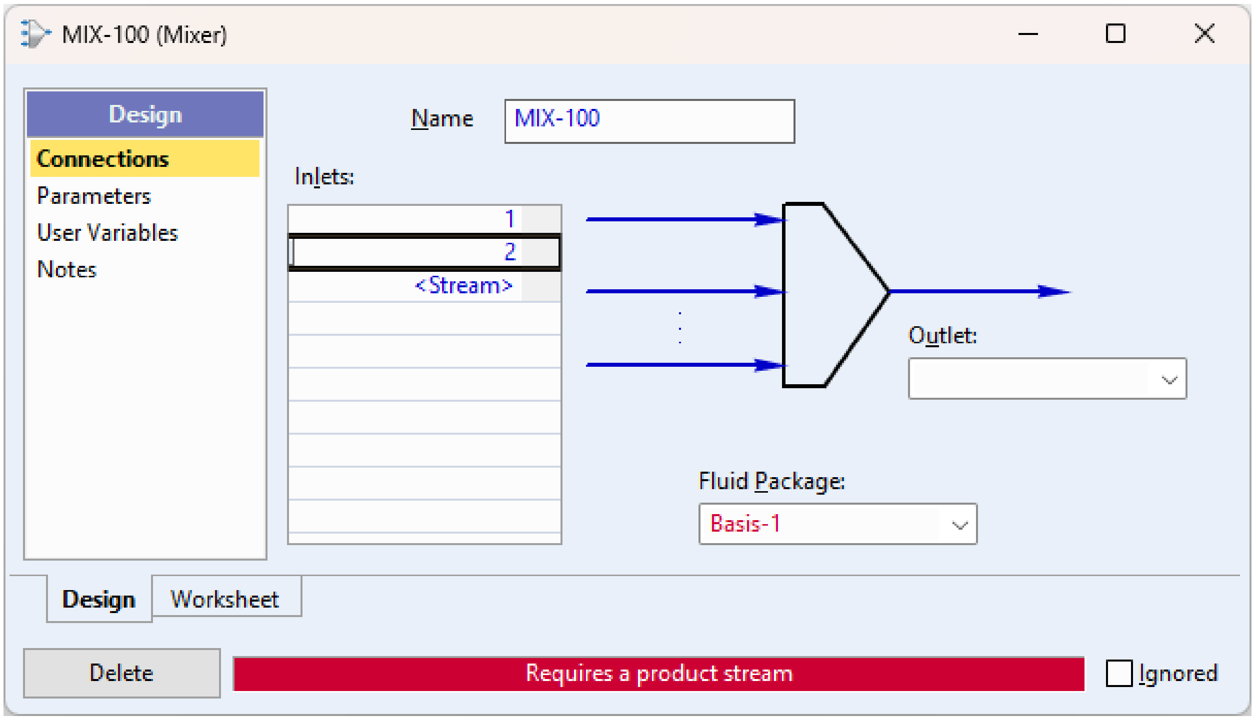
Click on the **Material Streams** arrows, and place two of them on the workspace.



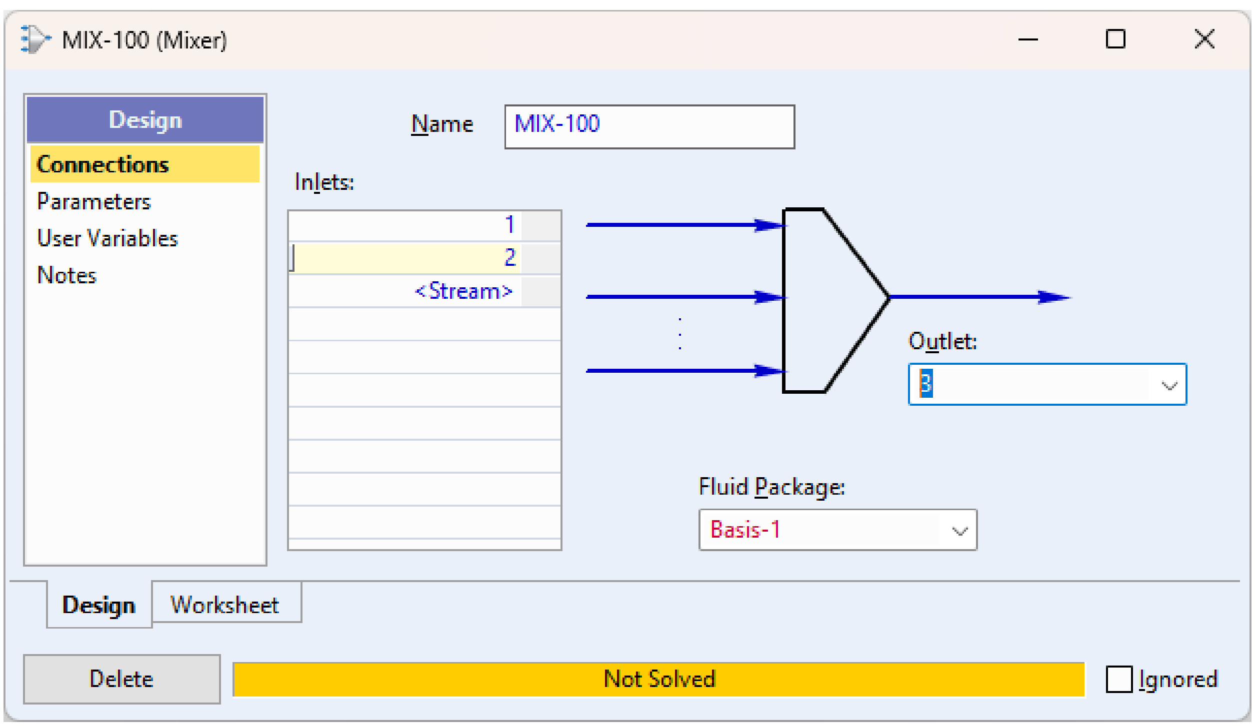
Double-click the Mixer Block. This will open another window.



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



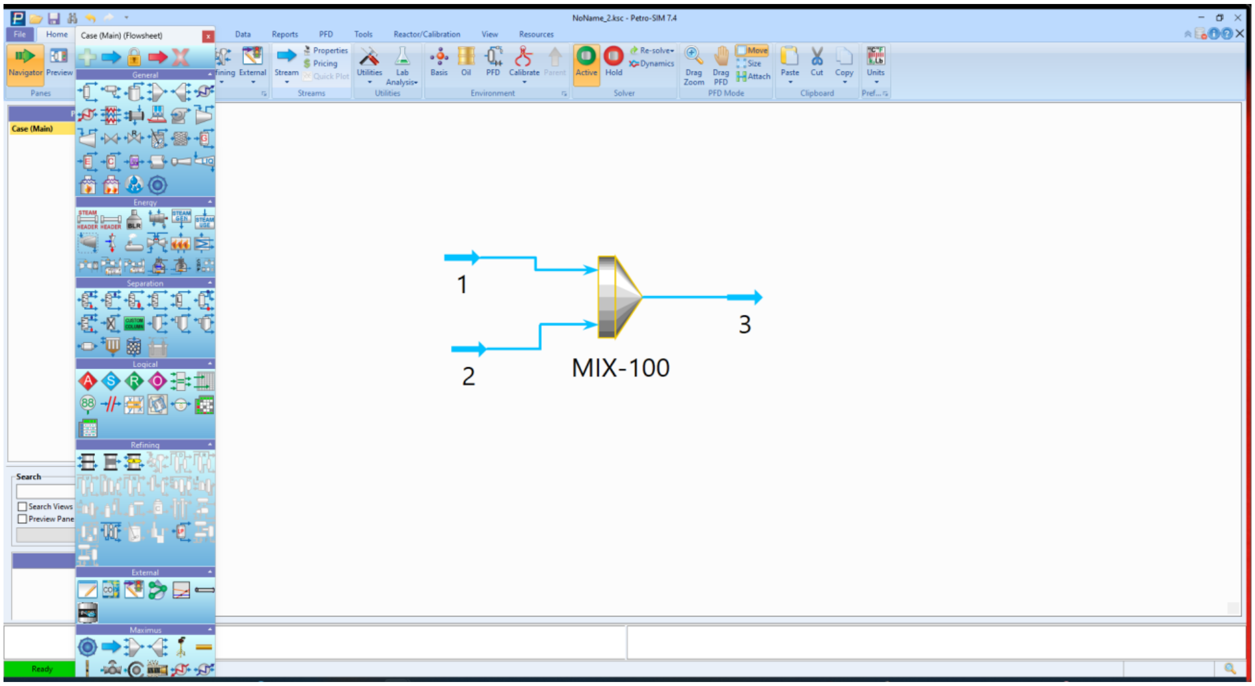
Locate the ***Outlet*** box and enter the number "**3**". This completes this block.



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

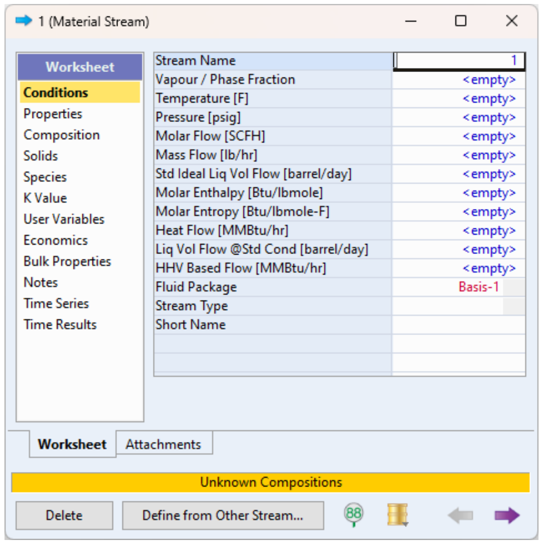
Click the ***x*** in the upper right-hand corner to close this dialog.

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



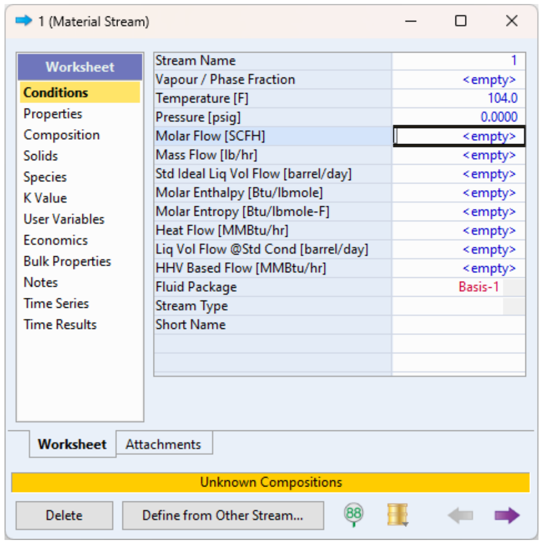
Entering Stream Composition Data

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

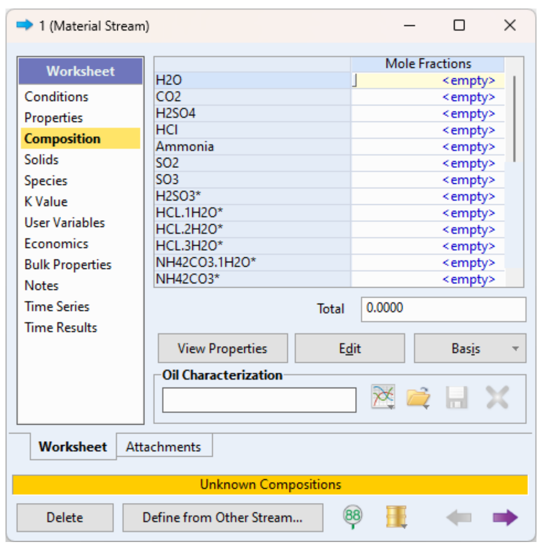


This is the standard input window for a stream. We will now add our conditions.

- Locate the cell for Temperature [F] and enter 104
- Locate the cell for Pressure [psig] and enter 0.0



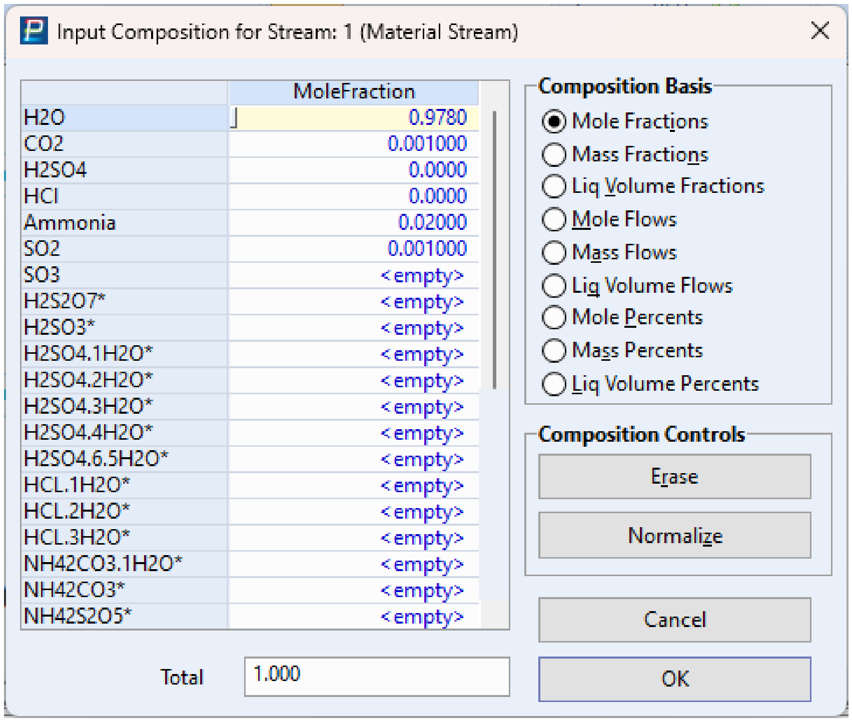
Now click the ***Composition*** line



We can now enter our composition for our components.

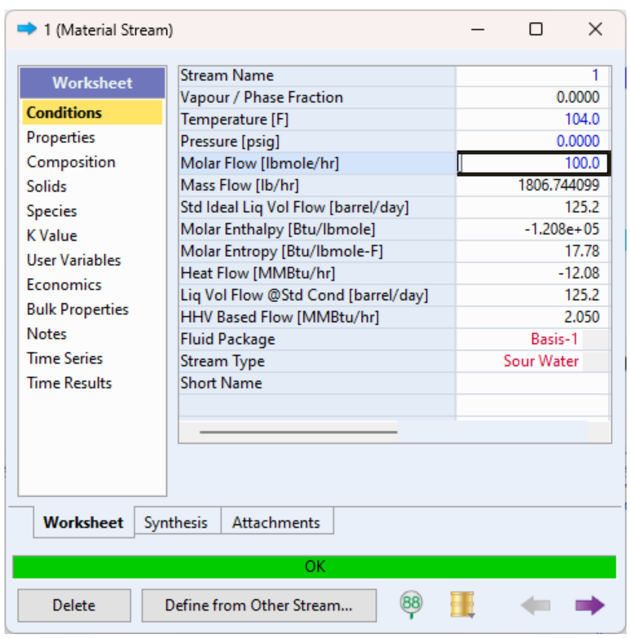
Now begin entering the value for **H2O** of 0.978

This will pop open another dialog.



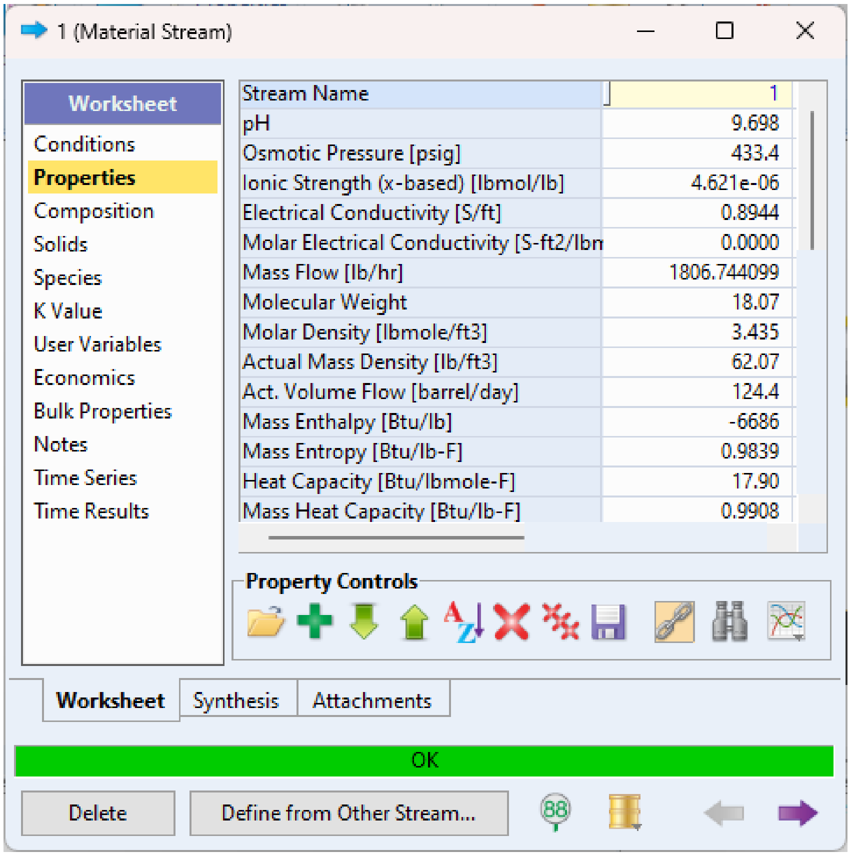
Enter the compositions as shown and then click the **OK** button.

Go back to the **Conditions** category, and enter a molar flow of 100 lbmole/hr.

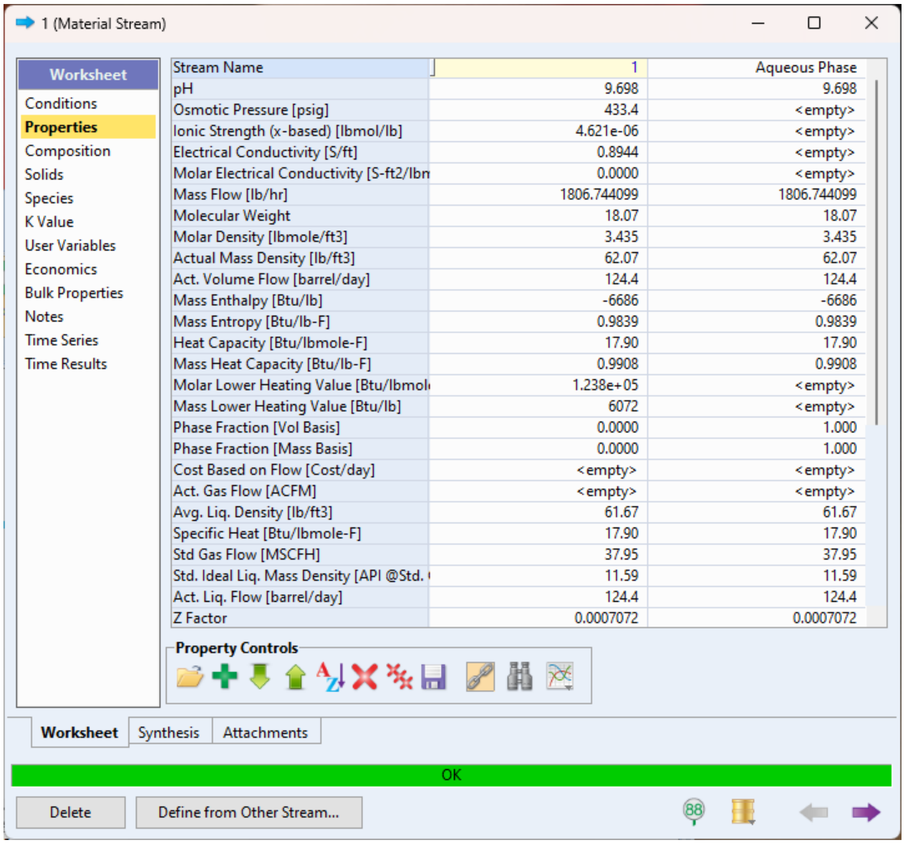


The status bar should turn green. This indicates that the program has already converged the stream. We can see some useful information at this time.

Click on the **Properties** line.

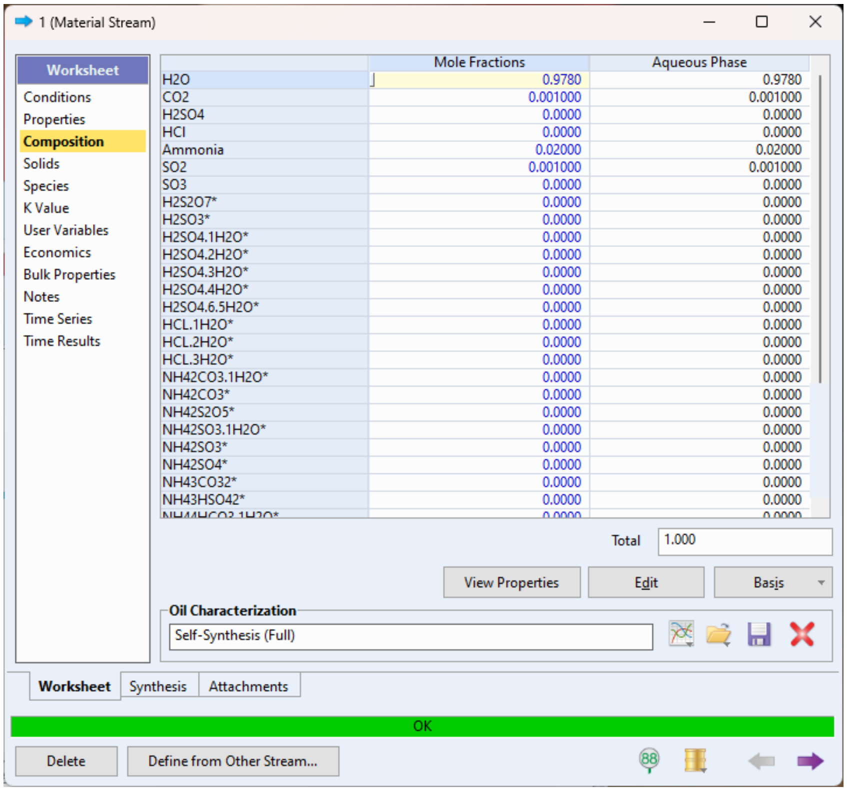


You can drag the dialog to the right to expand it to see more data.

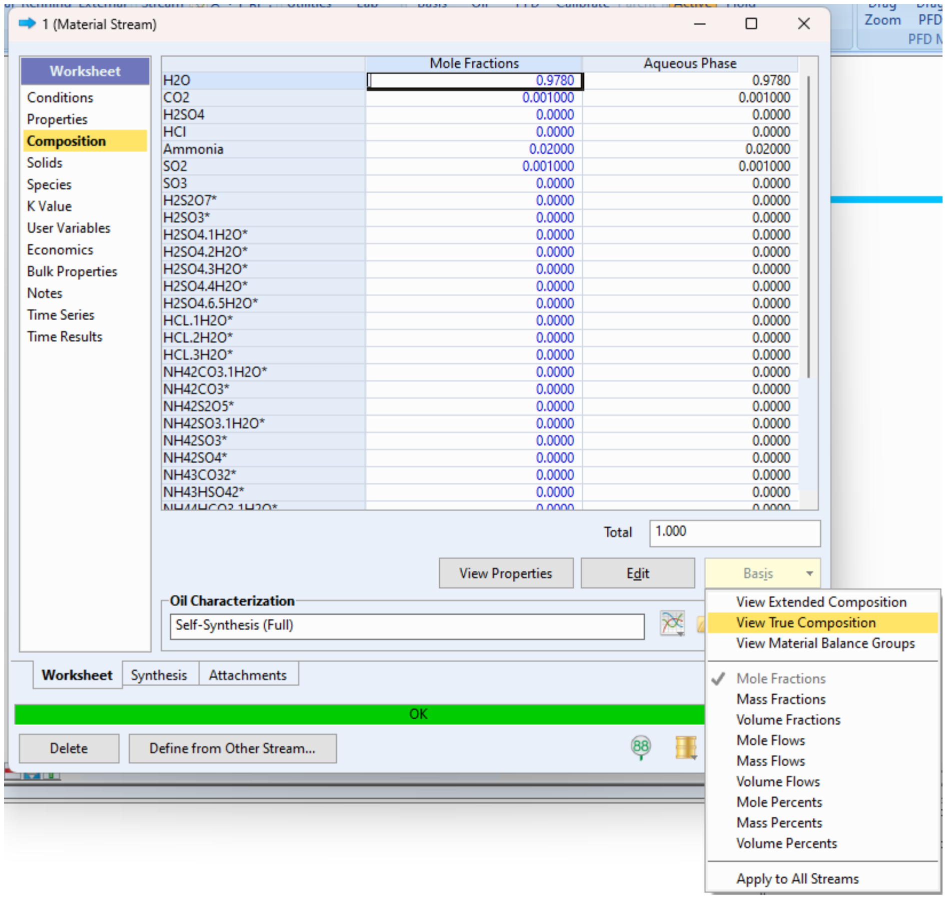


The pH of this solution is approximately 9.7. We also provide additional information. You can also explore other buttons, such as composition, to see more information about our report.

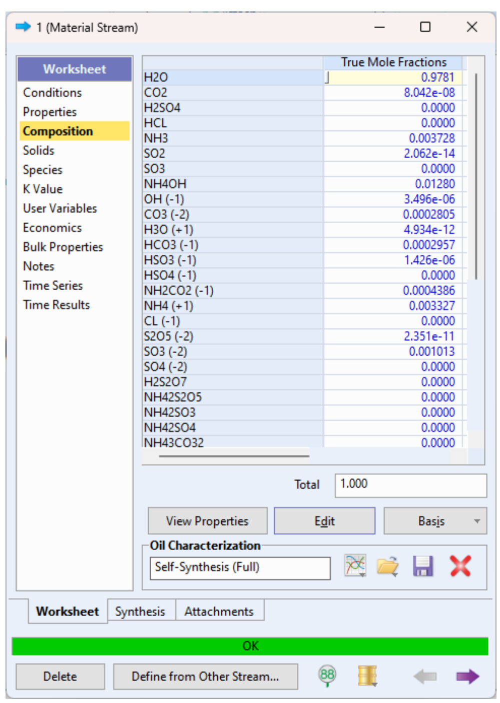
Click on the **Composition** line.



Click on the **Basis** button



Select **View True Composition**

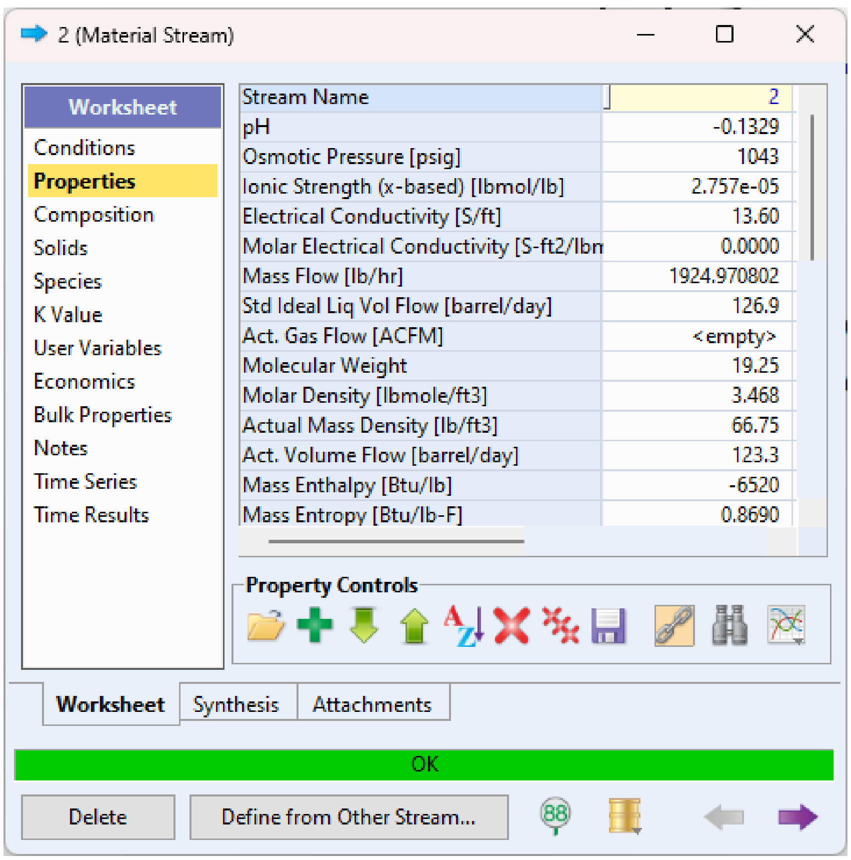


Now, you can see things like the solution ions. You can expand the dialog to see information about phases.

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

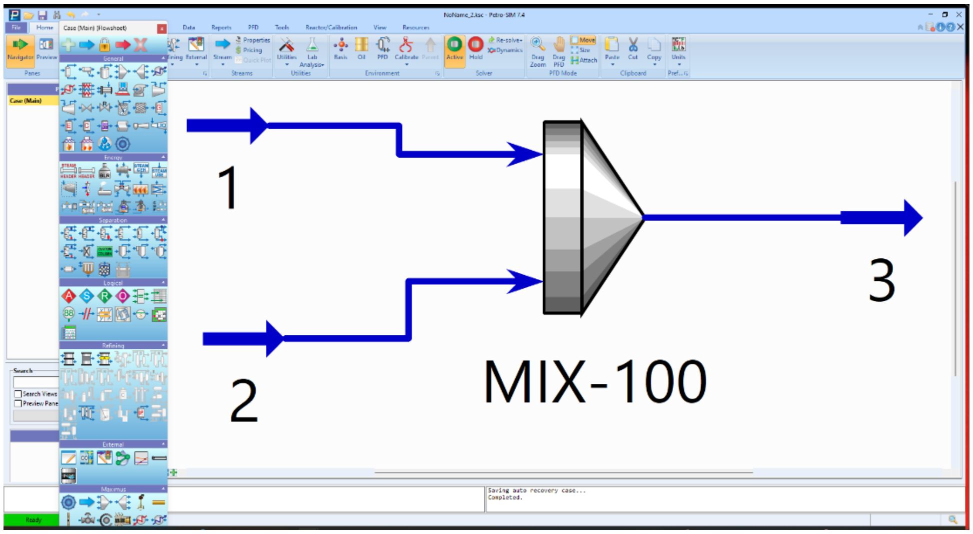
Temperature	77	[F]
Pressure	0	[psig]
H2O	0.979	
HCl	0.001	
H2SO4	0.02	
Total molar flow	100	[lbmole/hr]

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



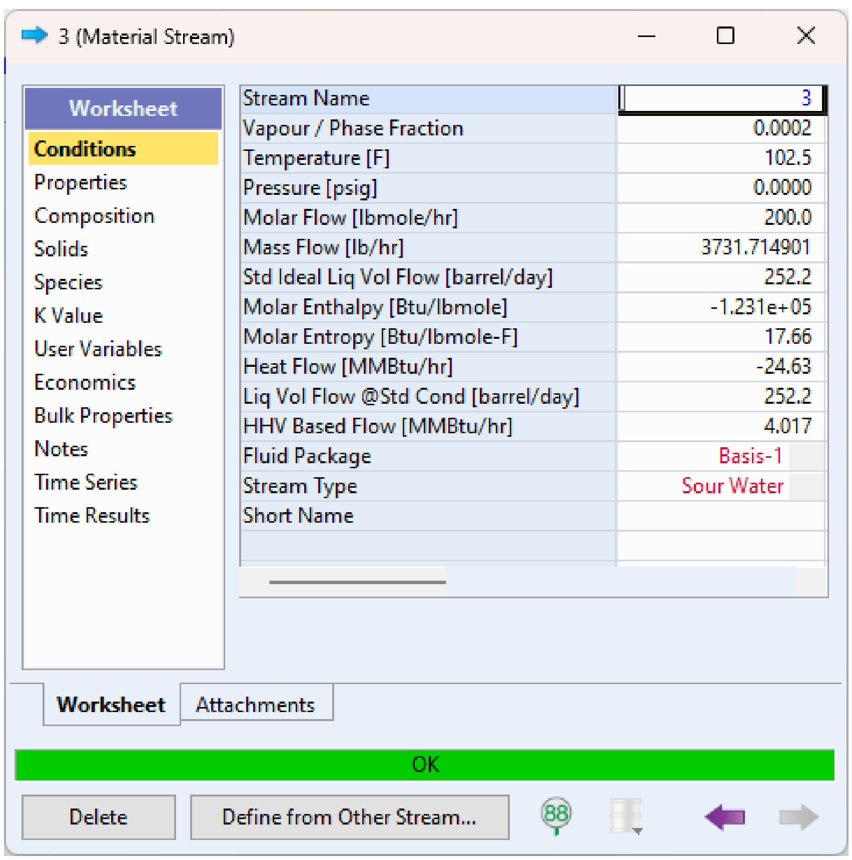
Click the ***x*** to close the dialog.

Petro-SIM 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.



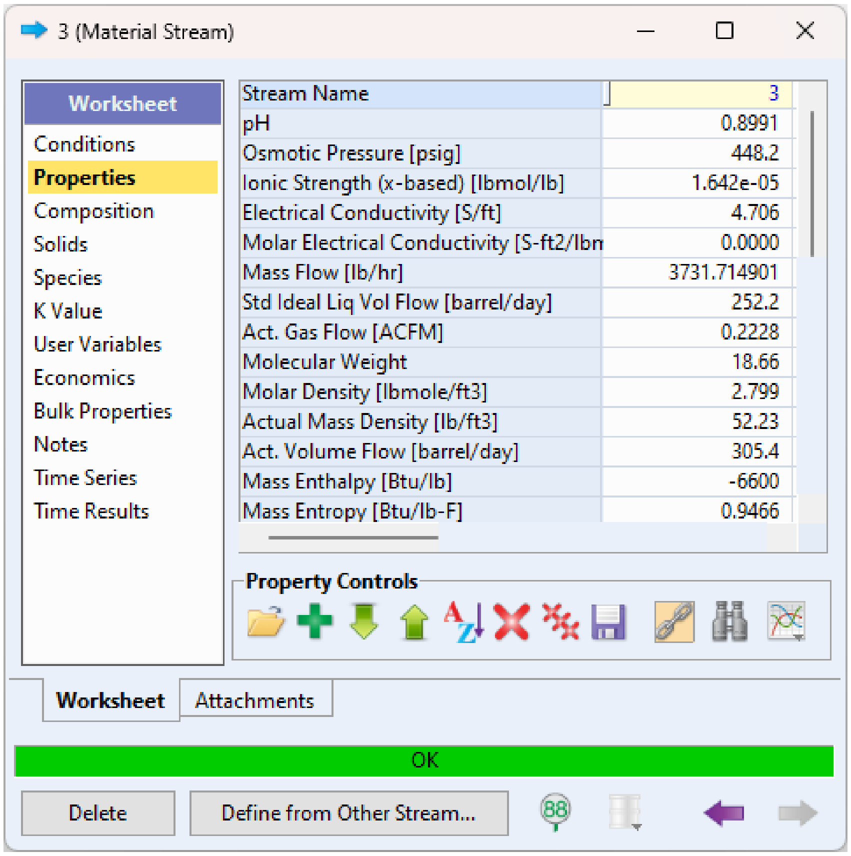
Reviewing the output

Double-click stream "3"



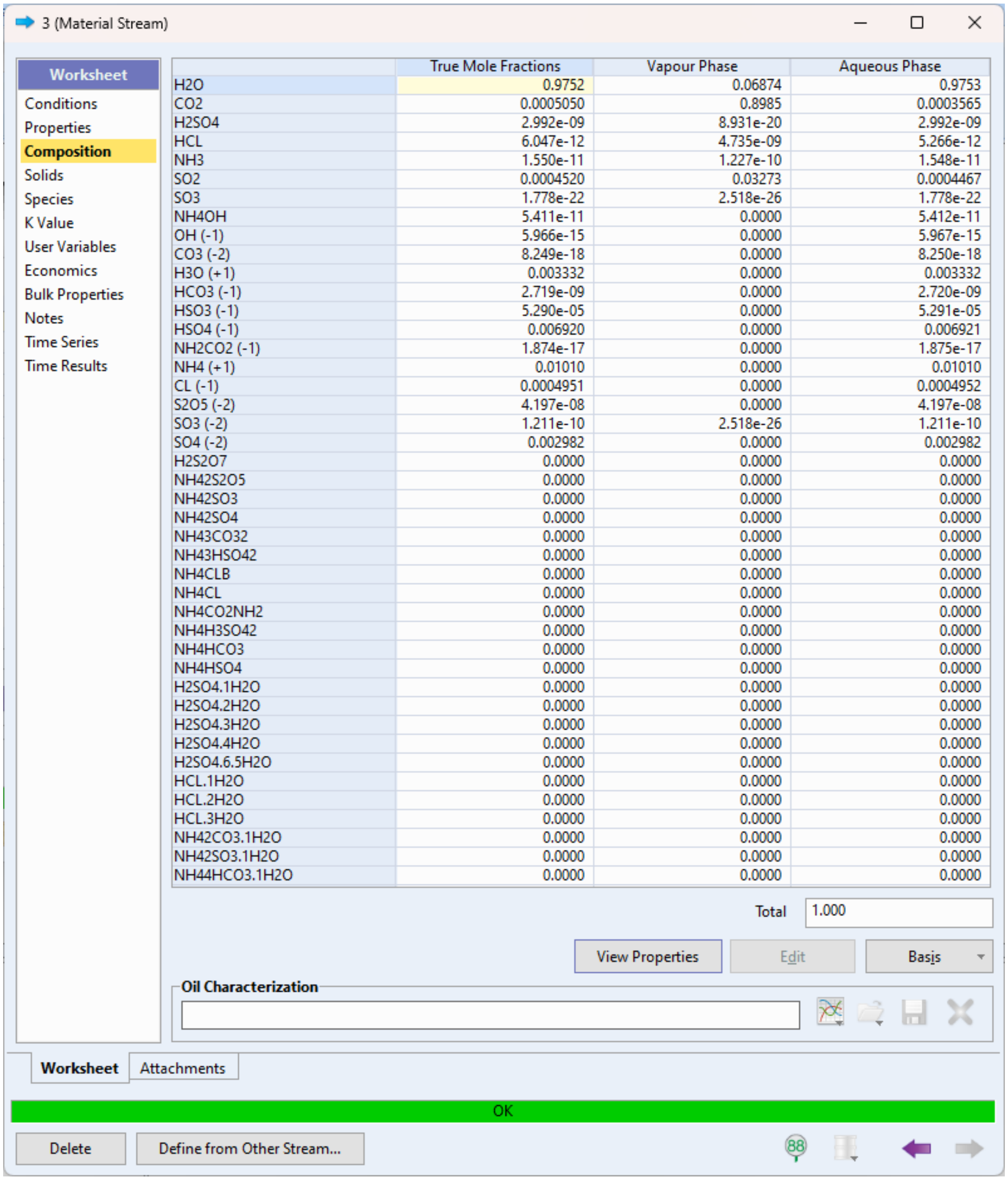
The converged process temperature is approximately 102.5 °F.

Click on the **Properties** line.



The converged pH is 0.9 indicating that some acid/base chemistry has taken place. What about the equilibrium compositions that have been calculated?

Click the ***Composition*** line and use the **Basis** button to **View True Composition**



	True Mole Fractions	Vapour Phase	Aqueous Phase
H2O	0.9752	0.06874	0.9753
CO2	0.0005050	0.8985	0.0003565
H2SO4	2.992e-09	8.931e-20	2.992e-09
HCL	6.047e-12	4.735e-09	5.266e-12
NH3	1.550e-11	1.227e-10	1.548e-11
SO2	0.0004520	0.03273	0.0004467
SO3	1.778e-22	2.518e-26	1.778e-22
NH4OH	5.411e-11	0.0000	5.412e-11
OH (-1)	5.966e-15	0.0000	5.967e-15
CO3 (-2)	8.249e-18	0.0000	8.250e-18
H3O (+1)	0.003332	0.0000	0.003332
HCO3 (-1)	2.719e-09	0.0000	2.720e-09
HSO3 (-1)	5.290e-05	0.0000	5.291e-05
HSO4 (-1)	0.006920	0.0000	0.006921
NH2CO2 (-1)	1.874e-17	0.0000	1.875e-17
NH4 (+1)	0.01010	0.0000	0.01010
CL (-1)	0.0004951	0.0000	0.0004952
S2O5 (-2)	4.197e-08	0.0000	4.197e-08
SO3 (-2)	1.211e-10	2.518e-26	1.211e-10
SO4 (-2)	0.002982	0.0000	0.002982
H2S2O7	0.0000	0.0000	0.0000
NH42S2O5	0.0000	0.0000	0.0000
NH42SO3	0.0000	0.0000	0.0000
NH42SO4	0.0000	0.0000	0.0000
NH43CO32	0.0000	0.0000	0.0000
NH43HSO42	0.0000	0.0000	0.0000
NH4CLB	0.0000	0.0000	0.0000
NH4CL	0.0000	0.0000	0.0000
NH4CO2NH2	0.0000	0.0000	0.0000
NH4H3SO42	0.0000	0.0000	0.0000
NH4HCO3	0.0000	0.0000	0.0000
NH4HSO4	0.0000	0.0000	0.0000
H2SO4.1H2O	0.0000	0.0000	0.0000
H2SO4.2H2O	0.0000	0.0000	0.0000
H2SO4.3H2O	0.0000	0.0000	0.0000
H2SO4.4H2O	0.0000	0.0000	0.0000
H2SO4.6.5H2O	0.0000	0.0000	0.0000
HCL.1H2O	0.0000	0.0000	0.0000
HCL.2H2O	0.0000	0.0000	0.0000
HCL.3H2O	0.0000	0.0000	0.0000
NH42CO3.1H2O	0.0000	0.0000	0.0000
NH42SO3.1H2O	0.0000	0.0000	0.0000
NH44HCO3.1H2O	0.0000	0.0000	0.0000

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

Additional Resources

Our [Support Center] has more articles for using the OLI Engine in Petro-SIM®. See more here:

- Using OLI Engine in Petro-SIM®: https://support.olisystems.com/hc/en-us/articles/37054530247955-Using-OLI-Engine-in-Petro-SIM
- OLI Engine V12 for Petro-SIM®: Getting Started User Guide: https://support.olisystems.com/hc/en-us/articles/37376053273107-OLI-Engine-V12-for-Petro-SIM-Getting-Started-User-Guide
- Using an OLI .dbs Chemistry File in Petro-SIM®: https://support.olisystems.com/hc/en-us/articles/37434861404179-Using-an-OLI-dbs-Chemistry-File-in-Petro-SIM
- OLI Engine in Petro-SIM® page: https://support.olisystems.com/hc/en-us/sections/37054468310035-OLI-Engine-in-Petro-SIM

Disclaimer

This tutorial was created with Petro-SIM 7.4 and the OLI Engine version 12.5.18.0. 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 Petro-SIM or OLI will yield the same results.

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