

# INTRODUCTION TO OLI Engine 12.x for Unisim Design

think simulation

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.

## **Trademarks**

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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



UniSim Design K491 le Tools Help Ctrl+N ٩ <u>N</u>ew Case **b** Refinery Case <u>O</u>pen Ctrl+S Save Template Save As... Ctrl+Shift+S -၀ိ္တ္ရွိ Co<u>l</u>umn Sa<u>v</u>e All... P<u>V</u>T Exp Template <u>C</u>lose Case Case Scenario Project Close All.

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

| 🔰 NoName.usc - UniSim Design R500 | -                                 | . 🗆      | ×          |
|-----------------------------------|-----------------------------------|----------|------------|
| File Edit Basis Tools Window Help |                                   |          |            |
| Ů ⊡ ⊟ ⊖ Ц ⊍ ≚ ≫ ♫ 🦕               | Environment: Basis<br>Mode: Stead | ly State | Ö          |
| 🛆 Simulation Basis Manager        |                                   |          | 5)         |
| Component Lists                   |                                   |          | õ          |
| Master Component List View        |                                   |          | (F1        |
| Add                               |                                   |          | $\bigcirc$ |
| Delete                            |                                   |          |            |
| Сору                              |                                   |          | 00         |
| Import                            |                                   |          |            |
| Export                            |                                   |          |            |
| Refresh                           |                                   |          |            |
| Re-import                         |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
| Enter PV I Environment            |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
|                                   |                                   |          |            |
| Application is not registered for | OLE Automation.                   |          |            |

## **Selecting Fluid Packages**

OLI recommends starting with adding a fluid package.

Select Fluid Packages

| A Simulation Basis Manager |                          |                       |             |           |                     |                 |
|----------------------------|--------------------------|-----------------------|-------------|-----------|---------------------|-----------------|
| Component Lists            |                          | 1                     |             |           |                     |                 |
| Master Component List      | View                     |                       |             |           |                     |                 |
|                            | Add                      |                       |             |           |                     |                 |
|                            | Delete                   |                       |             |           |                     |                 |
|                            | Сору                     |                       |             |           |                     |                 |
|                            | Import                   |                       |             |           |                     |                 |
|                            | Export                   |                       |             |           |                     |                 |
|                            | Refresh                  |                       |             |           |                     |                 |
|                            | Re-import                |                       |             |           |                     |                 |
| Components Fluid Pkgs      | Hypotheticals            | Hypo Correlation Sets | Oil Manager | Reactions | Component Maps      | Jser Properties |
| Enter PVT Environment      | <u>, , pouncileans</u> ) | Enter Regression En   | vironment   |           | Enter Simulation Er | vironment       |

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

#### Click the Add button

| 스 Simulation Basis Manager                                |  |
|---|--|
| Current Fluid Packages                                    | Flowsheet - Fluid Pkg Associatio <u>n</u> s                |
| View  | Flowsheet Fluid Pkg To Use                                 |
| Add   | Case (Main) <empty></empty>                                |
| Delete  |  |
| Сору  |  |
| View Users  | Default Fluid Pkg  |
| Import  | Fluid Pkg for New Sub-FlowSheets                           |
| Export  | Use Default Fluid Pkg     Use Parent's Fluid Pkg           |
| Components Fluid Pkgs Hypotheticals Hypo Correlation Sets | Oil Manager   Reactions   Component Maps   Jser Properties |
| Enter PVT Environment Enter Regression Env                | ironment Enter Simulation Environment                      |

Scroll down the window to find OLI\_Electrolyte

| 👙 Fluid Package: Basis-1   |   |
|--|---|
| Property Package Selection Kabadi-Danner Lee-Kesler-Plocker Margules MBWR NBS Steam NRTL OLI_Electrolyte Peng-Robinson PR-Twu PRSV REFPROP |   |
| Component List Selection Component List - 1 View   | Advanced Thermodynamics Switch To UniSim Thermo UniSim Thermo Regression Export |
| Set Up         Parameters         Parameters2         Binary Coeffs           Delete         Name         Basis-1         Property Pk      | Stab Test   Phase Order   Rxns   Tabular   Notes                                |

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**.

| Property Package Selection<br>Lee-Kesler-Plocker<br>MBWR<br>NBS Steam<br>NRTL<br>OLL_Electrolyte<br>Peng-Robinson<br>PR-Twu<br>PRSV<br>REFPROP | Property Package Filter<br>All Types<br>EOSs<br>Activity Models<br>Chao Seader Models<br>Vapour Pressure Models<br>Electrolyte Models<br>Miscellaneous Types | Initialize Electrolyte Environment         Phase Include         Vapour         Aqueous         Solid         2 <sup>nd</sup> Liquid             Redox Options    Included Redox Subsystem Selection |
|--|--|--|
| Component List Selection<br>Component List - 1   | <u>∨</u> iew   | View Electrolyte Reaction in Trace Window  |
| Set Up Parameters P<br>Delete <u>N</u> ame E   | arameters2   Binary Coeffs   Sta<br>lasis-1 Property Pkg   | b Test   Phase Order   Rxns   Tabular   Notes  <br>OLI_Electrolyte Edit Properties   |

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.

| 🎍 Fluid Package: Basis-1   |                                     |  |
|--|-------------------------------------|--|
| Propert <u>y</u> Package Selectio<br>Kabadi-Danner<br>Lee-Kesler-Plocker<br>Margules<br>MBWR<br>NBS Steam<br>NRTL<br>OLI_Electrolyte<br>Peng-Robinson<br>PR-Twu<br>PRSV<br>REFPROP | n<br>Property Package Filter        | Initialize Electrolytes Environment  Tase Option  apour  rganic  olid  queous  edox Options  cluded  Redox Subsystem Selection |
| Component List Selection   |                                     | View Electrolyte Reaction in Trace Window  |
| Component List - 1   | View                                | ○ AQ   MSE   |
| Set Up Parameters  | Parameters2 Binary Coeffs Stab Test | Phase Order Rxns Tabular Notes   |
| Delete Name  | Basis-1 Property Pkg                | OLI_Electrolyte Edit Properties  |

This will bring up the component list.

| ద Component List View:               | Component List - 1               |   |   |   |  |   |
|--------------------------------------|----------------------------------|---|---|---|--|---|
| Add Component                        | Selected Components              |   | -Components Av<br>Match   | ailable in the Library  | View Filters   |   |
| Hypo Components     Other Comp Lists |                                  | <add pure<br="">&lt;-Substitute-&gt;<br/>Remove&gt;<br/>Sort List<br/>iew Component</add> | Sim Name<br>Methane<br>Ethane<br>Propane<br>i-Butane<br>i-Pentane<br>n-Pentane<br>n-Hexane<br>n-Heptane<br>n-Heptane<br>n-Octane<br>n-Nonane<br>Nitrogen<br>CO2 | Full Name / Synonym          C1         C2         C3         i-C4         i-C5         n-C5         C6         C7         C8         C9         C10         N2         C02 | Formula<br>CH4<br>C2H6<br>C3H8<br>C4H10<br>C5H12<br>C5H12<br>C5H12<br>C5H12<br>C5H14<br>C7H16<br>C8H18<br>C9H20<br>C10H22<br>N2<br>CO2 | ^ |
| < >                                  |                                  |   | Show Syno   | nyms Cluste   | er   |   |
| Selected Compon                      | ent by Type J Component Database | is C  |   |   |  |   |

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*.

| Add Component List View: | Component List - 1 Selected Components  | Components Available in the Library-                          | Databank<br>Additional Databank |
|--------------------------|---|---|---------------------------------|
| OLI Electrolyte          |   | Sim Name Eull Name / Synonym                                  |                                 |
| Other Comp Lists         | <add f<="" th=""><th>ACENITRILE Acetonitrile<br/>ACET2 Acetic</th><th>CH3CN A<br/>C4H8O4</th></add> | ACENITRILE Acetonitrile<br>ACET2 Acetic                       | CH3CN A<br>C4H8O4               |
|                          | <-Substitu  | ACETALDEHD Acettic<br>ACETALDEHD Ethanal<br>ACETONE Acetone   | CH3COCH3<br>C2H4O<br>CH3COCH3   |
|                          | Remove  | ACEITLENE ACETIVENE<br>ACIDSO0 Acid<br>ACIDSO1 acid           | C2H2<br>C22H36<br>C10H16        |
|                          | Sort List.  | ACIDSO2 acid<br>ACIDSO3 acid<br>ACIDSO4 acid                  | C14H20<br>C18H28<br>C23H32      |
|                          | View Compo  | ACIDSO5 acid<br>ACRYL2 Acrylic<br>ACRYLONTRL 2-Propenenitrile | C25H34<br>C6H8O4<br>C3H3N       |
| < >                      |   | ADGLUC alpha-D-Glucose  | C6H12O6                         |
| Selected Compone         | ent by Type Component Databases   |   | J                               |
| Delete                   | Name  | Component List - 1  |                                 |

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.

| ≜ Component List View: | Component List - 1                      |   |                      |   |           |             | × |
|------------------------|---|---|----------------------|---|-----------|-------------|---|
| Add Component          | Selected Components                     |   | -Components Av       | ailable in the Library                      | Databank  |             |   |
| ✓ Library Components   |   |   | Match H2             | 20  | Addition  | al Databank |   |
| Traditional            |   |   |                      | •   | () AQ     | MSE         |   |
| > Hypo Components      |   |   | O Sim Name           | Full Name / Synonym                         | O Formula |             |   |
| Other Comp Lists       |   | <add pure<="" th=""><th>H2CO3</th><th>Carbonic H2CO3</th><th></th><th>~</th><th></th></add> | H2CO3                | Carbonic H2CO3                              |           | ~           |   |
|                        |   |   | H2CR2O7<br>H2CRO4    | Dichromic(VI) H2Cr2O7<br>Chromic(VI) H2CrO4 |           |             |   |
|                        |   | -Substitute->   | H2MNO4               | Manganic(VI) H2MnO4                         |           |             |   |
|                        |   |   | H2MOO4<br>H2O        | Molybdenic(VI) H2MoC<br>Water H2O           | )4        |             |   |
|                        | f i i i i i i i i i i i i i i i i i i i | Remove>   | H2O2                 | HYDROGEN H2O2                               |           |             |   |
|                        |   |   | H2RHVIO4<br>H2RUVIO4 | H2O4Rh<br>H2O4Ru                            |           |             |   |
|                        |   | Sort List   | H252O3               | Thiosulfuric H2S2O3                         |           |             |   |
|                        |   |   | H25204<br>H25206     | Dithionous H2S2O4<br>Dithionic H2S2O6       |           |             |   |
|                        | Vie                                     | w Component   | H252O8               | Peroxodisulfuric(VII) H2                    | 25208     |             |   |
|                        |   |   | H25506<br>H25E2O7    | Selenic(VI) H2SeO4.SeC                      | 03        | ~           |   |
| < >                    |   |   | Redox                |   |           |             |   |
| Selected Compon        | ent by Type Component Databases         | ]   |                      |   |           |             | J |
| Delete                 |   | Name Comp   | onent List - 1       |   |           |             |   |

You can either double-click the highlighted name or use the <u>Add Pure</u> button.

| Add Component List View: C<br>Add Component<br>V Library Components<br>Traditional<br>OLI Electrolyte | Selected Components            |   | -Components Av<br>Match H  | railable in the Library                                       | Addition  | nal Databank |
|---|--------------------------------|---|----------------------------|---|-----------|--------------|
| > Hypo Components   |                                |   | Sim Name                   | Full Name / Synonym   | O Formula |              |
| ····· Other Comp Lists  |                                | <add pure<="" th=""><th>H2CO3<br/>H2CR2O7<br/>H2CR04</th><th>Carbonic H2CO3<br/>Dichromic(VI) H2Cr2O7<br/>Chromic(VI) H2CrO4</th><th>7</th><th>^</th></add> | H2CO3<br>H2CR2O7<br>H2CR04 | Carbonic H2CO3<br>Dichromic(VI) H2Cr2O7<br>Chromic(VI) H2CrO4 | 7         | ^            |
|   |                                | <-Substitute->  | H2MNO4<br>H2MOO4           | Manganic(VI) H2MnO4<br>Molybdenic(VI) H2MnO4                  | 4<br>D4   |              |
|   |                                |   | H2O2                       | HYDROGEN H2O2   |           |              |
|   |                                | Remove>   | H2RHVIO4                   | H2O4Rh<br>H2O4Ru  |           |              |
|   |                                |   | H252O3                     | Thiosulfuric H2S2O3   |           |              |
|   |                                | Sort List   | H252O4                     | Dithionous H2S2O4   |           |              |
|   |                                |   | H2S2O6                     | Dithionic H2S2O6  |           |              |
|   |                                | Line Orene and  | H2S2O8                     | Peroxodisulfuric(VII) H                                       | 25208     |              |
|   |                                | view Component  | H25500                     | Selenic(VI) H2SeO4 Sel  | 03        |              |
|   |                                |   | H2SEO3                     | Selenious(IV) H2SeO3  |           | ×            |
| < >   |                                |   | Redox                      |   |           |              |
|   |                                |   |                            |   |           |              |
| Selected Compone  | ent by Type   Component Databa | ases  |                            |   |           |              |
|   |                                |   |                            |   |           |              |
| Delete  |                                | Name Comp   | onent List - 1             |   |           |              |
|   |                                |   |                            |   |           |              |

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:

| Å Component List View: (                                    | Component List - 1          |  |                   |                     |                     |
|---|-----------------------------|--|-------------------|---------------------|---------------------|
| Add Component   | Selected Components         |  | -Components Avail | able in the Library | Databank            |
| <ul> <li>Library Components</li> <li>Traditional</li> </ul> | H2O<br>NH3<br>CO2           |  | Match             |                     | Additional Databank |
| > Hypo Components   | SO2<br>HCL                  |  | O Sim Name (      | Full Name / Synonym | OFormula            |
| Other Comp Lists  | H2S04                       | <add pure<="" th=""><th>ACENITRILE</th><th>Acetonitrile</th><th>CH3CN</th></add> | ACENITRILE        | Acetonitrile        | CH3CN               |
|   |                             |  | ACET2             | Acetic              | C4H8O4              |
|   |                             |  | ACETACID          | Acetic              | СНЗСООН             |
|   |                             | <-Substitute->   | ACETALDEHD        | Ethanal             | C2H4O               |
|   |                             |  | ACETUNE           | Acetone             | CHSCOCHS            |
|   |                             | Demoura  | ACEITLENE         | Acetylene           | C2R2<br>C22H36      |
|   |                             | Remove>  | ACIDSOU           | acid                | C10H16              |
|   |                             |  | ACIDSO2           | acid                | C14H20              |
|   |                             | Sort List  | ACIDSO3           | acid                | C18H28              |
|   |                             | John Elst  | ACIDSO4           | acid                | C23H32              |
|   |                             |  | ACIDSO5           | acid                | C25H34              |
|   |                             | View Component   | ACRYL2            | Acrylic             | C6H8O4              |
|   |                             |  | ACRYLONTRL        | 2-Propenenitrile    | C3H3N               |
|   |                             |  | ADGLUC            | alpha-D-Glucose     | C6H12O6             |
| < >   |                             |  | Redox             |                     |                     |
| Selected Compone  | ent by Type Component Datab | ases   |                   |                     | J                   |
|   |                             |  |                   |                     |                     |
| Delete  |                             | Name Comp  | onent List - 1    |                     |                     |
|   |                             |  |                   |                     |                     |

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.

| A Component List View:   | Component List - 1                              |   |   |   |                                      | × |
|--|---|---|---|---|--------------------------------------|---|
| Add Component <ul> <li>Library Components</li> <li>Traditional</li> <li>OLI Electrolyte</li> </ul> | Selected Components<br>H2O<br>NH3<br>CO2<br>SO2 |   | Match   | able in the Library—                    | Additurel Databank                   |   |
| Other Comp Lists   | H2SO4   | <add pure<="" th=""><th>ACENITRILE<br/>ACET2<br/>ACETACID</th><th>Acetonitrile<br/>Acetic<br/>Acetic</th><th>CH3CN<br/>C4H804<br/>CH3COOH</th><th></th></add> | ACENITRILE<br>ACET2<br>ACETACID               | Acetonitrile<br>Acetic<br>Acetic        | CH3CN<br>C4H804<br>CH3COOH           |   |
|  |   | <-Substitute->  | ACETALDEHD<br>ACETONE<br>ACETYLENE<br>ACIDSO0 | Ethanal<br>Acetone<br>Acetylene<br>Acid | C2H4O<br>CH3COCH3<br>C2H2<br>C22H36  |   |
|  |   | Sort List   | ACIDSO1<br>ACIDSO2<br>ACIDSO3<br>ACIDSO4      | acid<br>acid<br>acid                    | C10H16<br>C14H20<br>C18H28<br>C23H32 |   |
|  | Vie   | ew Component  | ACIDSO5<br>ACRYL2<br>ACRYLONTRL               | acid<br>Acrylic<br>2-Propenenitrile     | C25H34<br>C6H8O4<br>C3H3N            |   |
| < >  |   |   | Redox   | alpha-D-Glucose                         | Conizoo                              |   |
| Selected Compone   | ent by Type ∫Component Databases                | Name Comp   | opent List - 1                                |   |                                      |   |
| Delete   |   | wane Compo  | Shent List - T                                |   |                                      |   |

This brings you back to the fluid package page.

| Propert <u>y</u> Package Selection<br>Kabadi-Danner<br>Lee-Kesler-Plocker<br>Margules<br>MBWR<br>NBS Steam<br>NRTL<br>OLI_Electrolyte<br>Peng-Robinson<br>PR-Twu<br>PRSV<br>REFPROP | <ul> <li>Property Package Filter</li> <li>All Types</li> <li>EOSs</li> <li>Activity Models</li> <li>Chao Seader Models</li> <li>Vapour Pressure Models</li> <li>Electrolyte Models</li> <li>Miscellaneous Types</li> </ul> | Initialize Electrolytes Environment  Phase Option Vapour Organic Solid Solid Aqueous  Redox Options Included Redox Subsystem Selection |  |  |
|---|--|--|--|--|
| Component List Selection     View Electrolyte Reaction in Trace Window       Component List - 1     View       O AQ     MSE   |  |  |  |  |
| Set Up Parameters Delete Name   | Parameters2 Binary Coeffs Sta<br>Basis-1 Property Pkg  | b Test Phase Order Rxns Tabular Notes OLL_Electrolyte Edit Properties  |  |  |

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.

| Simulation Ba             | sis Manager |                  |                |                                     |        | Flows        | heet - Fluid Pk                  | a Associations                       |                |
|---------------------------|-------------|------------------|----------------|-------------------------------------|--------|--------------|----------------------------------|--------------------------------------|----------------|
| Basis-1                   | NC: 6       | PP: OLI_Electrol | yte            | View<br>Add                         |        |              | Flowsheet<br>Case (Main          | Fluid Pkg To<br>n) Bas               | Use is-1       |
|                           |             |                  |                | Delete<br>Copy                      |        |              |                                  |                                      |                |
|                           |             |                  |                | View Users.                         |        | Fluid Pl     | Nefault Fluid Pl                 | kg Basis-1<br>ub-FlowSheets          | <b></b>        |
|                           | -           | [                |                | Export                              |        | 0 U          | se Default Flu<br>se Parent's Fl | iid Pkg 🔲 Includ<br>Iuid Pkg         | Column         |
| Components<br>Enter PVT E | Fluid Pkgs  | Hypotheticals    | Hypo C<br>Ente | orrelation Sets<br>er Regression En | Oil Ma | anager<br>nt | Reactions                        | Component Map.<br>Enter Simulation I | Ser Properties |

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.



#### The workspace now looks like this:

| NoName.usc - UniSim Design R491   | - 🗆 X   |
|---|---|
| File Edit Simulation Flowsheet PFD Tools Window Help  | Environment: Case (Main)  |
|   | Mode: Steady State  |
| bi dau Fi bi dù ⊕ A ∞ 47 ↔ 88   | → S Default Colou + A ×   |
|   | $\Rightarrow \Rightarrow$   |
|   |   |
|   |   |
|   |   |
|   |   |
|   |   |
| МІХ-100   |   |
|   | - E E - E   |
|   | T C C   |
|   |   |
|   |   |
|   |   |
|   | <b>♦</b>  |
| Required Info : MIX-100 Requires a feed stream<br>Required Info : MIX-100 Requires a product stream Saving case C:\Us | ers\JAMES~1.BER\AppData\Local\Temp\AutoRecovery save of NoName (0x251350).ahc |
| Completed.  |   |
| Solve Pass Comple   | sed   |
|   |   |
|   |   |
|   | Balance Tool Errors 🔺 🗸   |

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.

|     | Case (Main) |  |
|-----|-------------|--|
| lou | 🕂 🖰         |  |
|     | ->-         |  |
|     | n o         |  |

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.

| INIX-100       |                                |               |
|----------------|--------------------------------|---------------|
| Design         | Name MIX-100                   |               |
| Connections    |                                |               |
| Parameters     |                                |               |
| User Variables |                                |               |
| Notes          |                                |               |
|                | Inlets                         | Outlet        |
|                | < Stream >>                    | ~             |
|                |                                | Fluid Package |
|                |                                | Basis-1       |
|                | Ignore Selected Feed Stream(s) |               |
| Design Rating  | g Worksheet Dynamics Cost      |               |
| Delete         | Requires a feed s              | tream Ignored |

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

| I MIX-100  |  |                                    |
|--|--|------------------------------------|
| Design   | Name MIX-100                               |                                    |
| Connections<br>Parameters<br>User Variables<br>Notes |  |                                    |
|  | Inlets                                     | Outlet<br>Fluid Package<br>Basis-1 |
| Design Ratin   | g Worksheet Dynamics Cost Requires a produ | ct stream                          |

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

| ₱ MIX-100      |                                |               |
|----------------|--------------------------------|---------------|
| Design         | Name MIX-100                   |               |
| Connections    |                                |               |
| Parameters     |                                | $\backslash$  |
| User Variables | >                              | <b>≻</b> →    |
| Notes          |                                |               |
|                | Inlets                         | Outlet        |
|                | 1 -                            | 8             |
|                | 2                              | Fluid Package |
|                |                                | Basis-1       |
|                | Ignore Selected Feed Stream(s) | )             |
| Design Rating  | Worksheet Dynamics Cost        | ,'            |
| Delete         | Not Solve                      | d 🗌 Ignored   |
|                |                                |               |

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.

| ↑1  |   | - • ×   |
|---|---|---|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value<br>Electrolytes<br>User Variables<br>Notes<br>Cost Parameters | Stream Name Vapour / Phase Fraction [Mol. Basis] Temperature [C] Pressure [kPa] Molar Flow [kgmole/h] Mass Flow [kg/h] Std Ideal Liq Vol Flow [m3/h] Molar Enthalpy [kJ/kgmole] Molar Entropy [kJ/kgmole-C] Heat Flow [kJ/h] Liq Vol Flow @Std Cond [m3/h] Fluid Package Phase Option < | 1<br><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/>Basis-1<br/>Multiphase</empty></empty></empty></empty></empty></empty></empty></empty> |
| Worksheet Atta  | chments Dynamics Unknown Flow Rate  |   |
| Delete  | Define from Other Stream  | <b>+</b> +  |

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

| Worksheet         Stream Name         1           Conditions         Vapour / Phase Fraction [Mol. Basis] <empty>           Properties         Pressure [KPa]         101.3           Composition         Molar Flow [kg/h]         (empty&gt;)           K Value         Mass Flow [kg/h]         <empty>           Electrolytes         Molar Enthalpy [k]/kgmole]         <empty>           User Variables         Molar Enthalpy [k]/kgmole-C]         <empty>           Notes         Hoal ar Entropy [k]/kgmole-C]         <empty>           Liq Vol Flow @Std Cond [m3/h]         <empty>         Fluid Package           Phase Option         Multiphase         &lt;</empty></empty></empty></empty></empty></empty> | 1   |   |  |
|---|---|---|--|
| Phase Option Multiphase   | Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value<br>Electrolytes<br>User Variables<br>Notes<br>Cost Parameters | Stream Name<br>Vapour / Phase Fraction [Mol. Basis]<br>Temperature [C]<br>Pressure [kPa]<br>Molar Flow [kg/n]<br>Std Ideal Liq Vol Flow [m3/h]<br>Molar Enthalpy [k//kgmole]<br>Molar Enthopy [k//kgmole-C]<br>Heat Flow [kJ/h]<br>Liq Vol Flow @Std Cond [m3/h]<br>Eluid Parkana | 1<br><empty><br/>40.00<br/>101.3<br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><emp< th=""></emp<></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> |
|   |   | Fluid Package<br>Phase Option   | <empty><br/>Basis-1<br/>Multiphase</empty>   |
|   |   | Unknown Flow Rate   |  |
| Unknown Flow Rate   | Delete  | Define from Other Stream  | _ <u> </u>   |

Now click the Composition line

| 1   |  |  |
|---|--|--|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value<br>Electrolytes<br>User Variables<br>Notes<br>Cost Parameters | H2O<br>NH3<br>CO2<br>SO2<br>HCL<br>H2CO3<br>H2CO3<br>H2CO3<br>HCL02<br>H2CO3<br>HCL02<br>HCL02<br>HCL02<br>HCL02<br>HCL02<br>HCL02<br>HCL02<br>HCL02<br>HCL02<br>HCL02<br>HC02<br>HC02<br>HC02<br>HC02<br>HC02<br>HC02<br>HC02<br>HC | Mole Fractions Cempty> |
|   | Total  | <empty>       0.00000   roperties Basis</empty>  |
| Worksheet Atta  | chments Dynamics Unknown Flow Rat  | e  |
| Delete  | Define from Other Stre   | eam 🗢 🖨  |

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

| 峯 Stream: 1   | × |
|---|---|
| Compositional Basis     Mole Fractions     Mass Fractions     Mole Flows     Mass Flows |   |
|   |   |

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

Now begin entering the value for H2O of 55.51

| <b>→</b> 1  |  |   |          |
|---|--|---|----------|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value<br>Electrolytes<br>User Variables<br>Notes<br>Cost Parameters | H20<br>H10<br>S02<br>HCL<br>H2504<br>H2C03<br>H2C03<br>H2C03<br>HCL 1H20<br>HCL 1H20<br>HCL 2H20<br>HCL 3H20<br>KCL 3H20<br>KCL 3H20<br>KCL<br>KCL<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>H20<br>KCL<br>KCL<br>KCL<br>KCL<br>KCL<br>KCL<br>KCL<br>KCL | Motar Flows       55.51 <empty> <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | kgmole/h |
|   | Total<br>Edit Edit F   | 0.00000 kgmole/h<br>Properties Basis.   |          |
| Worksheet Atta  | chments Dynamics<br>Unknown Flow Ra  | te  | l        |
| Delete  | Define from Other Str  | eam 🗲   | •        |

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

| 🔰 Input Composit  | ion for Stream: 1  | ×   |
|---|--|---|
| H20<br>NH3<br>C02<br>S02<br>HCL<br>H2S04<br>H2C03<br>H2S03              | CompMoleFlow 55.510 <empty> &lt;</empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | Composition Basis<br>Mole Fractions<br>Mass Fractions<br>Mole Flows<br>Mass Flows |
| HCL.1H20<br>HCL.2H20<br>HCL.3H20<br>NH42C03<br>NH42C03.1H20<br>NH42S205 | <empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty><br/><empty></empty></empty></empty></empty></empty></empty></empty>  | Composition Controls  |
| NH42SO3<br>NH42SO3.1H2O<br>NH42SO4<br>NH43CO32                          | <empty><br/><empty><br/><empty><br/><empty></empty></empty></empty></empty>  | Cancel  |
| Equalize Composition  | Total 55.510 kgmole/ł  | ОК  |

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.

|                     | 43                   |                      |
|---------------------|----------------------|----------------------|
|                     | CompMoleFlow         | Composition Basis    |
| H2O                 | 55.510               | Mala Eractiona       |
| NH3                 | 1.0000               | O mole Practions     |
| CO2                 | 0.10000              | Mass Fractions       |
| S02                 | 0.10000              |                      |
| HCL                 | <empty></empty>      | <u>M</u> ole Flows   |
| H2SO4               | <empty></empty>      | Mass Flows           |
| H2CO3               | <empty></empty>      |                      |
| H2SO3               | <empty></empty>      |                      |
| HCL.1H2O            | <empty></empty>      |                      |
| HCL.2H2O            | <empty></empty>      |                      |
| HCL.3H2O            | <empty></empty>      | Composition Controls |
| NH42CO3             | <empty></empty>      | -                    |
| NH42CO3.1H2O        | <empty></empty>      | E <u>r</u> ase       |
| NH42S2O5            | <empty></empty>      |                      |
| NH42SO3             | <empty></empty>      | Normali <u>z</u> e   |
| NH42SO3.1H2O        | <empty></empty>      |                      |
| NH42SO4             | <empty></empty>      |                      |
| NH43CO32            | <empty> Y</empty>    | Cancel               |
| Faualiza Compositio | Total 56 710 kamole/ |                      |

Click the **OK** button.

|                  |                      | Molar Flows                           |
|------------------|----------------------|---------------------------------------|
| Worksheet        | H20                  | 55,510                                |
| ···· Conditions  | NH3                  | 1.0000                                |
| Properties       | C02                  | 0,10000                               |
| Composition      | S02                  | 0.10000                               |
| Composition      | HCL                  | 0.00000                               |
| K value          | H2SO4                | 0.00000                               |
| Electrolytes     | H2CO3                | 0.00000                               |
| — User Variables | H2SO3                | 0.00000                               |
| Notes            | HCL.1H2O             | 0.00000                               |
| Cost Parameters  | HCL.2H2O             | 0.00000                               |
| oost i arametero | HCL.3H2O             | 0.00000                               |
|                  | Total<br>Edit Edit P | 56.71000 kgmole/h<br>Properties Basis |
| Worksheet Atta   | chments Dynamics     |                                       |

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.

| <b>≯</b> 1  | ₽<br>₽   |   |
|---|--|---|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value<br>Electrolytes | Phase<br>© Aqueous<br>© Organic<br>Solid<br>Vapor<br>Property<br>Property  |   |
| User Variables<br>Notes<br>Cost Parameters                                      | pH         Osmotic Pressure [kPa]         Ionic Strength [kgmol/kg]         Heat Capacity [k/kgmole-C]         Viscosity [cP]         Ideal Std Liquid Density [kg/m3]         Specific Elec Conductivity [S/m]         Molar Elec Conductivity [S-m2/kgmole]         Thermal Conductivity [W/m-K]         Surface Tension [dyne/cm] | 9.340<br>2771<br>7.925e-006<br>74.66<br>0.6802<br>999.1<br>5.143<br>0.0000<br>0.6251<br>68.88 |
| Worksheet Attac   | hments Dynamics  |   |
| Delete  | Define from Other Stream   | <b>+</b> +  |

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.

| <b>→</b> 1  |   |  |   |                        |                         | -               | , • <mark>×</mark> |
|---|---|--|---|------------------------|-------------------------|-----------------|--------------------|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value | Phase<br>Aqueous<br>Organic<br>Solid<br>Vapor | True Species In<br>Properties<br>Composition | fo <u>C</u> onc. Basis<br>Molar<br>Mass |                        |                         |                 |                    |
| ···· Electrolytes<br>···· User Variables                        | True Species                                  | Mole Fraction                                | Molar Flow<br>[kgmole/h]                | Molality<br>[kgmol/kg] | Molarity<br>[kgmole/m3] | Activity Coeff. | ^                  |
| ···· Notes  | H2OAQ   | 0.979288                                     | 54.857                                  | 5.551e-002             | 55.21                   | 1.002           |                    |
| Cost Parameters   | CO2AQ   | 0.000000                                     | 2.1721e-005                             | 2.198e-008             | 2.186e-005              | 0.9821          |                    |
|   | H2SO4AQ                                       | 0.000000                                     | 0.00000                                 | 0.0000                 | 0.0000                  | 0.0000          |                    |
|   | HCLAQ   | 0.000000                                     | 0.00000                                 | 0.0000                 | 0.0000                  | 0.0000          |                    |
|   | NH3AQ   | 0.002593                                     | 0.14526                                 | 1.470e-004             | 0.1462                  | 1.036           |                    |
|   | NH40HAQ                                       | 0.008799                                     | 0.49288                                 | 4.987e-004             | 0.4961                  | 1.044           |                    |
|   | SO2AQ   | 0.000000                                     | 7.6309e-012                             | 7.722e-015             | 7.681e-012              | 0.9300          |                    |
|   | SO3AQ   | 0.000000                                     | 0.00000                                 | 0.0000                 | 0.0000                  | 0.0000          |                    |
|   | CLION   | 0.000000                                     | 0.00000                                 | 0.0000                 | 0.0000                  | 0.0000          |                    |
|   | CO3ION  | 0.000396                                     | 2.2169e-002                             | 2.243e-005             | 2.231e-002              | 0.1412          |                    |
|   | H30ION  | 0.000000                                     | 6.5945e-010                             | 6.673e-013             | 6.637e-010              | 0.6861          | ×                  |
| Worksheet Attac   | hments Dynam                                  | iics   |   |                        |                         |                 |                    |
|   |   |  | OK                                      |                        |                         |                 |                    |
| Delete  | Define from                                   | n Other Stream                               |   |                        |                         |                 | <b>+ +</b>         |

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

Click on the  $\boldsymbol{x}$  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    | С   |
|-------------|-------|-----|
| Pressure    | 101.3 | kPa |
| H2O         | 55.51 |     |
| HCI         | 0.1   |     |
| H2SO4       | 1.0   |     |

Click the *Electrolytes* line to see the pH.

| <b>*</b> 2  |  |   |
|---|--|---|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value<br>Electrolytes<br>User Variables<br>Notes<br>Cost Parameters | Phase       True Species Info         Organic       Orporties         Osolid       Composition         Property       Property         PH       Osmotic Pressure [kPa]         Ionic Strength [kgmol/kg]       Heat Capacity [k]/kgmole-C]         Viscosity [cP]       Ideal Std Liquid Density [kg/m3]         Specific Elec Conductivity [S-m2/kgmole]       Thermal Conductivity [W/m-k]         Surface Tension [dyne/cm]       Surface Tension [dyne/cm] | -8.112e-002<br>6582<br>2.514e-005<br>73.80<br>1.126<br>1036<br>41.58<br>0.0000<br>0.5844<br>72.94 |
| Worksheet Attac   | hments Dynamics  |   |
| Delete  | Define from Other Stream   | <b>+ +</b>  |

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.

| NoName.usc - UniSim Design R491                      |   | -                                    | - 0 ×                                 |
|--|---|--------------------------------------|---------------------------------------|
| File Edit Simulation Flowsheet PFD Tools Window Help |   |                                      |                                       |
| ŮŮВӘ《╨Ѱ∞╚▤♥◊◊•• 4                                    |   | Environment: Case (I<br>Mode: Steady | Main)<br>/ State                      |
| C PFD - Case (Main)                                  |   |                                      | Case (Main) 🛛 💌                       |
| 여여51 0000 ⊙ A ∞ 4 ↔ 品                                |   | → → Default Colou                    | + 6 ×                                 |
| 1<br>2<br>MIX-100                                    | 3   |                                      |                                       |
|  |   |                                      |                                       |
| PFD 1  |   |                                      | <b>A</b>                              |
|  | Soling Handwalloof_<br>Soling Hirlo<br>Soling Hirlo<br>Soling Hirlo<br>Soling Journel<br>Soling ProductBlock_J<br>Soling Fast Completed<br>Saving case Cr\Deers\JMME3-1.8ER\AppGata\Local\Temp\AutoRecovery save<br>Completed | of NoName (0x251350).ahc             | · · · · · · · · · · · · · · · · · · · |
|  | n •   | Balance Tool                         | <b>▲ </b> ▼                           |
|  |   |                                      |                                       |

#### **Reviewing the output**

#### Double-Click stream "3"

| • 3              |                                      |             |             | 5            | (             | - 0 💌      |
|------------------|--------------------------------------|-------------|-------------|--------------|---------------|------------|
| Worksheet        | Stream Name                          | 3           | 3_Elec      | Vapour Phase | Aqueous Phase |            |
| Conditions       | Vapour / Phase Fraction [Mol. Basis] | 0.0006      | 0.0006      | 0.0006       | 0.9994        |            |
| Conditions       | Temperature [C]                      | 36.99       | 36.99       | 36.99        | 36.99         |            |
| Properties       | Pressure [kPa]                       | 101.3       | 101.3       | 101.3        | 101.3         |            |
| ···· Composition | Molar Flow [kgmole/h]                | 114.3       | 114.3       | 6.574e-002   | 114.3         |            |
| - K Value        | Mass Flow [kg/h]                     | 2130        | 2130        | 2.857        | 2127          |            |
| Electrolytes     | Std Ideal Liq Vol Flow [m3/h]        | 2.092       | 2.092       | 2.395e-003   | 2.089         |            |
| User Variables   | Molar Enthalpy [kJ/kgmole]           | -2.865e+005 | -2.865e+005 | -3.787e+005  | -2.864e+005   |            |
| ···· Notes       | Molar Entropy [kJ/kgmole-C]          | 72.66       | 72.66       | 215.4        | 72.57         |            |
| Cost Parameters  | 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    |            |
|                  | JI                                   |             |             |              |               | 1          |
| Worksheet Atta   | chments Dynamics                     | OK          |             |              |               |            |
| Delete           | Define from Other Stream             |             |             |              |               | <b>+</b> + |

The converged process temperature is approximately 37.0 °C.

Click on the *Electrolytes* line.

| → 3   |  | - • ×   |
|---|--|---|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value<br>Electrolytes | Phase<br>Aqueous<br>Organic<br>Solid<br>Vapor<br>Property  |   |
| User Variables<br>Notes<br>Cost Parameters                                      | pH         Osmotic Pressure [kPa]         lonic Strength [kgmol/kg]         Heat Capacity [k/kgmole-C]         Viscosity [cP]         Ideal Std Liquid Density [kg/m3]         Specific Elec Conductivity [S/m]         Molar Elec Conductivity [S-m2/kgmole]         Thermal Conductivity [W/m-K]         Surface Tension [dyne/cm] | 0.8681<br>3013<br>1.488e-005<br>74.67<br>0.7624<br>1018<br>14.69<br>0.0000<br>0.6162<br>71.72 |
| Worksheet Atta  | chments Dynamics OK  |   |
| Delete  | Define from Other Stream   | <b>\$</b>   |

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.

| → 3   |   |                  |   |                        |                         |                 |            |
|---|---|------------------|---|------------------------|-------------------------|-----------------|------------|
| Worksheet<br>Conditions<br>Properties<br>Composition<br>K Value | Phase<br>Aqueous<br>Organic<br>Solid<br>Vapor | True Species Inf | io <u>C</u> onc. Basis<br>Molar<br>Mass |                        |                         |                 |            |
| <ul> <li>Electrolytes</li> <li>User Variables</li> </ul>        | True Species                                  | Mole Fraction    | Molar Flow<br>[kgmole/h]                | Molality<br>[kgmol/kg] | Molarity<br>[kgmole/m3] | Activity Coeff. | ^          |
| Notes   | H2OAQ   | 0.976725         | 110.61                                  | 5.551e-002             | 55.17                   | 1.002           |            |
| Cost Parameters   | CO2AQ   | 0.000369         | 4.1734e-002                             | 2.094e-005             | 2.082e-002              | 1.087           |            |
|   | H2SO4AQ                                       | 0.000000         | 2.8532e-007                             | 1.432e-010             | 1.423e-007              | 1.129           |            |
|   | HCLAQ   | 0.000000         | 8.9278e-010                             | 4.480e-013             | 4.453e-010              | 0.7357          |            |
|   | NH3AQ   | 0.000000         | 1.2435e-009                             | 6.240e-013             | 6.202e-010              | 1.039           |            |
|   | NH40HAQ                                       | 0.000000         | 4.4457e-009                             | 2.231e-012             | 2.217e-009              | 1.027           |            |
|   | SO2AQ   | 0.000764         | 8.6542e-002                             | 4.343e-005             | 4.316e-002              | 0.9311          |            |
|   | SO3AQ   | 0.000000         | 1.3335e-020                             | 6.692e-024             | 6.651e-021              | 1.123           |            |
|   | CLION   | 0.000883         | 0.10000                                 | 5.018e-005             | 4.988e-002              | 0.6901          |            |
|   | CO3ION  | 0.000000         | 7.1770e-016                             | 3.602e-019             | 3.580e-016              | 9.905e-002      |            |
|   | H30ION  | 0.003510         | 0.39744                                 | 1.995e-004             | 0.1982                  | 0.6809          |            |
|   | HC03ION                                       | 0.000000         | 2.8632e-007                             | 1.437e-010             | 1.428e-007              | 0.5837          |            |
|   |   | 0 000000         | 0.0007- 002                             | 5 01/2 006             | 1 002~ 002              | 0.6001          |            |
| Worksheet Attac   | hments Dynam                                  | iics             |   |                        |                         |                 | ,          |
|   |   |                  |   | ОК                     |                         |                 |            |
| Delete  | Define fror                                   | n Other Stream   |   |                        |                         |                 | <b>+ +</b> |

Click on the Composition line at the left.

| <b>→</b> 3          |  |                |                     |              |               |    | ×     |
|---------------------|--|----------------|---------------------|--------------|---------------|----|-------|
| Washahaat           |  | Mole Fractions | Mole Fractions Elec | Vapour Phase | Aqueous Phase |    | ~     |
| worksneet           | H2O                                      | 0.979881       | 0.979881            | 0.061316     | 0.980410      |    | - · · |
| Conditions          | NH3                                      | 0.008747       | 0.008747            | 0.000000     | 0.008752      |    |       |
| Properties          | CO2                                      | 0.000875       | 0.000875            | 0.886339     | 0.000365      |    |       |
| Composition         | S02                                      | 0.000875       | 0.000875            | 0.052346     | 0.000845      |    |       |
| K Value             | HCL                                      | 0.000875       | 0.000875            | 0.000000     | 0.000875      |    |       |
| K value             | H2SO4                                    | 0.000000       | 0.000000            | 0.000000     | 0.000000      |    |       |
| Electrolytes        | H2CO3                                    | 0.000000       | 0.000000            | 0.000000     | 0.000000      |    |       |
| ···· User Variables | H2S03                                    | 0.000000       | 0.000000            | 0.000000     | 0.000000      |    |       |
| ··· Notes           | HCL.1H20                                 | 0.000000       | 0.000000            | 0.000000     | 0.000000      |    |       |
| Cost Parameters     | HCL.2H20                                 | 0.000000       | 0.000000            | 0.000000     | 0.000000      |    |       |
|                     | NH42002                                  | 0.00000        | 0.00000             | 0.000000     | 0.000000      |    |       |
|                     | NH42CO3 1H20                             | 0.000000       | 0.000000            | 0.000000     | 0.000000      |    |       |
|                     | NH42C03.1120                             | 0.000000       | 0.000000            | 0.000000     | 0.000000      | N  | - v   |
|                     | 1111420200                               |                | -                   | (JAAAAAAA)   | ()            | 13 |       |
|                     | Total                                    | perties Basis  |                     |              |               |    |       |
| Worksheet Atta      | chments Dynamics Define from Other Strea | m              | OK                  |              |               | ¢  | `     |

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.

| Mandan hard     |              | Molar Flows    | Molar Flows Elec | Vapour Phase | Aqueous Phase |  |
|-----------------|--------------|----------------|------------------|--------------|---------------|--|
| worksneet       | H2O          | 112.02         | 112.02           | 4.0308e-003  | 112.02        |  |
| Conditions      | NH3          | 1.0000         | 1.0000           | 5.2729e-012  | 1.0000        |  |
| Properties      | CO2          | 0.10000        | 0.10000          | 5.8266e-002  | 4.1734e-002   |  |
| Composition     | S02          | 0.10000        | 0.10000          | 3.4411e-003  | 9.6559e-002   |  |
| Value           | HCL          | 0.10000        | 0.10000          | 4.8866e-010  | 0.10000       |  |
| K value         | H2SO4        | 0.00000        | 3.7521e-021      | 3.7521e-021  | 0.00000       |  |
| Electrolytes    | H2CO3        | 0.00000        | 0.00000          | 0.00000      | 0.00000       |  |
| User Variables  | H2SO3        | 0.00000        | 0.00000          | 0.00000      | 0.00000       |  |
| Notes           | HCL.1H2O     | 0.00000        | 0.00000          | 0.00000      | 0.00000       |  |
| Cost Parameters | HCL.2H2O     | 0.00000        | 0.00000          | 0.00000      | 0.00000       |  |
| cost runnictors | HCL.3H2O     | 0.00000        | 0.00000          | 0.00000      | 0.00000       |  |
|                 | NH42CO3      | 0.00000        | 0.00000          | 0.00000      | 0.00000       |  |
|                 | NH42CO3.1H2O | 0.00000        | 0.00000          | 0.00000      | 0.00000       |  |
|                 | Total        | operties Basis |                  |              |               |  |
|                 |              |                |                  |              |               |  |

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