

INTRODUCTION TO OLI Engine for Aspen Hysys

think simulation

getting the chemistry right

Introduction to OLI Engine for Aspen Hysys

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OLI Engine for Aspen Hysys

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Disclaimer

This manual was produced using the OLI Engine 12.0.0.6 for Aspen Hysys 14

As time progresses, new data and refinements to existing data sets can result in values that you obtain being slightly different than what is presented in this manual. This is a natural progress and cannot be avoided. When large systematic changes to the software occur, this manual will be updated.

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Overview

The OLI Engine for Aspen HYSYS interface greatly enhances Aspen HYSYS' capability to model electrolyte systems. A rigorous and self-consistent thermodynamic framework is employed to tame the mathematically stiff equations commonly found in electrolyte systems. Also, a database of over 10,000 components is available.

The OLI model is available as a property set within Aspen HYSYS. This "Getting Started" guide will show you how to create the electrolyte chemistry for a simple case and then create a simple flowsheet in Aspen HYSYS.

Assumptions

The following assumptions are made for this guide:

- 1. Aspen HYSYS is currently installed and running on your computer.
- 2. The license manager for Aspen HYSYS is currently set up.
- 3. The OLI Engine for Aspen HYSYS product has been installed.
- 4. The OLI security model is running.
- 5. Aspen HYSYS V14 is being used.
- 6. The user is expected to know how to run Aspen HYSYS.

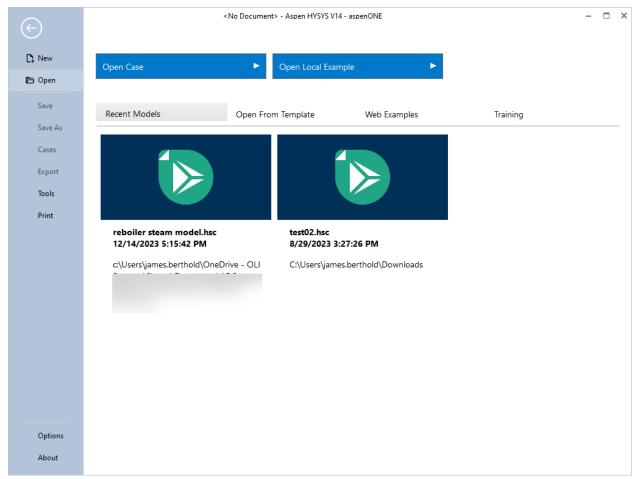
Application

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

Using the OLI Engine for Aspen HYSYS

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

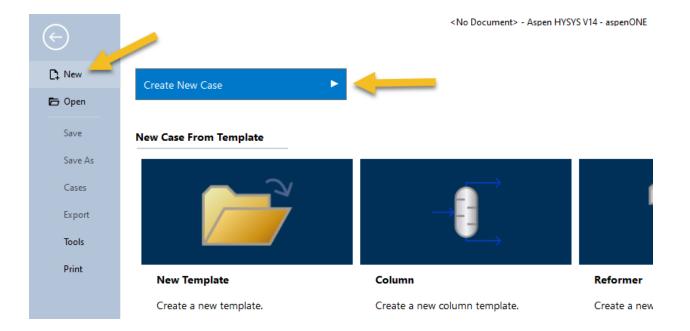




This will now display the Aspen HYSYS development environment.

Entering the Chemistry and fluid packages

Select New and then Create New Case



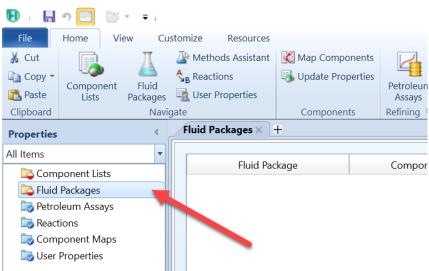
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This will bring up the Simulation Environment.

Selecting Fluid Packages

OLI recommends starting with adding a fluid package.

Select Fluid Packages



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

Click the **Add** button

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| 🔁 Fluid Packages | | | | | |
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Scroll down the window to find OLI_Electrolyte

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| Set Up | Binary Coe | ffs | StabTest | Phase Order |
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| MBV | VR | | | |
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| Sour | Water | | | |
| SRK | | | | |
| SRK- | Twu | | | |
| 1 | m (Sulfur R | | | * |

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**.

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| □-{□ Simulation | | " | • |
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| | | Respo | nsiveness: 5 100% \ominus ——— 🕀 |

You have two options to see the component list. Either click the Component List in the navigator

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

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| Image: Compose Mays Image: Compose | Component Lists Component Lists Discrete Section | Package Type: HYSYS | Component List Selection Component List - 1 [H | IYSYS Databanks] • View 2 | Î |
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| Inergy Analysis Messages Versage Versages Versage | Safety Analysis | * | m | • | |
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| | | Required Into : Components Empty component list | Updated fluid package xml data is invalid | | |

Here we are choosing Option 1, In the tree-view, click on *Component Lists*.

Click the small arrow to expand the list. This will expand the list to display all the component lists. Select **Component List -1**

| Home View Cu | stomize Resources | | | | | | | | | Se | earch Aspen Knowledge | 2 | ۵ |
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| ut opy - aste component Lists Navig | | | Petroleum Assays Refining 12 | Hypothetical Convert Remove Dup Hypotheti | licates M | Oil anager | Convert to | * Associate Fluid Package Definitions * Options | PVT Laboratory Measurements PVT Data | | | | |
| erties < | Component List View | : Component List - 1 [HY | SYS Databank | s] × + | | | | | | | | | |
| Component Lists Component List - 1 Fluid Packages | Source Databank: HYS | | | | | | Select: Search for: | Pure Components | Filter: Search | | All Families - | | |
| Petroleum Assays Reactions | Component | Туре | G | roup | | | Sim | ulation Name | Full Name / Synonyr | . (| Formula | - | |
| Component Maps User Properties | | | | | | ld. | 3 | Methane | rui Nuite / Synonyi | " C1 | CH4 | | |
| oser Properties | | | | | | | | Ethane | | C2 | C2H6 | | |
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| | | | | | Repla | ce | | i-Butane | | i-C4 | C4H10 | | |
| | | | | | | | | n-Butane | | n-C4 | C4H10 | | |
| | | | | | | | | i-Pentane | | i-C5 | C5H12 | | |
| | | | | | Remo | ve | | n-Pentane | | n-C5 | C5H12 | | |
| | | | | | | | | n-Hexane | | C6 | C6H14 | | |
| | | | | | | | | n-Heptane | | C7 | C7H16 | | |
| | | | | | | | | n-Octane | | C8 | C8H18 | | |
| Properties | | | | | | | | n-Nonane | | C9 | C9H20 | | |
| Simulation | | | | | | | | n-Decane | | C10 | C10H22 | * | |
| Safety Analysis | Status | Empty compos | aant liet | | | | | | | | | | |
| | Messages | | | | | | 61 | xml data is invalid | | | | | • |
| Energy Analysis | | ents Empty componer | | | | | | | | | | | |

Entering Components

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

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

| Select: | Pure Components | Filter: | All Families | | | | |
|---|-----------------|---------------------|--------------|---|--|--|--|
| earch for: Search by: Full Name/Synonym | | | | | | | |
| Simulat | ion Name | Full Name / Synonym | Formula | * | | | |
| | Methane | C | 1 CH4 | | | | |
| | Ethane | c | 2 C2H6 | | | | |
| | Propane | C | 3 C3H8 | | | | |
| | i-Butane | i-C4 | 4 C4H10 | | | | |

This will display several options:

| Select: | Pure Components | - | Filter: | 4 |
|-------------|---|---|---------------|----|
| Search for: | Pure Components OLI (Aqueous) OLI (MSE) | 4 | Search by: | F |
| Simula | tic Hypothetical Solid | | ame / Synonym | |
| | Methane | | | C1 |
| | Ethane | | | C2 |

For this example, we will use OLI (MSE)

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| ut opy v aste loard | | Map Components Update Properties Components | Petroleum | Hypotheticals Manager Convert Remove Duplicates Hypotheticals | Oil Manager | Convert to Refining Assay | Associate Fluid Pac Definitions - Options | kage PVT Laboratory Measurements PVT Data | | | |
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| :ms • | | | | | | | | | | | (|
| Component Lists | Source Databank: HYS | /S | | | | Select: | OLI (MSE) | • | | | |
| Fluid Packages | Component | Туре | G | roup | | Search f | or: | | Additional Database | | |
| Petroleum Assays | | | | | | | | | | | |
| Reactions Component Maps | | | | | | | Simulation Name | Full Name / Synonym | Formula | * | |
| User Properties | | | | | < Add | | ACENITRILE | Acet | onitrile CH3CN | | |
| | | | | | | | ACET2 | Acetic_acid, | _dimer C4H8O4 | | |
| | | | | | | | ACETACID | Acet | tic_acid CH3COOH | | |
| | | | | | Replace | | ACETALDEHD | 1 | Ethanal C2H4O | | |
| | | | | | | | ACETONE | A | cetone CH3COCH3 | | |
| | | | | | | _ | ACETYLENE | Ace | etylene C2H2 | | |
| | | | | | lemove | | ACIDSO0 | Acid_soluble | _oil_(0) C22H36 | | |
| | | | | | | | ACIDSO1 | acid_soluble_oil_ | light C10H16 | | |
| | | | | | | | ACIDSO2 | acid_soluble_oil2 | 20-30% C14H20 | | |
| | | | | | | | ACIDSO3 | acid_soluble_oil6 | 50-70% C18H28 | | |
| roperties | | | | | | | ACIDSO4 | acid_soluble_oil | _>70% C23H32 | | |
| imulation | | | | | | | ACIDSO5 | acid_soluble_oil | _>80% C25H34 | Ŧ | |
| | Status | Empty compos | ent list | | | | | | | | |
| afety Analysis | Messages | | | | | | | | | | |
| nergy Analysis | Required Info : Compor | | | - | Update | d fluid packa | ge xml data is inva ge xml data is inva | alid. | | | _ |
| * | Required Info : Compor | ient List - 1 [HYSYS Datab | anks] Empty | component list | Update | d fluid packa | ge xml data is inva | alid. | | | |

We can now begin to select our components from the OLI supplied species. You can either scroll down the rather large list or enter your species into the **Search For:** box.

Enter the species H2O into the Search For: box.

You can see the components list scrolls to the species. If the species highlighted is the correct species, click the *Add* button.

| Component Ruid Peter Lists Package National Nam | La Une Properties | plate Properties P | troleum & Convert | ficah Managar Di Displication Managar Displication | Canvetta Bi | Ameriate Pluid Package Definitions * Options | PVT Laboratory Measurementik PVT Outa | | | |
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| roperties C | Component List View: Comp | onent List - 1 (HYSY) | 5 Dutabankoj × [+ | | | | | | | |
| Reactions | | Select | | - | | 1 | 0 | | | |
| California Batoleum Assays Reactions | Component | Type | Group | | Search for | ation Name | Full Name / Synonym | Additional Database Formula | | |
| Component Maps | | | | 1 4.55 | | HRODE | Carbonic acid | NICOS | | |
| | | | | | | H208207 | Dichronic(VI)_acid | H20/207 | | |
| | | | | | | HICKOM | Overve(V), and | HECKOA | 11 | |
| | | | | Explain | | H2MNO4 | Manganic(VI)_acid | H2MvO4 | | |
| | | | | | | H2M004 | Molybdenc(VI),acid | H2MbO4 | 1 | |
| | | | | | | Hao | Water | H2D | | |
| | | | | Retorue | | H202 | HYDROGEN, PERCHEDE | 1002 | | |
| | | | | | | H2RHVIC4 | H2048h | | | |
| | | | | | | H2RLVIO4 | H2O4Ru | | | |
| | | | | | | H25208 | Thiosuffaric_acid | H25200 | | |
| | | | | | | H25204 | Dithionous_acid | H25204 | | |
| Properties | | | | | | H25206 | Othionic_acid | #25206 | 1 | |

As you type, the component list changes to search for the species. As you can see the species H2O is highlighted. Also, there is the species H2O2 (peroxide) which has a similar formula. Select the species you need.

You will notice that the component list no longer displays H2O in the available box. Rather it now appears in the Selected components.

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|--|--|--|-----------------------------------|---|-----------|----------------|---|----------|------------------|--|----------------|----------------------|--|---|
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| operties < | | component est i firi | 515 Dutabanic | | | | | | | | | | | |
| Component Lists Component List - 1 Fluid Packages | Source Databank: HYS | /S | | | | | | | OLI (MSE) | • | _ | | | U |
| Basis-1 | Component | Туре | G | roup | | | Search | for: | H20 | | | Additional Database | | |
| Reactions | H2 | 20 Electrolyte Compo | nent | | | | | | | | | | | |
| Component Maps | | | | | | | | Simulat | ion Name | Full Name / Syno | nym | Formula | <u></u> | |
| o User Properties | | | | | | < Add | | | H2CO3 | c | arbonic_acid | H2CO3 | | |
| | | | | | | | | | H2CR2O7 | Dichro | omic(VI)_acid | H2Cr2O7 | E | |
| | | | | | | | | | H2CRO4 | Chro | omic(VI)_acid | H2CrO4 | dditional Database Formula H2Cr03 H2Cr04 H2Mn04 H2M | |
| | | | | | R | eplace | | | H2MNO4 | Mang | anic(VI)_acid | H2MnO4 | | |
| | | | | | | | | | H2MOO4 | Molybd | enic(VI)_acid | H2MoO4 | | |
| | | | | | | | | | H2O2 | HYDROGE | N_PEROXIDE | H2O2 | | |
| | | | | Otie Otie Cenverto PVT Laboratory Remove Duplicate: Additional Database PVT Data VI Select: Oli (MSE) Select: Oli (MSE) Additional Database Select: Oli (MSE) Full Name / Synonym Search for: H2O H2C03 H2CR207 Dichromic(VI)_acid H2C02 H2CR04 Chromic(VI)_acid H2C03 Replace H2MNO4 Mangaric(VI)_acid H2MoO4 H2D02 HVDGEN_PEROXIDE H02 H2S2O3 Thiosufuric_acid H2S2O3 H2S2O4 H2S2O8 Peroxodisulfuric(VIII)_acid H2S2O8 H2S2O8 H2S2O8 Peroxodisulfuric(VIII)_acid H2S2O8 H2S2O8 Updated Third package m1 data is invalid; Invalid; H2S2O8 H2S2O8 | | | | | | | | | | |
| | | | | | | | Search Aspen Knowledge Search Aspen Knowledge Oil Search Aspen Knowledge Oil PVT Laboratory Weil Laboratory Measurements Oil PVT Data | | | | | | | |
| | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | |
| Properties | | | | | | | | | H2S2O6 | D | ithionic_acid | H2S2O6 | | |
| Simulation | | | | | | | | | H2S2O8 | Peroxodisulf | uric(VII)_acid | H2S2O8 | * | |
| Safety Analysis | Status | OK | | | | | | | | | | | | |
| | Messages | | | | | | | | | | | | | - |
| Energy Analysis | | | | | | Update | d fluid pack | ige xml | data is invalid. | | | | | _ |

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

Using the same procedure, add the following components¹.

- NH3
- CO2
- SO2
- HCL
- H2SO4

The input should look like this:

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

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| Cut Copy + Paste pboard | Subser Properties | Map Components Update Properties Components Refini | leum ays Remove D | icals Manager Duplicates Ma heticals | Oil Conver nager Refining | t to | ge PVT Laboratory Measurements PVT Data | | | |
| operties < | Component List View: C | Component List - 1 [HYSYS Da | atabanks] × + | | | | | | | |
| tems Component Lists Component List - 1 Fluid Packages | Source Databank: HYSYS | | | | Se | elect: OLI (MSE) | - | | | () |
| Basis-1 | Component | Туре | Group | | Se | arch for: | | Additional Database | | |
| Petroleum Assays | H2C | Electrolyte Component | | | _ | | | | | |
| Reactions | NH3 | B Electrolyte Component | | | | Simulation Name | Full Name / Synonym | Formula | - | |
| o User Properties | CO2 | 2 Electrolyte Component | | < Ad | ± | ACENITRILE | Acetonitril | e CH3CN | | |
| | SO2 | 2 Electrolyte Component | | | | ACET2 | Acetic_acid,_dime | er C4H8O4 | | |
| | HCL | Electrolyte Component | | | | ACETACID | Acetic_aci | d CH3COOH | | |
| | H2SO4 | Electrolyte Component | | Repla | :e | ACETALDEHD | Ethana | al C2H4O | | |
| | | | | | | ACETONE | Aceton | e CH3COCH3 | | |
| | | | | | | ACETYLENE | Acetylen | e C2H2 | | |
| | | | | Remo | /e | ACIDSO0 | Acid_soluble_oil_(0 | D) C22H36 | | |
| | | | | | | ACIDSO1 | acid_soluble_oilligh | nt C10H16 | | |
| | | | | | | ACIDSO2 | acid_soluble_oil20-309 | % C14H20 | | |
| | | | | | | ACIDSO3 | acid_soluble_oil60-709 | % C18H28 | | |
| Properties | | | | | | ACIDSO4 | acid_soluble_oil>709 | | | |
| Simulation | | | | | | ACIDSO5 | acid_soluble_oil>809 | % C25H34 | * | |
| Safety Analysis | Statuc | ٥ĸ | | | | | | | | |
| Energy Analysis | Messages | | | u | pdated fluid p | ackage xml data is inval ackage xml data is inval ackage xml data is inval | id. | | | • |

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

Creating the Simulation

Click on the Simulation section

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| File Home View Cu | ustomize Resources | | | | | | | | Search Aspen Knowledge | 2 | \$ |
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| operties < | Component List View: Co | | | | | | | | | | |
| l Items + | | | | | | | | | | | G |
| Component Lists | Source Databank: HYSYS | | | | | Select: | OLI (MSE) | • | | | |
| Basis-1 | Component | Туре | Group | | | Search for | : | | Additional Database | | |
| Retroleum Assays | H2O | Electrolyte Component | | | | | | | | | |
| Reactions | NH3 | Electrolyte Component | | | | Si | nulation Name | Full Name / Synonym | Formula | * | |
| User Properties | CO2 | Electrolyte Component | | < / | Add | | ACENITRILE | Acetonitril | e CH3CN | | |
| | SO2 | Electrolyte Component | | | | | ACET2 | Acetic_acid,_dime | r C4H8O4 | | |
| | HCL | Electrolyte Component | | | | | ACETACID | Acetic_acio | d CH3COOH | | |
| | H2SO4 | Electrolyte Component | | Rep | place | | ACETALDEHD | Ethana | I C2H4O | | |
| | | | | | | | ACETONE | Aceton | e CH3COCH3 | | |
| | | | | | | | ACETYLENE | Acetylen | e C2H2 | | |
| | | | | Ren | move | | ACIDSO0 | Acid_soluble_oil_(0 |) C22H36 | | |
| | | | | | | | ACIDSO1 | acid_soluble_oilligh | t C10H16 | | |
| | | | | | | | ACIDSO2 | acid_soluble_oil20-309 | 6 C14H20 | | |
| | | | | | | | ACIDSO3 | acid_soluble_oil60-709 | 6 C18H28 | | |
| Properties | | | | D. | | | ACIDSO4 | acid_soluble_oil>709 | 6 C23H32 | | |
| Simulation | | | | | | | ACIDSO5 | acid_soluble_oil>809 | 6 C25H34 | * | |
| | Status | OK. | | | | | | | | | |
| Safety Analysis | | | | | | | | | | | |
| Energy Analysis | Messages | | | | Updated | fluid package | xml data is invalid. xml data is invalid. xml data is invalid. | | | | |

As you click this button, Aspen HYSYS temporarily passes control to the OLI software to create the electrolyte model. Progress messages can be seen in the status line at the bottom of the window as well as in the summary box. After a few moments, the standard ASPEN HYSYS development window is displayed.

| 関 i 🔒 🤊 🎨 📃 🐷 🗸 🗸 | Unitled - Aspen HYSYS V11 - aspen ONE Powelleet - CD × |
|--|--|
| File Home Economics | Dynamics Plant Data Equation Oriented View Customize Resources Flowsheet/Modify Format |
| 👗 Cut 🛛 si 🔹 🔮 | 🛛 Utility Manager 🔽 Active 📰 🚰 🗹 Model 📈 🗠 Case Studies 🚔 Stream Analysis - 🎉 Pressure Relief 🔗 Emissions |
| | Adjust Manager 📢 On Hold Workbook, Reports 🔄 Flowsheet Compression Zata Fits 🔐 Equipment Design - 🎇 BLOWDOWN and Depressuring - |
| | Fluid Packages sinulation 1 Soher 1 Summaries Analysis Analysis Safety |
| Simulation 4 | |
| All Items | Capital:USD_Utilities:USD_Viear U Energy Savings:MW (%) U Exchangers - Unknown: 0 OK: 0 Risk: 0 🕑 V |
| Contraction with the second se | |
| 🔯 UnitOps | Model Palette 🗰 🖬 1 |
| Constreams | Streams Flowsheets |
| Contraction Equipment Design | |
| Nodel Analysis | |
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| Case Studies | |
| 🗔 Data Fits | |
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| Properties | |
| - Simulation | |
| Safety Analysis | Messages |
| S Energy Analysis | Updated Fluid package xml data is invalid. Updated Fluid package xml data is invalid. Updated Fluid package xml data is invalid. Updated Fluid package xml data is invalid. |
| | |
| | The PIPESIM Enhanced Link Extension is not registered. Please register it to gain access to this operation. |
| Solver (Main) - Ready View Converge | ence Responsiveness: 5 25% \odot |

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

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

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

Selecting the mixer

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

| - | Model Palette | ≁ # × |
|------------|------------------------|--------------------|
| i ^ | Views | Streams Flowsheets |
| | | P |
| | All | |
| | Dynamics & Control | ✐₽₽ |
| | External Model | |
| | Heat Transfer | <u>747</u> |
| | Manipulator | |
| | Piping & Hydraulics | |
| | Pressure Changer | ±~ ± \$ |

The workspace now looks like this:

| B = B = 86 = = ≠ | Untitled - Aspen HYSYS V12.1 - aspenONE | Flowsheet – 🗆 🗙 |
|--|---|---|
| File Home Economics | Dynamics Plant Data Equation Oriented View Customize Resource | |
| لل Cut Copy → ∰ Unit Sets Paste → | | 🗠 Case Studies 🚔 Stream Analysis 👻 🌆 Pressure Relief 💦 Emissions 👔 🎒 |
| Simulation < | Capital:USD_Utilities:USD/Year OEnergy Savings:MW (| %) 💽 Exchangers - Unknown: 0 OK: 0 Risk: 0 💽 |
| All Items 🔹 | Flowsheet Case (Main) - Solver Active × + | ▼ Model Palette |
| © Workbook ▷ Qurkbook ▷ Churtops ▷ Stream Analysis ▷ Equipment Design ▷ Model Analysis ▷ Data Tables ▷ Strip Charts ▷ Case Studies ▷ Data Fits ▷ Data Tits ▷ Data Tits ▷ Data Al | MIX-100 | Views Streams Piowsheets Image: Stream S |
| Properties | | Changer Cn(A) |
| C Simulation | <u> </u> | Reactor |
| a - Salety Analysis | Messages | • 4 x |
| Strengy Analysis | Required Info : MIX-100 Requires a feed stream Required Info : MIX-100 Requires a product stream Optional Info : MIX-100 Not Solved | Operation. Saving case C:\users\JAMES~1.8ER\AppData\Local\Temp\AutoRecovery save of NoName (0x170368).ahc Completed. Flowsheet Object MIX-100 is created on the Main flowsheet |
| olver (Main) - Ready View Converg | ence | Responsiveness: 5 115% 👄 🛛 🕀 🔛 |

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.

| | - | | 1 |
|---|----|---|-----|
| | | | - 1 |
| - | 20 | ~ | - 1 |
| | - | | _ 1 |

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

| /Flowsheet Case (Main) - Solver Active × + | Model Palette | ↓ 4 × |
|--|------------------------|--------------------|
| | Views | Streams Flowsheets |
| | | 2 |
| | All | €>+€¢ |
| 1 | Dynamics & Control | ∯₽₽₽ |
| 2 MIX-100 | External Mode | ⊨ •₩•€• |
| - | Heat Transfer | ~ ? fJ |
| | Manipulator | |
| | Piping & Hydraulics | |
| | Pressure Changer | ±// 🖽 🕰 |
| ۷ ۲ | Reactor | Cn(A) |

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

| Mixer: MIX-100 | | 13 |
|--|------------------------|--------|
| Design Rating | Worksheet Dynamics | |
| Design Connections Parameters User Variables Notes | Name MIX-100 | |
| Delete | Requires a feed stream | gnored |

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

| xer: MIX- | 100 | | | | - 0 : |
|--|---------------|-----------|----------|---------------------------|-----------|
| Design | Rating | Worksheet | Dynamics | | |
| Desi Connecto Parameter User Vau Notes | tions ters | Inlets | Name | MIX-100 | |
| [| Delete | | | Requires a product stream |] Ignored |

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

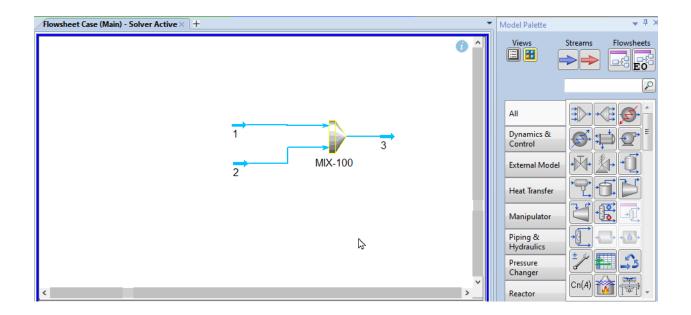
Locate the *Outlet* box and enter the number "3". This completes this block.

| Ν | /lixer: MIX-100 | | | | - E 13 |
|---|-----------------|---------------------|---------|---|---------|
| | Design Rating | Worksheet Dynamics | | | |
| | Design | Name | MIX-100 | | |
| н | Connections | | | | |
| | Parameters | | | | |
| L | User Variables | | | | |
| | Notes | inlets << Stream | | Outlet 3 Fluid Package Basis-1 | |
| | | | | | |
| | Delete | | Not S | Solved | 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.

| | Stream Name | 1 | 1 Elec | |
|---|-------------------------------|-----------------|-----------------|--|
| Conditions | Vapour / Phase Fraction | <empty></empty> | <empty></empty> | |
| Properties | Temperature [C] | <empty></empty> | <empty></empty> | |
| Composition | Pressure [kPa] | <empty></empty> | <empty></empty> | |
| Oil & Gas Feed | Molar Flow [kgmole/h] | <empty></empty> | <empty></empty> | |
| Petroleum Assay K Value | Mass Flow [kg/h] | <empty></empty> | <empty></empty> | |
| Electrolytes | Std Ideal Liq Vol Flow [m3/h] | <empty></empty> | <empty></empty> | |
| User Variables | Molar Enthalpy [kJ/kgmole] | <empty></empty> | <empty></empty> | |
| Notes | Molar Entropy [kJ/kgmole-C] | <empty></empty> | <empty></empty> | |
| Cost Parameters Normalized Yields Emissions | Heat Flow [kJ/h] | <empty></empty> | <empty></empty> | |
| | Liq Vol Flow @Std Cond [m3/h] | <empty></empty> | <empty></empty> | |
| Emissions | Fluid Package | Basis-1 | | |
| | Utility Type | | | |
| | | | | |
| | | | | |

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

| orksheet Attachm | ents Dynamics | | | |
|--|-------------------------------|-----------------|-----------------|--|
| Worksheet | Stream Name | 1 | 1_Elec | |
| Conditions | Vapour / Phase Fraction | <empty></empty> | <empty></empty> | |
| Properties | Temperature [C] | 40.00 | 40.00 | |
| Composition | Pressure [kPa] | 101.3 | 101.3 | |
| Oil & Gas Feed Petroleum Assay | Molar Flow [kgmole/h] | <empty></empty> | <empty></empty> | |
| Petroleum Assay K Value Electrolytes User Variables Notes Cost Parameters Normalized Yields ▷ Emissions | Mass Flow [kg/h] | <empty></empty> | <empty></empty> | |
| | Std Ideal Liq Vol Flow [m3/h] | <empty></empty> | <empty></empty> | |
| | Molar Enthalpy [kJ/kgmole] | <empty></empty> | <empty></empty> | |
| | Molar Entropy [kJ/kgmole-C] | <empty></empty> | <empty></empty> | |
| | Heat Flow [kJ/h] | <empty></empty> | <empty></empty> | |
| | Liq Vol Flow @Std Cond [m3/h] | <empty></empty> | <empty></empty> | |
| Emissions | Fluid Package | Basis-1 | | |
| | Utility Type | | | |
| | | | | |
| | Co- | | | |

Now click the *Composition* line

| Worksheet | | Mole Fractions | Mole Fractions Elec | |
|-------------------------|--------------|------------------|---------------------|--|
| Conditions | H2O | <empty></empty> | <empty></empty> | |
| Properties | NH3 | <empty></empty> | <empty></empty> | |
| Composition | CO2 | <empty></empty> | <empty></empty> | |
| Oil & Gas Feod | SO2 | <empty></empty> | <empty></empty> | |
| Petroleum Assay | HCL | <empty></empty> | <empty></empty> | |
| K Value Electrolytes | H2SO4 | <empty></empty> | <empty></empty> | |
| User Variables | H2CO3 | <empty></empty> | <empty></empty> | |
| Notes | H2SO3 | <empty></empty> | <empty></empty> | |
| Cost Parameters | HNH2CO2 | <empty></empty> | <empty></empty> | |
| Normalized Yields | NH42CO3 | <empty></empty> | <empty></empty> | |
| Emissions | NH42SO3 | <empty></empty> | <empty></empty> | |
| | NH42SO3.1H2O | <empty></empty> | <empty></empty> | |
| | NH42SO4 | <empty></empty> | <empty></empty> | |
| | NH43HSO42 | <empty></empty> | <empty></empty> | |
| | NH44H2CO33 | <empty></empty> | <empty></empty> | |
| | NH4CL | <empty></empty> | <empty></empty> | |
| | NH4CLB | <empty></empty> | <empty></empty> | |
| | NH4CO2NH2 | <empty></empty> | <empty></empty> | |
| | NH4H3SO42 | <empty></empty> | <empty></empty> | |
| | NH4HCO3 | <empty></empty> | <empty></empty> | |
| | NH4HSO3 | <empty></empty> | <empty></empty> | |
| | NH4HSO4 | <empty></empty> | <empty></empty> | |
| | NH4OH | <empty></empty> | <empty></empty> | |
| | Total | 0.0000 | 00 | |
| | Edit View | Properties Basis | | |

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

| Worksheet | | Mole Fractions | Mole Fractions Elec | |
|-------------------------|----------------|--------------------------|---------------------|--|
| Conditions | H2O | <empty></empty> | <empty></empty> | |
| Properties | NH3 | <empty></empty> | <empty></empty> | |
| Composition | CO2 | <empty></empty> | <empty></empty> | |
| Oil & Gas Feed | SO2 | <empty></empty> | <empty></empty> | |
| Petroleum Assay | HCL | <empty></empty> | <empty></empty> | |
| K Value Electrolytes | H2SO4 | <empty></empty> | <empty></empty> | |
| User Variables | H2CO3 | <empty></empty> | <empty></empty> | |
| Notes | H2SO3 | <empty></empty> | <empty></empty> | |
| Cost Parameters | HNH2CO2 | <empty></empty> | <empty></empty> | |
| Normalized Yields | NH42CO3 | <empty></empty> | <empty></empty> | |
| Emissions | NH42SO3 | <empty></empty> | <empty></empty> | |
| | NH42SO3.1H2O | <empty></empty> | <empty></empty> | |
| | NH42SO4 | <empty></empty> | <empty></empty> | |
| | NH43HSO42 | <empty></empty> | <empty></empty> | |
| | NH44H2CO33 | <empty></empty> | <empty></empty> | |
| | NH4CL | <empty></empty> | <empty></empty> | |
| | NH4CLB | <empty></empty> | <empty></empty> | |
| | NH4CO2NH2 | <empty></empty> | <empty></empty> | |
| | NH4H3SO42 | <empty></empty> | <empty></empty> | |
| | NH4HCO3 | <empty></empty> | <empty></empty> | |
| | NH4HSO3 | <empty></empty> | <empty></empty> | |
| | NH4HSO4 | <empty></empty> | <empty></empty> | |
| | NH4OH | <empty></empty> | <empty></empty> | |
| | Total | 0.000 | 00 | |
| | Edit View Prop | erties | | |
| | | | | |
| | Edit View Prop | Change Compositional Bas | | |

This will open a new window

| 된 Stream: Materi | — | \times |
|---------------------|---|----------|
| Compositional Basis | | |
| O Mole Fractions | | |
| O Mass Fractions | | |
| Mole Flows | | |
| O Mass Flows | | |
| | | |
| | | |
| | 6 | |
| | | |

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

Now begin entering the value for H2O of 55.51

| Worksheet | | Molar Flows | Molar Flows_Elec | |
|----------------------------|--------------|---------------------|----------------------|--|
| Conditions | H2O kan | nole/h 🔻 55.51 | _ <empty></empty> | |
| Properties | NH3 | wempty> | <empty></empty> | |
| Composition | CO2 | <empty></empty> | <empty></empty> | |
| Oil & Gas Feed | SO2 | <empty></empty> | <empty></empty> | |
| Petroleum Assay K Value | HCL | <empty></empty> | <empty></empty> | |
| Electrolytes | H2SO4 | <empty></empty> | <empty></empty> | |
| User Variables | H2CO3 | <empty></empty> | <empty></empty> | |
| Notes | H2SO3 | <empty></empty> | <empty></empty> | |
| Cost Parameters | HNH2CO2 | <empty></empty> | <empty></empty> | |
| Normalized Yields | NH42CO3 | <empty></empty> | <empty></empty> | |
| Emissions | NH42SO3 | <empty></empty> | <empty></empty> | |
| | NH42SO3.1H2O | <empty></empty> | <empty></empty> | |
| | NH42SO4 | <empty></empty> | <empty></empty> | |
| | NH43HSO42 | <empty></empty> | <empty></empty> | |
| | NH44H2CO33 | <empty></empty> | <empty></empty> | |
| | NH4CL | <empty></empty> | <empty></empty> | |
| | NH4CLB | <empty></empty> | <empty></empty> | |
| | NH4CO2NH2 | <empty></empty> | <empty></empty> | |
| | NH4H3SO42 | <empty></empty> | <empty></empty> | |
| | NH4HCO3 | <empty></empty> | <empty></empty> | |
| | Tota | al 0.00000 kgmole/h | | |

Once you hit enter it will prompt you to a new window to finish entering the composition of the stream. A fly-out unit selection box appears near the composition. Use the defaults at this time.

| | Comp Mole Flow | | Composition Basis |
|--------------|-------------------|-------|------------------------|
| kgmole/h 🔻 | 55.51 | | Mole Fractions |
| NH3 | <empty></empty> | | Mass Fractions |
| CO2 | <empty></empty> | | |
| SO2 | <empty></empty> | | C Liq Volume Fractions |
| HCL | <empty></empty> | | Mole Flows |
| H2SO4 | <empty></empty> | | |
| H2CO3 | <empty></empty> | | Mass Flows |
| H2SO3 | cempty> | | C Lig Volume Flows |
| HNH2CO2 | <empty></empty> | = | C Elq Volume Hows |
| NH42CO3 | <empty></empty> | | |
| NH42SO3 | <empty></empty> | | Composition Controls |
| NH42SO3.1H2O | <empty></empty> | | Erase |
| NH42SO4 | <empty></empty> | | Erase |
| NH43HSO42 | <empty></empty> | | |
| NH44H2CO33 | <empty></empty> | | Equalize Composition |
| NH4CL | <empty></empty> | | |
| NH4CLB | <empty></empty> | | |
| NH4CO2NH2 | <empty></empty> | | |
| NH4H3SO42 | <empty></empty> | | |
| NH4HCO3 | <empty></empty> | - | |
| | | Ť | Cancel |
| | | | Cancer |
| Normalize | Total 55.5100 kgm | ole/h | ОК |

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

| | CompMoleFlow | | Composition Basis |
|--------------|--------------------|------|-----------------------|
| H2O | 55.5100 | | Mole Fractions |
| NH3 | 0.0000 | | Mass Fractions |
| CO2 | 0.0000 | | |
| SO2 | 0.0000 | | Liq Volume Fractions |
| HCL | 0.0000 | | Mole Flows |
| H2SO4 | 0.0000 | | |
| H2CO3 | 0.0000 | | Mass Flows |
| H2SO3 | 0.0000 | = | C Lig Volume Flows |
| HNH2CO2 | 0.0000 | - | C Lq foldine fibility |
| NH42CO3 | 0.0000 | | |
| NH42SO3 | 0.0000 | | Composition Controls |
| NH42SO3.1H2O | 0.0000 | | Erase |
| NH42SO4 | 0.0000 | | Liase |
| NH43HSO42 | 0.0000 | | |
| NH44H2CO33 | 0.0000 | | Equalize Composition |
| NH4CL | 0.0000 | | |
| NH4CLB | 0.0000 | | |
| NH4CO2NH2 | 0.0000 | | |
| NH4H3SO42 | 0.0000 | | |
| NH4HCO3 | 0.0000 | * | |
| | | | Cancel |
| Normalize | Total 55.5100 kgmo | le/h | 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.

| NH31.0000CO20.1000SO20.1000HCL <empty>H2SO4<empty>H2CO3<empty>HNH2CO2<empty>NH42CO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO3<empty>NH42SO4<empty>NH4CLB<empty>NH4CLB<empty>NH4CLB<empty>NH4CB3<empty>NH4H3SO42<empty>NH4CO3<empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | | Comp M | ole Flow | | Composition Basis |
|---|--------------|--------|-----------------|---|-----------------------|
| CO2 0.1000 SO2 0.1000 HCL <empty> H2SO4 <empty> H2CO3 <empty> HNH2CO2 <empty> NH42CO3 <empty> NH42SO3.1H2O <empty> NH42SO3.1H2O <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO3.1H2O <empty> NH44H2CO33 <empty> NH44H2CO33 <empty> NH4CLB <empty> NH4CO2NH2 <empty> NH4HO3 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | H2O | | 55.5100 | ~ | O Mole Fractions |
| 0.1000 Iliq Volume Fractions HCL <empty> H2SO4 <empty> H2CO3 <empty> H2SO3 <empty> HNH2CO2 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO4 <empty> NH42SO3 <empty> NH42SO4 <empty> NH43HSO42 <empty> NH4CL <empty> NH4CL <empty> NH4CO2NH2 <empty> NH4HDO3 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | NH3 | | 1.0000 | | Mass Fractions |
| SO2 0.1000 HCL <empty> H2SO3 <empty> H2SO3 <empty> HNH2CO2 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO4 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO4 <empty> NH44H2CO33 <empty> NH4CL <empty> NH4CD3 <empty> NH4HD3 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | CO2 | | 0.1000 | | |
| H2SO4 < cempty> H2SO3 < cempty> H2SO3 < cempty> HNH2CO2 < cempty> NH42SO3 < cempty> NH42SO3 < cempty> NH42SO3 < cempty> NH42SO3 < cempty> NH42SO4 < cempty> NH42SO3 < cempty> NH42SO4 < cempty> NH42SO4 < cempty> NH42SO4 < cempty> NH42SO4 < cempty> NH42SO4 < cempty> NH44H2CO33 < cempty> NH4CL < cempty> NH4CL < cempty> NH4CD2NH2 < cempty> NH4CO2NH2 < cempty> NH4CO2NH2 < cempty> NH4HCO3 < cempty> | SO2 | | 0.1000 | | Cliq Volume Fractions |
| H2CO3 < <empty> H2SO3 < <empty> HNH2CO2 < <empty> NH42SO3 < <empty> NH42SO3 < <empty> NH42SO3 < <empty> NH42SO3 < <empty> NH42SO4 < <empty> NH43SO42 < <empty> NH44H2CO33 <<empty> NH4CL < <empty> NH4CLB < <empty> NH4CO2NH2 < <empty> NH4CO2NH2 <<empty> NH4CO2NH2 <<empty> NH4CO2NH2 <<empty> NH4HCO3 <<empty> NH4HCO3 <<empty> Composition Controls Equalize Composition</empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | HCL | | <empty></empty> | | Mole Flows |
| NH2CO3 <empty> HNH2CO2 <empty> NH42CO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO4 <empty> NH44H2CO33 <empty> NH44H2CO33 <empty> NH44H2CO33 <empty> NH4CLB <empty> NH4CO2NH2 <empty> NH4H033 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | H2SO4 | | <empty></empty> | | |
| HNH2CO2 <empty> NH42CO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO4 <empty> NH44SO42 <empty> NH44H2CO33 <empty> NH4CLB <empty> NH4CO2NH2 <empty> NH4CO3 <empty> NH4HCO3 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | H2CO3 | | <empty></empty> | | Mass Flows |
| HNH2CO2 <empty> NH42CO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO3 <empty> NH42SO4 <empty> NH43HSO42 <empty> NH44H2CO33 <empty> NH4CL <empty> NH4CL <empty> NH4C203H2 <empty> NH4HSO42 <empty> NH4HC02NH2 <empty> NH4HC03 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | H2SO3 | | <empty></empty> | | C Lig Volume Flows |
| NH42SO3 <empty> NH42SO3.1H2O <empty> NH42SO4 <empty> NH43HSO42 <empty> NH44H2C033 <empty> NH4CL <empty> NH4CLB <empty> NH4C02NH2 <empty> NH4H03 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | HNH2CO2 | | <empty></empty> | = | |
| NH42SO3 <empty> NH42SO3.1H2O <empty> NH42SO4 <empty> NH43SO42 <empty> NH44H2CO33 <empty> NH4CL <empty> NH4CO2NH2 <empty> NH4H2SO4 <empty> NH4CO2NH2 <empty> NH4H03 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | NH42CO3 | | <empty></empty> | | |
| NH42S04 <empty> NH43HS042 <empty> NH43HS042 <empty> NH44H2C033 <empty> NH4CL <empty> NH4CLB <empty> NH4C02NH2 <empty> NH4H03 <empty></empty></empty></empty></empty></empty></empty></empty></empty> | NH42SO3 | | <empty></empty> | | Composition Controls |
| NH42S04 <empty> NH43HS042 <empty> NH44H2C033 <empty> NH4CL <empty> NH4CLB <empty> NH4C02NH2 <empty> NH4H203 <empty> NH4C02NH2 <empty> NH4H03 <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty> | NH42SO3.1H2O | | <empty></empty> | | Fraço |
| NH44H2CO33 <empty> Equalize Composition NH4CL <empty> NH4CLB <empty> NH4CO2NH2 <empty> NH4H2SO42 <empty> NH4HCO3 <empty></empty></empty></empty></empty></empty></empty> | NH42SO4 | | <empty></empty> | | Liase |
| NH4CLS <empty> NH4CLB <empty> NH4CO2NH2 <empty> NH4H2O3 <empty></empty></empty></empty></empty> | NH43HSO42 | | <empty></empty> | | |
| NH4CLB <mpty> NH4CO2NH2 <mpty> NH4H3SO42 <mpty> NH4HCO3 <mpty> NH4HCO3 <mpty></mpty></mpty></mpty></mpty></mpty> | NH44H2CO33 | | <empty></empty> | | Equalize Composition |
| NH4CO2NH2 <empty> NH4H3SO42 <empty> NH4HCO3 <empty></empty></empty></empty> | NH4CL | | <empty></empty> | | |
| NH4H3SO42 <empty> NH4HCO3 <empty></empty></empty> | NH4CLB | | <empty></empty> | _ | |
| NH4HCO3 <empty></empty> | NH4CO2NH2 | | <empty></empty> | | |
| | NH4H3SO42 | | <empty></empty> | | |
| Cancel | NH4HCO3 | | <empty></empty> | - | |
| | NUAUCO2 | | | | Cancel |

Click the **OK** button.

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

Click on the *Electrolytes* line.

| Vaterial Stream: 1 | | | - E |
|--|--|----------------------|------------|
| Worksheet Attachme | ents Dynamics | | |
| Worksheet Conditions Properties Composition Oil & Gas Feed | True Species Info Properties Composition Phase Aqu Soli | d | _ |
| Petroleum Assay | рН | 9.3400 | |
| K Value PSD Property | Osmotic Pressure | 2770.9 kPa | |
| Electrolytes | Ionic Strength | 7.9249e-006 kgmol/kg | |
| User Variables Notes | Heat Capacity | 74.660 kJ/kgmole-C | |
| Cost Parameters | Viscosity | 0.68024 cP | |
| Normalized Yields | Specific Electrical Conductivity | 5.1431 S/m | |
| Emissions | Molar Electrical Conductivity | 0.00000 S-m2/kgmole | |
| | | | |
| | | ОК | |
| Delete | Define from Stream | View Assay | + + |

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.

| Worksheet Conditions Properties Composition | True Species Info Properties Composition | Phase Aqueous Solid | Conc. Basis Molar Mass | | | |
|--|--|---------------------------|------------------------------|------------------------|-------------------------|--|
| Oil & Gas Feed Petroleum Assay K Value | True Species | Mole Fraction | Molar Flow [kgmole/h] | Molality [kgmol/kg] | Molarity [kgmole/m3] | |
| PSD Property | H2O | 0.97929 | 54.8569 | 5.55081e-002 | 55.2144 | |
| Electrolytes | CO2AQ | 0.00000 | 2.17211e-005 | 2.19789e-008 | 2.18626e-005 | |
| User Variables Notes | H2SO4AQ | 0.00000 | 0.000000 | 0.000000 | 0.000000 | |
| Cost Parameters | HCLAQ | 0.00000 | 0.000000 | 0.000000 | 0.000000 | |
| Normalized Yields | NH3AQ | 0.00259 | 0.145256 | 1.46980e-004 | 0.146202 | |
| Emissions | NH4OHAQ | 0.00880 | 0.492882 | 4.98732e-004 | 0.496094 | |
| | SO2AQ | 0.00000 | 7.63093e-012 | 7.72151e-015 | 7.68065e-012 | |
| | SO3AQ | 0.00000 | 0.000000 | 0.000000 | 0.000000 | |
| | CLION | 0.00000 | 0.000000 | 0.000000 | 0.000000 | |
| | CO3ION | 0.00040 | 2.21690e-002 | 2.24322e-005 | 2.23135e-002 | |
| | H3OION | 0.00000 | 6.59448e-010 | 6.67276e-013 | 6.63745e-010 | |
| | HCO3ION | 0.00068 | 3.79443e-002 | 3.83947e-005 | 3.81915e-002 | |
| | HSO3ION | 0.00000 | 2.38525e-004 | 2.41356e-007 | 2.40079e-004 | |
| | HSO4ION | 0.00000 | 0.000000 | 0.000000 | 0.000000 | |
| | NH2CO2ION | 0.00071 | 3.98650e-002 | 4.03382e-005 | 4.01247e-002 | |
| | NH4ION | 0.00575 | 0.321997 | 3.25820e-004 | 0.324096 | |
| | OHION | 0.00000 | 8.87369e-005 | 8.97902e-008 | 8.93151e-005 | |
| | \$205ION | 0.00000 | 1.32696e-008 | 1.34271e-011 | 1.33561e-008 | |
| | | | OK | | | |

Click on the *x* to close this dialog.

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

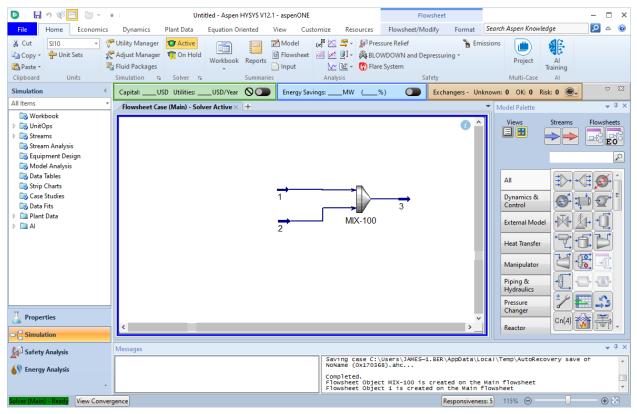
| Temperature | 25 | С |
|-------------|-------|-----|
| Pressure | 101.3 | kPa |
| H2O | 55.51 | |
| HCI | 0.1 | |
| H2SO4 | 1.0 | |

Click the *Electrolytes* line to see the pH.

| Vlaterial Stream: 2 | | | | - 6 % |
|--|--|----------------------|---------|-------------|
| Worksheet Attachme | nts Dynamics | | | 0 |
| Worksheet Conditions Properties Composition Oil & Gas Feed | True Species Info Properties Composition | | | |
| Petroleum Assay | pН | -0.0811 |] | |
| K Value PSD Property | Osmotic Pressure | 6582.5 kPa | | |
| Electrolytes | Ionic Strength | 2.5144e-005 kgmol/kg | | |
| User Variables Notes | Heat Capacity | 73.805 kJ/kgmole-C | | |
| Notes Cost Parameters | Viscosity | 1.1257 cP | | |
| Normalized Yields | Specific Electrical Conductivity | 41.582 S/m | | |
| Emissions | Molar Electrical Conductivity | 0.00000 S-m2/kgmole | | |
| | | | N | |
| | | ОК | | |
| Delete | Define from Stream | View Assay | | > |

Click the *x* to close the dialog.

Hysys will attempt to converge the process as you create it. As you close the final dialog box for data entry you will see that the output stream "3" is "Blue" which means it has converged.



Reviewing the output

Double-Click stream "3"

| | Stream Name | 3 | 3_Elec | Vapour Phase |
|--------------------------------------|-------------------------------|-----------------|-----------------|-----------------|
| Conditions | Vapour / Phase Fraction | 0.0006 | 0.0006 | 0.0006 |
| Properties | Temperature [C] | 36.99 | 36.99 | 36.99 |
| Composition | Pressure [kPa] | 101.3 | 101.3 | 101.3 |
| Oil & Gas Feed Petroleum Assav | Molar Flow [kgmole/h] | 114.3 | 114.3 | 6.574e-002 |
| K Value | Mass Flow [kg/h] | 2130 | 2130 | <empty></empty> |
| PSD Property | Std Ideal Liq Vol Flow [m3/h] | <empty></empty> | <empty></empty> | <empty></empty> |
| Electrolytes | Molar Enthalpy [kJ/kgmole] | -2.865e+005 | -2.865e+005 | -3.787e+005 |
| User Variables | Molar Entropy [kJ/kgmole-C] | 72.66 | 72.66 | 215.4 |
| Notes | Heat Flow [kJ/h] | -3.275e+007 | -3.275e+007 | -2.490e+004 |
| Cost Parameters Normalized Yields | Liq Vol Flow @Std Cond [m3/h] | <enpty></enpty> | <empty></empty> | <empty></empty> |
| Emissions | Fluid Package | Basis-1 | | |
| cimpatona | Utility Type | | | |
| | | | | |
| | | | | |

The converged process temperature is approximately 37.0 °C.

Click on the *Electrolytes* line.

| Material Stream: 3 | | | |
|--|--|------------|----------|
| Worksheet Attachme | ents Dynamics | | 0 |
| Worksheet Conditions Properties Composition Oil & Gas Feed | True Species Info Properties Composition | d | |
| Petroleum Assay | pН | 0.8681 | |
| K Value PSD Property | Osmotic Pressure | | |
| Electrolytes | Ionic Strength | | |
| User Variables Notes | Heat Capacity | - | |
| Cost Parameters | Viscosity | | |
| Normalized Yields | Specific Electrical Conductivity | | |
| Emissions | | | |
| | | | Þ |
| | | ОК | |
| Delete | Define from Stream | View Assay | \ |

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.

| Worksheet Conditions Properties Composition Oil & Gas Feed Petroleum Assay K Value | True Species Info – Properties Composition | Phase Aqueous Solid | Conc. Basis Molar Mass | | | |
|--|--|---------------------------|------------------------------|------------------------|-------------------------|--|
| | True Species | Mole Fraction | Molar Flow [kgmole/h] | Molality [kgmol/kg] | Molarity [kgmole/m3] | |
| PSD Property | H2O | 0.97673 | 110.609 | 5.55081e-002 | 55.1678 | |
| Electrolytes | CO2AQ | 0.00037 | 4.17338e-002 | 2.09438e-005 | 2.08154e-002 | |
| User Variables Notes | H2SO4AQ | 0.00000 | 2.85323e-007 | 1.43187e-010 | 1.42309e-007 | |
| Cost Parameters | HCLAQ | 0.00000 | 8.92784e-010 | 4.48037e-013 | 4.45290e-010 | |
| Normalized Yields | NH3AQ | 0.00000 | 1.24349e-009 | 6.24038e-013 | 6.20213e-010 | |
| Emissions | NH4OHAQ | 0.00000 | 4.44573e-009 | 2.23106e-012 | 2.21738e-009 | |
| | SO2AQ | 0.00076 | 8.65423e-002 | 4.34306e-005 | 4.31644e-002 | |
| | SO3AQ | 0.00000 | 1.33354e-020 | 6.69225e-024 | 6.65122e-021 | |
| | CLION | 0.00088 | 1.00000e-001 | 5.01843e-005 | 4.98766e-002 | |
| | CO3ION | 0.00000 | 7.17700e-016 | 3.60172e-019 | 3.57964e-016 | |
| | H3OION | 0.00351 | 0.397437 | 1.99451e-004 | 0.198228 | |
| | HCO3ION | 0.00000 | 2.86323e-007 | 1.43689e-010 | 1.42808e-007 | |
| | HSO3ION | 0.00009 | 9.99071e-003 | 5.01376e-006 | 4.98303e-003 | |
| | HSO4ION | 0.00629 | 0.712580 | 3.57603e-004 | 0.355411 | |
| | NH2CO2ION | 0.00000 | 31.46321e-015 | 7.34300e-019 | 7.29798e-016 | |
| | NH4ION | 0.00883 | 1.00000 | 5.01843e-004 | 0.498766 | |
| | OHION | 0.00000 | 5.40518e-013 | 2.71255e-016 | 2.69592e-013 | |
| | S2O5ION | 0.00000 | 1.29468e-005 | 6.49723e-009 | 6.45740e-006 | |
| | | | OK | | | |

Click on the *Composition* line at the left.

| Worksheet | | Mole Fractions | Mole Fractions_Elec | Vapour Phase | Aqueous Phase | |
|--|---------------|--------------------------|---------------------|--------------|---------------|--|
| Conditions Properties Composition Oil & Gas Feed Petroleum Assay K Value PSD Property Electrolytes User Variables Notes | H2O | 0.9799 | 0.9799 | 0.0613 | 0.9804 | |
| | NH3 | 0.0087 | 0.0087 | 0.0000 | 0.0088 | |
| | CO2 | 0.0009 | 0.0009 | 0.8863 | 0.0004 | |
| | SO2 | 0.0009 | 0.0009 | 0.0523 | 0.0008 | |
| | HCL | 0.0009 | 0.0009 | 0.0000 | 0.0009 | |
| | H2SO4 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | H2CO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | H2SO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | HCL.1H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| Cost Parameters | HCL2H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| Normalized Yields | HCL3H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| Emissions | NH42CO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42CO3.1H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42S2O5 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42SO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42SO3.1H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42SO4 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH43CO32 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH43HSO42 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH44HCO3.1H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | Total | 1.0000 operties Basis | 0 | | | |

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.

| Worksheet | | Molar Flows | Molar Flows_Elec | Vapour Phase | Aqueous Phase | |
|---|--------------|--------------------|------------------|--------------|---------------|--|
| Conditions Properties Composition Oil & Gas Feed Petroleum Assay K Value PSD Property Electrolytes | H2O | 112.0200 | 112.0200 | 0.0040 | 112.0160 | |
| | NH3 | 1.0000 | 1.0000 | 0.0000 | 1.0000 | |
| | CO2 | 0.1000 | 0.1000 | 0.0583 | 0.0417 | |
| | SO2 | 0.1000 | 0.1000 | 0.0034 | 0.0966 | |
| | HCL | 0.1000 | 0.1000 | 0.0000 | 0.1000 | |
| | H2SO4 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | H2CO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| User Variables | H2SO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| Notes | HCL1H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| Cost Parameters | HCL2H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| Normalized Yields | HCL3H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| Emissions | NH42CO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42CO3.1H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42S2O5 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42SO3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42SO3.1H2O | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | NH42SO4 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| | Total | 114.32000 kgmole/h | | | | |

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