

# OLI Engine for Aspen Hysys Version 12

think simulation

getting the chemistry right

## Introduction to OLI Engine for Aspen Hysys

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OLI Engine for Aspen Hysys Version 12

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If you need to contact Support, you can submit an online request via OLI Portal: <u>https://portal.olisystems.com/</u>

Other useful links and resources are:

OLI Systems Portal – How to create and account: <u>https://info.olisystems.com/portal-instructions</u> Product Downloads: <u>http://downloads.olisystems.com/</u> OLI Systems YouTube Channel: <u>https://www.youtube.com/OLISystems</u> OLI Systems Wiki page: <u>http://wiki.olisystems.com/wiki/Main\_Page</u>

# **Disclaimer**

This manual was produced using the OLI Engine for Aspen Hysys Version 12 and OLI Engine 11.5.1.

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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# **Table of Contents**

DISCLAIMER	2
TRADEMARKS	2
TABLE OF CONTENTS	3
OVERVIEW	4
Assumptions	4
Application Using the OLI Engine for Aspen HYSYS	<b>5</b> 5
Entering the Chemistry and fluid packages Selecting Fluid Packages Entering Components	7
Creating the Simulation Selecting the mixer Entering Stream Composition Data	
Reviewing the output	

# **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:

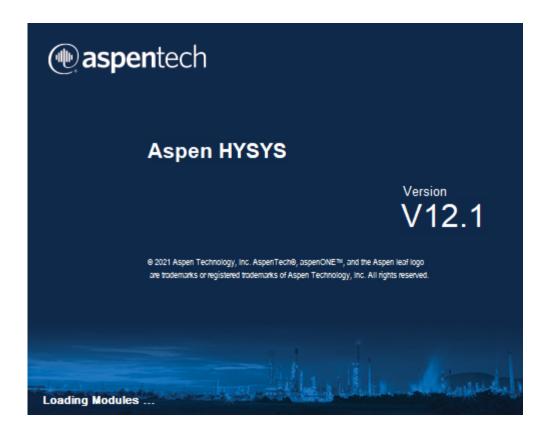
- 1. Aspen HYSYS is currently installed and running on your computer.
- 2. The license manager for Aspen HYSYS is currently set up.
- 3. The OLI Engine for Aspen HYSYS product has been installed.
- 4. The OLI security model is running.
- 5. Aspen HYSYS V12 is being used.
- 6. The user is expected to know how to run Aspen HYSYS.

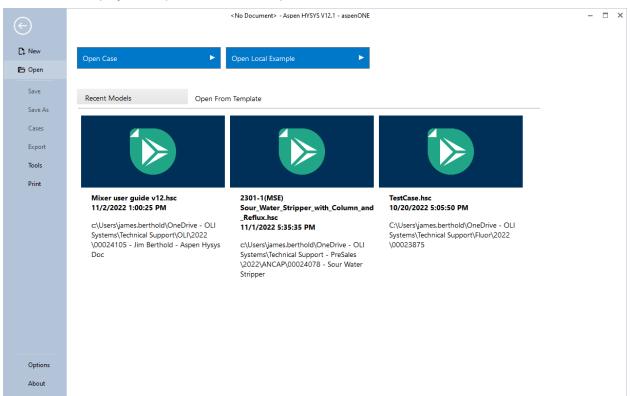
# Application

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.

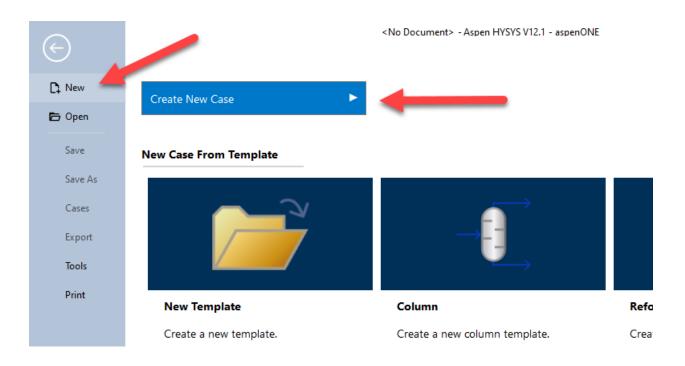




### This will now display the Aspen HYSYS development environment.

# 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

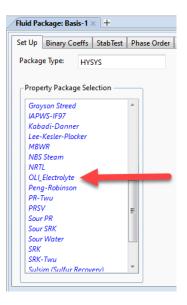
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There are no fluid packages currently defined for this simulation. We need to add a package.

#### Click the Add button

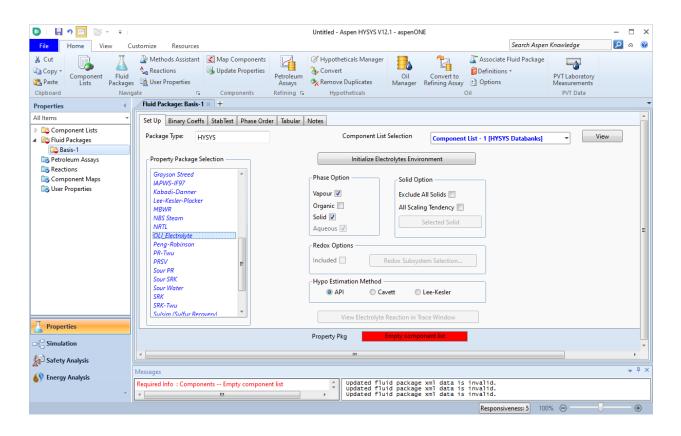
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Scroll down the window to find OLI\_Electrolyte

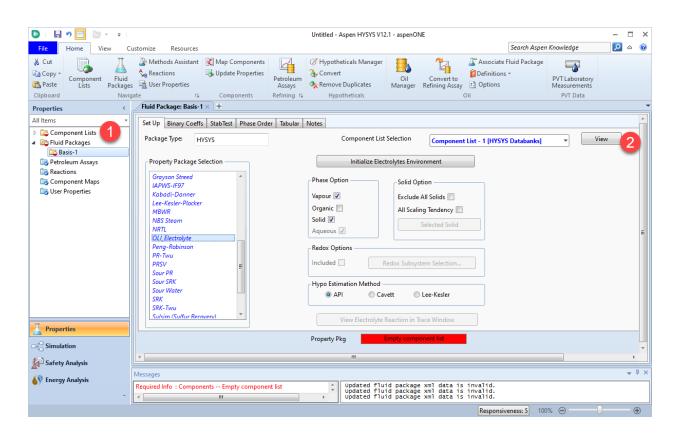


Highlight the object **OLI\_Electrolyte**.

The window changes to display some OLI specific options. It is beyond the scope of this document to explain those options currently. Notice that the name of the component list is **Component List -1**.



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)



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** 

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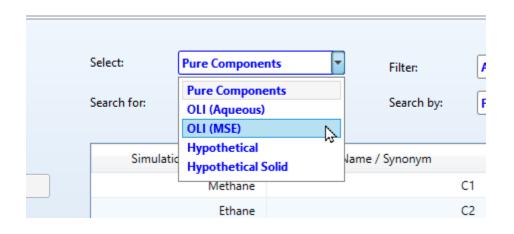
# **Entering Components**

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	-
Search for:		Search by:	Full Name/Synonym	·
Simulat	ion Name	Full Name / Synonym	Formula	*
	Methane	C1	I CH4	
		C	2 C2H6	
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This will display several options:



## For this example, we will use OLI (MSE)

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							ACIDSO2	acid_soluble_oil20-309	6 C14H20		
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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.

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				Replace		H2MNO4	Manganic(VI)_acid	H2MnO4		
						H2MOO4	Molybdenic(VI)_acid	H2MoO4		
						H2O	Water	H2O		
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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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							÷	H2S2O3	Thio	sulfuric_acid	H2S2O3		
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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 components<sup>1</sup>.

- NH3
- CO2
- SO2
- HCL
- H2SO4

The input should look like this:

<sup>&</sup>lt;sup>1</sup> 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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o User Properties	CO2 SO2	Electrolyte Component Electrolyte Component		< Add		ACENTRILE ACET2	Acetic acid, dimer			
	HCL	Electrolyte Component				ACETACID	Acetic acid			
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						ACIDSO1	acid_soluble_oillight	C10H16		
						ACIDSO2	acid_soluble_oil20-30%	C14H20		
						ACIDSO3	acid_soluble_oil60-70%	C18H28		
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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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	SO2	Electrolyte Component				ACET2	Acetic_acid,_dimer	C4H8O4		
	HCL	Electrolyte Component			_	ACETACID	Acetic_acid	CH3COOH		
	H2SO4	Electrolyte Component		Replace		ACETALDEHD	Ethanal	C2H4O		
						ACETONE	Acetone	CH3COCH3		
						ACETYLENE	Acetylene	C2H2		
				Remove		ACIDSO0	Acid_soluble_oil_(0)	C22H36		
						ACIDSO1	acid_soluble_oillight	C10H16		
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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.

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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.

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#### The workspace now looks like this:

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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.

_	<u> </u>
~	

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

/Flowsheet Case (Main) - Solver Active × [+	Model Palette	<b>▼</b> # ×
3 ^	Views	Streams Flowsheets
<b>⊾</b>	All	
1	Dynamics & Control	∯₽₫
2 MIX-100	External Model	×₩₽€
	Heat Transfer	755
	Manipulator	
	Piping & Hydraulics	
	Pressure Changer	* 🖽 🕰
< ×	Reactor	Cn(A)

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

Mixer: MIX-1	100				13
Design	Rating	Worksheet	Dynamics		
Connecti Paramete User Vari Notes	in ons ers	Injets	Name	MIX-100	
D	elete			Requires a feed stream	ored

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

xer: MIX-	100				
Design	Rating	Worksheet	Dynamics		
Desi Connect Paramel User Val Notes	<b>gn</b> tions ters	Inlets	Name	MIX-100	
[	Delete			Requires a product stream	Ignored

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

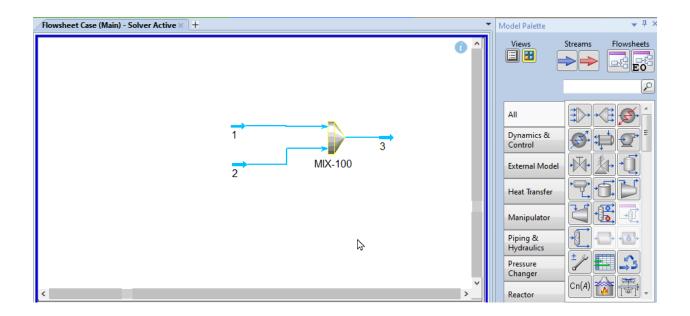
Locate the *Outlet* box and enter the number "3". This completes this block.

Mixer: MIX-100				13
Design Rating	Worksheet Dynamics			
Design Connections	Name	MIX-100		
Parameters User Variables Notes		$\rightarrow$		
	Iniets << Stream		Outlet 3 Fluid Package Basis-1	
			DdSIS-1	
Delete		Not Solv	ed	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.

Worksheet	Stream Name	1	1_Elec	
Conditions	Vapour / Phase Fraction	<empty></empty>	<empty></empty>	
Properties Composition Oil & Gas Feed	Temperature [C]	<empty></empty>	<empty></empty>	
	Pressure [kPa]	<empty></empty>	<empty></empty>	
	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	Heat Flow [kJ/h]	<empty></empty>	<empty></empty>	
Finissions	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 Attachme	ents Dynamics			
Worksheet	Stream Name	1	1_Elec	
Conditions	Vapour / Phase Fraction	<empty></empty>	<empty></empty>	
Properties	Temperature [C]	40.00	40.00	
Composition Oil & Gas Feed	Pressure [kPa]	101.3	101.3	
	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	Heat Flow [kJ/h]	<empty></empty>	<empty></empty>	
Normalized Yields Emissions	Liq Vol Flow @Std Cond [m3/h]	<empty></empty>	<empty></empty>	
EITIISSIOTIS	Fluid Package	Basis-1		
	Utility Type			
	Ç≠			

## 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 Petroleum Assay K Value Electrolytes	SO2	<empty></empty>	<empty></empty>	
	HCL	<empty></empty>	<empty></empty>	
	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 Pr	roperties 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 Petroleum Assay	SO2	<empty></empty>	<empty></empty>	
	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 Pro			
		Change Compositional Bas	is	

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

Material Stream: 1					- 8
Worksheet Attachme	ents Dynamics				
Worksheet Conditions			Molar Flows	Molar Flows_Elec	
Properties Composition Oil & Gas Feed Petroleum Assay K Value Electrolytes User Variables	H2O NH3 CO2 SO2 HCL H2SO4 H2CO3	kgmole/h ▼	55.51 sempty> <empty> <empty> <empty> <empty></empty></empty></empty></empty>	<empty> <empty> <empty> <empty> <empty> <empty></empty></empty></empty></empty></empty></empty>	· · · · · · · · · · · · · · · · · · ·
User Variables Notes Cost Parameters Normalized Yields ▷ Emissions	H2SO3 HNH2CO2 NH42CO3 NH42SO3 NH42SO3 NH42SO4 NH42SO4 NH43HSO42 NH44H2CO33 NH4CL NH4CLB NH4CC2NH2 NH4CLB NH4CO2NH2		<pre><mptv> <mptv> <mpt< td=""><td><empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></td><td>E</td></mpt<></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></mptv></pre>	<empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	E
	Edit	Total View Properti Unkno	<empty></empty>	<empty></empty>	
Delete	Define from Str	eam	View Assay	<b>+ +</b>	

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>		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>	=	eld volume nows
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>		
		Ŧ	Cancel
			Current
Normalize	Total 55.5100 kgmo		ОК

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

Input Composition fo	r Stream: Material Stream: 1		
	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	=	Ciq volume riows
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	*	Canad
			Cancel
Normalize	Total 55.5100 kgmol	e/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.

H2O     55,5100       NH3     1.0000       CO2     0.1000       SO2     0.1000       HCL <empty>       H2CO3     <empty>       H2SO4     <empty>       H2CO3     <empty>       H2SO3     <empty>       HVH2CO2     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO4     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO4     <empty>       NH42SO4     <empty>       NH42LB     <empty>       NH4CD2     <empty>       NH4CB     <empty>       NH4CO2NH2     <empty>       NH4HO3     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>		Comp Mole F	low	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	5	5.5100 🔺	Mole Fractions
SO2     0.1000       HCL <empty>       H2SO4     <empty>       H2C03     <empty>       H2SO3     <empty>       HNH2C02     <empty>       NH42SO3     <empty>       NH42SO4     <empty>       NH42SO3     <empty>       NH42LO33     <empty>       NH44H2CO33     <empty>       NH4CLB     <empty>       NH4CO2NH2     <empty>       NH4HO3     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	NH3		1.0000	Mass Fractions
SO2     U. 1000       HCL <empty>       H2SO4     <empty>       H2CO3     <empty>       H2SO3     <empty>       HNH2CO2     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO4     <empty>       NH43SO42     <empty>       NH4CD3     <empty>       NH4CD2NH2     <empty>       NH4HD30     <empty>       NH4HC03     <empty>       NH4HC03     <empty>       NH4HC03     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	CO2		0.1000	
H2SO4 < <empty> H2SO3 &lt; empty&gt; H2SO3 &lt; empty&gt; HNH2CO2 &lt; empty&gt; NH42SO3 &lt; empty&gt; NH42SO3 &lt; empty&gt; NH42SO3 &lt; empty&gt; NH42SO3 &lt; empty&gt; NH42SO4 &lt; e</empty>	SO2		0.1000	Liq Volume Fractions
H2CO3 <empty>       H2SO3     <empty>       HNH2CO2     <empty>       NH42CO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO4     <empty>       NH43SO42     <empty>       NH4CD33     <empty>       NH4CL     <empty>       NH4CD34     <empty>       NH4CD3     <empty>       NH4CO2NH2     <empty>       NH4HO3     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	HCL	<6	empty>	Mole Flows
H2SO3 <empty>       H2SO3     <empty>       HNH2CO2     <empty>       NH42CO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO4     <empty>       NH44H2CO33     <empty>       NH44H2CO33     <empty>       NH4CL     <empty>       NH4CL     <empty>       NH4CO2NH2     <empty>       NH4HO3     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	H2SO4	<6	empty>	
HNH2CO2 < <empty> NH42CO3 &lt; empty&gt; NH42SO3 &lt; empty&gt; NH42SO3 &lt; empty&gt; NH42SO4 &lt; empty&gt; NH42SO4 &lt; empty&gt; NH44H2CO33 &lt; empty&gt; NH4CLB &lt; empty&gt; NH4CLB &lt; empty&gt; NH4CO2NH2 &lt; empty&gt; NH4HCO3 &lt; empty&gt;</empty>	H2CO3	<	mpty>	Mass Flows
HNH2CO2 <empty>       NH42CO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO3     <empty>       NH42SO4     <empty>       NH43HSO42     <empty>       NH44H2CO33     <empty>       NH4CL     <empty>       NH4CL     <empty>       NH4C1     <empty>       NH4C02NH2     <empty>       NH4HC03     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	H2SO3	<6	empty>	C Lia Volume Flows
NH42SO3 <empty>       NH42SO3.1H2O     <empty>       NH42SO4     <empty>       NH43HSO42     <empty>       NH44H2CO33     <empty>       NH4CL     <empty>       NH4CLB     <empty>       NH4CO2NH2     <empty>       NH4HO3     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	HNH2CO2	<6	empty> =	
NH42SO3 <empty>       NH42SO3.1H2O     <empty>       NH42SO3.1H2O     <empty>       NH42SO4     <empty>       NH43HSO42     <empty>       NH44H2CO33     <empty>       NH4CL     <empty>       NH4C2NH2     <empty>       NH4H2O3     <empty>       NH4HO3     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	NH42CO3	<6	empty>	
NH42SO4 <empty>       NH43HSO42     <empty>       NH43HSO42     <empty>       NH44H2C033     <empty>       NH4CL     <empty>       NH4CL     <empty>       NH4CL     <empty>       NH4C02NH2     <empty>       NH4HC03     <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	NH42SO3	<6	empty>	Composition Controls
NH42S04 <empty>       NH43HS042     <empty>       NH4H2C033     <empty>       NH4CL     <empty>       NH4CLB     <empty>       NH4C02NH2     <empty>       NH4HC03     <empty>       NH4HC03     <empty></empty></empty></empty></empty></empty></empty></empty></empty>	NH42SO3.1H2O	<6	empty>	Eraco
NH44H2CO33 <empty>     Equalize Composition       NH4CL     <empty>       NH4CLB     <empty>       NH4CO2NH2     <empty>       NH4H2SO42     <empty>       NH4HCO3     <empty></empty></empty></empty></empty></empty></empty>	NH42SO4	<6	empty>	Elase
NH4CL <empty>       NH4CL     <empty>       NH4CLB     <empty>       NH4CO2NH2     <empty>       NH4H3SO42     <empty>       NH4HCO3     <empty></empty></empty></empty></empty></empty></empty>	NH43HSO42	<6	mpty>	
NH4CLB <a href="https://www.selfacture.com">wmmundle</a> NH4CO2NH2 <a href="https://www.selfacture.com">wmmundle</a> NH4H3SO42 <a href="https://www.selfacture.com">wmmundle</a> NH4HCO3 <a href="https://www.selfacture.com">wmmundle</a> NH4HCO3 <a href="https://www.selfacture.com">wmmundle</a>	NH44H2CO33	<	empty>	Equalize Composition
NH4CO2NH2 <empty>       NH4H3SO42     <empty>       NH4HCO3     <empty></empty></empty></empty>	NH4CL	<6	empty>	
NH4H3SO42 <empty> NH4HCO3 <empty></empty></empty>	NH4CLB	<	empty>	
NH4HCO3 <empty></empty>	NH4CO2NH2	<6	empty>	
	NH4H3SO42	<6	empty>	
	NH4HCO3	<6	empty>	
Cancel				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.

erial Stream: 1			- 8
orksheet Attachme	ents Dynamics		
Worksheet Conditions Properties Composition	True Species Info Properties Composition  Phase  Phase  Aque  Solid	ous	
Oil & Gas Feed Petroleum Assay	pH	9.3400	
K Value	Osmotic Pressure	2770.9 kPa	
PSD Property Electrolytes	Ionic Strength	7.9249e-006 kgmol/kg	
User Variables	Heat Capacity	74.660 kJ/kgmole-C	
Notes	Viscosity	0.68024 cP	
Cost Parameters Normalized Yields	Specific Electrical Conductivity	5.1431 S/m	
Emissions	Molar Electrical Conductivity	0.00000 S-m2/kgmole	
		ОК	

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	True Species Info -	Phase Aqueous	Conc. Basis Molar			
Properties Composition	<ul> <li>Composition</li> </ul>	Solid	C 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.

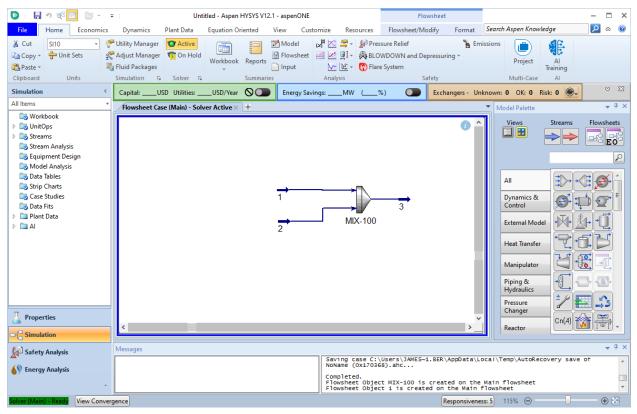
Temperature	25	С
Pressure	101.3	kPa
H2O	55.51	
HCI	0.1	
H2SO4	1.0	

Click the *Electrolytes* line to see the pH.

terial Stream: 2			- 0
Worksheet Attachme	nts Dynamics		
Worksheet Conditions Properties Composition Oil & Gas Feed	True Species Info Properties Composition Phase — Aque Solid		
Petroleum Assay	рН	-0.0811	
K Value PSD Property	Osmotic Pressure	6582.5 kPa	
Electrolytes	Ionic Strength	2.5144e-005 kgmol/kg	
User Variables	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	
		OK	
Delete	Define from Stream	View Assay	<b>+ +</b>

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"

Worksheet	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	Molar Flow [kgmole/h]	114.3	114.3	6.574e-002	
Petroleum Assay 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 User Variables	Molar Enthalpy [kJ/kgmole]	-2.865e+005	-2.865e+005	-3.787e+005	
	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]	<empty></empty>	<empty></empty>	<empty></empty>	
Emissions	Fluid Package	Basis-1			
	Utility Type				

The converged process temperature is approximately 37.0 °C.

Click on the *Electrolytes* line.

Material Stream: 3			- B 8
Worksheet Attachme	ents Dynamics		0
Worksheet Conditions Properties Composition Oil & Gas Feed	True Species Info Properties Composition		
Petroleum Assay	рН	0.8681	
K Value	Osmotic Pressure	3013.0 kPa	
PSD Property Electrolytes	Ionic Strength	1.4878e-005 kgmol/kg	
User Variables	Heat Capacity	74.667 kJ/kgmole-C	
Notes Cost Parameters	Viscosity	0.76241 cP	
Normalized Yields	Specific Electrical Conductivity	14.687 S/m	
Emissions	Molar Electrical Conductivity	0.00000 S-m2/kgmole	
			ß
		OK	
Delete	Define from Stream	View Assay	<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.

Worksheet Attachme	nts Dynamics					
Worksheet Conditions Properties Composition Oil & Gas Feed Petroleum Assay K Value	True Species Info — O Properties O 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			
Delete	Define from S	tream	/iew Assav		<b>(</b>	

Click on the Composition line at the left.

Worksheet		Mole Fractions	Mole Fractions_Elec	Vapour Phase	Aqueous Phase	
Conditions	H2O	0.9799	0.9799	0.0613	0.9804	
Properties	NH3	0.0087	0.0087	0.0000	0.0088	
Composition	CO2	0.0009	0.0009	0.8863	0.0004	
Oil & Gas Feed Petroleum Assay	SO2	0.0009	0.0009	0.0523	0.0008	
K Value	HCL	0.0009	0.0009	0.0000	0.0009	
PSD Property	H2SO4	0.0000	0.0000	0.0000	0.0000	
Electrolytes	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	
	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 roperties	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 & Cas Feed Petroleum Assay K Value PSD Property Electrolytes User Variables Notes Cost Parameters Normalized Yields Emissions	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	
	H2SO3	0.0000	0.0000	0.0000	0.0000	
	HCL.1H2O	0.0000	0.0000	0.0000	0.0000	
	HCL2H2O	0.0000	0.0000	0.0000	0.0000	
	HCL3H2O	0.0000	0.0000	0.0000	0.0000	
	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	7			

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