

OLI Engine for Petro-SIM V7.4

Getting Started Guide

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Overview

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

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

Assumptions

The following assumptions are made for this guide:

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



Application

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

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

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

Using the OLI Engine for Petro-SIM

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

💀 Simulation Basis Manager				-		\times
Cu <u>r</u> rent Fluid Packages		Flowshe	et - Fluid Pkg Associatio <u>n</u>	5		
	<u>V</u> iew		FlowSheet	Fluid Pkg	g To Use	
	<u>A</u> dd		Case (Main)	<(empty>	
	Delete					
	Сор <u>у</u>					
	<u>I</u> mport					
	E <u>x</u> port	D	efault Fluid Pkg			~
Fluid Packages Components Hypo	otheticals Oil Manager	Reactions	Component Maps Us	er Properties		
Ī			Enter Si <u>m</u> ulation Envir	onment		

Click the **<u>Add...</u>** button.

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



🔏 Fluid Package: Basis-1 –	×
Property Package Selection Kabadi Danner Lee-Kesler Plocker Margules MFL File (Multiflash) NBS Steam NRTL OLI Electrolytes Peng Robinson PRSV RKSA (Multiflash) Sour PR Component List Selection	
Component List - 1 View	
Set Up Parameters Binary Coeffs StabTest Rxns Tabular Notes Phase Order	
Delete <u>N</u> ame Basis-1 Property Pkg <none></none>	

This will display a new panel:

🛓 Fluid Package: Basis-1	_		×
Property Package Selection \$	ne 12.0		
Component List Selection Component List - 1 View Prote	ect Interactio	on Parame	ters
Set Up Parameters Binary Coeffs StabTest Rxns Tabular Notes Phase Order Delete Name Basis-1 Property Pkg OLI Electrolytes			

You can use multiple versions of the OLI Engine. Currently displayed is OLI Engine 12.0. If you have more than one OLI Engine, you can select from an older version. Click the drop-down button:



🛓 Fluid Package: Basis-1		– 🗆 X
Property Package Selection Margules MFL File (Multiflash) NBS Steam NRTL OLI Electrolytes Peng Robinson PRSV RKSA (Multiflash) Sour PR Sour SRK SRK	Property Package Filter All Types Multiflash EOSs Activity Models Chao Seader Models Vapour Press Models Miscellaneous Types OLI Vers	ion: OLI Engine 12.0
Component List Selection Component List - 1	View	
Set Up Parameters Bind Delete <u>N</u> ame Ba	ary Coeffs StabTest Rxns Tabular No sis-1 Property Pkg Ol	utes Phase Order

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

👗 Fluid Package: Basis-1		-		\times
Property Package Selection Margules MFL File (Multiflash) NBS Steam NRTL OLI Electrolytes Peng Robinson PRSV RKSA (Multiflash) Sour SRK Sour SRK	OLI systems, inc.	ne 12 0	õ	
Component List Selection Component List - 1 Set Up Parameters Binary Coeffs StabTest Rxns Tabular Delete Name Basis-1 Property Pkg	OLI Electrolytes	der		

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



Fluid Package: Basis-1 Property Package Selection Margules MFL File (Multiflash) NBS Steam	Property Package Filter		
NRTL OLI Electrolytes Peng Robinson PRSV RKSA (Multiflash) Sour PR Sour SRK SRK	 Multiflash EOSs Activity Models Chao Seader Models Vapour Press Models Miscellaneous Types 	OLI Version: OLI Engine 12.0	یا خ و ب
Component List Selection	Vie	w	
Set Up Parameters Bina Delete Name Base	sis-1 Property Pkg	abular Notes Phase Order OLI Electrolytes	

Click the indicated icon.

🔳 Chemistry Bu	ilder	-	_		×
- Databanks Available	Thermodynamic Framework MSE (H3O+ ion)	 ∽ Selected			
Corrosion (MSE Geochemical (M Total Suspended Urea (MSE) Surface Comple) 1SE) 1 Solids xation Double Layer Model (MS	MSE (H3O+ ion) Databank search order is from top t	to botto	m.	•
	Next >	 search order.		Can	cel



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

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

		Add	I Remov
Name	CAS Number	Databank	Tag
Water	7732-18-5	PUB	

Click the <u>Next></u> button.

On this dialog, we will enter our components. H₂O is required for all models regardless if there is no flowrate for the component. You cannot remove this species. It will show its databank as PUB (AQ); however, it will actually be using the thermodynamic framework selected in the previous screen (MSE).

Click the <u>Add</u> button.



Components				;	×
Add Component Components	Match		D. I. I.	Show Synonym	15
Hypothetical	Name	CAS Number	Databank	Tag	
	Ammonium aluminum sulfate	7784-26-1	MSE	AALSO42.12H2O	
	Acetonitrile	75-05-8	MSE	ACENITRILE	
	Acetic acid, dimer		MSE	ACET2	
	Acetic acid	64-19-7	MSE	ACETACID	
	Ethanal	75-07-0	MSE	ACETALDEHD	
	Acetone	67-64-1	MSE	ACETONE	
	Acetylene	74-86-2	MSE	ACETYLENE	
	Acid soluble oil (0)		MSE	ACIDSO0	
	acid soluble oil - light		MSE	ACIDSO1	
	acid soluble oil - 20-30%		MSE	ACIDSO2	
	acid soluble oil - 60-70%		MSE	ACIDSO3	
	acid soluble oil - >70%		MSE	ACIDSO4	
	acid soluble oil - >80%		MSE	ACIDSO5	
	Add Selected Component			Close	

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

Components				– 🗆 X
Add Component	Match CO2			Show Synonyms
Hypothetical	Name	CAS Number	Databank	Tag
riypotrictical	Carbon dioxide	124-38-9	MSE	CO2
	Dicobalt(II) trihydroxide glucona		MSE	CO2OH3GLU
	Dicobalt(II) trihydroxide glucona		MSE	CO2OH3GLU.4H2O
	Add Selected Component			Close

Click the Add Selected Component button.



cted Components		Add	Remove		
Name	CAS Number	Databank	Tag		
Water	7732-18-5	PUB	H2O		
Carbon dioxide	124-38-9	MSE	CO2		
(Components				- 0
	Add Component	Match			Show Synonyr
	Components	Name	CAS Number	Databank	Tag
	Hypothetical	Ammonium aluminum sulfate	7784-26-1	MSE	AALSO42.12H2O
		Acetonitrile	75-05-8	MSE	ACENITRILE
		Acetic acid, dimer		MSE	ACET2
		Acetic acid	64-19-7	MSE	ACETACID
		Ethanal	75-07-0	MSE	ACETALDEHD
		Acetone	67-64-1	MSE	ACETONE
		Acetylene	74-86-2	MSE	ACETYLENE
< Back		Acid soluble oil (0)		MSE	ACIDSO
		acid soluble oil - light		MSE	ACIDS01
		acid soluble oil - 20-30%		MSE	ACIDSO2
		acid soluble oil - 60-70%		MSE	ACIDSO
		acid soluble oil - >70%		MSE	ACIDSO4
		acid soluble oil - >80%		MSE	ACIDSOS
		Add Selected Component			Close

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

NH₃ SO₂ H₂SO₄ HCI

Click the **<u>Close</u>** button when finished.



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

Click <u>Next></u>

Chemistry Builder	_		×
Redox Chemistry			
Enable Redox			
Included Subsystems			
🕞 Sulfur			
S(-2)			
S(+2)			
S(+3)			
S(+4)			
S(+5)			
S(+6)			
S(+7)			
S(+8)			
S(0)			
Chlorine			
CI(-1)			
CI(+1)			
< Back Next > Finish		Cance	el



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

Chemistry Builder			_		×
Phases					
Included Phases	Included Solid Phases				
Aqueous		Include?			
	H2O				
Vapour	HCL.1H2O	V			
Solids	HCL.2H2O	V			
	HCL.3H2O	✓			
Second Liquid	NH42CO3.1H2O	V			
	NH42S2O5	✓			
	NH42SO3	V 1			
	NH42SO3.1H2O	✓			
	NH42SO4	✓			
	NH43CO32	✓			
	NH43HSO42	✓			
	Calculate Scaling Ten	dencies for excluded so	olids		
< Back		Finish		Canc	el

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



Simulation Basis	Manager					_	o x
-Cu <u>r</u> rent Fluid Pac	kages			Flowshe	et - Fluid Pkg Associa	atio <u>n</u> s	
Basis-1 NC: 2	29 PP: OLI Elec	trolytes	<u>V</u> iew		FlowSheet	Fluid Pkg	To Use
					Case (M	ain)	Basis-1
			<u>A</u> dd				
			Delete				
			Сору				
			<u>I</u> mport				
			E <u>x</u> port	D	efault Fluid Pkg	Basis-1	~
Fluid Packages	Components	Hypotheticals	Oil Manager	Reactions	Component Maps	User Properties	
Î					Enter Si <u>m</u> ulation	Environment	

Click the Enter Simulation Environment... button.

Creating the Simulation

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





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

Selecting the mixer

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



The workspace now looks like this:





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

We need to create two inlet streams.

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



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



IV MIX-100 (Mixer)	_		<
Design Connections Parameters User Variables Notes	Name MIX-100 Inlets: Stream> Control of the second seco	~	
Design Workshee	t		
Delete	Requires a feed stream	<u>Ignore</u>	d

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



> MIX-100 (Mixer) -		x
Design Name MIX-100 Connections Inlets: 1 2 Variables 2 Outlet: Notes <stream> : Outlet: Fluid Package: Basis-1 Design Worksheet</stream>	~	
Delete Requires a product stream	<u>Ignor</u>	red

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

DIX-100 (Mixer)	_	o x
Design Connections Parameters User Variables Notes	Name MIX-100	~
Design Workshee	et	
Delete	Not Solved	<u>Ig</u> nored

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

Click the \boldsymbol{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

中 1 (Material Stream	n)	-		×
Worksheet Conditions Properties Composition Solids Species K Value User Variables Economics Bulk Properties Notes Time Series Time Results	Stream Name Vapour / Phase Fraction Temperature [F] Pressure [pig] Molar Flow [SCFH] Mass Flow [Ib/hr] Std Ideal Liq Vol Flow [Barrel/day] Molar Entropy [Btu/Ibmole] Molar Entropy [Btu/Ibmole] Heat Flow [MMBtu/hr] Heat Flow @Std Cond [barrel/day] HHV Based Flow [MMBtu/hr] Fluid Package Stream Type Short Name		<em <em <em <em <em <em <em sems satis</em </em </em </em </em </em </em 	1 pty> pty> pty> pty> pty> pty> pty> pty> pty> pty> pty> pty> pty> pty> pty>
Worksheet At	tachments Unknown Compositions			
Delete	Define from Other Stream 🚳	II.	-	⇒

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

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

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



Worksheet	Stream Name			1
Carallelana	Vapour / Phase Fraction		<en< td=""><td>npty></td></en<>	npty>
Conditions	Temperature [F]			104.0
Properties	Pressure [psig]		().0000
Composition	Molar Flow [SCFH]		<en< td=""><td>npty></td></en<>	npty>
Solids	Mass Flow [lb/hr]		<en< td=""><td>npty></td></en<>	npty>
Species	Std Ideal Liq Vol Flow [barrel/day]		<en< td=""><td>npty></td></en<>	npty>
K Value User Variables	Molar Enthalpy [Btu/Ibmole]		<en< td=""><td>mpty></td></en<>	mpty>
	Molar Entropy [Btu/Ibmole-F]	<emp< td=""></emp<>		
	Heat Flow [MMBtu/hr]	<em< td=""><td>npty></td></em<>		npty>
	Liq Vol Flow @Std Cond [barrel/day]		<en< td=""><td>npty></td></en<>	npty>
Bulk Properties	HHV Based Flow [MMBtu/hr]		<en< td=""><td>npty></td></en<>	npty>
Notes	Fluid Package		Basis	s-1
Time Series	Stream Type			
Time Results	Short Name			
Worksheet A	ttachments			
	Unknown Compositions			

Now click the **Composition** line

中 1 (Material Strear	n)		-	- 0	×
Workshoot			Mol	e Fractions	
worksneet	H2O]	<empty< td=""><td>> </td></empty<>	>
Conditions	CO2			<empty< td=""><td>></td></empty<>	>
Properties	H2SO4			<empty< td=""><td><u>></u></td></empty<>	<u>></u>
Composition	HCI			<empty< td=""><td>2</td></empty<>	2
Solids	Ammonia SO2			< empty	<u> </u>
Species	SO3			<empty <empty< td=""><td>5</td></empty<></empty 	5
Value Value	H2SO3*			<empty< td=""><td>></td></empty<>	>
K value	HCL.1H2O*			< empty	>
User Variables	HCL.2H2O*			< empty	>
Economics	HCL.3H2O*			<empty< td=""><td>></td></empty<>	>
Bulk Properties	NH42C03.1H20*			<empty< td=""><td>></td></empty<>	>
Notes	NH42CO3*			<empty< td=""><td>></td></empty<>	>
Time Series		Total	0.0000		
Time Results					
	View Properties	Eg	lit	Bas <u>i</u> s	٣
	Oil Characterization				
			M 1	2	X
Worksheet At	tachments				
	Unknown Com	positions			
Delete	Define from Other Stream		8	-	•

We can now enter our composition for our components.

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

This will pop open another dialog.



	MoleFraction	Composition Basis
H2O J	0.9780	Mole Fractions
CO2	0.001000	Mass Fractions
H2SO4	0.0000	
HCI	0.0000	Cliq volume Fractions
Ammonia	0.02000	O Mole Flows
502	0.001000	Mass Flows
SO3	<empty></empty>	O Lig Volume Flows
H2SO3*	<empty></empty>	Mala Parcente
HCL.1H2O*	<empty></empty>	O Mole Percents
HCL.2H2O*	<empty></empty>	Mass Percents
HCL.3H2O*	<empty></empty>	Liq Volume Percents
NH42CO3.1H2O*	<empty></empty>	
NH42CO3*	<empty></empty>	Composition Controls
NH42S2O5*	<empty></empty>	Frace
NH42SO3.1H2O*	<empty></empty>	Liase
NH42SO3*	<empty></empty>	
NH42SO4*	<empty></empty>	Normalize
NH43CO32*	<empty></empty>	
NH43HSO42*	<empty></empty>	
NH44HC03.1H20*	<empty></empty>	Cancel

Enter the compositions as shown and then click the **<u>OK</u>** button.

Go back to the **Conditions** category, and enter a molar flow of 100 MMSCFD

🔿 1 (Material Strea	n)	-		×
Worksheet	Stream Name Vapour / Phase Fraction		0	1 .0000
Properties Composition Solids Species K Value User Variables Economics Bulk Properties Notes Time Series Time Results	I emperature [F] Pressure [psig] Molar Flow [IMSCFD] Molar Enthalpy [Btu/Ibmole] Molar Enthalpy [Btu/Ibmole] Molar Entropy [Btu/Ibmole-F] Heat Flow [MMBtu/hr] Hity Based Flow [MMBtu/hr] Fluid Package Stream Type Short Name		0 198380 1.375 -1.208 1.375 Basis Sour Wat	104.0 .0000 100.0 .6330 e+04 e+05 17.78 .1326 ie+04 225.1 -1 .eer
Worksheet Sy	nthesis Attachments			
Delete	OK Define from Other Stream		-	-

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 **<u>Properties</u>** line.

➡ 1 (Material Stream	1)	- 0	×
Worksheet	Stream Name	1	
	рН	9.698	
Conditions	Osmotic Pressure [psig]	433.4	
Properties	lonic Strength (x-based) [lbmol/lb]	4.621e-06	
Composition	Electrical Conductivity [S/ft]	0.8944	
Solids	Molar Electrical Conductivity [S-ft2/lbn	0.0000	
Species	Mass Flow [lb/hr]	198380.6330	
K Value	Std Ideal Liq Vol Flow [barrel/day]	1.375e+04	
User Variables	Act. Gas Flow [ACFM]	<empty></empty>	
Economics	Molecular Weight	18.07	
D II D III II	Molar Density [lbmole/ft3]	3.435	
Bulk Properties	Actual Mass Density [lb/ft3]	62.07	
Notes	Act. Volume Flow [barrel/day]	1.366e+04	
Time Series	Mass Enthalpy [Btu/lb]	-6686	
Time Results	Mass Entropy [Btu/Ib-F]	0.9839	
	Property Controls	J 🖋 H 🖻	6
Worksheet Syn	Attachments		
Delete	Define from Other Stream 8		٠

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



Worksheet	Stream Name	1	A guessus Dhase
	J	0.609	Aqueous Phase
onditions	Osmotic Processo (nois)	9.098	9.090
roperties	lonic Strength (v-based) [lbmol/lb]	453.4	<empty></empty>
omnosition	Electrical Conductivity [S/ft]	4.0210-00	<empty></empty>
olide	Molar Electrical Conductivity [5/11]	0.0000	<empty></empty>
unus	Mass Flow [lb/br]	198380 6330	108380 6330
pecies	Std Ideal Lig Vol Flow [barrel/day]	1 375e+04	1 375e+04
Value	Act. Gas Flow [ACEM]	<empty></empty>	<emnty></emnty>
lser Variables	Molecular Weight	18.07	18.07
conomics	Molar Density [lbmole/ft3]	3,435	3.435
ulk Properties	Actual Mass Density [lb/ft3]	62.07	62.07
lotes	Act. Volume Flow [barrel/dav]	1.366e+04	1.366e+04
îme Series	Mass Enthalpy [Btu/lb]	-6686	-6686
ïme Results	Mass Entropy [Btu/Ib-F]	0.9839	0.9839
	Heat Capacity [Btu/lbmole-F]	17.90	17.90
	Mass Heat Capacity [Btu/Ib-F]	0.9908	0.9908
	Phase Fraction [Vol Basis]	0.0000	1.000
	Phase Fraction [Mass Basis]	0.0000	1.000
	Cost Based on Flow [Cost/day]	<empty></empty>	<empty></empty>
	Specific Heat [Btu/lbmole-F]	17.90	17.90
	Std Gas Flow [SCFH 1atm 15C]	4.159e+06	4.159e+06
	Std. Ideal Liq. Mass Density [API @Std. I	11.59	11.59
	Act. Liq. Flow [barrel/day]	1.366e+04	1.366e+04
	Z Factor	0.0007072	0.0007072

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

		Mole F	ractions	Aqueous Phase	
Worksheet	H2O	1110101	0.9780	0	9780
onditions	CO2	-	0.001000	0.00	1000
ropertier	H2SO4		0.0000	0	.0000
iopenties	HCI		0.0000	0	.0000
omposition	Ammonia		0.02000	0.0	2000
olids	SO2		0.001000	0.00	100
pecies	SO3		0.0000	0	.000
Value	H2SO3*		0.0000	0	.0000
Value	HCL.1H2O*		0.0000	0	.0000
ser Variables	HCL.2H2O*		0.0000	0	.0000
conomics	HCL.3H2O*		0.0000	0	.0000
ulk Properties	NH42CO3.1H2O*		0.0000	0	.0000
oter	NH42CO3*		0.0000	0	.0000
	NH42S2O5*		0.0000	0	.000
ime Series	NH42SO3.1H2O*		0.0000	0	.0000
ime Results	NH42SO3*		0.0000	0	.0000
	NH42SO4*		0.0000	0	.0000
	NH43CO32*		0.0000	0	.000
	NH43HSO42*		0.0000	0	.000
	NH44HCO3.1H2O*		0.0000	0	.000
	NH4CLB*		0.0000	0	.0000
	NH4CL*		0.0000	0	.0000
	NH4CO2NH2*		0.0000	0	.0000
	NH4H3SO42*		0.0000	0	.0000
	NH4HCO3*		0.0000	0	.0000
	NH4HSO3*		0.0000	0	.0000
	NH4HSO4*		0.0000	0	.0000
	NH4OH*		0.0000	0	.0000
	H2CO3*		0.0000	0	.0000
			Total 1.	000	
		View Properties	E <u>d</u> it	Basjs	
	-Oil Characterization-				
	Salf-Synthesis (Eull)		5	🗑 🛁 🕷	v
	Sea Synchesis (ruii)				~
Worksheet S	ynthesis Attachments				
		OK			
		UK			
			00	100	

Click on the **<u>Composition</u>** line.



Click on the **<u>Basis</u>** button

1 (Material Stream	n)		-		×	
		Mole Eractions	Agu	oour Phar		
Worksheet	H20	0.07	RO	Cous Filase	0780	
onditions	C02	0.0010	00	0.0	01000	
	H2SO4	0.00	00	0.0	0000	
roperties	HCI	0.00	00	0	00000	
omposition	Ammonia	0.020	00	0	02000	
olids	502	0.0010	00	0.0	01000	
necies	502	0.00	00	0.0	0000	
pecies	H2SO3*	0.00	00	0	0000	
Value	HCL 1H20*	0.00	00	0	0000	
lser Variables	HCL 2H2O*	0.00	00	0	0000	
conomics	HCL 3H2O*	0.00	00	0	0000	
ulli Deservation	NH42CO3 1H2O*	0.00	00	0	0000	
uik Properties	NH42CO2*	0.00	00	0	0000	
lotes	NH42C03	0.00	00	0	0000	
ime Series	NH425205 NH42502 1H20*	0.00	00	0	0000	
ime Results	NH42503.1120	0.00	00	0	0000	
ine results	NH42505	0.00	00	0	0000	
	NH42504"	0.00	00	0	0000	
	NH45CU52"	0.00	00	0	0000	
	NH45H5042"	0.00	00	0	0000	
	NH44HCU3.1H2U"	0.00	00	0	.0000	
	NH4CLB"	0.00	00	0	.0000	
	NH4CL [*]	0.00	00	0	.0000	
	NH4CO2NH2"	0.00	00	0	.0000	
	NH4H3SO42*	0.000	00	0	.0000	
	NH4HCO3*	0.00	00	0	0.0000	
	NH4HSO3*	0.000	00	0	.0000	
	NH4HSO4*	0.00	00	0	00000	
	NH40H*	0.00	00	0	0.0000	
	H2CO3*	0.00	00	0	0.0000	
		Total	1.000			
	Vic		dit	Bas <u>i</u> s	Ŧ	
	Oil Characterization			View E	xtended Co	mposition
	Self-Synthesis (Full)			View Tr	rue Compo	sition
				View N	Interial Ral	ance Group
				VIEWIV		ance oroup:
Worksheet Sy	nthesis Attachments			🗸 🛛 Mole F	ractions	
				Mass F	ractions	
	0	K		Volum	e Fractions	
				Mole F	lows	
Delete	Define from Other Stream		🤓 🧰	Mara E	1	
				IVIDSS F	10/05	
				Volum	e Flows	
				Mole P	ercents	
				Mass P	ercents	
				Volum	e Percents	
			-	Apple	to All Stree	me

Select View True Composition



⇒ 1 (Material Strea	m)	- 0	×
Worksheet		True Mole Fractions	
6 m	H2O	0.9/81	1
Conditions	02	8.042e-08	- 11
Properties	H2SU4	0.0000	- 11
Composition	HCL	0.0000	- 11
Solids	NH5	0.005728	- 11
Casalas	502	2.0028-14	- 11
Species	NHAOH	0.0000	- 1 1
K Value		2 4060 06	- 1
User Variables	CO3 (-2)	0.0002805	- 1
Economics	H3O (+1)	/ 03/e-12	- 11
Dulle Deservation	HC03 (-1)	0.0002057	- 11
buik Properties	HSO3 (-1)	1.426e-06	- 11
Notes	HS04 (-1)	0.0000	- 11
Time Series	NH2CO2 (-1)	0.0004386	
Time Results	NH4 (+1)	0.003327	
	CL (-1)	0.0000	
	S2O5 (-2)	2.351e-11	
	SO3 (-2)	0.001013	
	SO4 (-2)	0.0000	
	NH42S2O5	0.0000	
	NH42SO3	0.0000	
	NH42SO4	0.0000	
	Total	1.000	
	View Properties Ec	ļit Bas <u>i</u> s	Ŧ
	Oil Characterization		_
	Self-Synthesis (Full)] 🕅 🚔 🗎 🕻	<
Worksheet Sy	nthesis Attachments		
	ОК		
Delete	Define from Other Stream) 📕 🦛 🖬	•

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

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

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

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



➡ 2 (Material Strear	n)	– o ×	<
Worksheet	Stream Name	2	
Conditions	Osmotic Pressure [psig]	1043	
Properties	Ionic Strength (x-based) [lbmol/lb]	2.757e-05	
Composition	Electrical Conductivity [S/ft]	13.60	
Solids	Molar Electrical Conductivity [S-ft2/lbn	0.0000	
Species	Mass Flow [lb/hr]	211361.9337	1
K Value	Std Ideal Lig Vol Flow [barrel/day]	1.394e+04	
User Variables	Act. Gas Flow [ACFM]	<empty></empty>	
	Molecular Weight	19.25	
Economics	Molar Density [lbmole/ft3]	3.468	
Bulk Properties	Actual Mass Density [lb/ft3]	66.75	
Notes	Act. Volume Flow [barrel/day]	1.354e+04	
Time Series	Mass Enthalpy [Btu/lb]	-6520	
Time Results	Mass Entropy [Btu/Ib-F]	0.8690	
	Property Controls	J 🎤 🖡 🖄	
Worksheet Sy	nthesis Attachments		
	ОК		
Delete	Define from Other Stream	🎚 🔶 🔿	•

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

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





Reviewing the output

Double-click stream "3"

➡ 3 (Material Stream	-		×			
Worksheet Conditions	Stream Name Vapour / Phase Fraction Temperature [F]		0	3 .0002 102.5		
Composition Solids Species K Value User Variables Economics Bulk Properties Notes Time Series Time Results	Molar Flow [MMSCFD] Mass Flow [Ib/hr] Std Ideal Liq Vol Flow [barrel/day] Molar Enthalpy [Btu/Ibmole] Molar Entropy [Btu/Ibmole-F] Heat Flow [MMBtu/hr] Liq Vol Flow @Std Cond [barrel/day] HHV Based Flow [MMBtu/hr] Fluid Package Stream Type Short Name		409742 2.769 -1.231 2.769 Basis Sour Wat	200.0 .5667 he+04 le+05 17.66 -2704 he+04 441.1 -1 ter		
Worksheet Attachments OK Delete Define from Other Stream						

The converged process temperature is approximately 102.5 °F.

Click on the **<u>Properties</u>** line.



➡ 3 (Material Strea	am)	>	×
Worksheet	Stream Name pH	3 0.8991	
Properties	Osmotic Pressure [psig]	448.2	
roperties	Ionic Strength (x-based) [Ibmol/Ib]	1.642e-05	
Composition	Electrical Conductivity [S/ft]	4.706	
Solids	Molar Electrical Conductivity [S-ft2/lbn	0.0000	
Species	Mass Flow [lb/hr]	409742.5667	
K Value	Std Ideal Liq Vol Flow [barrel/day]	2.769e+04	
User Variables	Act. Gas Flow [ACFM]	24.46	
Economics	Molecular Weight	18.66	
D II D II I	Molar Density [lbmole/ft3]	2.799	
Bulk Properties	Actual Mass Density [lb/ft3]	52.23	
Notes	Act. Volume Flow [barrel/day]	3.353e+04	
Time Series	Mass Enthalpy [Btu/lb]	-6600	
Time Results	Mass Entropy [Btu/Ib-F]	0.9466	
	Property Controls	. / / 🖄	
Worksheet A	ttachments		
	ОК		
Delete	Define from Other Stream 88	1. 🔶 🗏	

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

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



🔿 3 (Material Strea	ım)			– 🗆 X
		True Mole Fractions	Vapour Phase	Aqueous Phase
Worksheet	H20	0.9752	0.06874	0.9753
Conditions	CO2	0.0005050	0.8985	0.0003565
Droportion	H2SO4	2.992e-09	8.931e-20	2.992e-09
Properties	HCL	6.047e-12	4.735e-09	5.266e-12
Composition	NH3	1.550e-11	1.227e-10	1.548e-11
Solids	SO2	0.0004520	0.03273	0.0004467
Species	SO3	1.778e-22	2.518e-26	1.778e-22
K Value	NH40H	5.411e-11	0.0000	5.412e-11
K value	OH (-1)	5.966e-15	0.0000	5.967e-15
User Variables	CO3 (-2)	8.249e-18	0.0000	8.250e-18
Economics	H3O (+1)	0.003332	0.0000	0.003332
Bulk Properties	HCO3 (-1)	2.719e-09	0.0000	2.720e-09
Noter	HSO3 (-1)	5.290e-05	0.0000	5.291e-05
T	HSO4 (-1)	0.006920	0.0000	0.006921
Time Series	NH2CO2 (-1)	1.874e-17	0.0000	1.875e-17
Time Results	NH4 (+1)	0.01010	0.0000	0.01010
	CL (-1)	0.0004951	0.0000	0.0004952
	S2O5 (-2)	4.197e-08	0.0000	4.197e-08
	SO3 (-2)	1.211e-10	2.518e-26	1.211e-10
	SO4 (-2)	0.002982	0.0000	0.002982
	NH42S2O5	0.0000	0.0000	0.0000
	NH42SO3	0.0000	0.0000	0.0000
	NH42SO4	0.0000	0.0000	0.0000
	NH43CO32	0.0000	0.0000	0.0000
	NH43HSO42	0.0000	0.0000	0.0000
	NH4CLB	0.0000	0.0000	0.0000
	NH4CL	0.0000	0.0000	0.0000
	NH4CO2NH2	0.0000	0.0000	0.0000
	NH4H3SO42	0.0000	0.0000	0.0000
	NH4HCO3	0.0000	0.0000	0.0000
	NH4HSO4	0.0000	0.0000	0.0000
	HCL.1H2O	0.0000	0.0000	0.0000
	HCL.2H2O	0.0000	0.0000	0.0000
	HCL.3H2O	0.0000	0.0000	0.0000
	NH42CO3.1H2O	0.0000	0.0000	0.0000
	NH42SO3.1H2O	0.0000	0.0000	0.0000
	NH44HCO3.1H2O	0.0000	0.0000	0.0000
			Total	1.000
		Vi	iew Properties E <u>d</u> it	Bas <u>i</u> s 🔻
	Oil Characterization			
				🔀 🛋 🗶
Worksheet A	ttachments			
		ОК		
Delete	Define from Other Stream		88	📃 🔶 🔶

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



Disclaimer

This tutorial was created with Petro-SIM 7.4 and the OLI Engine version 12.0.0.11. As time progresses, updates to the OLI databanks and engine may result in changes to the results displayed here. It is not guaranteed that later versions of either Petro-SIM or OLI will yield the same results.

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