

OLI SYSTEMS, INC.

A Guide to Using the OLI Engine in Aspen Plus

Featuring Aspen Plus V12.1

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1/9/2023

How to use the OLI Engine in Aspen PLUS.

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Disclaimer:

This manual was produced using the **OLI Engine 11.5.1 in Aspen Plus**. 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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Chapter 1 An Overview of the Aspen-OLI Interface

Advantages of Aspen-OLI

- The user interface is familiar to Aspen Plus users
- Learn one flow sheeting system
- Multiple Property Options in same flowsheet
- Well established non-electrolyte capability
- Sizing
- Costing
- Two Software Vendors, can get answers more quickly

Disadvantages of Aspen-OLI

- No Corrosion
- No Ion-exchange
- No Surface Complexation
- No Scaling Tendencies
- Two Software Vendors (who answers the question?)

Aspen-OLI Interface Layout

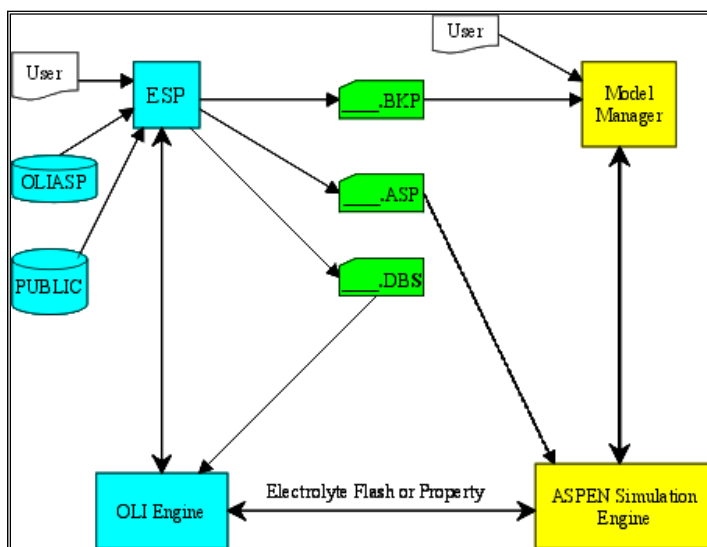


Figure 1-1 The layout of the Aspen OLI Interface

Aspen OLI Unit Operations

- MIXERS
- FSPLIT
- SEP
- SEP2
- HEATER
- FLASH2
- FLASH3
- HEATX
- MHEATX
- RADFRAC
- RSTOIC
- RYIELD
- RCSTR
- RPLUG
- PUMP
- COMPR

Aspen Property Set

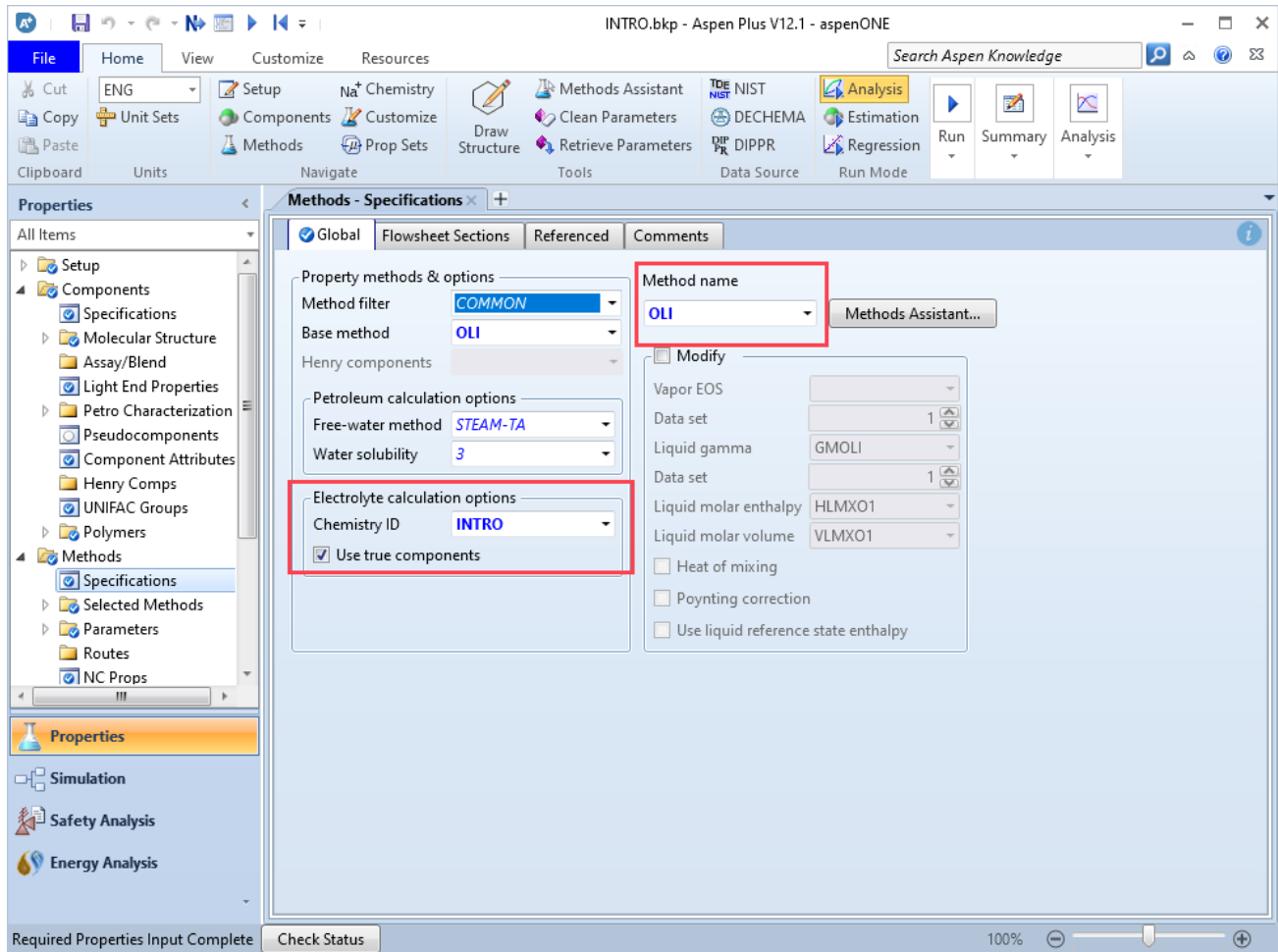


Figure 1-2 OLI Property Set, the boxed areas show that OLI is enabled

Property	Route ID	Property	Route ID
PHIVMX	PHIVMX01	MUVMXL	MUVMXLP1
PHILMX	PHILMX01	MUVLP	MUVLP01
HVMX	HVMX01	KVMXLP	KVMXLP01
HLMX	HLMX01	KVLP	KVLP01
GVMX	GVMX01	DHV	DHV00
GLMX	GLMX01	DHL	DHL00
SVMX	SVMX01	DHLPC	DHLPC00
SLMX	SLMX01	DGV	DGV00
VVMX	VVMX01	DGL	DGL00
VLMX	VLMX01	PHILPC	PHILPC00
MUVMX	MUVMX01	DSV	DSV00
MULMX	MULMX01	KVPC	KVPC01
KVMX	KVMX01		
KLMX	KLMX01		
DVMX	DVMX01		
DLMX	DLMX02		
SIGLMX	SIGLMX01		
PHIV	PHIV00		
PHIL	PHILO1		
HV	HV00		
HL	HL00		
GV	GV00		
GL	GL00		
SV	SV00		
SL	SL00		
VV	VV00		
VL	VL01		
MUV	MUV01		
MUL	MUL01		
KV	KV01		
KL	KL01		
DV	DV01		
DL	DL01		
SIGL	SIGL01		
HSMX	HSMX01		
PHIL	PHIL00		

Property Model	Set	OpCodes		Affected Properties
PHIVMX	PHVMXOLI	1		PHIVMX
PHILMX	PHLMXOLI	1		PHILMX
HVMX	HVMXOLI	1		HVMX
HLMX	HLMXOLI	1		HLMX
GVMX	GVMXOLI	1		GVMX
GLMX	GLMXOLI	1		GLMX
SVMX	SVMXOLI	1		SVMX
SLMX	SLMXOLI	1		SLMX
VVMX	VVMXOLI	1		VVMX
VLMX	VLMXOLI	1		VLMX
MUVMXL	MUV2WILK	1		MUVMX
MUVLP	MUV0CEB	1		MUVMX KVMX MUV KV
MULMX	MUL2ANDR	1		MULMX
KVMXLP	KV2WMSM	1		KVMX
KVLP	KV0STLP	1		KVMX KV
KLMX	KL2SRVR	1		KLMX
DVMX	DV1CEWL	1		DVMX
DLMX	DL1WCA	1		DLMX
SIGLMX	SIG2HSS	1	1	SIGLMX
PHIV	ESIG0	1		PHIV GL SL
PHIL	PHILOLI	1		PHIL
DHV	ESIG0	1		HV HL SL
PL	PL0XANT	1		HL GL SL
DHVL	DHVLWTSN	1		HL SL
DHLPC	DHLPC00	1		HL SL
DGV	ESIG0	1		GV
PHILPC	PHILPC00	1		GL SL
DSV	ESIG0	1		SV
VV	ESIG0	1		VV
VL	VL0RKT	1		VL
MUL	MUL0ANDR	1		MUL
KVPC	KV0STPC	1		KV
VV	ESRK0	1		KV
KL	KL0SR	1		KL
DV	DV0CEWL	1		DV
DL	DL0WCA	1		DL
SIGL	SIG0HSS	1		SIGL
HSMX	HSMXOLI	1		HSMX

Using the Aspen OLI Interface

New property option in ASPEN named OLI:

```
PROPERTIES OLI CHEMISTRY=xxxxx TRUE-COMPS=YES
```

The following ASPEN paragraphs are created when the chemistry model is generated:

```
    DATABANKS          PROP-DATA
    COMPONENTS        PROPERTIES
    CHEMISTRY          PROP-SET pH
```

ASPEN user is then required to add the additional paragraphs to run the simulation such as:

```
    FLOWSHEET
    STREAMS
    BLOCKS
```

```
ESP-NAME   DB 8-CHAR  ASP-ALIAS  ASP-NAME
=====
AR         P AR      AR        ARGON
BCL3       V BCL3   BCL3      BORON-TRICHLORIDE
BF3        V BF3    BF3        BORON-TRIFLUORIDE
BR2        V BR2    BR2        BROMINE
CLNO       V CLNO   CLNO      NITROSYL-CHLORIDE
CL2        P CL2    CL2        CHLORINE
PCL3       V PCL3   CL3P      PHOSPHORUS-TRICHLORIDE
SICL4      V SICL4  CL4SI     SILICON-TETRACHLORIDE
D2         V D2     D2        DEUTERIUM
D2O        V D2O   D2O       DEUTERIUM-OXIDE

F2         V F2     F2        FLUORINE
NF3        V NF3    F3N       NITROGEN-TRIFLUORIDE
SIF4       V SIF4   F4SI      SILICON-TETRAFLUORIDE
SF6        V SF6    F6S       SULFUR-HEXAFLUORIDE
HBR        V HBR    HBR       HYDROGEN-BROMIDE
HCL        P HCL    HCL       HYDROGEN-CHLORIDE
HF         P HF     HF        HYDROGEN-FLUORIDE
AGION      P AG+   AG+       AG+
AGCL2ION   P AGCL2- AGCL2-2  AGCL2--
AGSO4ION   P AGSO4- AGSO4-   AGSO4-
ALION      P AL+3  AL+3     AL+++
ALFION     P ALF+2 ALF+2    ALF++
ALF2ION    P ALF2+ ALF2+    ALF2+
```

Potential Problems

Mixing property options in the same flowsheet The user can mix property options in the same flowsheet, using OLI in one block and an Aspen sysopt such as SYSOP3 in another block. However, the user must be aware of the potential problem of enthalpy mis-matches in switching property options. Even though the base enthalpy for both Aspen and OLI is the heat of formation of the pure component at 25 C, a mis-match will occur due to differences in heat capacity and excess enthalpy calculations. If an isothermal calculation is made at the point of property option change, the effect will be to have an artificial duty on the block. An adiabatic calculation could cause major problems in convergence and result in erroneous results.

Chemistry model location (xxxx.DBS file) By default, ASPEN looks for the .DBS file in the directory where the BKP file has been created.

8 Character Component Names at chemistry model generation, an 8-character name will be created for each species and cross referenced to both OLI component names and Aspen component names. This cross referencing is made based on a table (OLIASP.XRF) supplied with the installation. **Do Not** change the names after the chemistry model is created. It is okay to add additional names to the components paragraph providing these components will have zero flow rates for any block using the OLI property option.

Chemistry ParagraphThe chemistry paragraph created and placed in the Aspen input file is only used by the RADFRAC block. All other blocks chemistry is defined by the information in the xxx.DBS file

Added Unit Blocks (OLI)

Four phase flash block (EFLASH)

OLI Distillation program (FraChem¹)

New run command (RUNASP)

¹ This is also known as EFRACH

Reads xxx.ASP file and converts keyword input to positional input and outputs xxx.INP.
 Executes the standard Aspen run command to run the simulation.

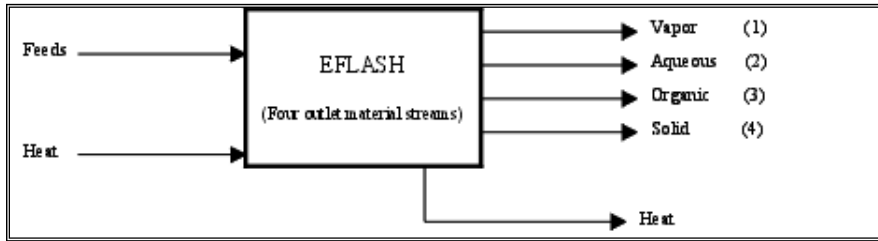


Figure 1-3 EFLASH unit operation

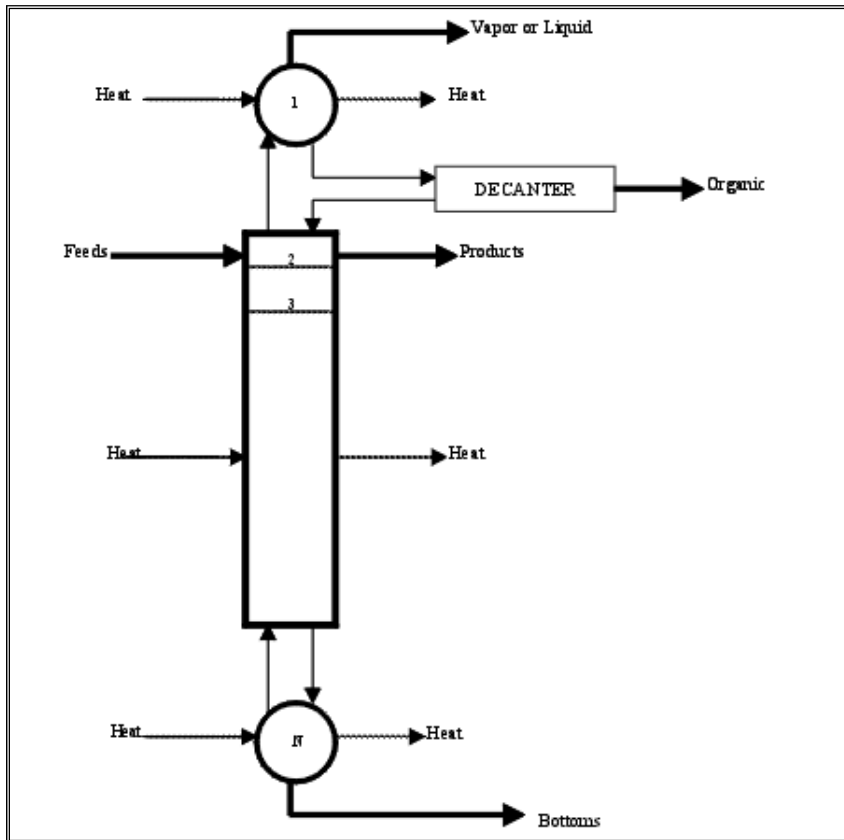


Figure 1-4 EFRACH Block

Chapter 2 ASPEN Neutralization Flowsheet

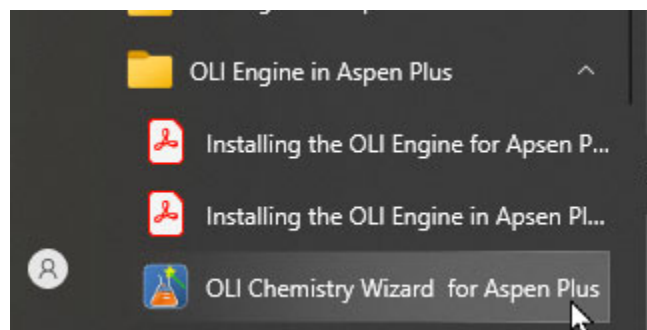
A Tour of the OLI-ASPEN Interface

The following example is flowsheet simulation of an acid-base neutralization process. An acid stream and a base stream are mixed together and then caustic is added to raise the pH to 9. Solid NaCl is added to precipitate out Na₂SO₄. The resulting stream is split, removing 75% and recycling 25%.

Generating Chemistry Model

There are two methods to create an OLI chemistry model to be used with Aspen PLUS. These are the Chemistry Wizard and the OLI Engine². We will concentrate on the OLI Chemistry Wizard.

Use the Start Button and locate the **OLI Chemistry Wizard**. Typical installation paths will put the program here:



The Chemistry Wizard information dialog is now displayed. You can enter the name of the model and change the location where the model files will be located. Here we will enter the name **Neutral1** for the model name and change the location of the files.

² The OLI Engine chemistry generator is supplied with the OLI Engine for Aspen PLUS and is very similar to the chemistry generator used for ESP. This will be shown in Chapter 6.

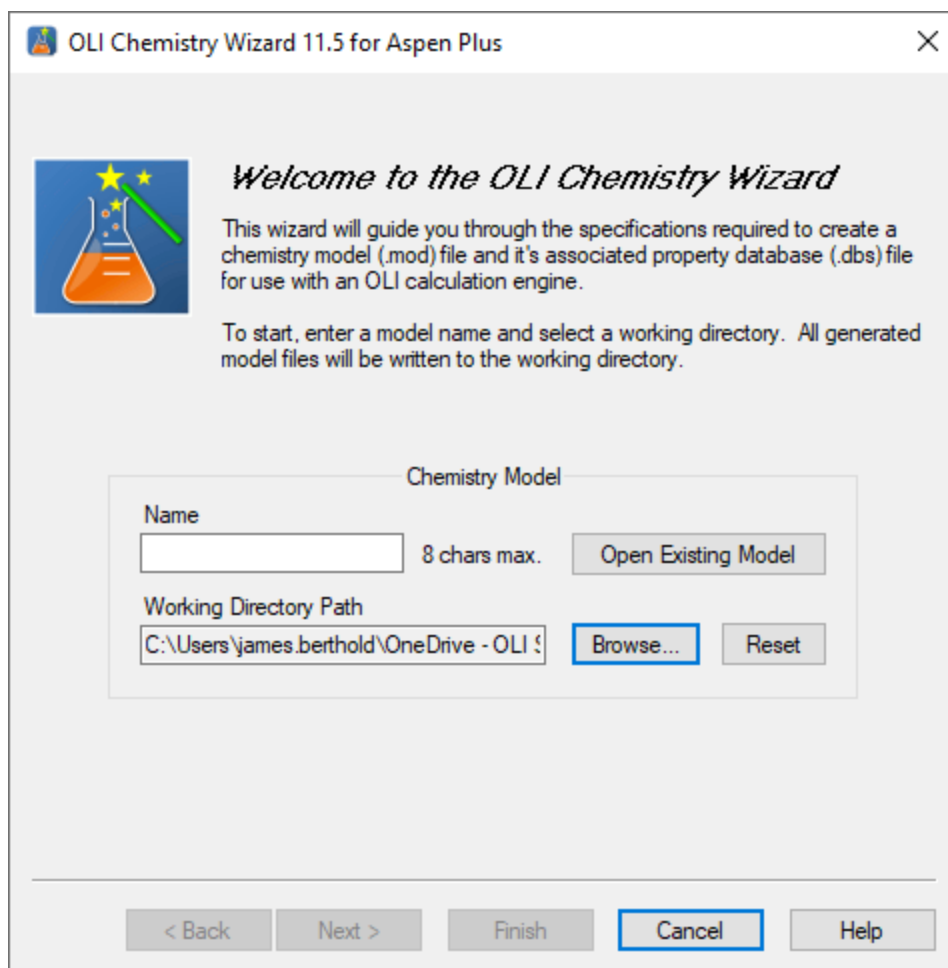
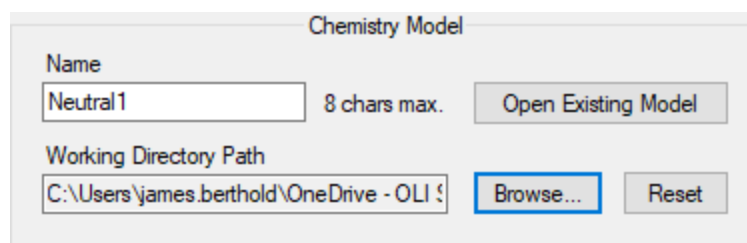
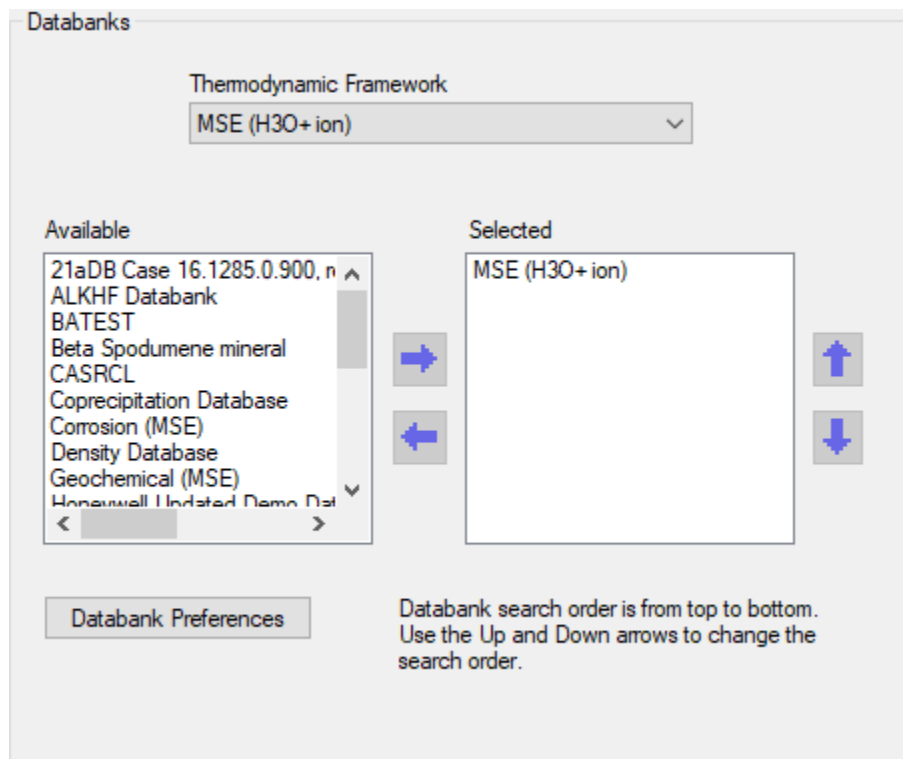


Figure 2-1 Specifying the model name and location



Click the **Next>** button to continue



Here we can select the thermodynamic framework. The default is MSE. There are two offered by OLI: the traditional aqueous model and the mixed-solvent electrolyte framework. This latter framework is also known as the H₃O⁺ (hydronium ion) framework.

We can also select databases in addition to the PUBLIC database. These databases listed contain data that limited to a more specific region of thermodynamic space than the PUBLIC database or contains data that is missing from the public database. For this example, we will only use the PUBLIC database.

Click the **Next>** button to continue

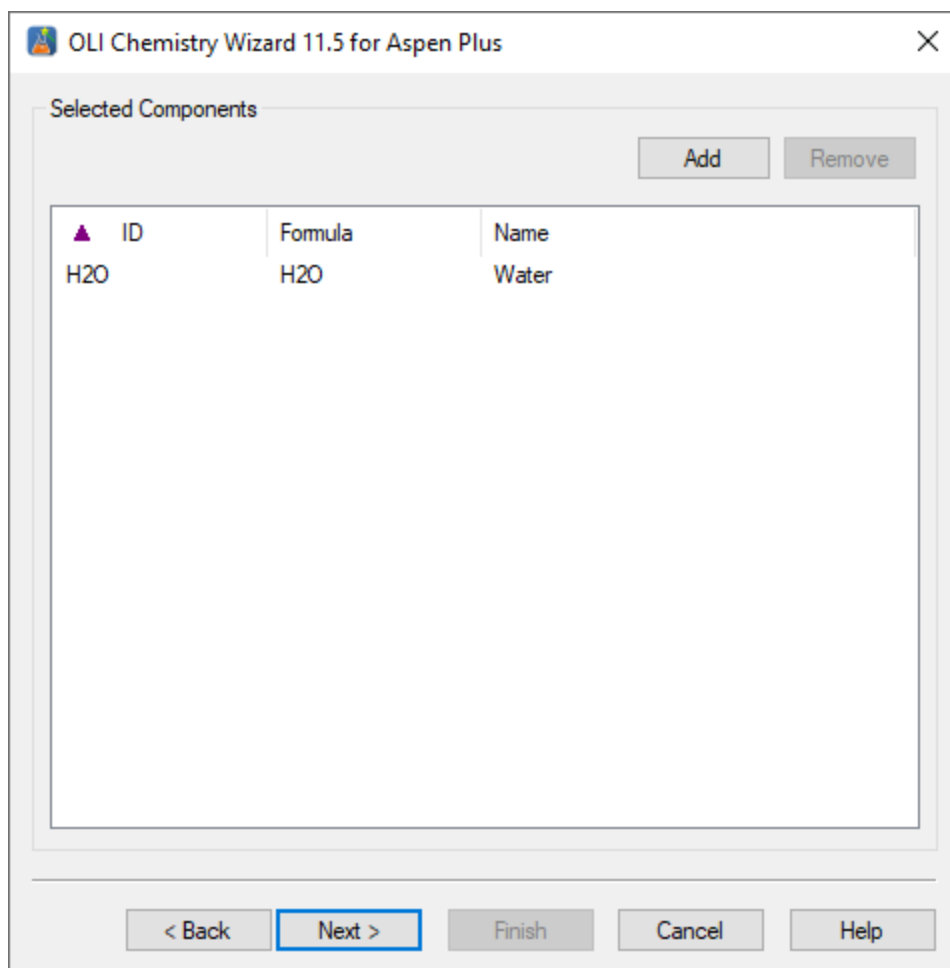


Figure 2-2 Adding components

We are now ready to add the components for this example. Click the **Add** button.

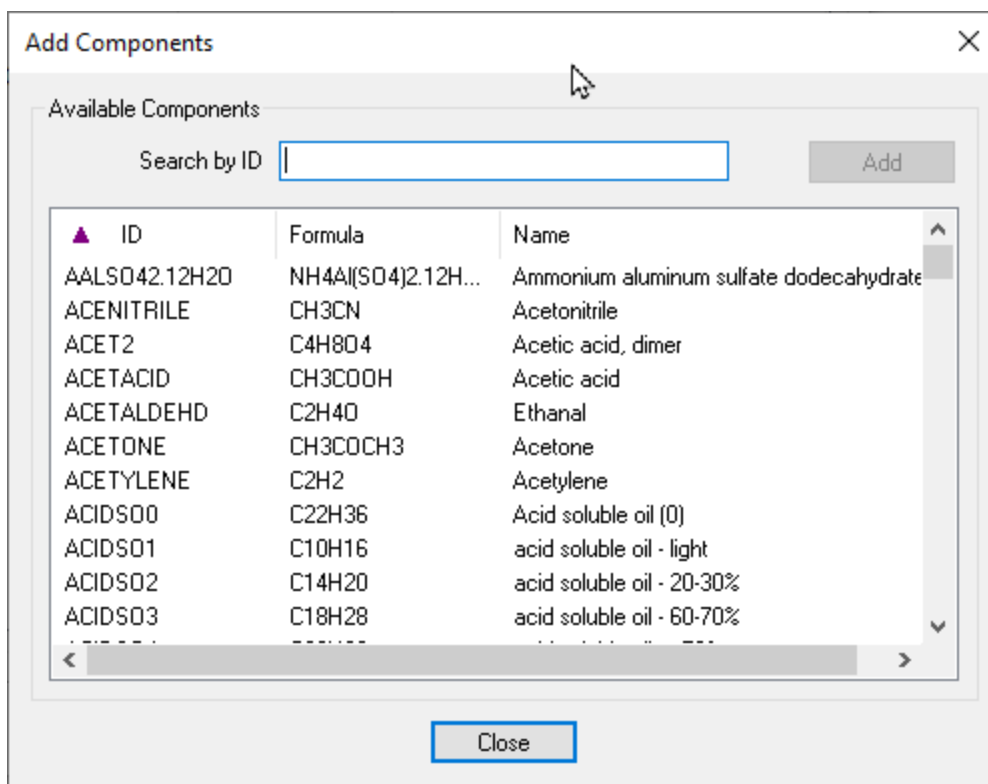


Figure 2-3 Select Components

We now need to add our components of ammonia (NH₃), carbon dioxide (CO₂), sulfur dioxide (SO₂), hydrochloric acid (HCL), sulfuric acid (H₂SO₄) and sodium hydroxide (NAOH).

We can scroll through the list or enter the component ID and let the software find the component. We will try the latter technique, enter the component ID NH₃

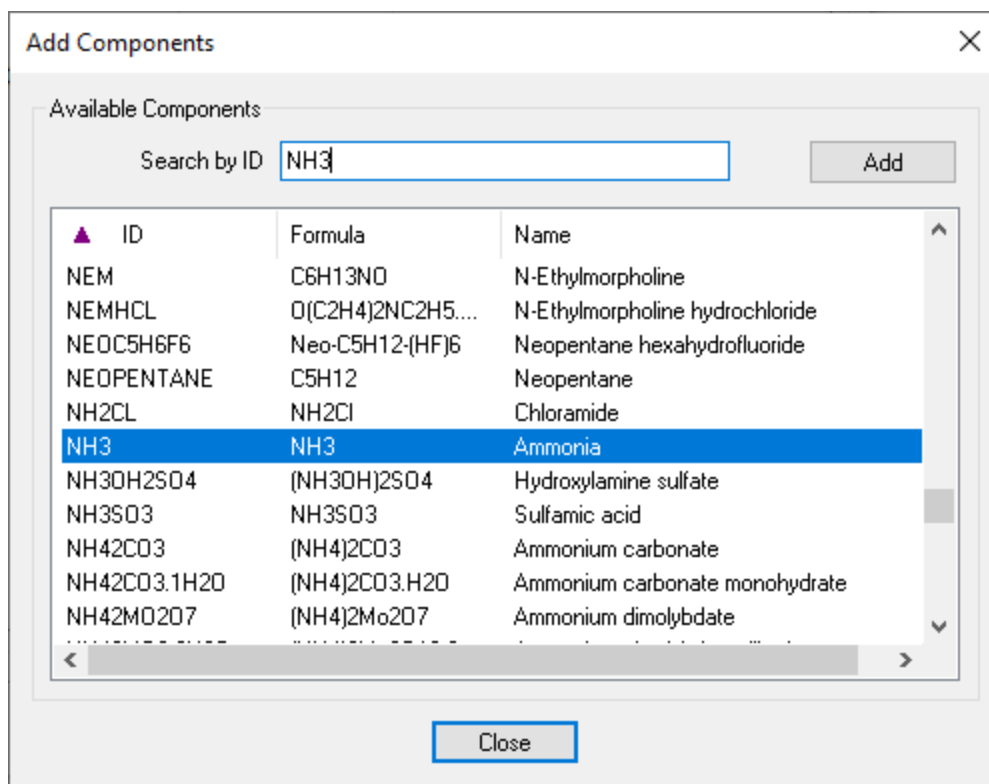


Figure 2-4 Adding NH3, ammonia

You can see that the screen automatically scrolled as you entered letters. The current component NH3 is highlighted. Click the **Add** button. Repeat this action for the remaining components. Click the **Close** button when done.

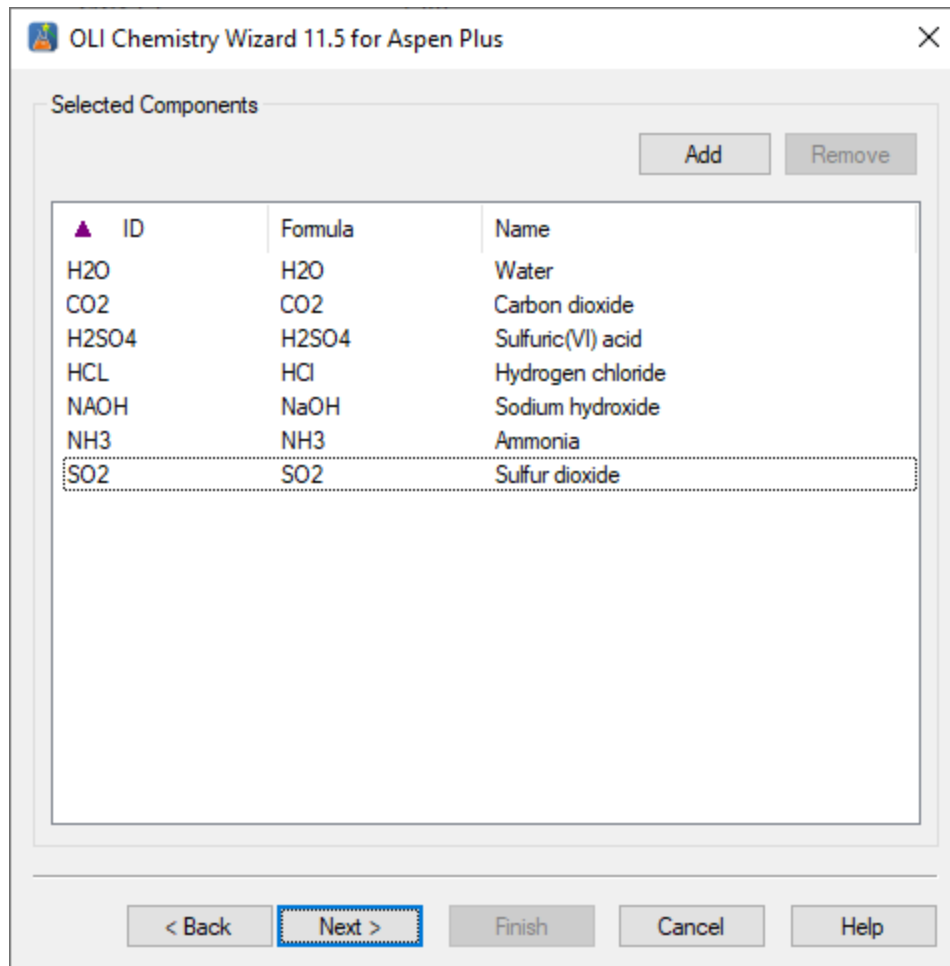


Figure 2-5 the added components

Click the **Next>** button.

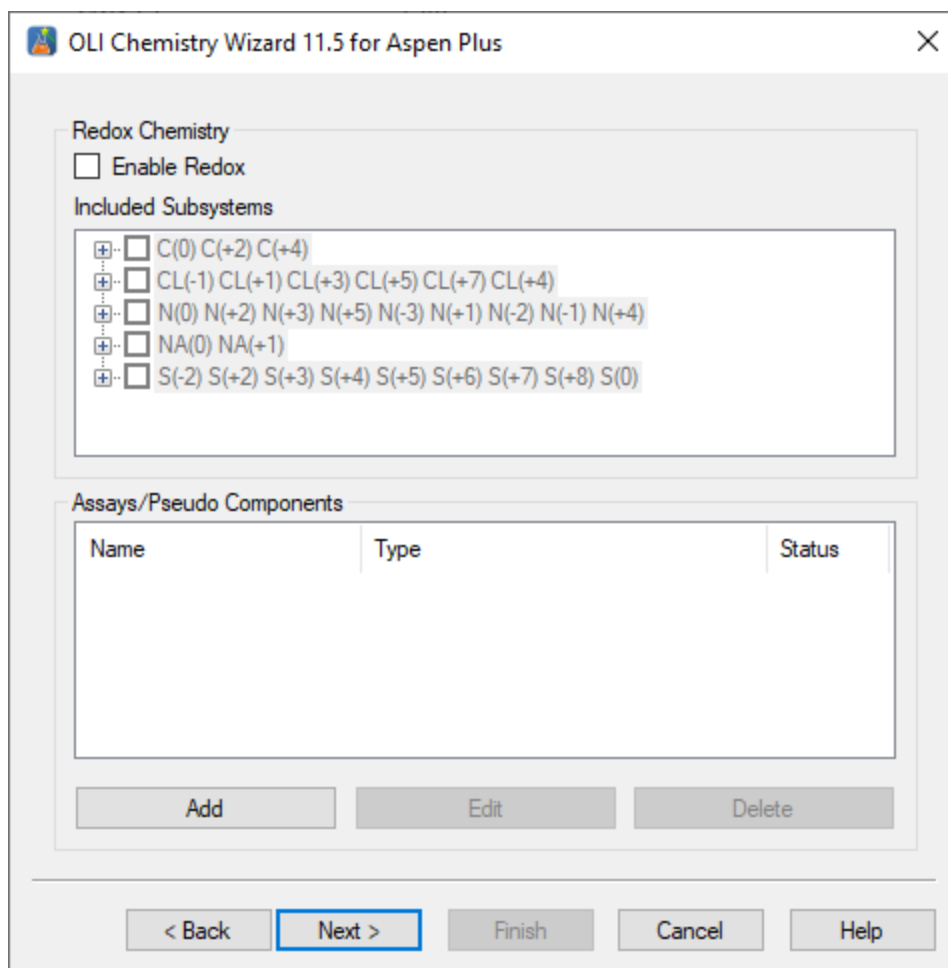


Figure 2-6 adding redox

On this screen we can add oxidation and reduction to the chemistry. We will not do so for this example. Click the **Next>** button.

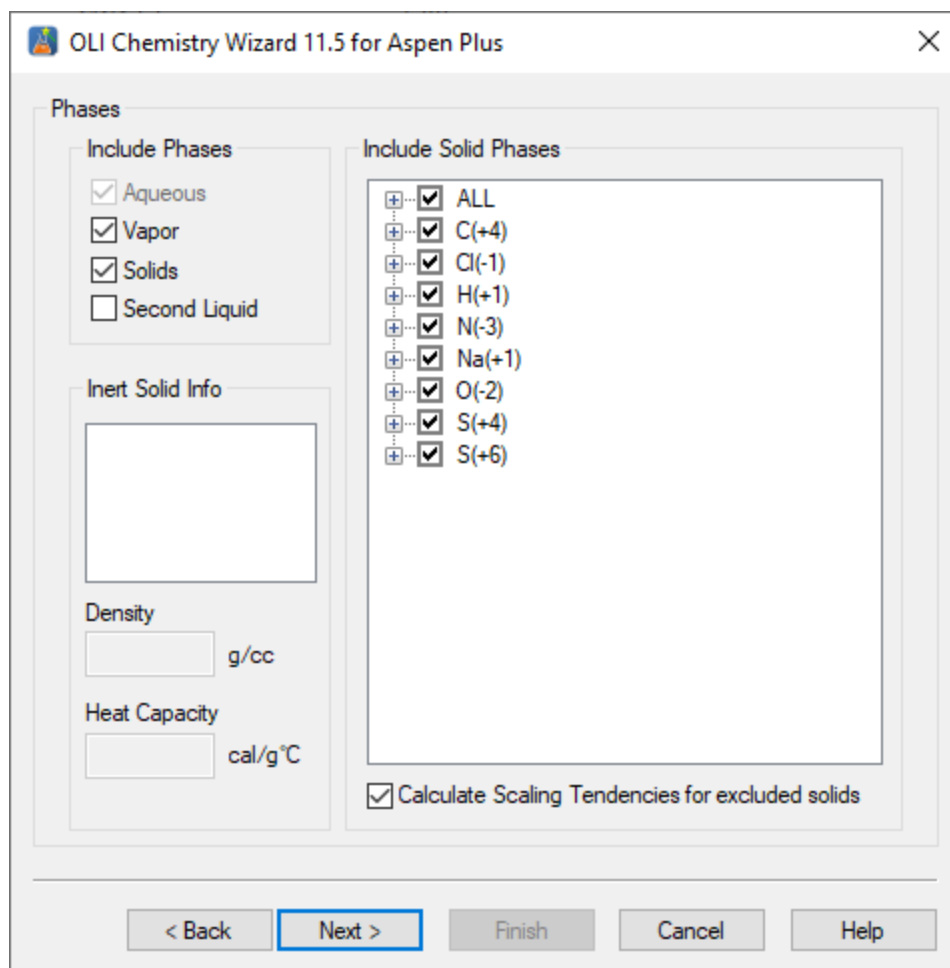


Figure 2-7 Selecting phases, including solids

On this screen we can enable vapor and second liquid (non-aqueous) phases.

By default, the vapor phase is enabled, and the second liquid phase is disabled. We can also turn off all potential solid phases or select individual solids to exclude. Occasionally the user will have prior knowledge of which solid phases will be present.

Eliminating solids that are not possible can dramatically reduce the execution time of the program.

Click **Next>** to continue.

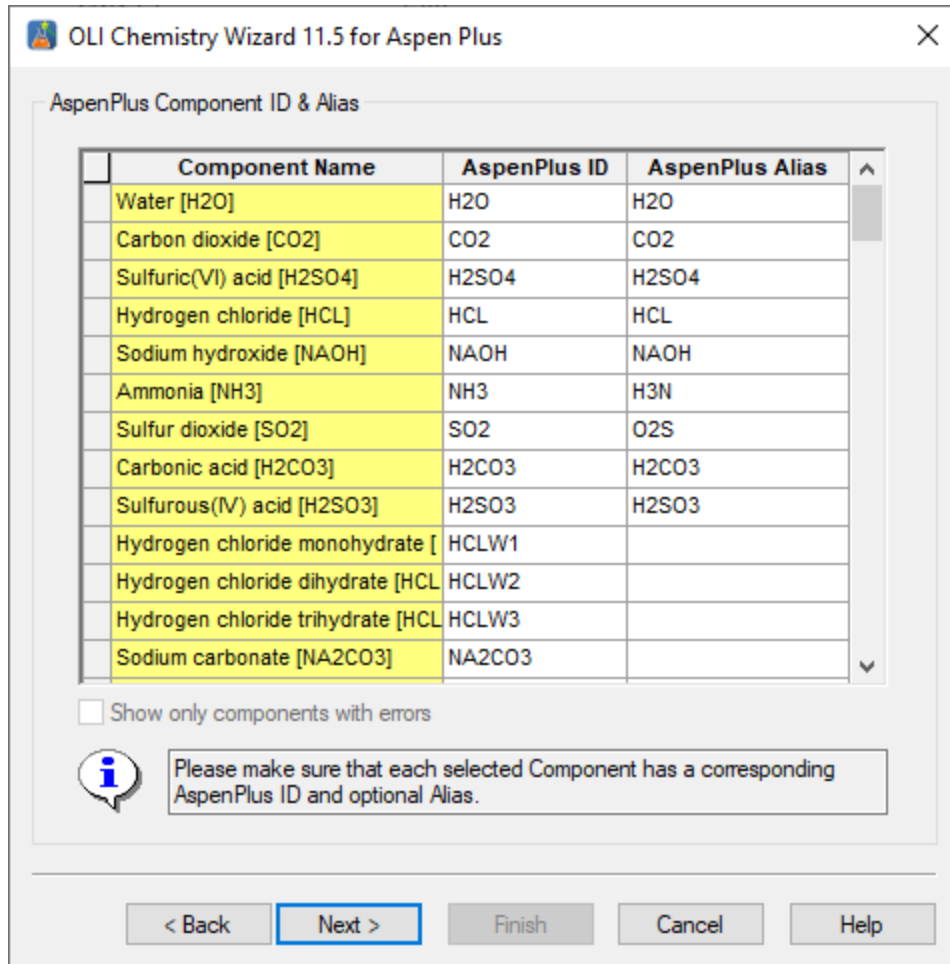


Figure 2-8 Aspen Alias names

Many times, OLI will have a component that Aspen PLUS will not. For those cases an alias name has to be provided to allow the two programs to properly communicate.

Click the **Next>** button.

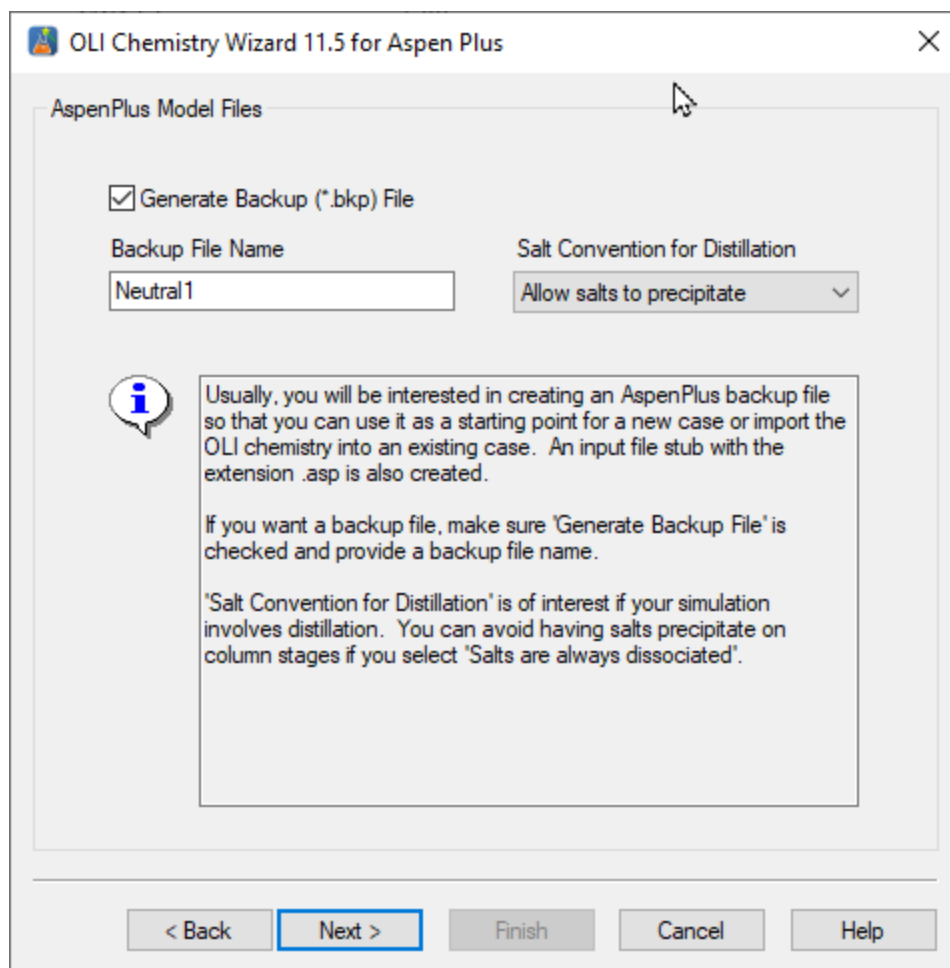


Figure 2-9 BKP file options

OLI initially communicates to Aspen PLUS via the BKP file. We will shortly create a flowsheet without any unit operations. The BKP file will initially have the same name as the chemistry model, but you may change the name if you wish.

A second option is to allow the solid salts to precipitate. This is the default option. Alternatively, you can dramatically increase the speed of execution by setting the salts to be dissociated. It is recommended for OLI models that you accept the default choices.

Click the **Next>** button.

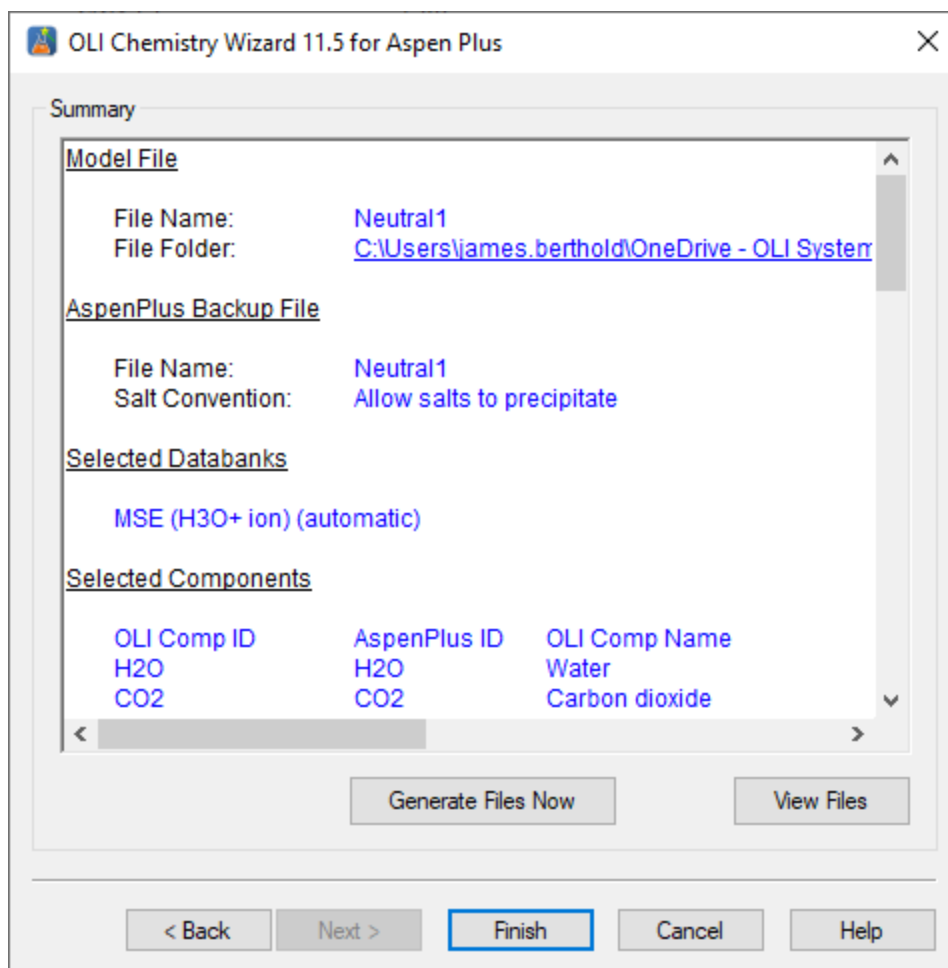


Figure 2-10 Almost done

We are almost done with the chemistry model generation. This is the summary screen of what we have selected. Please review it to make sure you have made the choices you require. Click the **Generate Files Now** button.

If the model was successfully generated, you will receive this message (you will have a different set of folders):

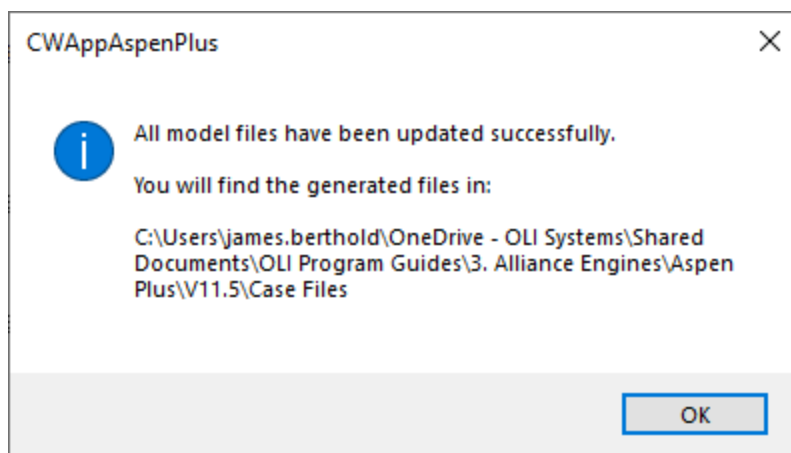


Figure 2-11 completed

Click the **OK** button.

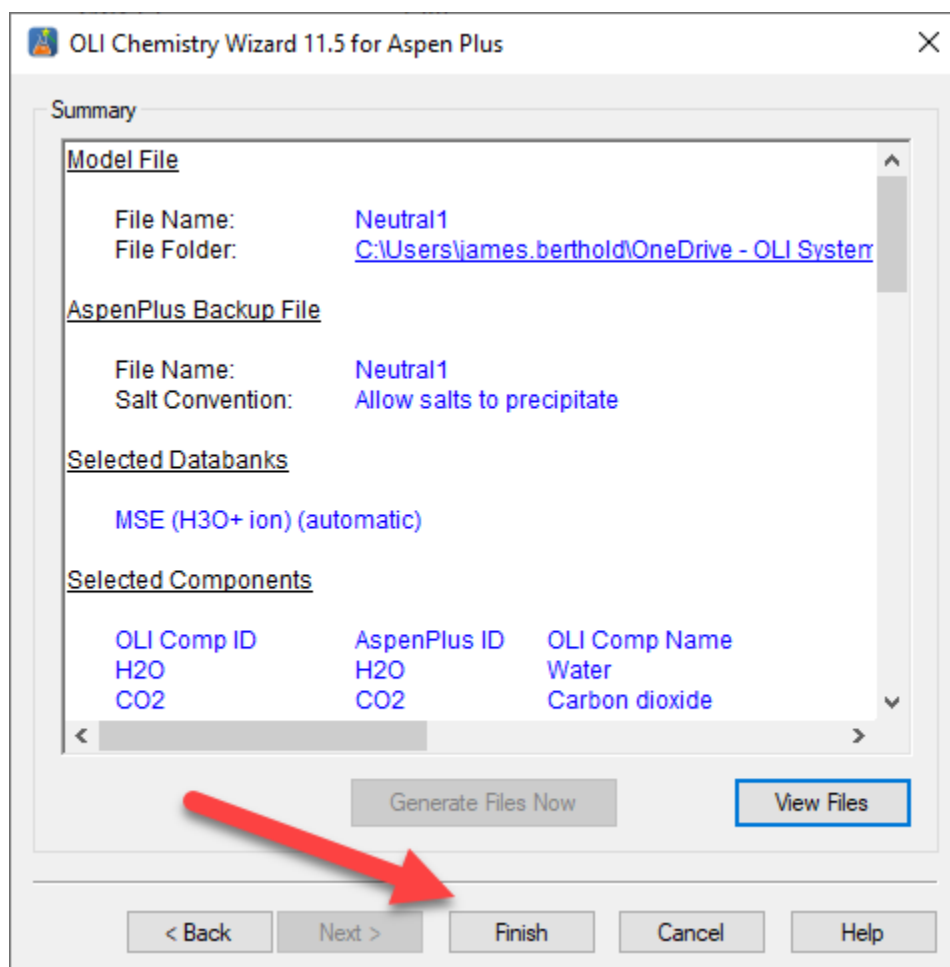


Figure 2-12 Done

We are now done with the chemistry model generation. Notice that the **Generate Files Now** button and the **Next>** button are gray. Click the **Finish** button.

We create a BKP file and an ASP file. We will use the BKP file in a moment. The ASP file is the old Aspen INP file. We have renamed the file from INP to ASP since OLI also uses a file with extension INP.³ Here is the contents of the file. It can be renamed to INP to be used with the Aspen PLUS Simulation Engine.

Creating the Aspen Flowsheet

It is beyond the scope of this manual to instruct the user in how to run Aspen PLUS. We will just concentrate on the issues unique to OLI. Start Aspen PLUS in the normal manner.

We first need to load the BKP file we just created. Use the standard file/open dialogs to open the NEUTRAL1.BKP file.

Accept whatever local or network setting you must to activate the Aspen PLUS program. You may see the following warning:

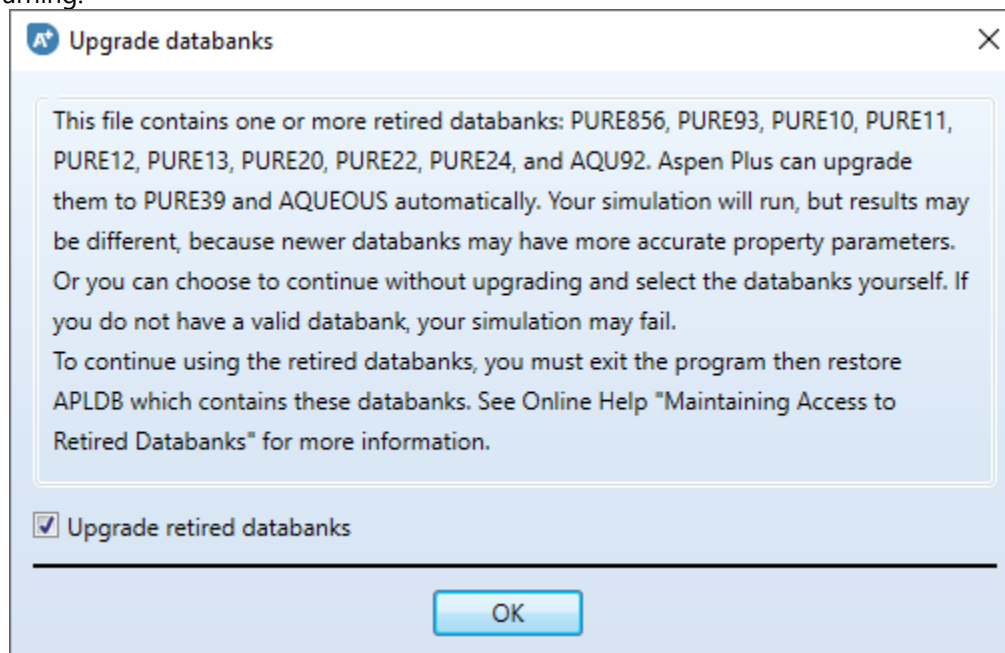


Figure 2-13 Compatibility warning

The BKP file generated by OLI is a very simple format file without any of the features available in latter versions Aspen PLUS. Keep the **Upgrade retired databanks** check box selected.

Click the **OK** button.

³ The INP file is used with OLI's ProChem software.

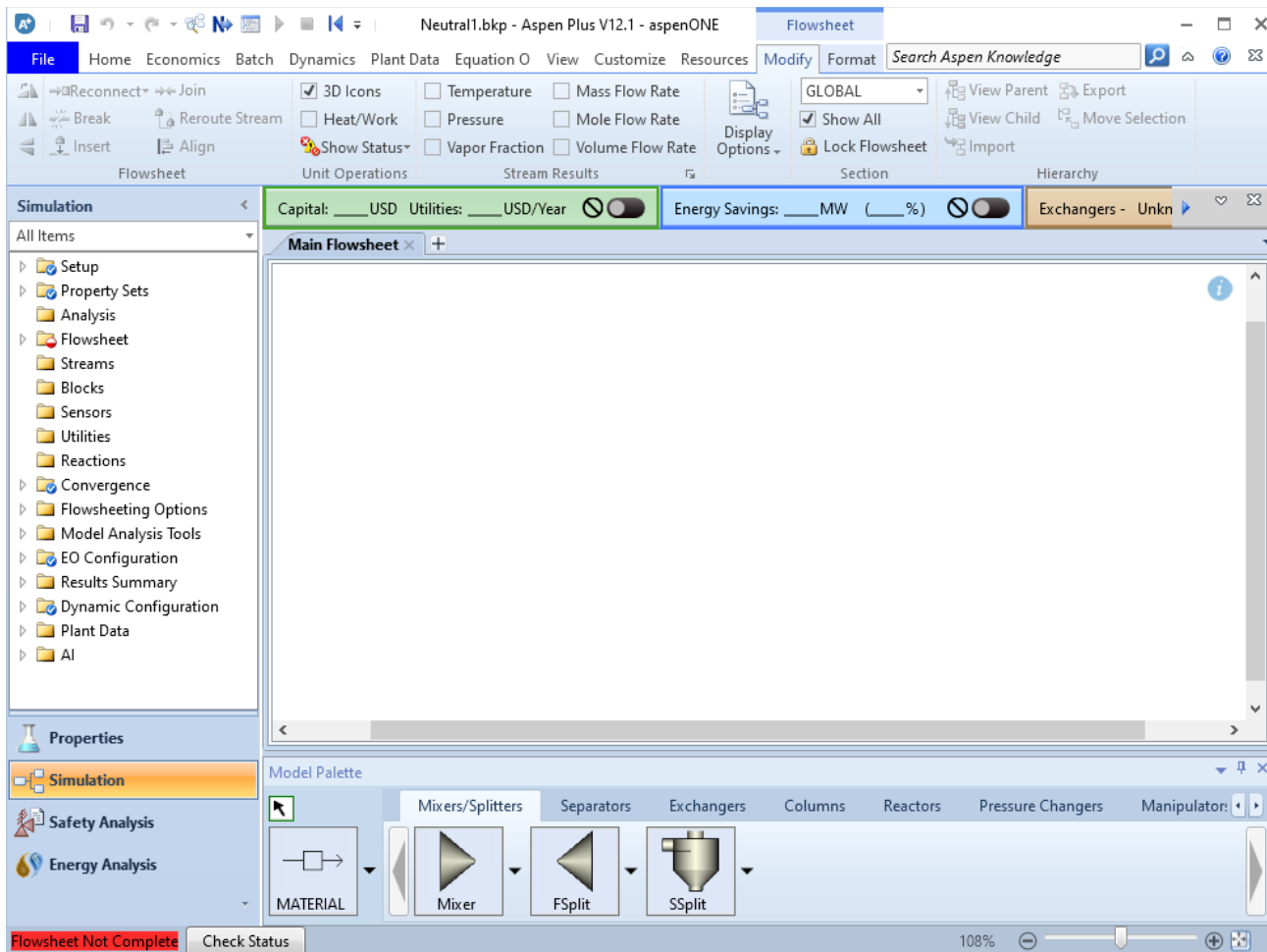


Figure 2-14 A blank flowsheet

We will create the following process:

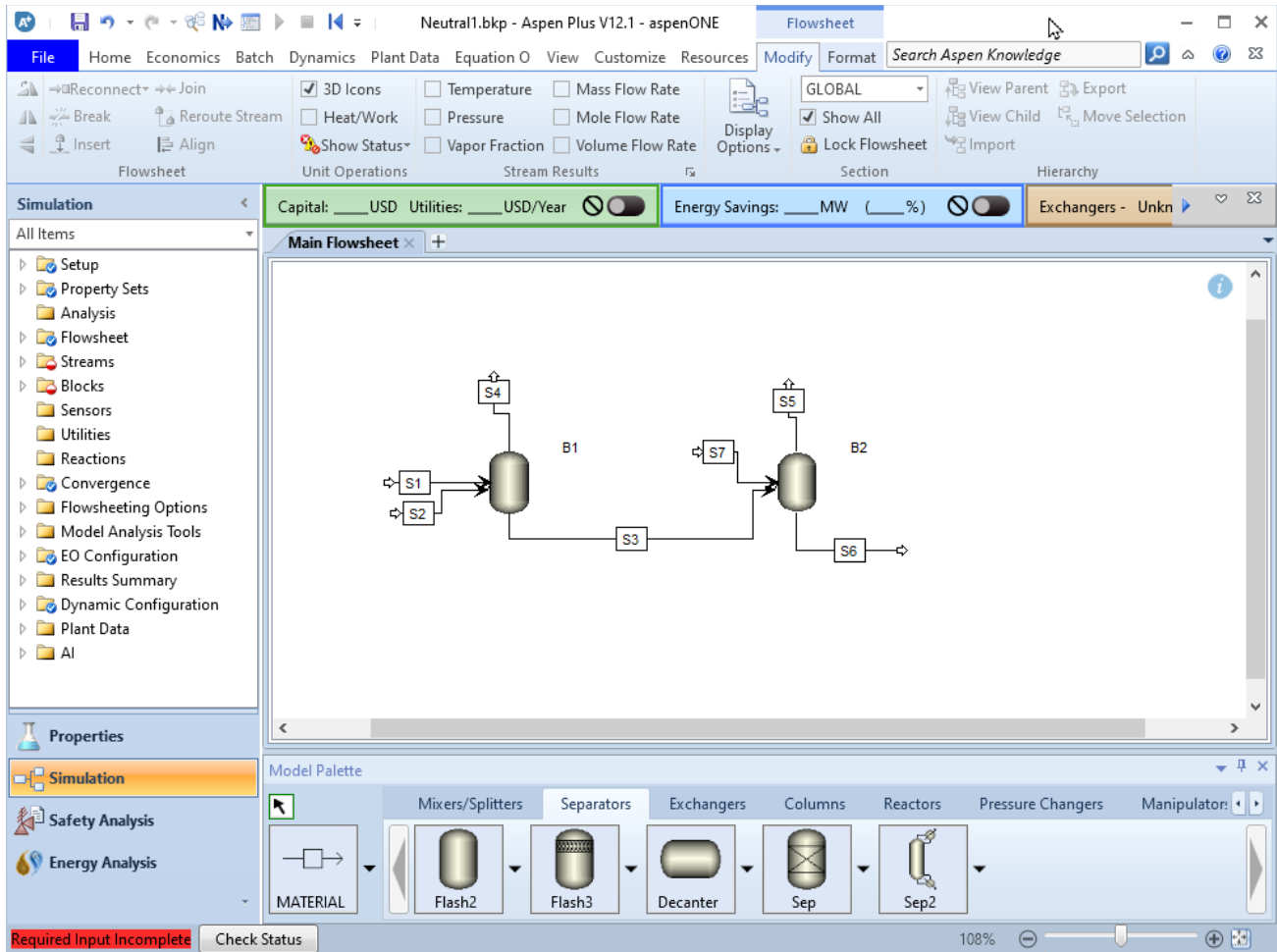


Figure 2-15 Neutral 1 Process

This process mixes a basic stream (S1) with an acidic stream (S2) adiabatically in block B1. The resultant vapor stream (S3) is drawn off and the mixed liquid (S4) is neutralized with a sodium hydroxide stream (S5) adiabatically in block B2. A design specification is that stream 7 is to be held to a pH of 9.0 within 0.01 pH units. The following tables contain the Stream conditions:

Table 2-1 Stream Definitions

Stream	S1	S2	S7
Temperature (°C)	40	25	30
Pressure (atm)	1	1	1
Total flow (lbmole/hr)	200	150	100
H2O (lbmole/hr)	55.5	55.5	55.5
NH3	1	0	0
CO2	0.1	0	0
SO2	0.1	0	0
HCL	0	0.1	0
H2SO4	0	1.0	0
NAOH	0	0	1

Table 2-2 Block Definition

Block	B1	B2
Duty (Btu/hr)	0	0
Pressure (atm)	1	1

Table 2-3 Design Specifications⁴

Design Specification	DS-1
Variable Name	PH
Variable Type	Stream-Prop
Variable Target	S6
Prop-Set	PH
Variable Target Value	9.0
Tolerance	0.01
Vary	S5
Vary Option	Type: Stream-Var Substream: Mixed Variable: Mole-Flow Lower Bound: 50 Upper Bound: 400

After entering the parameters, run the case as you would normally.

Below are the stream results from this case.

Table 2-4 Stream Results⁵

Stream Name	Units	Material						
		S1	S2	S3	S4	S5	S6	S7
Description								
From				B1	B1	B2	B2	
To		B1	B1	B2				B2
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Maximum Relative Error								
Cost Flow	\$/hr							

⁴ In the OLI terminology, these are controllers

⁵ Many zero rows have been eliminated from this report.

MIXED Substream							
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase	Liquid Phase	Liquid Phase
Temperature	F	104	77	101.9425 509	101.9425 509	103.4933 075	86
Pressure	psia	14.69594 878	14.69594 878	14.69594 878	14.69594 878	14.69594 878	14.69594 878
Molar Vapor Fraction		0	0	0	1	0	0
Molar Liquid Fraction		1	1	1	0	1	1
Molar Solid Fraction		0	0	0	0	0	0
Mass Vapor Fraction		0	0	0	1	0	0
Mass Liquid Fraction		1	1	1	0	1	1
Mass Solid Fraction		0	0	0	0	0	0
Molar Enthalpy	Btu/lbmol	122696.8 402	127456.7 837	123875.6 391	162299.5 724	123432.8 376	122057.3 314
Mass Enthalpy	Btu/lb	6686.769 197	6548.862 52	6630.212 564	3741.617 84	6678.842 426	6749.366 956
Molar Entropy	Btu/lbmol-R	17.66396 49	16.51379 181	17.46261 958	51.52829 97	17.36737 312	16.31316 405
Mass Entropy	Btu/lb-R	0.962656 057	0.848495 852	0.934654 146	1.187921 833	0.939733 305	0.902064 048
Molar Density	lbmol/cuft	3.404801 353	3.406140 669	3.418696 925	0.002450 691	3.456876 839	3.582951 805
Mass Density	lb/cuft	62.47536 82	66.29177 711	63.87325 633	0.106303 22	63.88713 644	64.79504 504
Enthalpy Flow	Btu/hr	2423950 4.37	1911851 7.56	4331595 9.51	42062.42 507	7372105 2.44	3040509 2.91
Average MW		18.34919 624	19.46243 081	18.68350 946	43.37684 373	18.48117 229	18.08426 364
Mole Flows	lbmol/hr	197.5560 603	150	349.6729 446	0.259165 347	597.2564 019	249.1050 112
H2O	lbmol/hr	193.4635 711	143.7410 383	342.1455 427	0.017617 916	586.0373 248	240.4404 912
CO2	lbmol/hr	7.66061E-05	0	0.125840 463	0.226891 287	8.33514E-05	0
H2SO4	lbmol/hr	0	3.61682E-06	3.07301E-07	6.24244E-21 -21	2.16611E-22	0

HCL	lbmol/h		5.13859E	1.3437E-	8.71308E		1.89949E	
	r	0	-09	09	-10	0	-17	0
NH3	lbmol/h	0.512364		1.06816E	6.22188E		0.323057	
	r	133	0	-08	-11	0	445	0
SO2	lbmol/h	2.69133E		0.270189	0.014656		7.68539E	
	r	-11	0	477	143	0	-11	0
SO3	lbmol/h		4.285E-	1.76611E	1.72293E			
	r	0	20	-20	-27	0	0	0
NA3HSO4	lbmol/h						1.96287E	
	r	0	0	0	0	0	-11	0
NH4OH	lbmol/h	1.738548		3.7603E-			1.125609	
	r	888	0	08	0	0	53	0
NA3OHSO4	lbmol/h						2.12271E	
	r	0	0	0	0	0	-09	0
NAOH	lbmol/h						2.44234E	2.18245E
	r	0	0	0	0	0	-10	-06
OH-	lbmol/h	0.000312	3.29618E	4.30429E			0.000533	4.332258
	r	961	-14	-12	0	0	753	921
CO3-2	lbmol/h	0.078199		1.20386E			0.024175	
	r	932	0	-14	0	0	316	0
H3O+	lbmol/h	2.32562E	3.343767	0.621144			1.8625E-	1.13406E
	r	-09	367	698	0	0	08	-13
HCO3-	lbmol/h	0.133829		1.9365E-			0.081414	
	r	287	0	06	0	0	867	0
HSO3-	lbmol/h	0.000841		0.067499			0.001231	
	r	27	0	883	0	0	96	0
HSO4-	lbmol/h		2.221596	1.484779			6.35528E	
	r	0	419	22	0	0	-08	0
NA+	lbmol/h						4.332261	4.332258
	r	0	0	0	0	0	083	921
NAOHCO-2	lbmol/h						1.29627E	
	r	0	0	0	0	0	-08	0
NH2CO2-	lbmol/h	0.140627		2.64846E			0.020168	
	r	861	0	-14	0	0	852	0
NH4+	lbmol/h	1.135795		3.527336			2.058501	
	r	979	0	812	0	0	034	0
CL-	lbmol/h		0.265017	0.265017			0.265017	
	r	0	663	666	0	0	667	0
S2O5-2	lbmol/h	4.68072E		0.000193			3.71615E	
	r	-08	0	931	0	0	-08	0
SO3-2	lbmol/h	0.351892		3.20464E			0.336845	
	r	323	0	-07	0	0	509	0
SO4-2	lbmol/h		0.428576	1.165397			2.650176	
	r	0	642	151	0	0	613	0

pH is not a standard Aspen Plus stream variable you must add the property to the report. Here we have added pH to the S6 stream report.

The screenshot displays the Aspen Plus V12.1 interface. The main window shows a 'Stream Summary' report for stream S6 (MATERIAL). The report table includes various properties such as Molar Density, Mass Density, Enthalpy Flow, Average MW, Mole Flows, Mole Fractions, Mass Flows, Mass Fractions, Volume Flow, and pH. The pH value is 9.00132, which is highlighted with a red box. The 'Model Palette' at the bottom shows various unit operations like Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, and Manipulators.

Property	Units	S6
Molar Density	lbmol/cuft	3.45688
Mass Density	lb/cuft	63.8871
Enthalpy Flow	Btu/hr	-7.37211e+07
Average MW		18.4812
+ Mole Flows	lbmol/hr	597.256
+ Mole Fractions		
+ Mass Flows	lb/hr	11038
+ Mass Fractions		
Volume Flow	cuft/hr	173.773
pH		9.00132

As you can see, the pH of stream S6 is 9.0 within the tolerance we defined.

Chapter 3 ASPEN Emergency Chlorine Scrubber Flowsheet

A Tour of the OLI-ASPEN Interface (RADFRAC example)

The following example is a simulation of a Chlorine scrubber. Caustic is used to remove chlorine from a gas stream. The caustic feed rate to the column is adjusted to reduce the chlorine in the column overhead gas to 0.5 moles/hr.

Generating Chemistry Model

Using the OLI Chemistry Wizard, create a chemistry model with the following components. We recommend the name of the model to be CHLORINE. Turn off all solids in this model.

H₂O, CO₂, Cl₂, N₂, NaOH

Creating the Aspen Flowsheet

Start Aspen normally and open the Chlorine.BKP file just created.

Create the following flowsheet

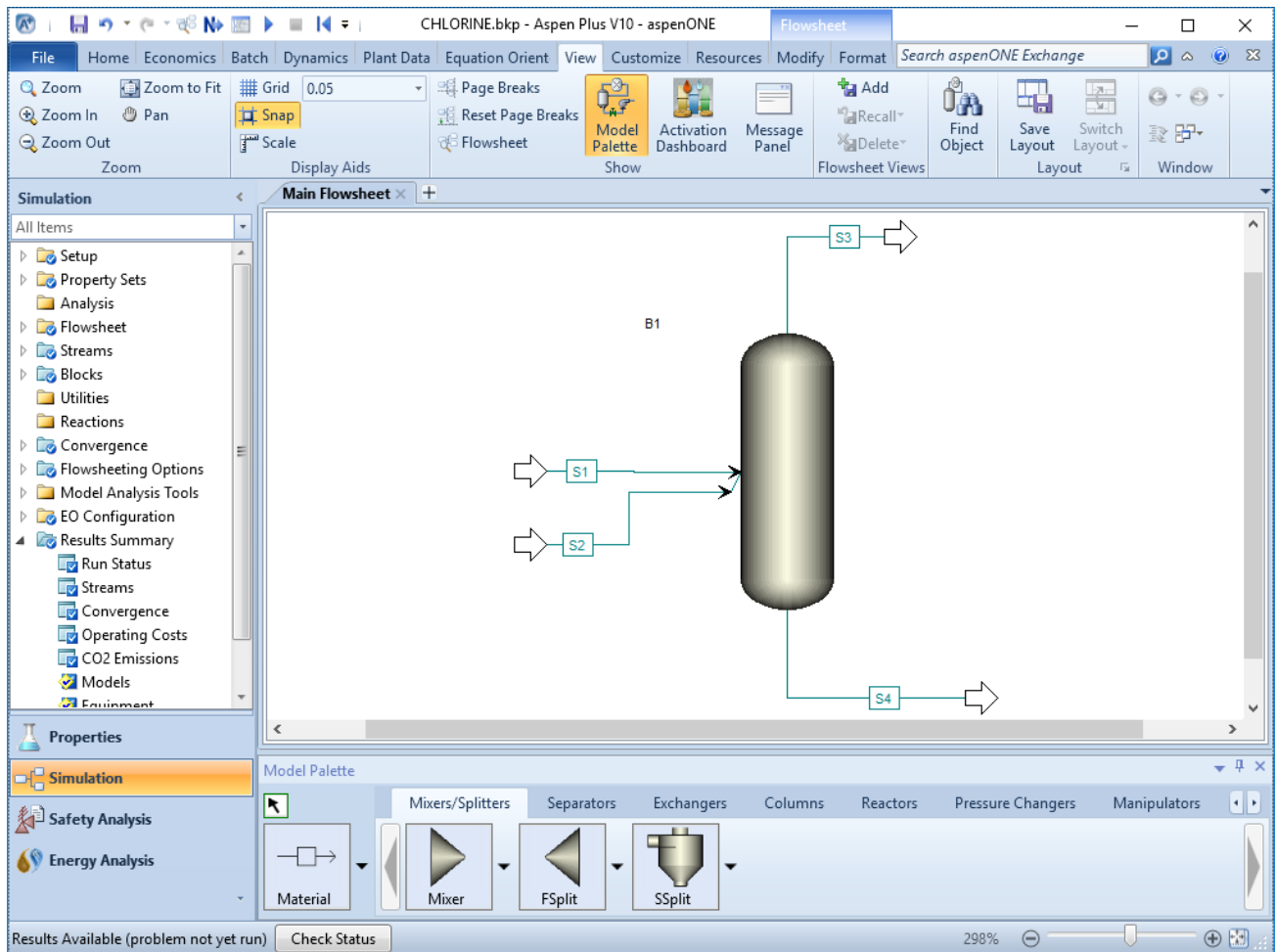


Figure 3-1

Caustic Feed Stream (S1)

Main Flowsheet × S1 (MATERIAL) - Input × +

Mixed | CI Solid | NC Solid | Flash Options | EO Options | Costing | Information

Specifications

Flash Type: Temperature Pressure

State variables

Temperature: 25 C

Pressure: 1 atm

Vapor fraction: []

Total flow basis: Mole

Total flow rate: [] lbmol/hr

Solvent: []

Reference Temperature

Volume flow reference temperature: [] F

Component concentration reference temperature: [] F

Composition

Mole-Flow lbmol/hr

Component	Value
H2O	48.8
CO2	
CL2	
HClO	
HCL	
N2	
NAHCO3	
NAOH	2.57
H2CO3IN	
Total	51.37

Component Attributes

Particle Size Distribution

Feed Stream (S2)

Main Flowsheet × S2 (MATERIAL) × +

Mixed | CI Solid | NC Solid | Flash Options | EO Options | Costing | Information

Specifications

Flash Type: Temperature Pressure

State variables

Temperature: 33 C

Pressure: 1.01 atm

Vapor fraction: []

Total flow basis: Mole

Total flow rate: [] lbmol/hr

Solvent: []

Reference Temperature

Volume flow reference temperature: [] F

Component concentration reference temperature: [] F

Composition

Mole-Flow lbmol/hr

Component	Value
H2O	2.27
CO2	23.59
CL2	2.27
HClO	
HCL	
N2	26.3
NAHCO3	
NAOH	
H2CO3IN	
Total	54.43

Component Attributes

Particle Size Distribution

RADFRAC (Block B1) configuration (5 stages)

The screenshot shows the configuration window for RADFRAC (Block B1) with 5 stages. The 'Configuration' tab is active. The 'Setup options' section includes:

- Calculation type: Equilibrium
- Number of stages: 5
- Condenser: None
- Reboiler: None
- Valid phases: Vapor-Liquid
- Convergence: Standard

The 'Operating specifications' section includes a 'Free water reflux ratio' set to 0 on a 'Feed Basis'.

RADFRAC (Block B1) streams

The screenshot shows the streams window for RADFRAC (Block B1). It displays feed streams, product streams, and pseudo streams.

Feed streams

Name	Stage	Convention
S1	1	Above-Stage
S2	5	On-Stage

Product streams

Name	Stage	Phase	Basis	Flow	Units	Flow Ratio	Feed Specs
S3	1	Vapor	Mole		lbmol/hr		Feed basis
S4	5	Liquid	Mole		lbmol/hr		Feed basis

Pseudo streams

Name	Pseudo Stream Type	Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparound ID	Pumparound Conditions	Flow	Units

RADFRAC (Block B1) pressure

Main Flowsheet × B1 (RadFrac) × +

Configuration Streams Pressure Condenser Reboiler 3-Phase Information

View Top / Bottom

Top stage / Condenser pressure
Stage 1 / Condenser pressure 1 atm

Stage 2 pressure (optional)
 Stage 2 pressure 1 atm
 Condenser pressure drop psi

Pressure drop for rest of column (optional)
 Stage pressure drop 1 atm
 Column pressure drop psi

RADFRAC (Block B1) estimates

Simulation Main Flowsheet × B1 Convergence - Estimates × +

Temperature Flows Liquid Composition Vapor Composition

Temperature estimates (optional) Generate Estimates...

Stage	Temperature
1	35
5	35

Properties

Design Specs for BLOCK B1

Define Spec Vary Fortran Declarations EO Options Information

Active

^ Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
FLOW	Mole-Flow Stream=S3 Substream=MIXED Component=CL2 Units=lbmol/hr

New... Delete Copy Paste Move Up Move Down View Variables

^ Edit selected variable

Variable: FLOW

Category: All Blocks Streams Model Utility Property Parameters Reactions

Reference:

Type: Mole-Flow

Stream: S3

Substream: MIXED

Component: CL2

Units: lbmol/hr

EO input:

Open variable:

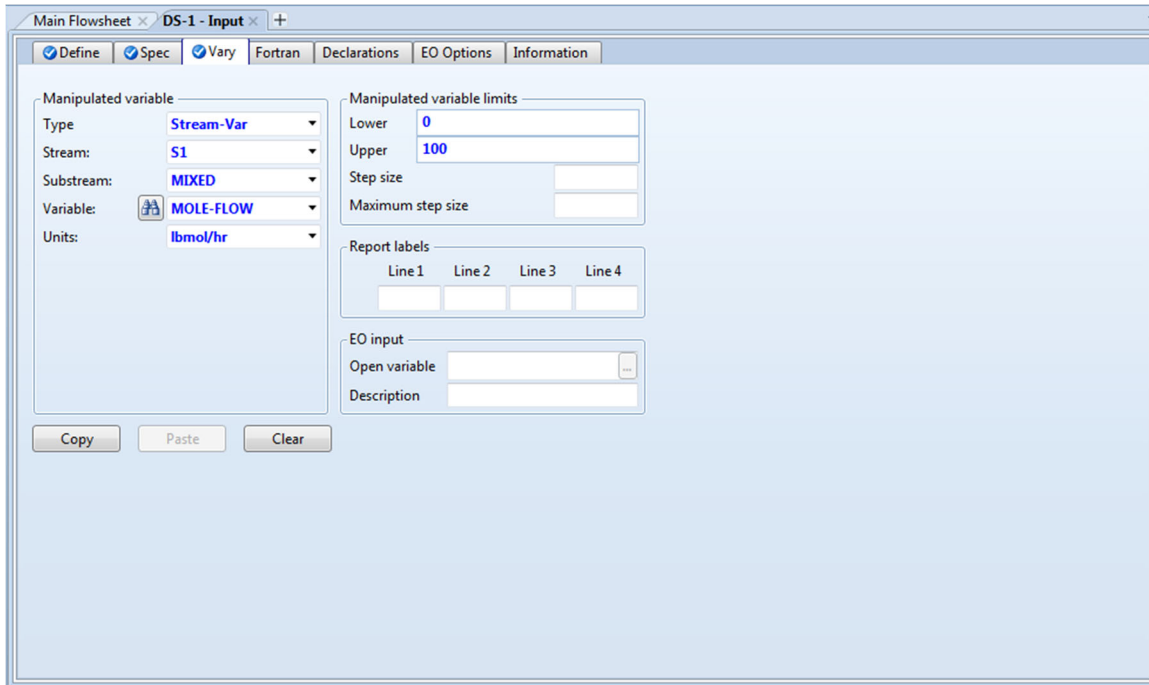
Description:

Main Flowsheet DS-1 - Input

Define Spec Vary Fortran Declarations EO Options Information

Design specification expressions

Spec	FLOW
Target	0.05
Tolerance	0.001



Now select the Vary Object

Now run the case

Stream Results

	S 1	S 2	S 3	S 4
	LIQUID	VAPOR	VAPOR	LIQUID
Substream: MIXED				
Mole Flow lbmol/hr				
H2O	55.37699	2 . 2 7	4.946512	53.29557
CO2	0	2 3 . 5 9	23.48042	6.66E-03
CL2	0	2 . 2 7	0.050656	9.90E-04
HCLO	0	0	0.128111	1.495381
HCL	0	0	7.55E-12	1.56E-13
N2	0	2 6 . 3	26.29985	1.52E-04
NAHCO3	0	0	3.76E-32	0.035227
OH-	2.91637	0	0	6.90E-08
CLO-	0	0	0	0.594862
CO3-2	0	0	0	1.39E-04
HCO3-	0	0	0	0.067459
H+	6.20E-15	0	0	2.00E-07
NACO3-	0	0	0	9.47E-05
NA+	2.91637	0	0	2.881048
CL-	0	0	0	2.218354
Total Flow lbmol/hr	61.20973	5 4 . 4 3	54.90554	60.59594
Total Flow lb/hr	1114.282	1976.797	1869.545	1221.535
Total Flow cuft/hr	16.23819	21639.56	22999.46	17.62484
Temperature F	7 7	9 1 . 4	115.0552	88.8305
Pressure psia	14.69595	14.84291	14.69595	14.69595
Vapor Frac	0	1	1	0
Liquid Frac	1	0	0	1
Solid Frac	0	0	0	0
Enthalpy Btu/lbmol	-1.21E+05	-77605.4	-81553.4	-1.18E+05
Enthalpy Btu/lb	-6633.57	-2136.82	-2395.09	-5843.47
Enthalpy Btu/hr	-7.39E+06	-4.22E+06	-4.48E+06	-7.14E+06
Entropy Btu/lbmol-R	15.08149	48.53608	48.5468	16.28609
Entropy Btu/lb-R	0.828456	1.336413	1.425742	0.807894
Density lbmol/cuft	3.769493	2.52E-03	2.39E-03	3.438099
Density lb/cuft	68.6211	0.091351	0.081286	69.30758
Average MW	18.20433	36.31816	34.0502	20.1587
Liq Vol 60F cuft/hr	16.51118	5.12638	5.711628	16.03514
*** LIQUID PHASE ***				
PH	14.52949			6.705763

The flowrate of the caustic stream (S1) was adjusted and that the specified flowrate of chlorine in the vapor stream S3 was achieved.

Chapter 4 EFLASH and EFRACH (FraChem)

Overview

Two OLI Electrolyte blocks have been added to enable the use of OLI's 4 phase flash (EFLASH) and OLI's distillation tower (FRACHEM). These two blocks were added through ASPEN user added blocks capability and are available via the **Customize Tab | Manage Libraries** feature of Aspen PLUS.

The ability to separate a 4-phase system into 4 streams does not exist in Aspen PLUS. This operation allows you to make complete phase separation.

EFLASH (Electrolyte Flash)



Figure 4-1 EFLASH diagram

Four Outlet Material Streams

- (1) - VAPOR
- (2) - AQUEOUS
- (3) - ORGANIC
- (4) - SOLID

Three Outlet Material Streams

- (1) - VAPOR
- (2) - AQUEOUS & ORGANIC
- (3) - SOLID

Two Outlet Material Streams

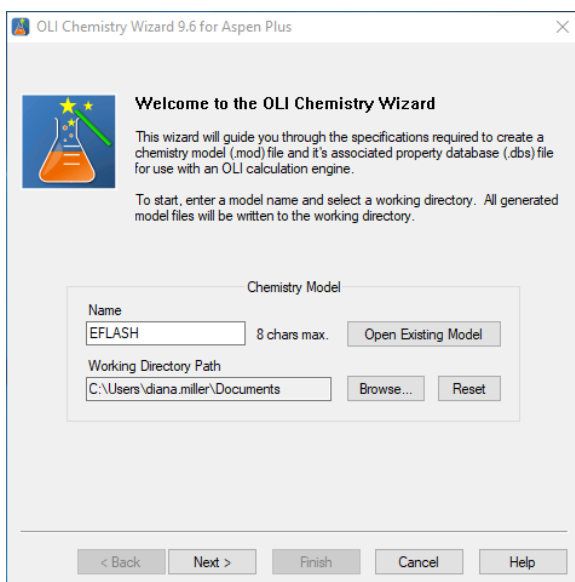
- (1) - VAPOR
- (2) - AQUEOUS & ORGANIC & SOLID

One Outlet Material Stream

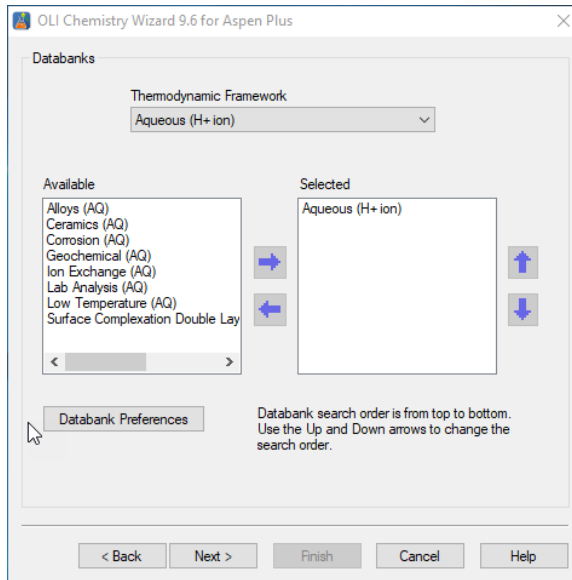
- (1) - ALL PHASES

Example

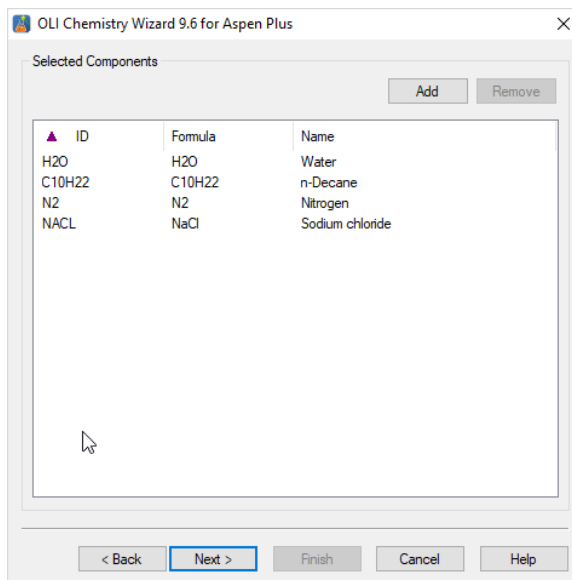
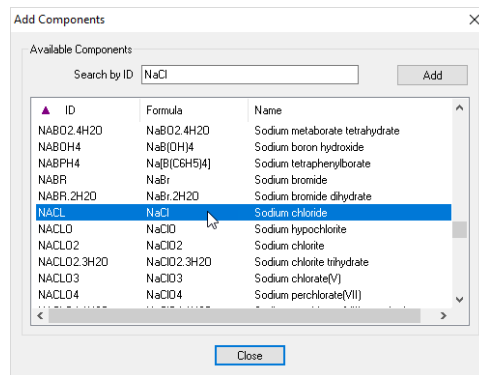
In this case we will create a chemistry model called EFLASH.



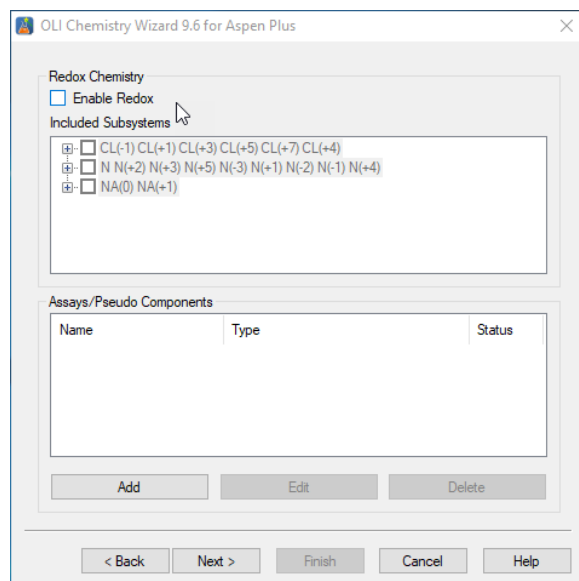
Select the Aqueous (H+ ion)



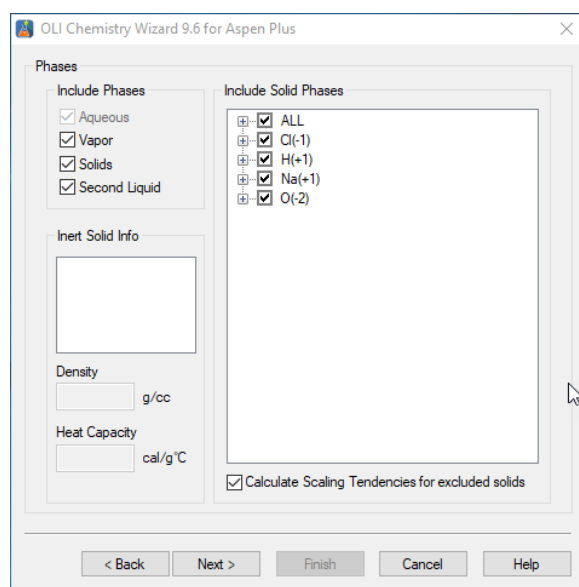
This model will contain H₂O, NaCl, C₁₀H₂₂ and N₂.



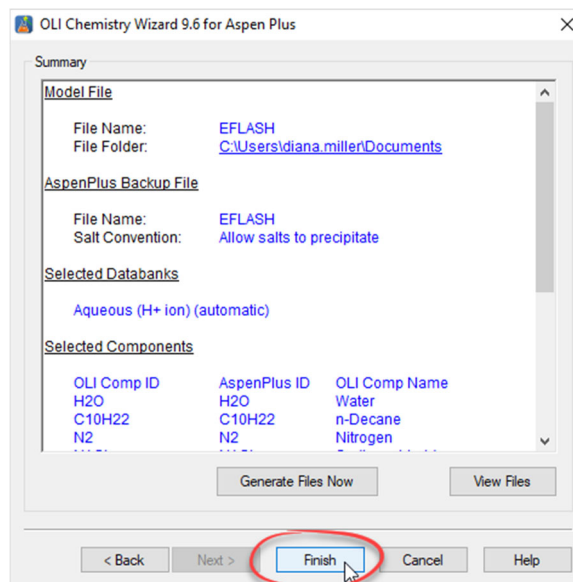
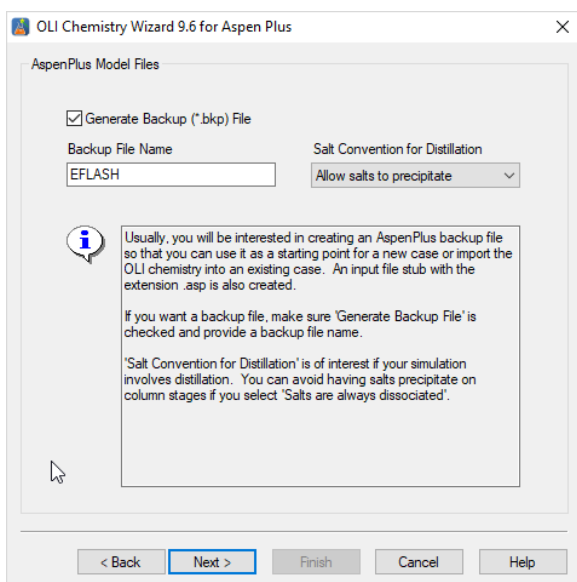
Do not Enable Redox reactions



When prompted, select the second liquid (organic) phase as well as the aqueous, vapor and solid phases.

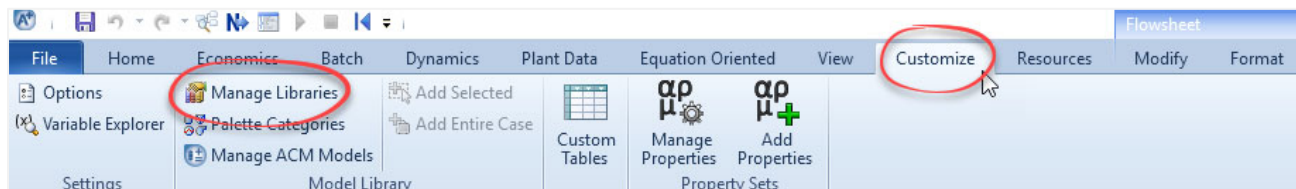


Generate the *.bkp file, and select finish.

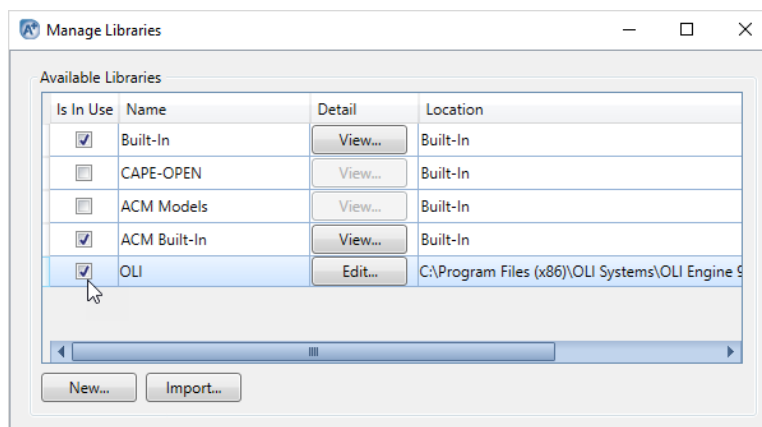


Start Aspen PLUS as you would normally and open the BKP file you just created using either the OLI Chemistry Wizard or OLI Chemistry Generator.

Select the **Customize** menu tab, and then select **Manage Libraries**.



If the OLI option has been purchased and the OLI Alliance Suite for Aspen PLUS has been installed, then the OLI option will appear in this dialog. **Check the OLI box and then close the window (X).**



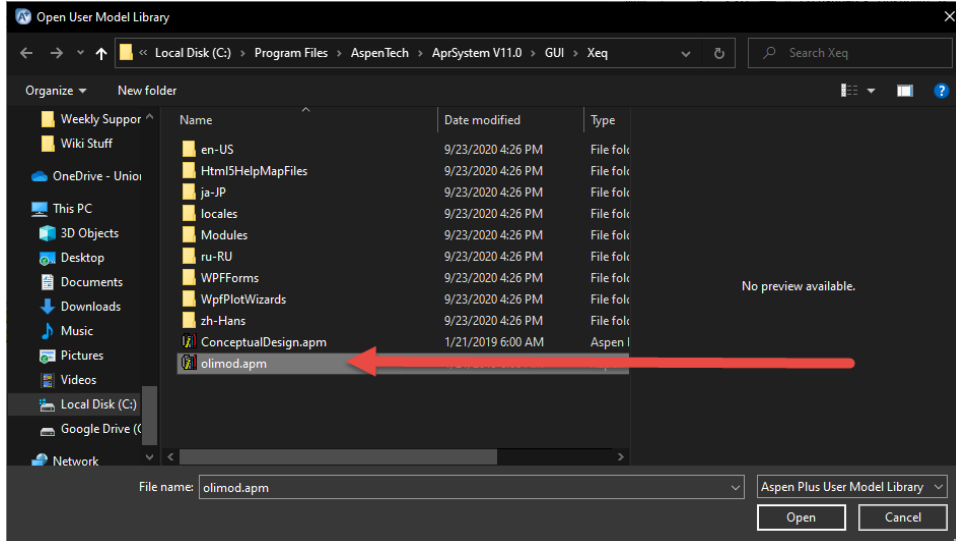
If the OLI library is not available, you will have to import it. Click the **Import...** button

Search for the following folder:

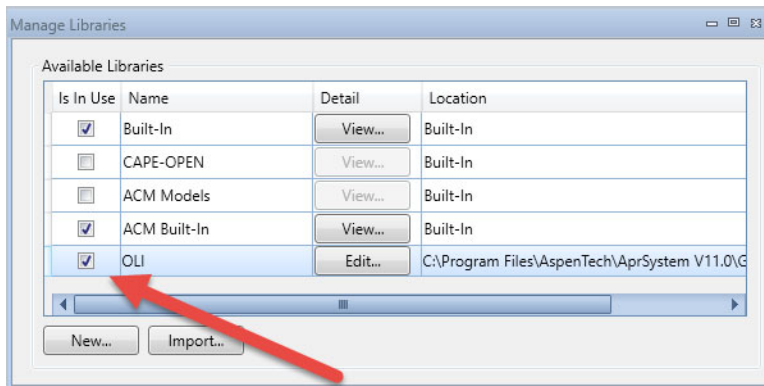
C:\Program Files\AspenTech\AprSystem V11.0\GUI\XeQ

This is for Aspen Plus V11. If you have a different version, search for the appropriate version.

Then select the **olimod.apm** library

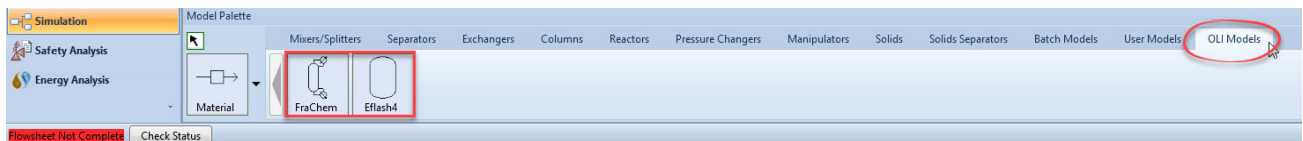


Once added, or if it had been added previously, click the check box to activate the library:



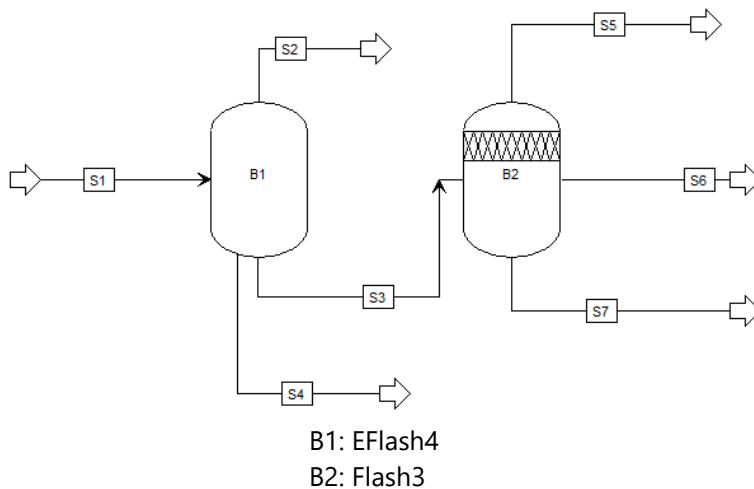
Once loaded, this library will always be available for this version on this computer.

The library has been added to the library tool bar at the bottom of the Aspen PLUS user interface. The icons for the library appear at the left-hand side. The EFLASH and EFRACH (a/k/a FraChem) appear on this library palette.



Like any other icon, we can drag the icon to the work sheet.

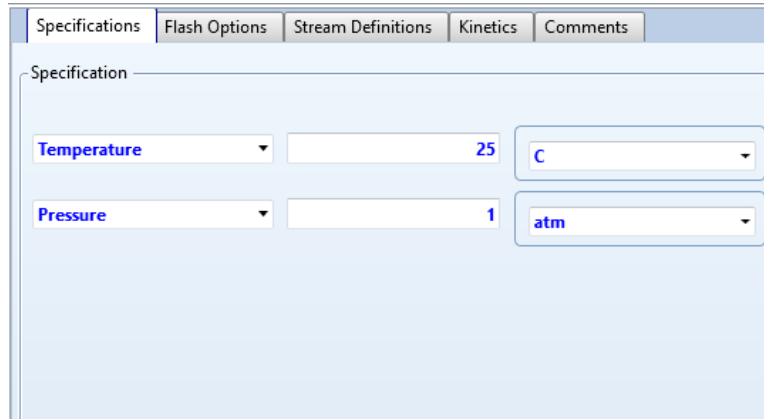
Please create the following worksheet:



Enter the following composition for STREAM 1

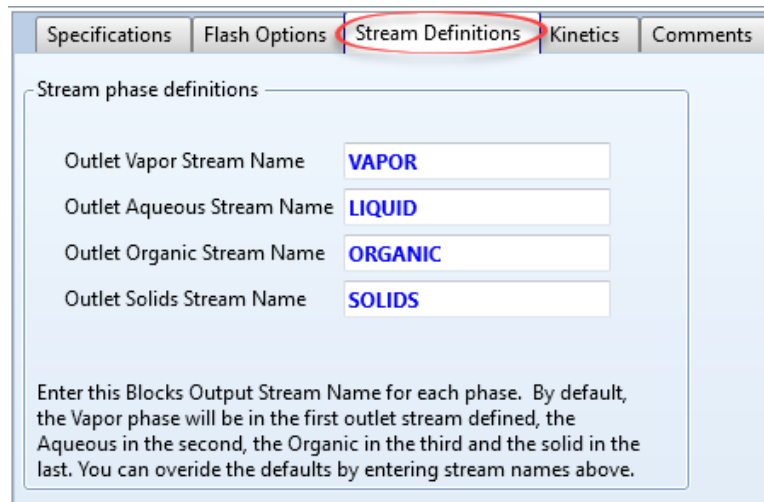
Temperature	25	C
Pressure	1	atm
H2O	100	kmol/hr
C10H22	10	kmol/hr
N2	1	kmol/hr
NaCl	20	kmol/hr

Double-click on block B1. Add the indicated temperature and pressure in the correct units.



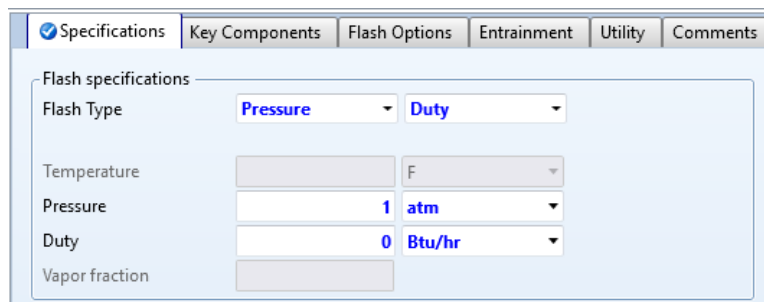
The screenshot shows the 'Specifications' tab of a software interface. It contains two rows of input fields. The first row is for 'Temperature', with a dropdown menu set to 'C', a text box containing '25', and a unit dropdown set to 'C'. The second row is for 'Pressure', with a dropdown menu set to 'atm', a text box containing '1', and a unit dropdown set to 'atm'.

Click on the **Stream Definitions** tab, and fill out the four streams.



The screenshot shows the 'Stream Definitions' tab. It has four text input fields for outlet stream names: 'VAPOR', 'LIQUID', 'ORGANIC', and 'SOLIDS'. Below these fields is a paragraph of text: 'Enter this Blocks Output Stream Name for each phase. By default, the Vapor phase will be in the first outlet stream defined, the Aqueous in the second, the Organic in the third and the solid in the last. You can override the defaults by entering stream names above.'

Close the block and open Block B2. Change the default **Temperature** value to **Pressure and Heat Duty**, 1 atm and 0 Btu/hr. then, close the block.



The screenshot shows the 'Specifications' tab for Block B2. The 'Flash Type' is set to 'Pressure' and 'Duty'. The 'Temperature' field is empty, with a unit dropdown set to 'F'. The 'Pressure' field contains '1' and the unit dropdown is set to 'atm'. The 'Duty' field contains '0' and the unit dropdown is set to 'Btu/hr'. The 'Vapor fraction' field is empty.

Run the simulation.

We have separated the solid phase into STREAM 4, the vapor into STREAM 2 and a mixed stream (aqueous and organic) into STREAM 3. The Mixed Stream is then further separated by phase.

EFLASH Results

	S1	S2	S3	S4	S5	S6	S7
	MIXED	VAPOR	LIQUID	SOLID	MISSING	LIQUID	LIQUID
Substream: MIXED							
Mole Flow lbmol/hr							
H2O	220.4623	0.0530786	220.4092	0	0	7.97E-03	220.4012
C10H22	22.04623	4.00E-03	22.04223	0	0	22.04222	4.80E-07
HCL	1.80E-12	9.96E-13	8.03E-13	0	0	0	0
N2	2.204623	2.162302	0.0423205	0	0	0.0415593	7.61E-04
NACL	0	0	0	0	0	0	0
NAOHW1	0	0	0	0	0	0	0
NAOH	0	0	0	0	0	0	0
NACL-S	19.66807	0	0	19.66807	0	0	0
NAOH-S	0	0	0	0	0	0	0
OH-	1.39E-07	0	1.39E-07	0	0	0	1.39E-07
H+	1.39E-07	0	1.39E-07	0	0	0	1.39E-07
NA+	24.42438	0	24.42438	0	0	0	24.42438
CL-	24.42438	0	24.42438	0	0	0	24.42438
Total Flow lbmol/hr	313.23	2.219382	291.3425	19.66807	0	22.09175	269.2507
Total Flow lb/hr	9747.232	62.09899	8535.672	1149.46	0	3137.614	5398.058
Total Flow cuft/hr	1018.273	869.6067	140.1569	8.509561	0	68.20093	71.95598
Temperature F	77	77	77	77		77	77
Pressure psia	14.69595	14.69595	14.69595	14.69595	14.69595	14.69595	14.69595
Vapor Frac	7.09E-03	1	0	0		0	0
Liquid Frac	0.9301234	0	1	0		1	1
Solid Frac	0.0627911	0	0	1		0	0
Enthalpy Btu/lbmol	-1.20E+05	-2684.868	-1.17E+05	-1.77E+05		-1.29E+05	-1.16E+05
Enthalpy Btu/lb	-3867.461	-95.95564	-4008.032	-3027.367		-908.7212	-5809.502
Enthalpy Btu/hr	-3.77E+07	-5958.748	-3.42E+07	-3.48E+06		-2.85E+06	-3.14E+07
Entropy Btu/lbmol-R	21.65743	45.90025	21.46558	21.76371		101.8803	14.90378
Entropy Btu/lb-R	0.6959674	1.640449	0.7326705	0.3723923		0.7173327	0.7433884
Density lbmol/cuft	0.307609	2.55E-03	2.078688	2.311291		0.3239216	3.741882
Density lb/cuft	9.572315	0.0714104	60.90083	135.0787		46.00545	75.01889
Average MW	31.11845	27.9803	29.29772	58.44297		142.0265	20.04844
Liq Vol 60F cuft/hr		1.882868		11.88138	0	68.63595	
*** LIQUID PHASE ***							
PH	6.945542		6.945544				6.9455

Input Language

BLOCK blockid EFLASH

PARAM keyword=value

Optional keywords: TEMP PRES DUTY VFRAC PH MOLEC PHASE

PARAM Default flash is adiabatic at inlet pressure. The user must specify two of the state variables. The valid combinations are:

TEMP, PRES - Constant TP flash
DUTY, PRES - Adiabatic flash to calculate TEMP
DUTY, TEMP - Adiabatic flash to calculate PRES
VFRAC, PRES - Fixed vapor fraction, calculate TEMP
VFRAC, TEMP - Fixed vapor fraction, calculate PRES
PH, PRES - Fixed pH, calculate TEMP
PH, TEMP - Fixed pH, calculate PRES
TEMP - Temperature
PRES - Pressure, zero or negative indicates pressure drop
VFRAC - Molar vapor fraction
DUTY - Heat duty
PH - pH of the outlet
MOLEC - Default outlet streams are in the true ionic form provided all species names have been defined in the COMPONENTS paragraph. If MOLEC is specified in the PARAM sentence, stream output will be in molecular form (all ions combined to molecular components)
PHASE - No equilibrium calculation, evaluate enthalpy at T,P and Specified phase conditions (V,L,S)
PHASE=V - ALL VAPOR PRODUCT
PHASE=L - ALL LIQUID PRODUCT
PHASE=S - ALL SOLID PRODUCT

EFLASH Examples

Example 1 Flash at a temperature=100 and pressure=14.7. Put vapor product in stream S1, aqueous product in stream S2, organic liquid phase in stream S3 and solid phase in stream S4..

FLWSHEET

BLOCK FLSH IN=FEED1 FEED2 OUT=S1 S2 S3 S4

BLOCK FLSH EFLASH

PARAM TEMP=100 PRES=1

Example 2 Adiabatic flash to calculate temperature. All phases put in stream S1.

FLWSHEET

BLOCK FLSH IN=FEED1 FEED2 OUT=S1

BLOCK FLSH EFLASH

PARAM DUTY=0. PRES=0

Example 3 Flash to a vapor fraction=.2 at the inlet pressure. Put vapor phase in stream S1, aqueous and organic in stream S2 and solid in S3.

FLWSHEET

BLOCK FLSH IN=FEED1 FEED2 OUT=S1 S2 S3

BLOCK FLSH EFLASH

PARAM VFRAC=.2 PRES=0.

Example 4 All vapor stream at 300 F and 14.7 psia

FLWSHEET

BLOCK FLSH IN=FEED1 OUT=S1

BLOCK FLSH EFLASH

PARAM TEMP=300 PRES=14.7 PHASE=V

NOTE: There is no equilibrium calculation in this block. The outlet is assumed to be vapor at this condition and the enthalpy is evaluated at the specified temp and pres.

EFRACH (Electrolyte Distillation, Frachem)

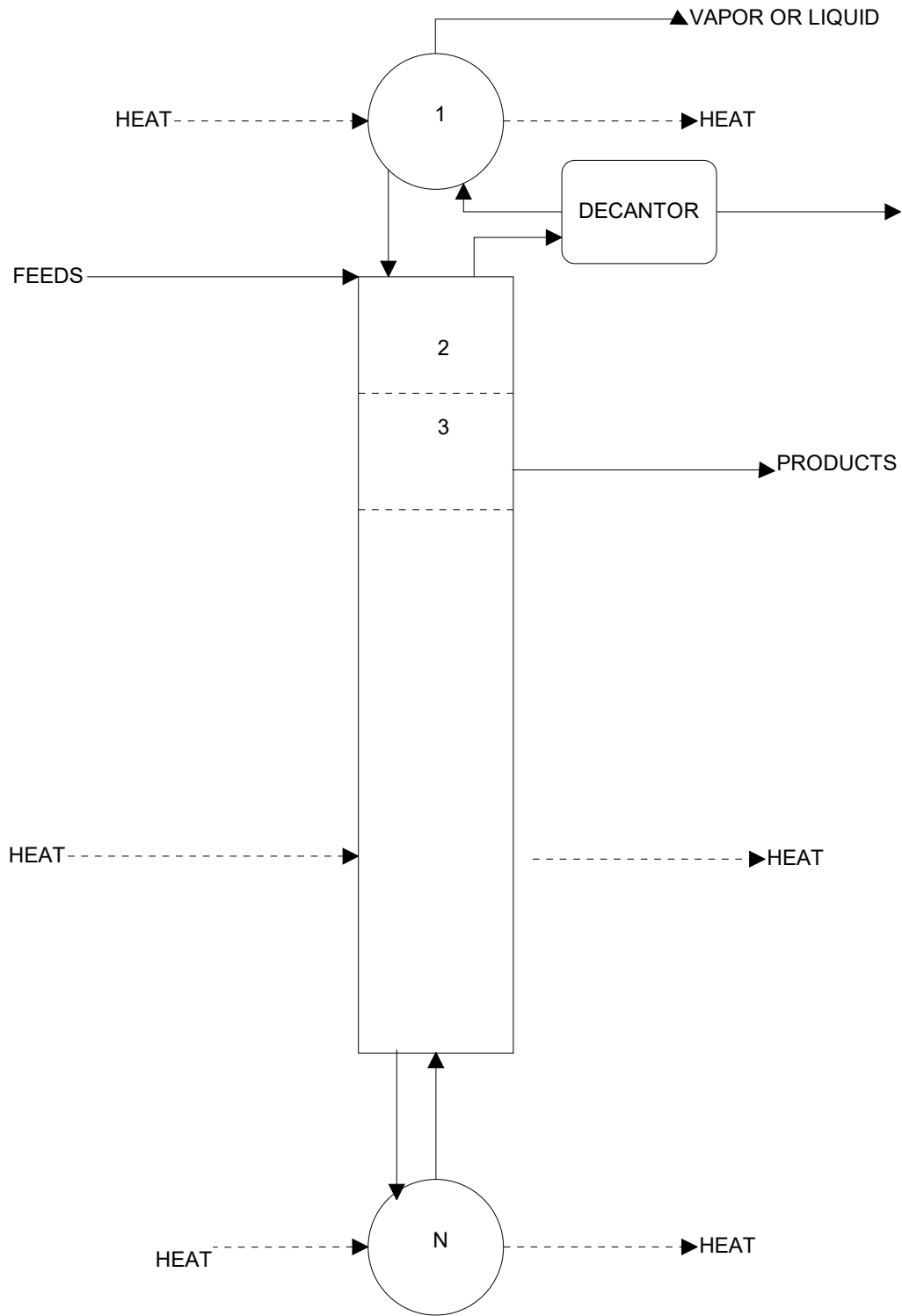
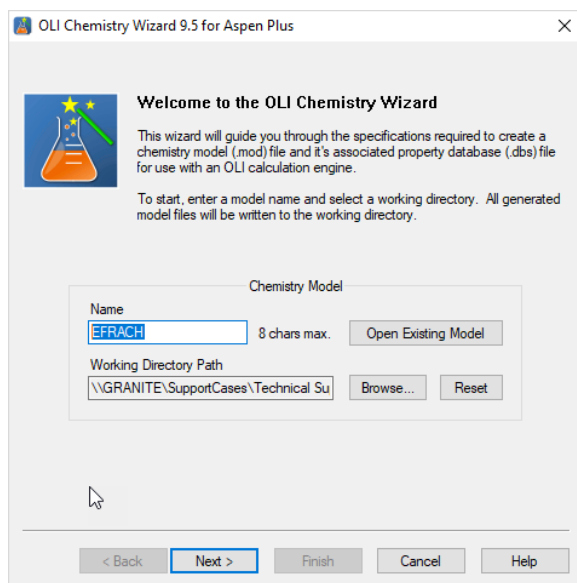


Figure 4-2 EFRACH diagram

Example: Chlorine Scrubber

Using the OLI Chemistry Wizard, create a chemistry model with the following components for the FRACHEM unit operation: H₂O, CO₂, CL₂, N₂, NaOH. We recommend the name EFRACH. Don't enable Redox reactions and turn off all the solids in this model.

Note: This is the same chemistry as the one used in Chapter 3, called CLORINE.



Follow the same steps, as shown in the EFlash example above to create the *.bkg file.

Open the newly created *.bkg file in Aspen Plus. Remember to go to **Customize** Tab > **Manage Library** and enable OLI.

Create the following flowsheet using the FraChem block.

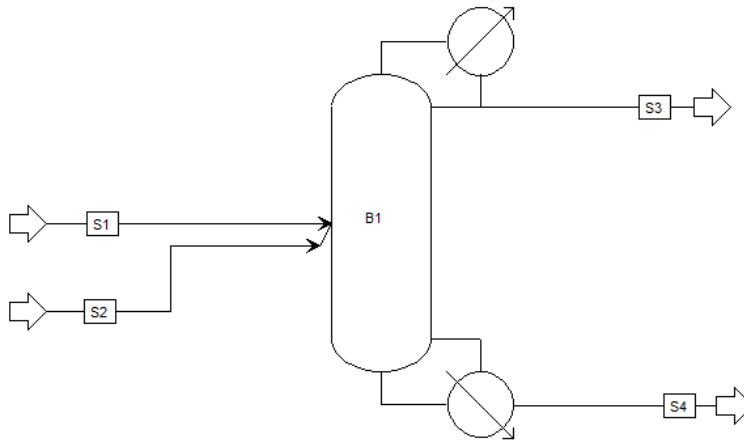


Figure 4-3 FraChem Diagram

Enter the compositions for Streams 1 and 2.
The composition for Stream 1 is shown below:

Main Flowsheet x S1 (MATERIAL) x +

Mixed CI Solid NC Solid Flash Options EO Options Costing Comments

Specifications

Flash Type: Temperature Pressure

State variables

Temperature: 25 C

Pressure: 1 atm

Vapor fraction: []

Total flow basis: Mole

Total flow rate: [] lbmol/hr

Solvent: []

Reference Temperature

Volume flow reference temperature: [] F

Component concentration reference temperature: [] F

Composition

Mole-Flow lbmol/hr

Component	Value
H2O	48.8
CO2	
CL2	
HCLO	
HCL	
N2	
NAHCO3	
NAOH	2.57
H2CO3IN	
NA2CO3	
NA2O	
NA3HCO32	
NA5H3C34	
NACL	
NACLOIN	
TRONA	
WEGSCH	
OH-	
CLO-	
...	
Total	51.37

Composition for Stream 2:

Main Flowsheet | S1 (MATERIAL) | S2 (MATERIAL) | +

Mixed | CI Solid | NC Solid | Flash Options | EO Options | Costing | Comments

Specifications

Flash Type: Temperature Pressure

State variables

Temperature: 33 C

Pressure: 1.01 atm

Vapor fraction: []

Total flow basis: Mole

Total flow rate: [] lbmol/hr

Solvent: []

Reference Temperature

Volume flow reference temperature: [] F

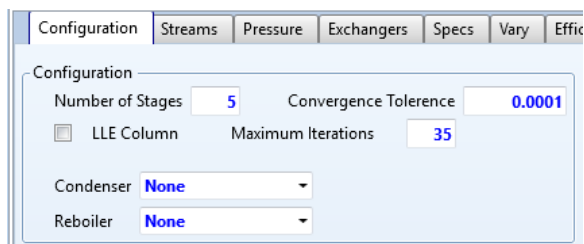
Component concentration reference temperature: [] F

Composition

Mole-Flow lbmol/hr

Component	Value
H2O	2.27
CO2	23.59
CL2	2.27
HClO	
HCL	
N2	26.3
NAHCO3	
NAOH	
H2CO3IN	
NA2CO3	
NA2O	
NA3HCO32	
NA5H3C34	
NACL	
NACLOIN	
TRONA	
WEGSCH	
OH-	
CLO-	
CO3-	
Total	54.43

Now we need to define the EFRACH (FraChem) block. Double click the block. There are 5 stages without a condenser or reboiler. We will be using the default tolerances and iterations. Please update the **Configuration** tab to look as follows:



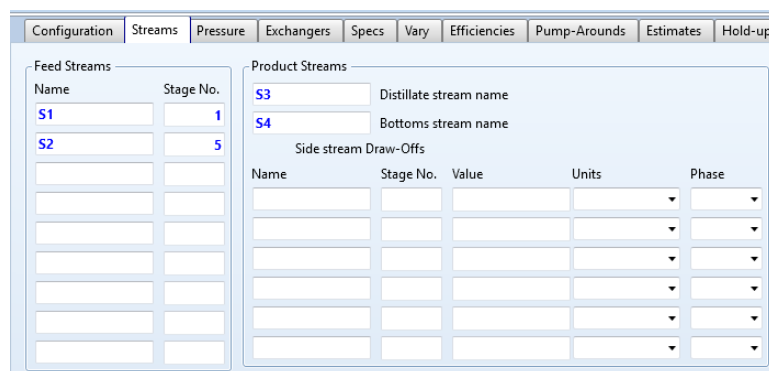
Now click on the **Streams** tab

A note to OLI/ESP users, although this is an OLI block we have adopted Aspen PLUS's convention that the top stage is number 1⁶. Stream 1 is the caustic stream and is a liquid stream. Liquid streams should enter above the vapor streams. In our case it will enter on Stage 1.

Stream 2 is the vapor stream containing the chlorine gas. Vapor streams should enter below liquid streams. We will have Stream 2 enter on the bottom stage 5.

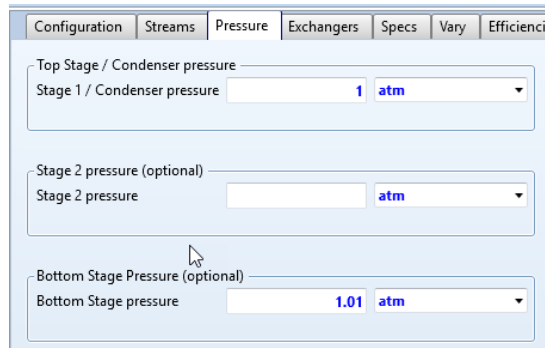
The vapor distillate stream is Stream 3 and the liquid bottoms are Stream 4. We are not using any side draws for this example.

Please update the **Streams** tab to match the image below.



Click on the **Pressure** tab. There is a small pressure drop across the column. Please enter the top and bottom stage pressures.

⁶ In ESP, the bottom stage is stage 1, just the opposite of Aspen PLUS.

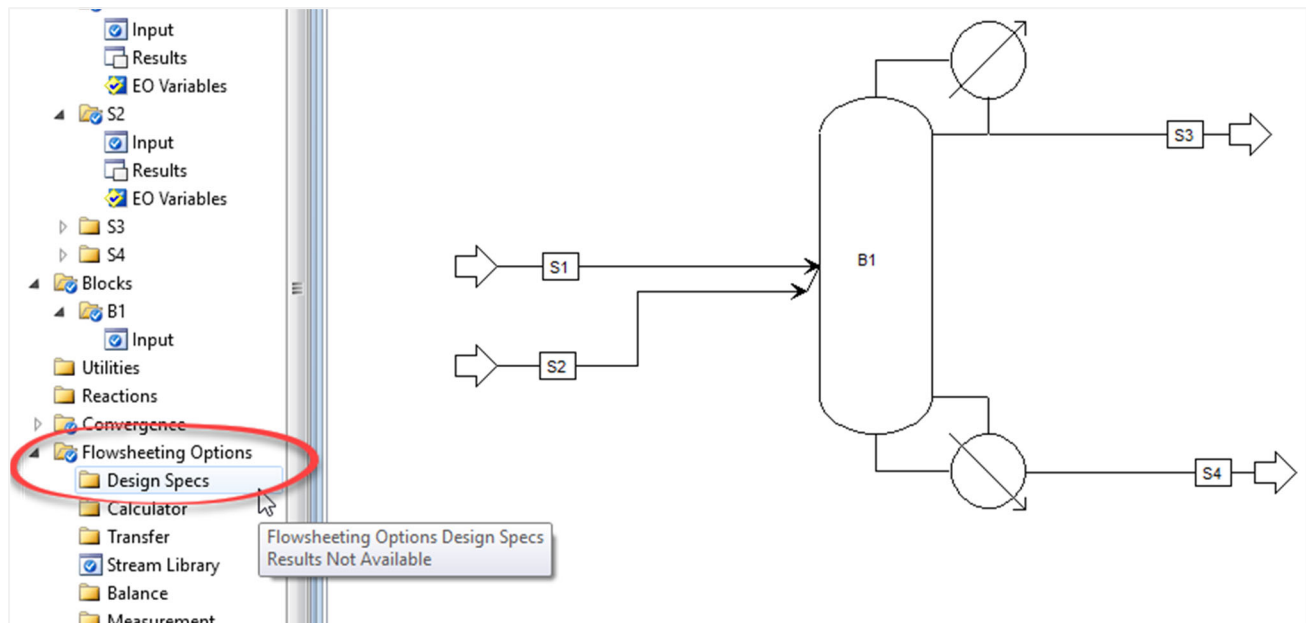


There are no exchangers or internal specifications for this unit.

Design Spec...

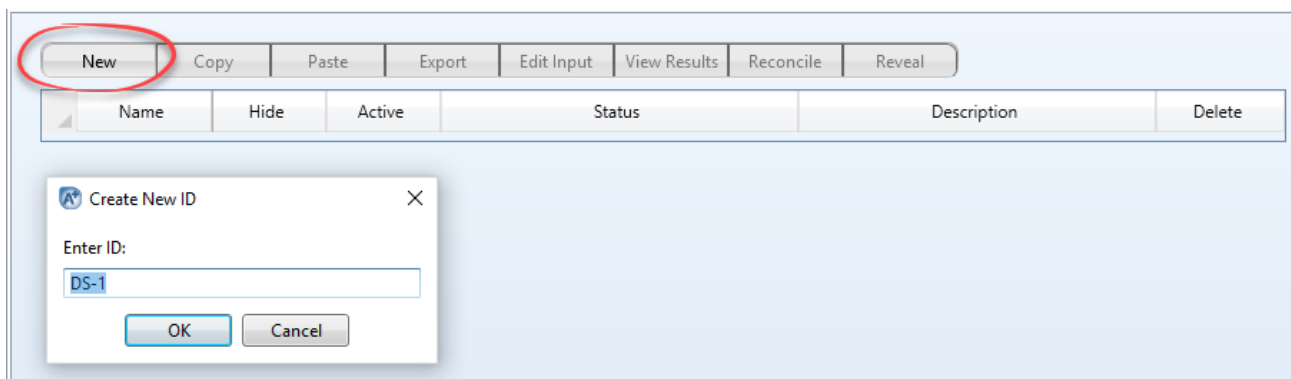
As with the example in Chapter 3, there is a design specification for this case. We will repeat the design specification here.

Start by adding the design specification. In the left hand tree look for **Flowsheeting Options**, and then click on **Design Specs**.



The image below is displayed. Click the **New...** button.

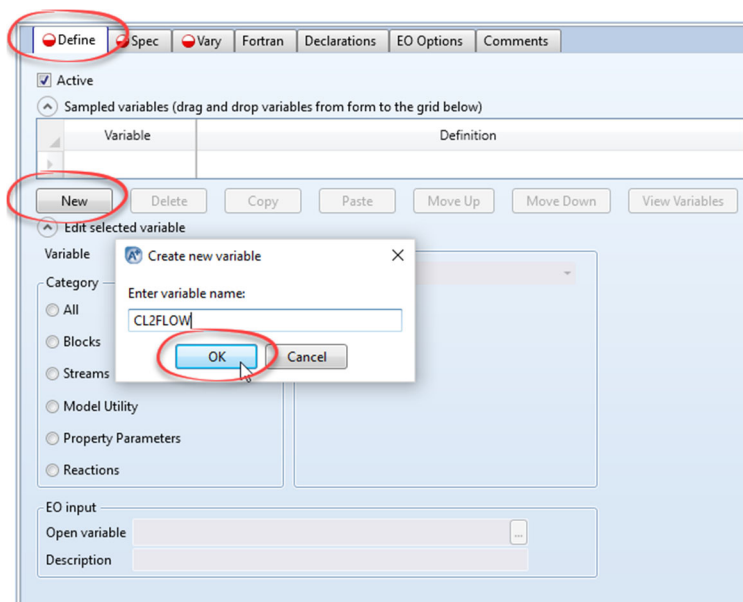
We will accept the default name DS-1. Click the **OK** button.



A new window is open.

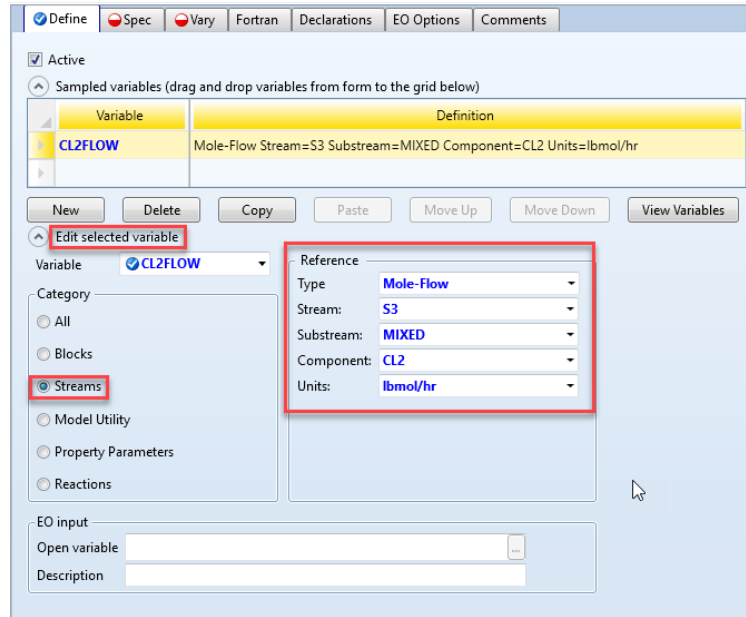
Now, we need to **Define** the variable for the specification.

We are defining the variable CL2FLOW. This will be the specified variable of 0.5 lbmol/hr of Chlorine in the distillate flow.

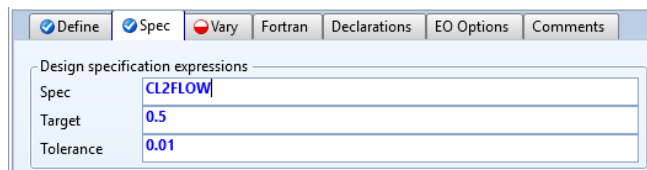


Now go to the **Edit Selected Variable section**. The variable is part of the stream. The type is **Mole-Flow** and we are referring to Stream 3. The component is CL2.

Update this dialog as shown.



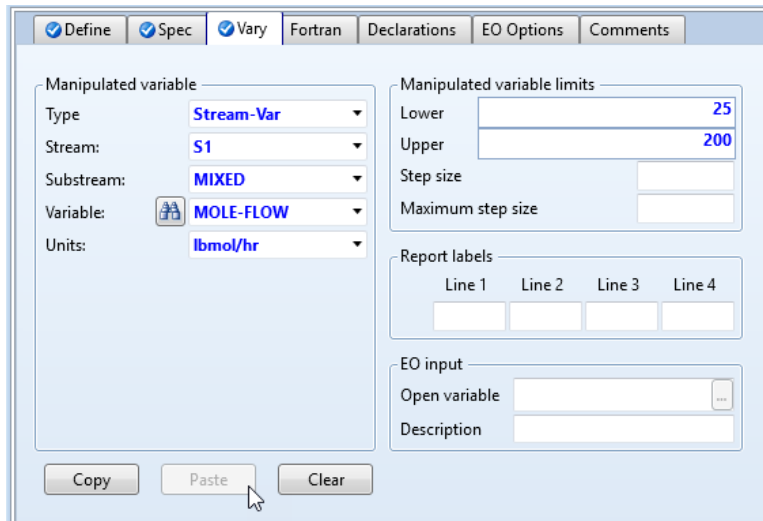
Next click the **Spec** tab. The spec variable is CL2FLOW at a value of 0.5 (in lbmol/hr). We will allow the variable to be between 0.49 and 0.51 lbmol/hr.



Next click on the **Vary** tab.

In here we will adjust the liquid stream flow rate to match the specification. The variable type is **StreamVar** for Stream 1. We are adjusting the **MOLE-FLOW** of the stream. We need to set some reasonable bounds for the varied variable. In this case we will not let the stream flow rate go below 25 lbmole/hr or more than 200 lbmole/hr.

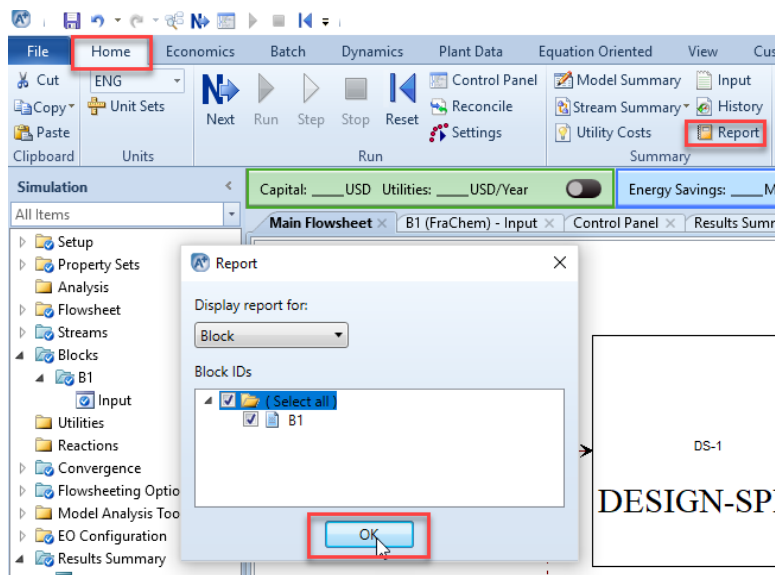
Please update the dialog as shown below.



We are now ready to run the calculation. Please run the simulation.

EFRACH Results

You can review the results as normal except that there is not block report for an OLI block. The data is available however. You need to create a report. Go to **Home** tab, **Report**, Select the Block **B1** and Click **OK**.



This will display the block report directly from the OLI solver. Unfortunately, unit conversion is not possible in this text file.

BLOCK: B1 MODEL: USER2

INLET STREAMS: S1 S2
 OUTLET STREAMS: S3 S4
 FIRST PROPERTY SPECS
 PROPERTY OPTION SET: OLI
 CHEMISTRY ID: EFRACH - TRUE SPECIES
 SECOND PROPERTY SPECS
 PROPERTY OPTION SET: OLI
 CHEMISTRY ID: EFRACH - TRUE SPECIES

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	101.270	101.168	0.100737E-02
MASS(LB/HR)	2829.48	2829.48	-0.284499E-07
ENTHALPY(BTU/HR)	-0.988040E+07	-0.988045E+07	0.522327E-05

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	1038.19	LB/HR
PRODUCT STREAMS CO2E	1034.85	LB/HR
NET STREAMS CO2E PRODUCTION	-3.34052	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	-3.34052	LB/HR

Column Profile

Stage	Temperature F	Liquid Rate LBMOL/HR	Vapor Rate LBMOL/HR
1	109.53477	46.84241	54.76289
2	96.14059	46.64215	54.92256
3	91.08846	46.50228	54.66516
4	89.13355	46.44296	54.52868
5	88.53795	46.40463	54.47251

Aqueous Composition (mole fractions)

Stage	H2O	CO2	CL2	HCLO	HCL
1	0.88978	8.821431E-05	2.627191E-06	1.556907E-02	2.025672E-15
2	0.88043	1.010818E-04	1.238996E-05	2.428213E-02	3.022983E-15
3	0.87918	1.073444E-04	1.545304E-05	2.527008E-02	2.765462E-15
4	0.87909	1.103697E-04	1.635401E-05	2.525866E-02	2.637146E-15
5	0.88101	1.122432E-04	1.678233E-05	2.323816E-02	2.871383E-15

Aqueous Composition (mole fractions)

Stage	N2	NAOH	H2CO3	NA2CO3	NA2O
1	2.277042E-06	0.0	0.0	0.0	0.0
2	2.399740E-06	0.0	0.0	0.0	0.0
3	2.485220E-06	0.0	0.0	0.0	0.0
4	2.528510E-06	0.0	0.0	0.0	0.0
5	2.560856E-06	0.0	0.0	0.0	0.0

Aqueous Composition (mole fractions)

Stage	NA3HCO32	NA5H3CO34	NACL	NACLO	NAHCO3
1	0.0	0.0	0.0	0.0	7.093167E-04
2	0.0	0.0	0.0	0.0	5.133475E-04
3	0.0	0.0	0.0	0.0	5.547109E-04
4	0.0	0.0	0.0	0.0	5.812645E-04
5	0.0	0.0	0.0	0.0	5.613581E-04

Aqueous Composition (mole fractions)

Stage	TRONA	WEGSCHEIDER	OH-1	CLO-1	CO3-2
1	0.0	0.0	5.939414E-09	1.493619E-02	1.109771E-05
2	0.0	0.0	1.687639E-09	1.082434E-02	2.720043E-06
3	0.0	0.0	1.273216E-09	1.019529E-02	2.370144E-06
4	0.0	0.0	1.156253E-09	9.919940E-03	2.312654E-06
5	0.0	0.0	1.064736E-09	8.513549E-03	2.055105E-06

Aqueous Composition (mole fractions)

Stage	HCO3-1	H+1	NACO3-1	NA+1	CL-1
1	1.906723E-03	1.911661E-09	5.453994E-06	4.692785E-02	3.005728E-02
2	1.104030E-03	3.216044E-09	1.654501E-06	4.733217E-02	3.539670E-02
3	1.101185E-03	3.324143E-09	1.558991E-06	4.743482E-02	3.613205E-02
4	1.118766E-03	3.322609E-09	1.567946E-06	4.746955E-02	3.642466E-02
5	1.070891E-03	3.385240E-09	1.405945E-06	4.752931E-02	3.793936E-02

Vapor Composition (mole fractions)

Stage	H2O	CO2	CL2	HCLO	HCL
1	7.593340E-02	0.42928	9.288394E-03	5.243251E-03	4.372068E-13
2	5.027767E-02	0.43036	3.489892E-02	5.610078E-03	5.257991E-13
3	4.284472E-02	0.43152	3.951723E-02	5.004990E-03	4.402945E-13
4	4.019696E-02	0.43264	4.015503E-02	4.697222E-03	4.046567E-13
5	3.945139E-02	0.43312	4.040731E-02	4.208825E-03	4.325753E-13

Vapor Composition (mole fractions)

Stage	N2	NAOH	H2CO3	NA2CO3	NA2O
1	0.48025	0.0	0.0	0.0	0.0
2	0.47886	0.0	0.0	0.0	0.0
3	0.48111	0.0	0.0	0.0	0.0
4	0.48231	0.0	0.0	0.0	0.0
5	0.48281	0.0	0.0	0.0	0.0

Vapor Composition (mole fractions)

Stage	NA3HCO32	NA5H3CO34	NACL	NACLO	NAHCO3
1	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.0

Vapor Composition (mole fractions)

Stage	TRONA	WEGSCHEIDER
1	0.0	0.0
2	0.0	0.0
3	0.0	0.0
4	0.0	0.0
5	0.0	0.0