

OLI SYSTEMS, INC.

A Guide to Using the OLI Engine in Aspen Plus

Featuring Aspen Plus V14.5

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How to use the OLI Engine in Aspen PLUS.

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Disclaimer:

This manual was produced using the **OLI Engine 12.5.23 in Aspen Plus (version 14.5)**. 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

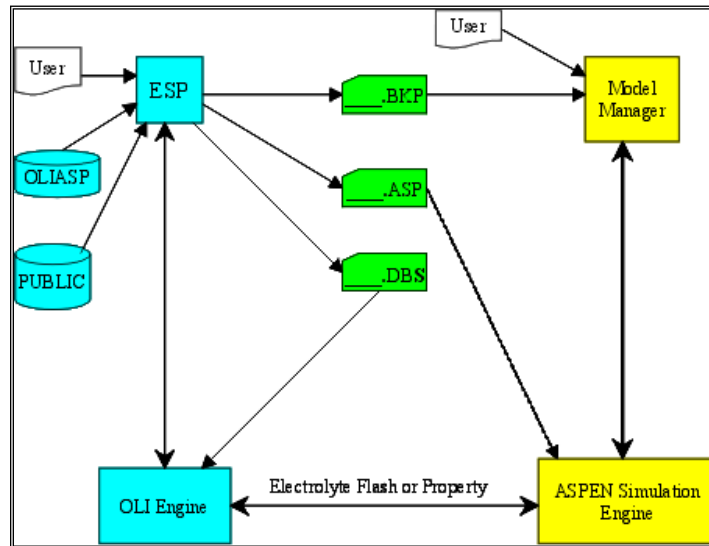


Figure 1-1 The layout of the Aspen OLI Interface

Aspen OLI Unit Operations

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

Aspen Property Set

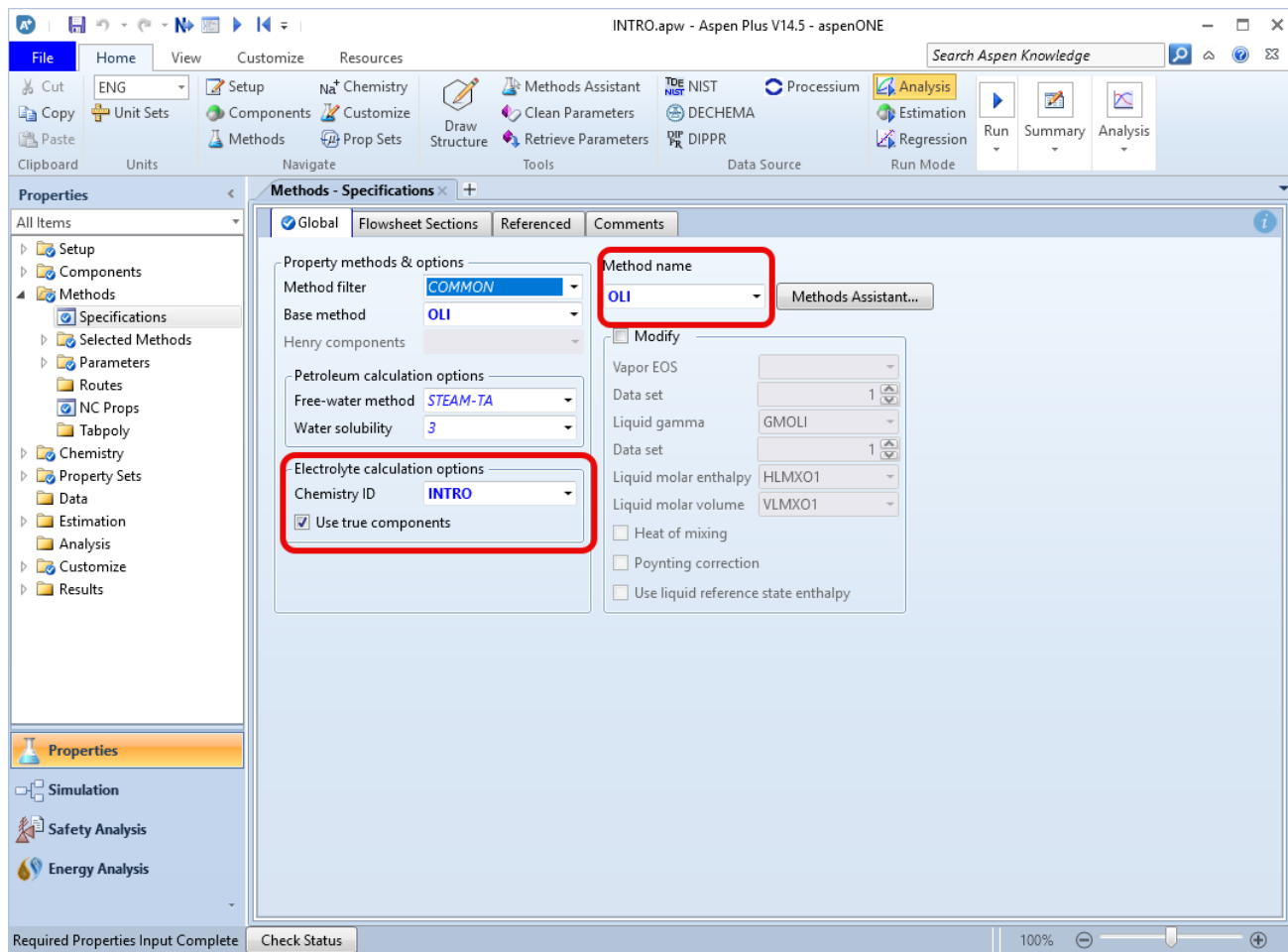


Figure 1-2 OLI Property Set, the boxed areas show that OLI is enabled.

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	PHIOLI	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:

```
FLWSHEET
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)

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

¹ This is also known as EFRACH

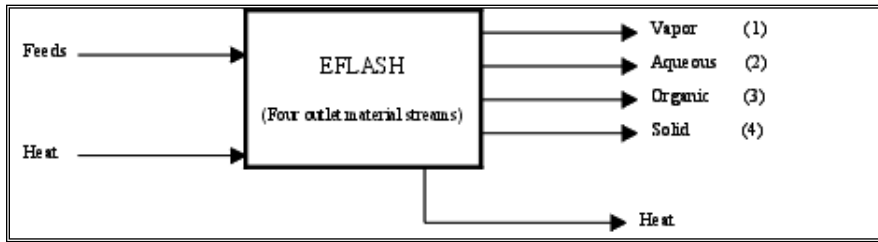


Figure 1-3 EFLASH unit operation

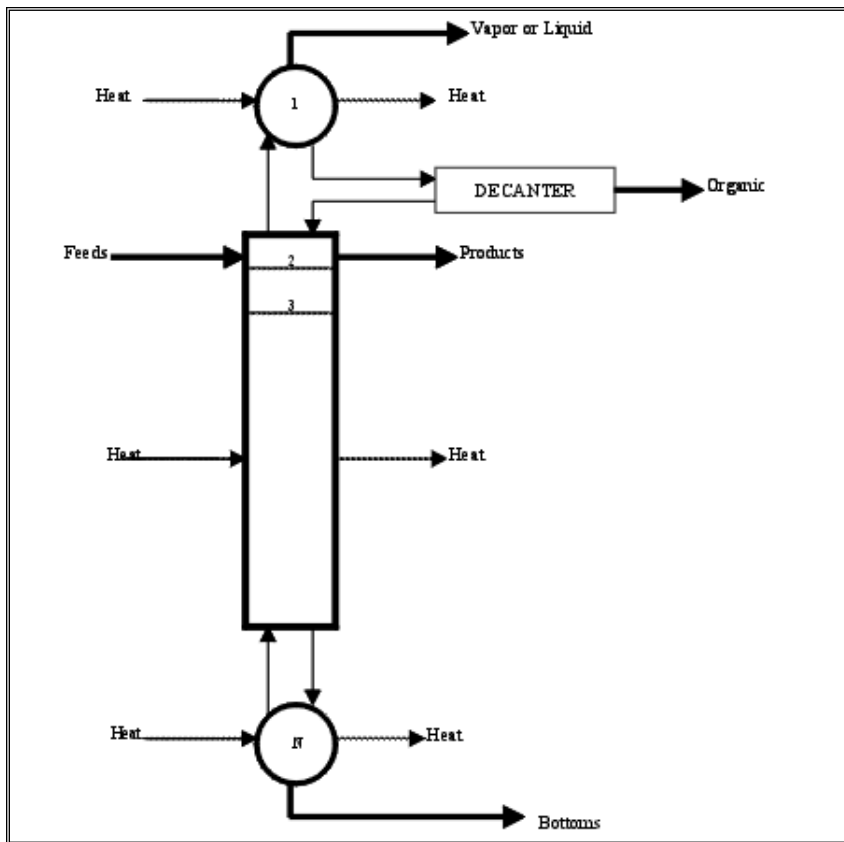


Figure 1-4 EFRACH Block

Chapter 2 ASPEN Neutralization Flowsheet

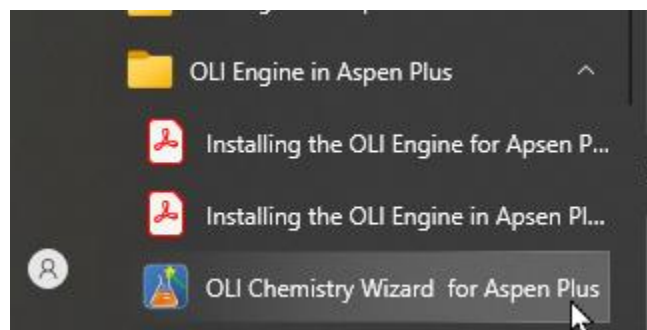
A Tour of the OLI-ASPEN Interface

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 for Aspen Plus**. 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.

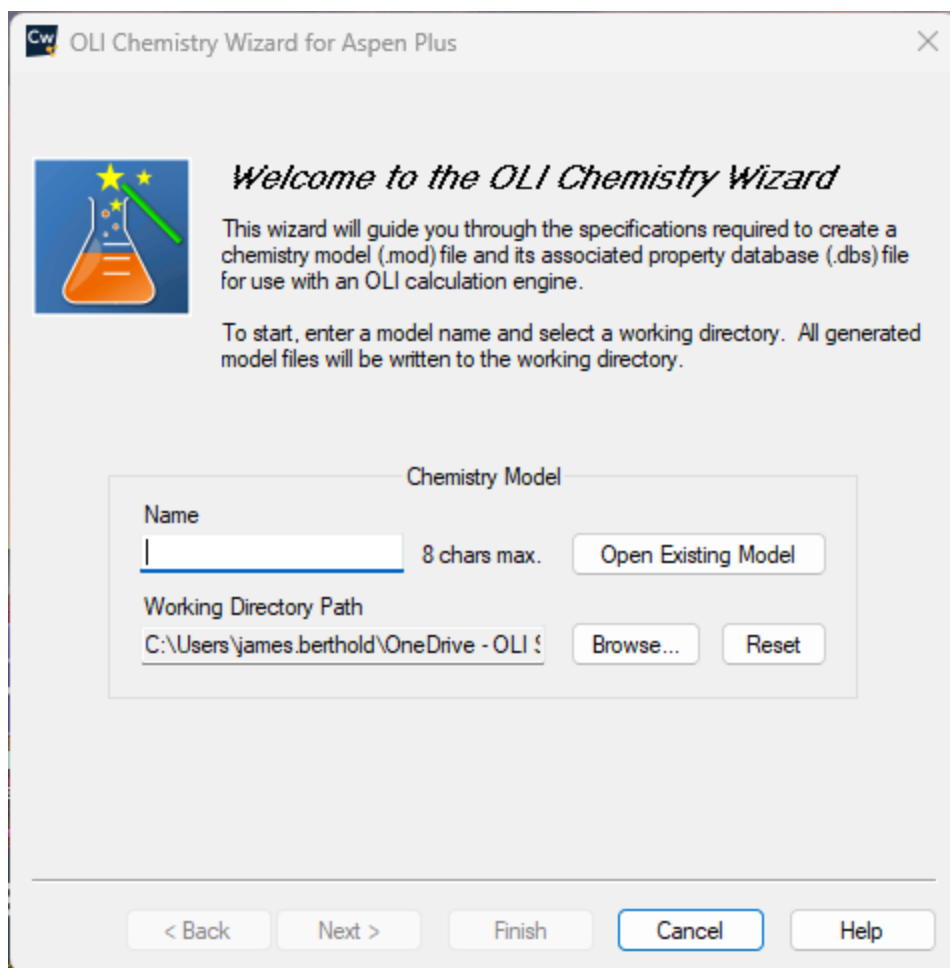
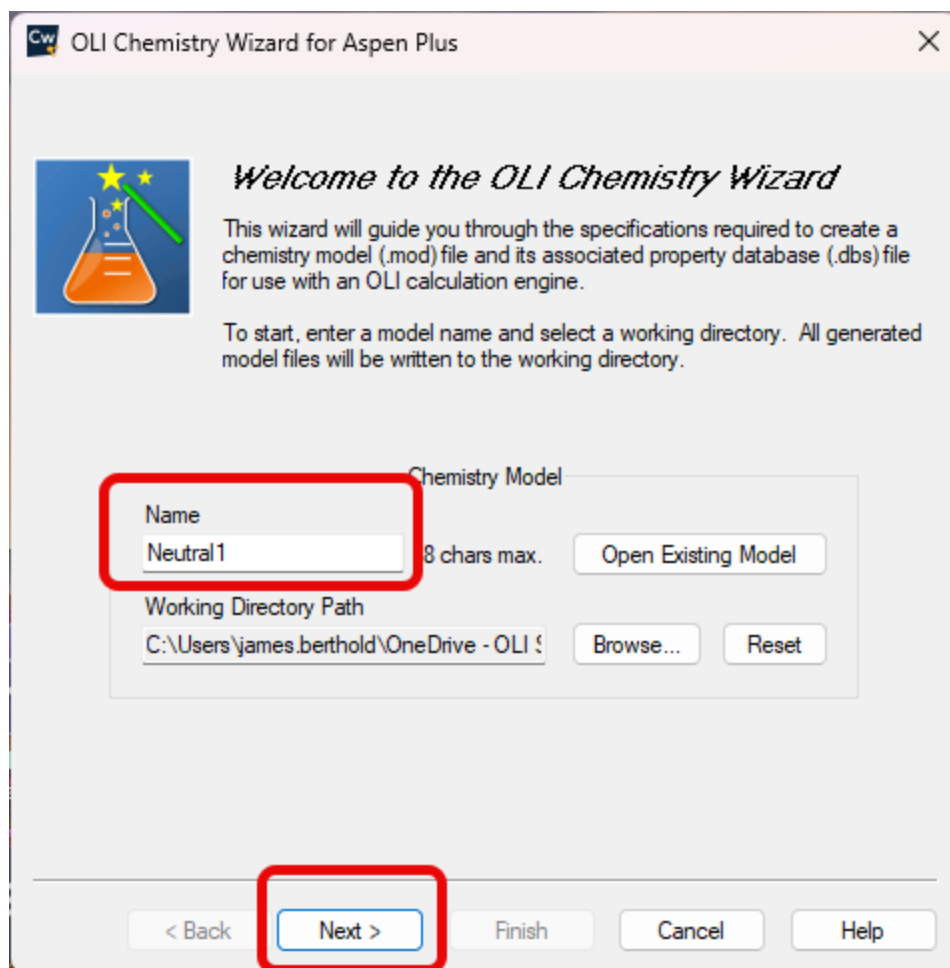
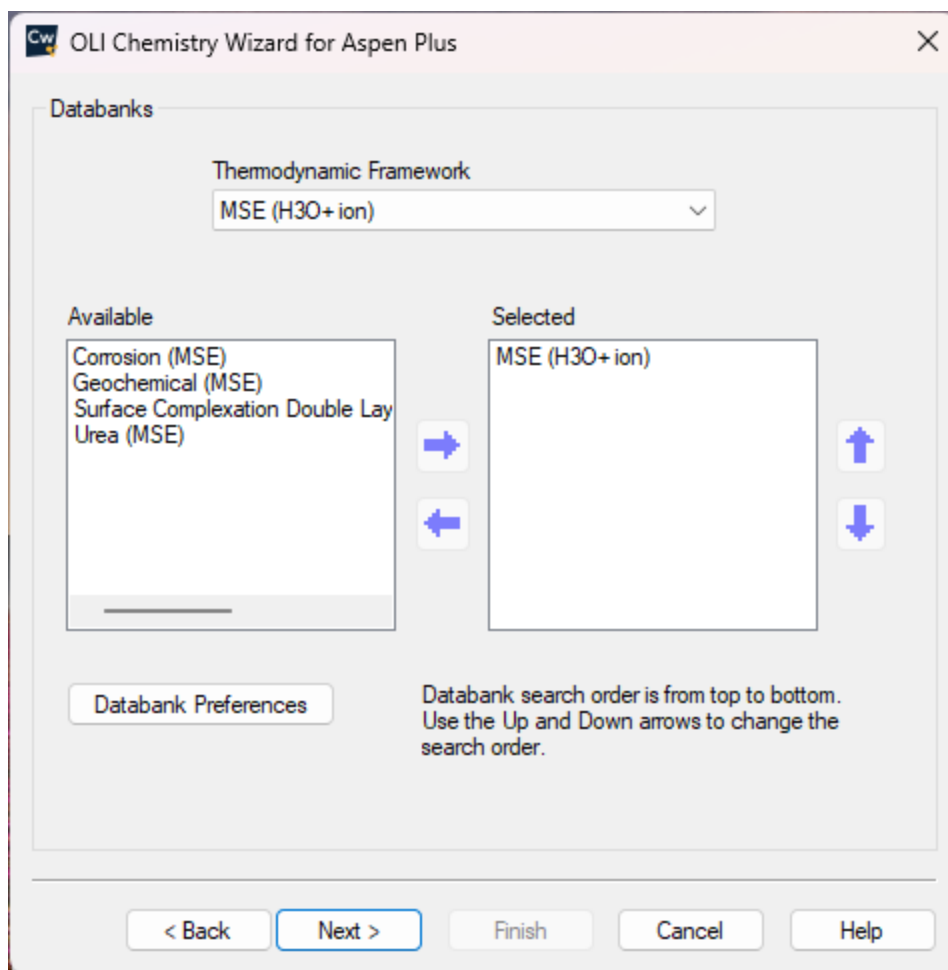


Figure 2-1 Specifying the model name and location



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 are 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

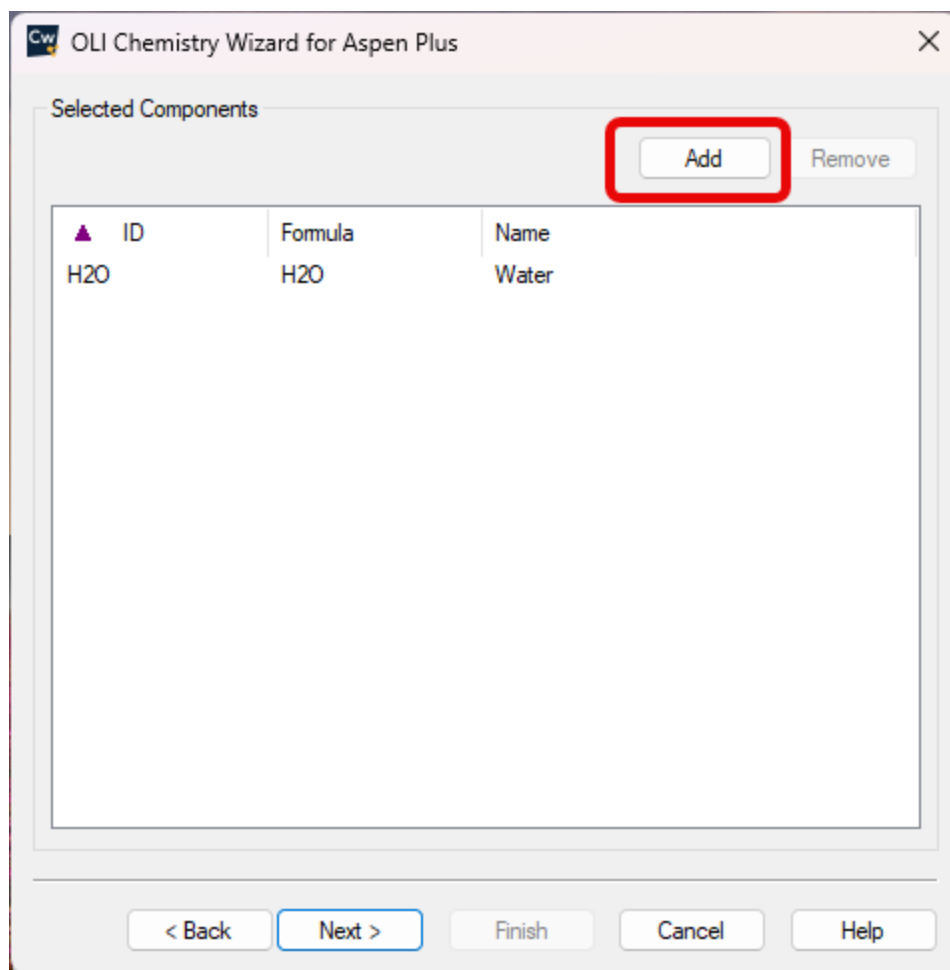


Figure 2-2 Adding components

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

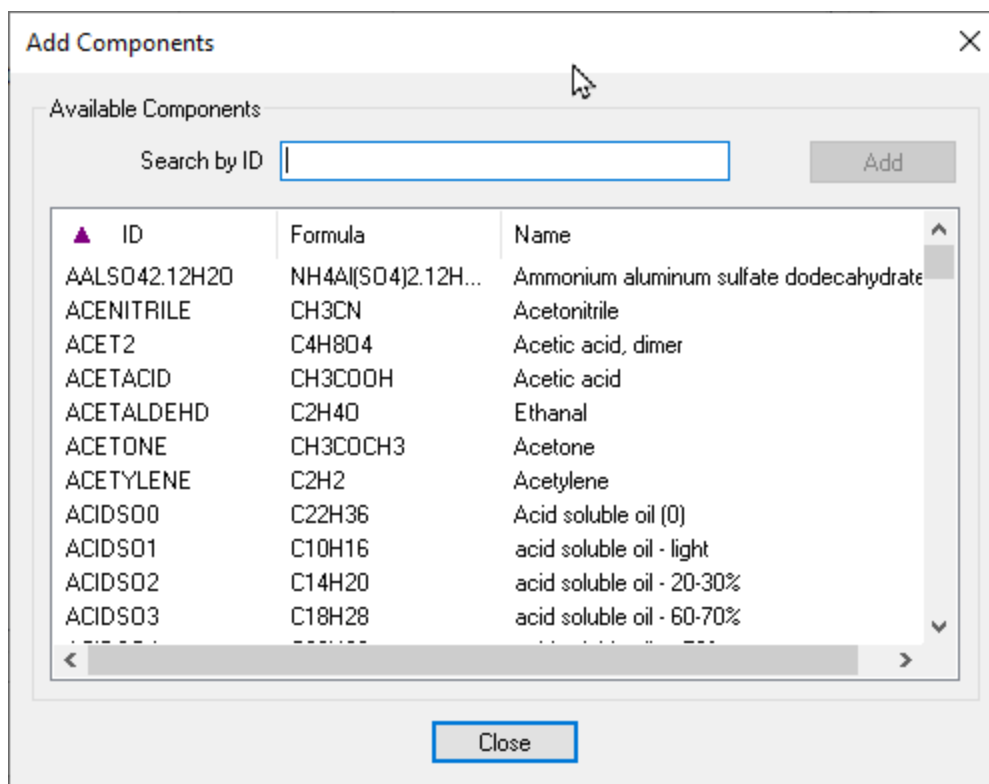


Figure 2-3 Select Components

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

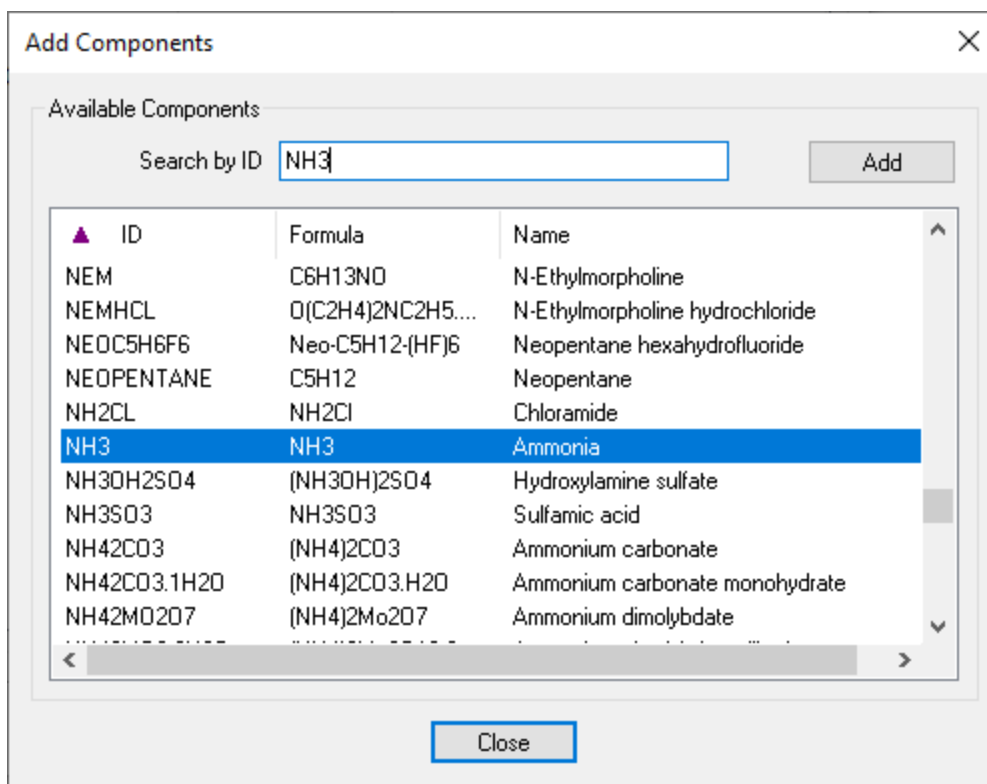


Figure 2-4 Adding NH3, ammonia

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.

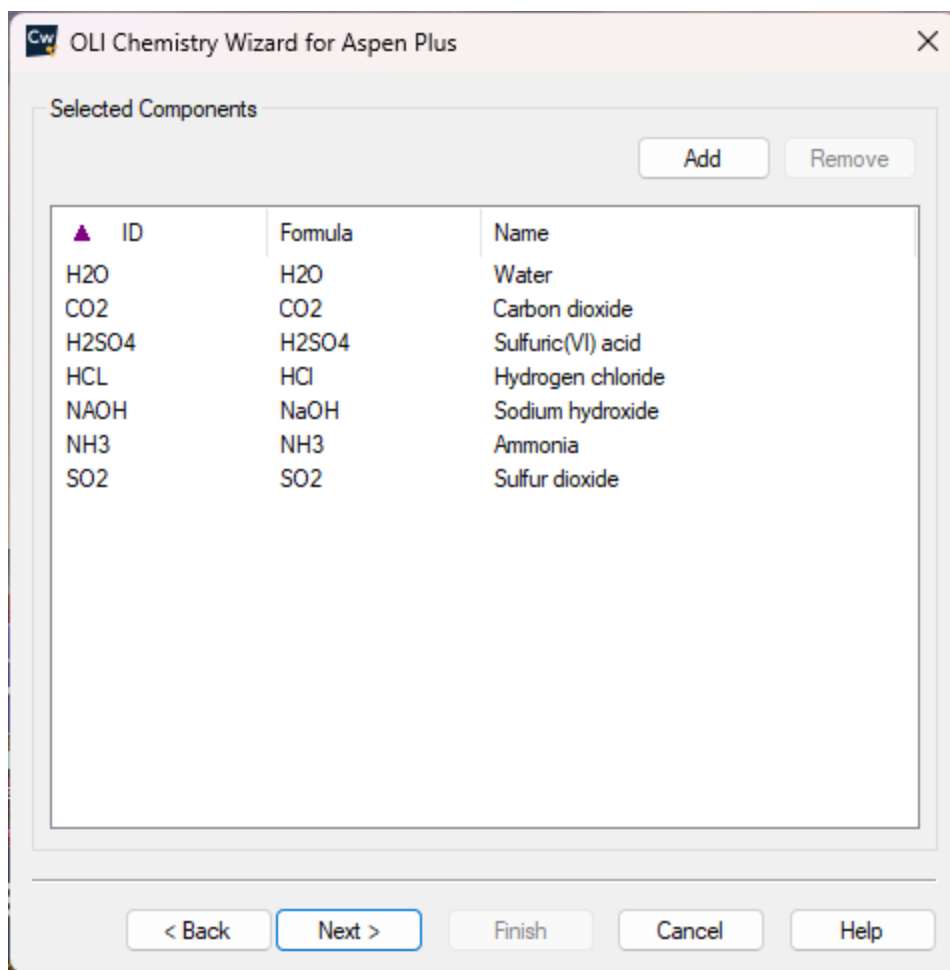


Figure 2-5 the added components

Click the **Next>** button.

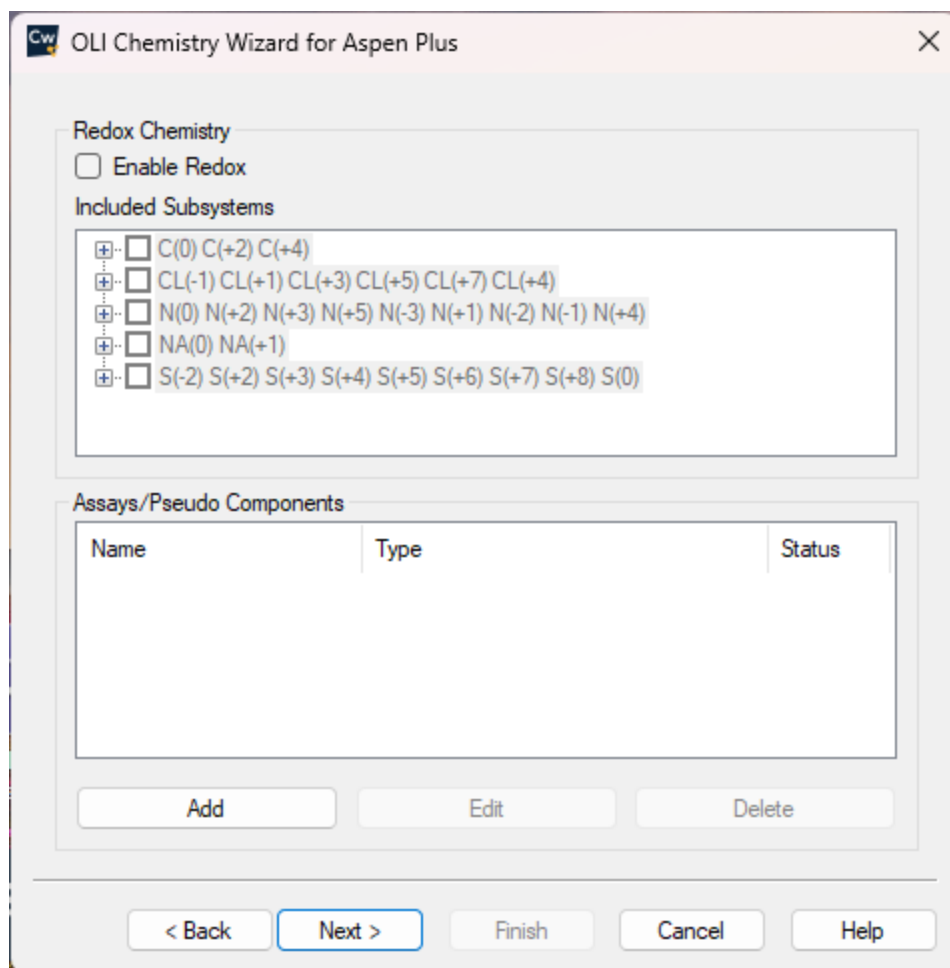


Figure 2-6 adding redox

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

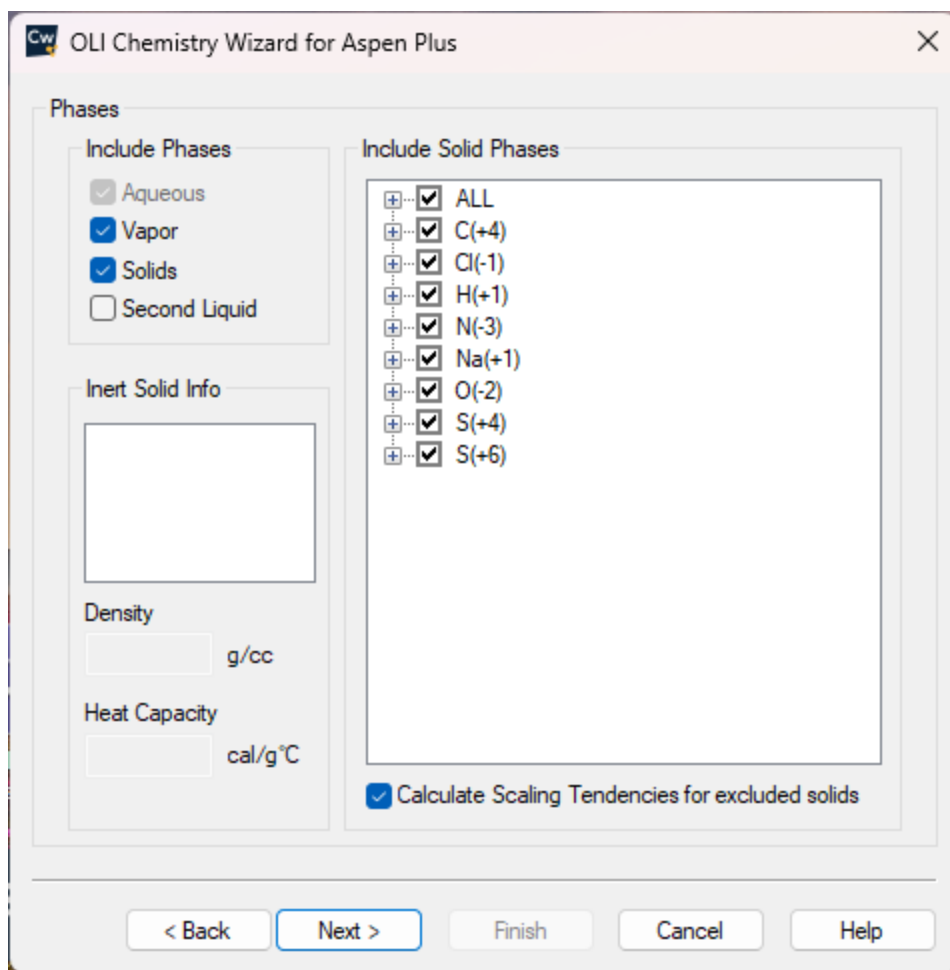


Figure 2-7 Selecting phases, including solids

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.

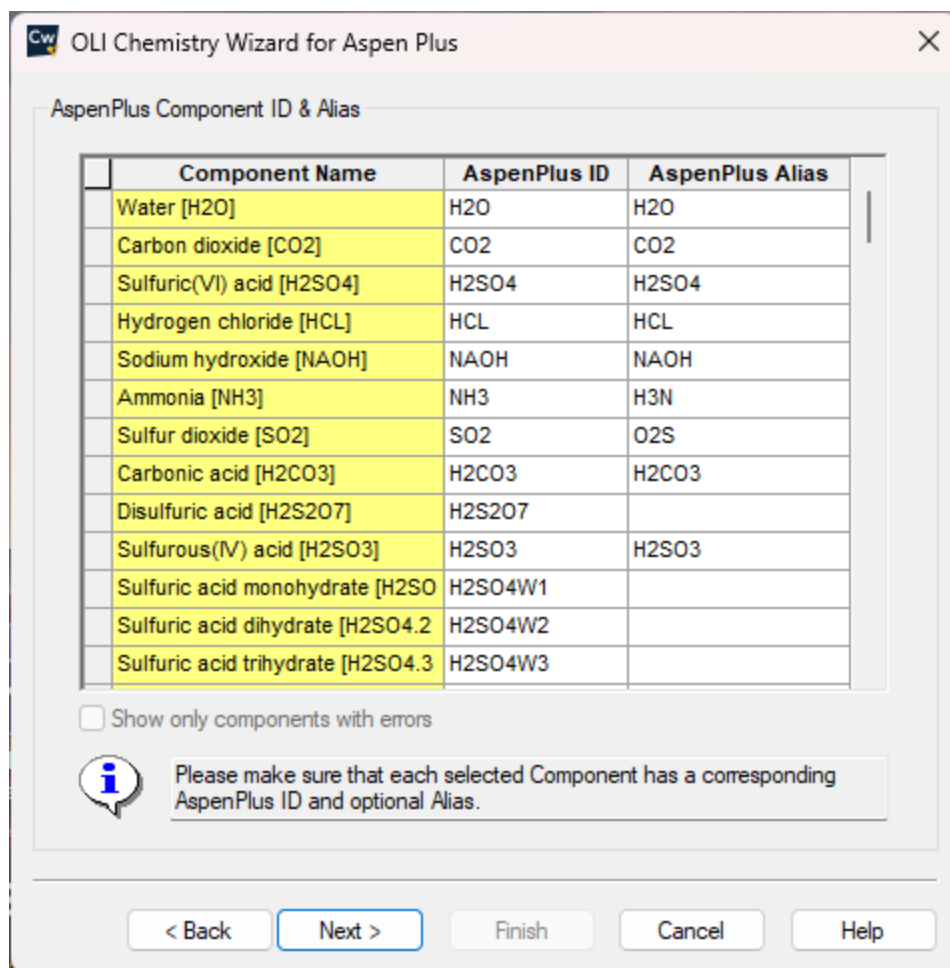


Figure 2-8 Aspen Alias names

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.

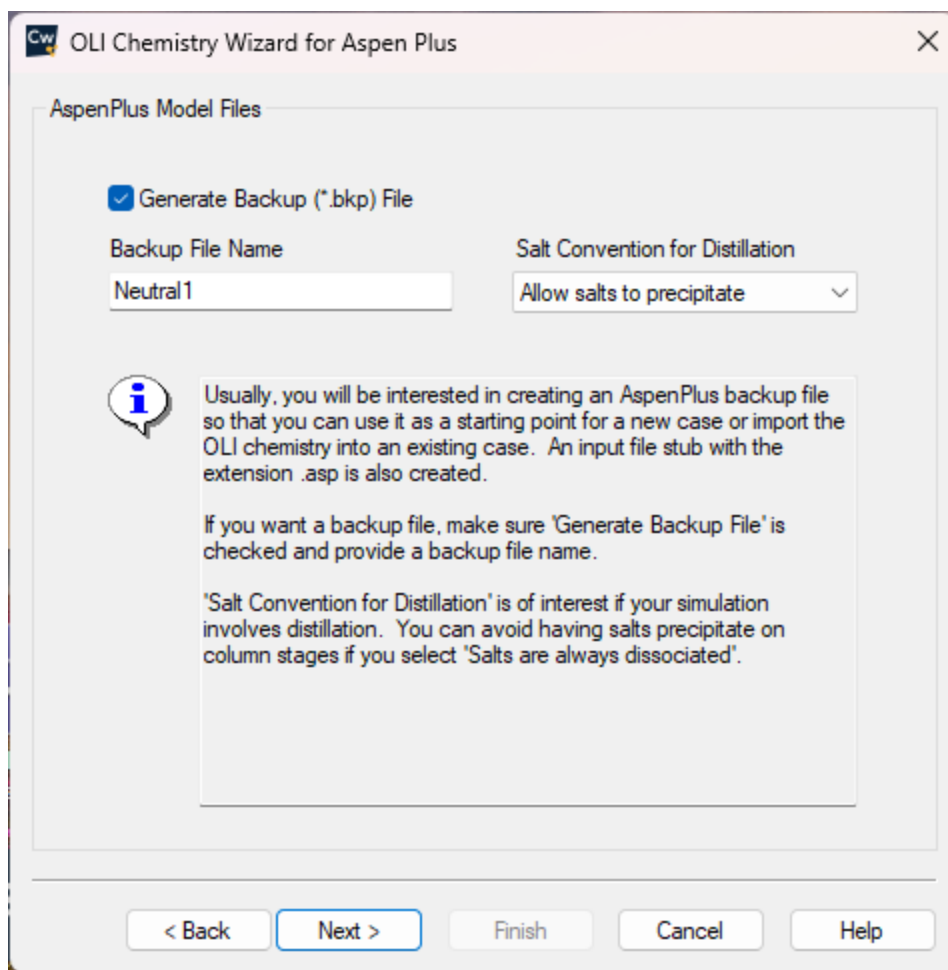


Figure 2-9 BKP file options

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.

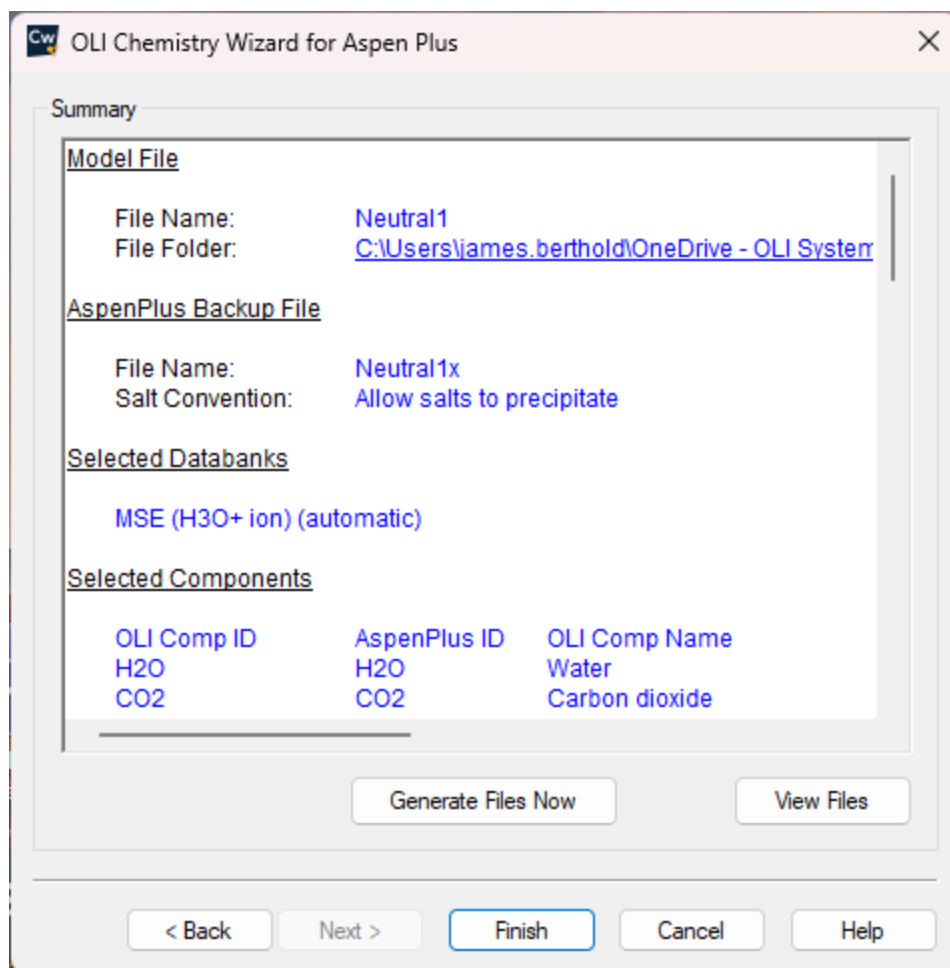


Figure 2-10 Almost done

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):

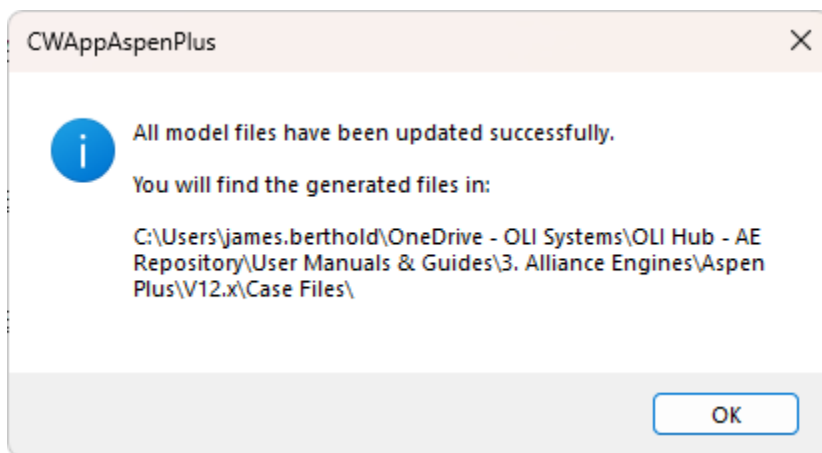


Figure 2-11 completed

Click the **OK** button.

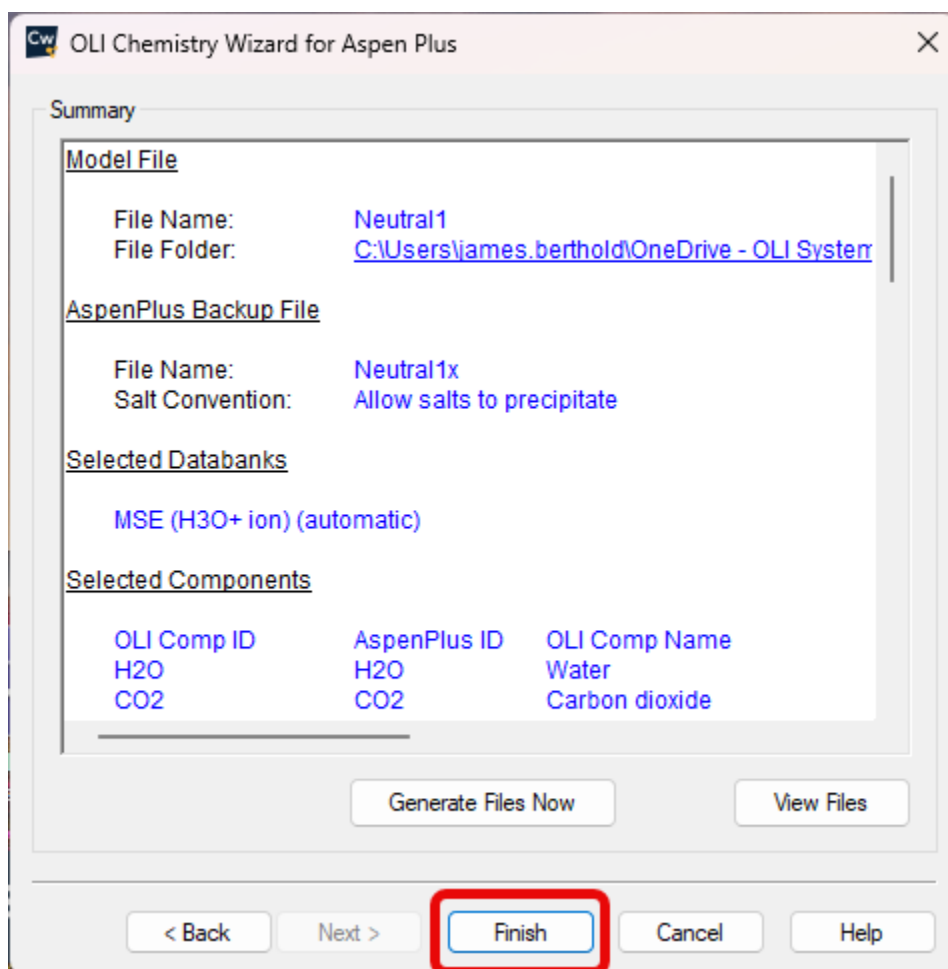


Figure 2-12 Done

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 settings you must in which to activate the Aspen PLUS program. You may see the following warning:

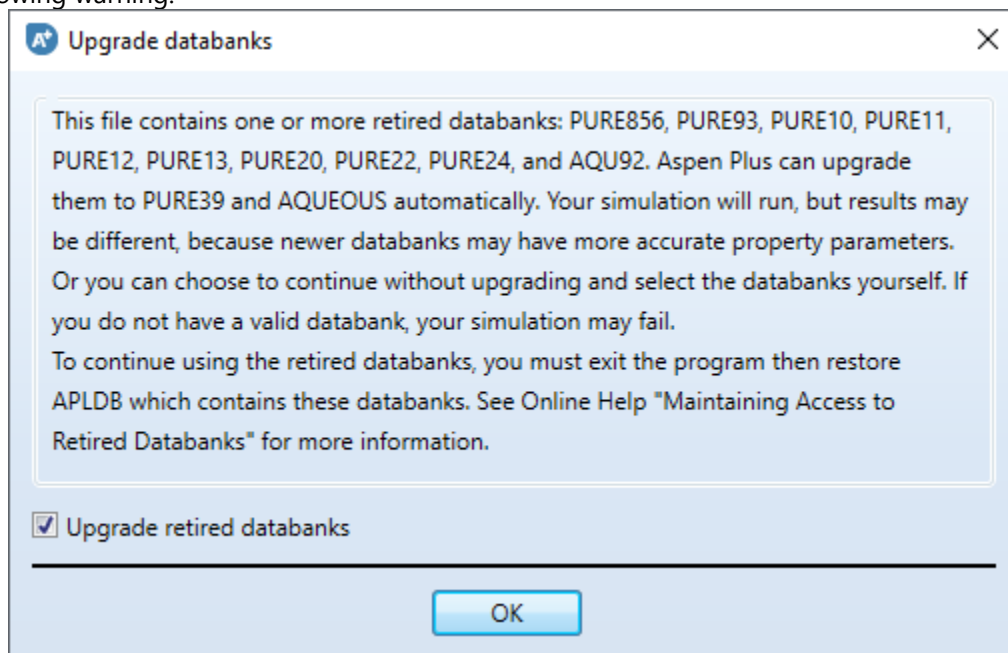


Figure 2-13 Compatibility warning

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.

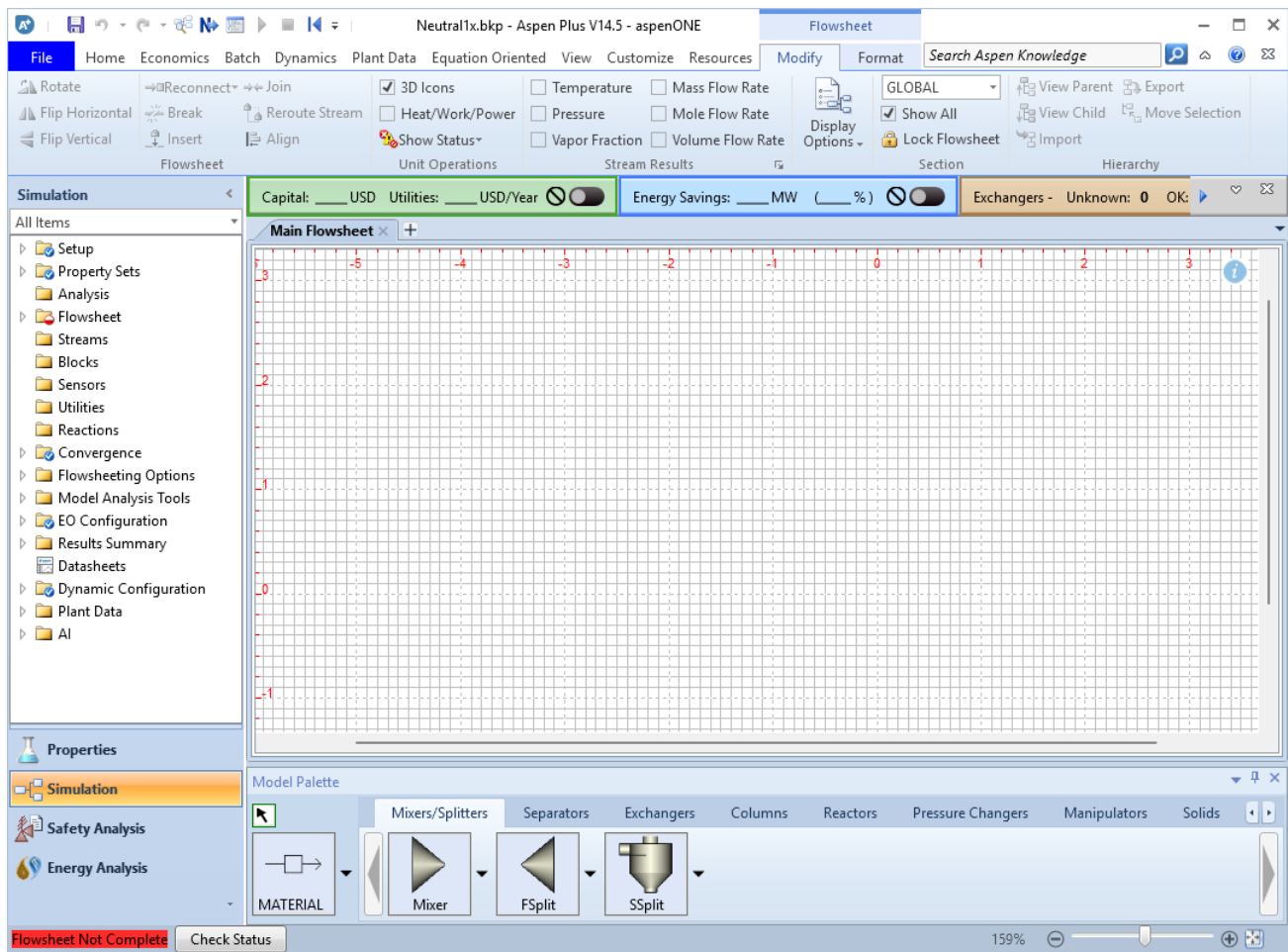


Figure 2-14 A blank flowsheet

You should already be familiar with Aspen Plus. Here we will remove the PFD grid lines to make the image more readable.

We will create the following process:

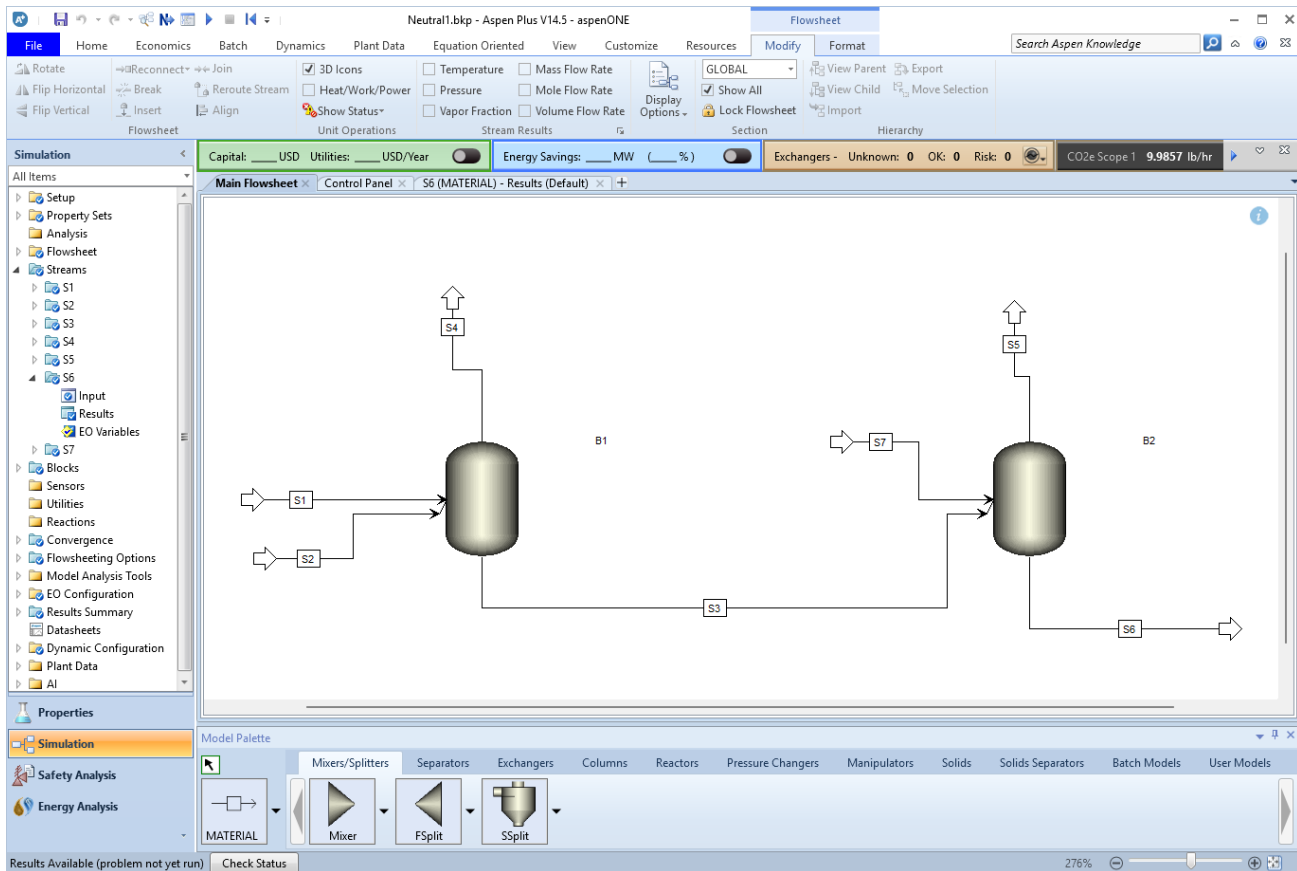


Figure 2-15 Neutral 1 Process

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.

⁴ In the OLI terminology, these are controllers

Table 2-4 Stream Results⁵

Material								
Stream Name	Units	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							
MIXED Substream								
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase		Liquid Phase	Liquid Phase
Temperature	F	104	77	101.9425509	101.9425509		103.4933075	86
Pressure	psia	14.69594878	14.69594878	14.69594878	14.69594878		14.69594878	14.69594878
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	-122696.8402	-127456.7837	-123875.6391	-162299.5724		-123432.8376	-122057.3314
Mass Enthalpy	Btu/lb	-6686.769197	-6548.86252	-6630.212564	-3741.61784		-6678.842426	-6749.366956
Molar Entropy	Btu/lbmol-R	17.6639649	16.51379181	17.46261958	51.5282997		17.36737312	16.31316405
Mass Entropy	Btu/lb-R	0.962656057	0.848495852	0.934654146	1.187921833		0.939733305	0.902064048
Molar Density	lbmol/cuft	3.404801353	3.406140669	3.418696925	0.002450691		3.456876839	3.582951805
Mass Density	lb/cuft	62.4753682	66.29177711	63.87325633	0.10630322		63.88713644	64.79504504
Enthalpy Flow	Btu/hr	-24239504.37	-19118517.56	-43315959.51	-42062.42507		-73721052.44	-30405092.91
Average MW		18.34919624	19.46243081	18.68350946	43.37684373		18.48117229	18.08426364
Mole Flows	lbmol/hr	197.5560603	150	349.6729446	0.259165347	0	597.2564019	249.1050112
H2O	lbmol/hr	193.4635711	143.7410383	342.1455427	0.017617916	0	586.0373248	240.4404912
CO2	lbmol/hr	7.66061E-05	0	0.125840463	0.226891287	0	8.33514E-05	0
H2SO4	lbmol/hr	0	3.61682E-06	3.07301E-07	6.24244E-21	0	2.16611E-22	0
HCL	lbmol/hr	0	5.13859E-09	1.3437E-09	8.71308E-10	0	1.89949E-17	0
NH3	lbmol/hr	0.512364133	0	1.06816E-08	6.22188E-11	0	0.323057445	0
SO2	lbmol/hr	2.69133E-11	0	0.270189477	0.014656143	0	7.68539E-11	0
SO3	lbmol/hr	0	4.285E-20	1.76611E-20	1.72293E-27	0	0	0
NA3HSO4	lbmol/hr	0	0	0	0	0	1.96287E-11	0
NH4OH	lbmol/hr	1.738548888	0	3.7603E-08	0	0	1.12560953	0

⁵ Many zero rows have been eliminated from this report.

NA3OHSO4	lbmol/hr	0	0	0	0	0	2.12271E-09	0
NAOH	lbmol/hr	0	0	0	0	0	2.44234E-10	2.18245E-06
OH-	lbmol/hr	0.000312961	3.29618E-14	4.30429E-12	0	0	0.000533753	4.332258921
CO3-2	lbmol/hr	0.078199932	0	1.20386E-14	0	0	0.024175316	0
H3O+	lbmol/hr	2.32562E-09	3.343767367	0.621144698	0	0	1.8625E-08	1.13406E-13
HCO3-	lbmol/hr	0.133829287	0	1.9365E-06	0	0	0.081414867	0
HSO3-	lbmol/hr	0.00084127	0	0.067499883	0	0	0.00123196	0
HSO4-	lbmol/hr	0	2.221596419	1.48477922	0	0	6.35528E-08	0
NA+	lbmol/hr	0	0	0	0	0	4.332261083	4.332258921
NAOHCO-2	lbmol/hr	0	0	0	0	0	1.29627E-08	0
NH2CO2-	lbmol/hr	0.140627861	0	2.64846E-14	0	0	0.020168852	0
NH4+	lbmol/hr	1.135795979	0	3.527336812	0	0	2.058501034	0
CL-	lbmol/hr	0	0.265017663	0.265017666	0	0	0.265017667	0
S2O5-2	lbmol/hr	4.68072E-08	0	0.000193931	0	0	3.71615E-08	0
SO3-2	lbmol/hr	0.351892323	0	3.20464E-07	0	0	0.336845509	0
SO4-2	lbmol/hr	0	0.428576642	1.165397151	0	0	2.650176613	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 the 'Stream Summary' for stream S6. The 'pH' property is highlighted with a red rectangular box, showing a value of 9.00132. The 'Volume Flow' property is also visible, with a value of 173.773 cuft/hr. The 'Mole Fractions' and 'Mass Fractions' sections are expanded, showing various flow properties.

Property	Units	Value
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

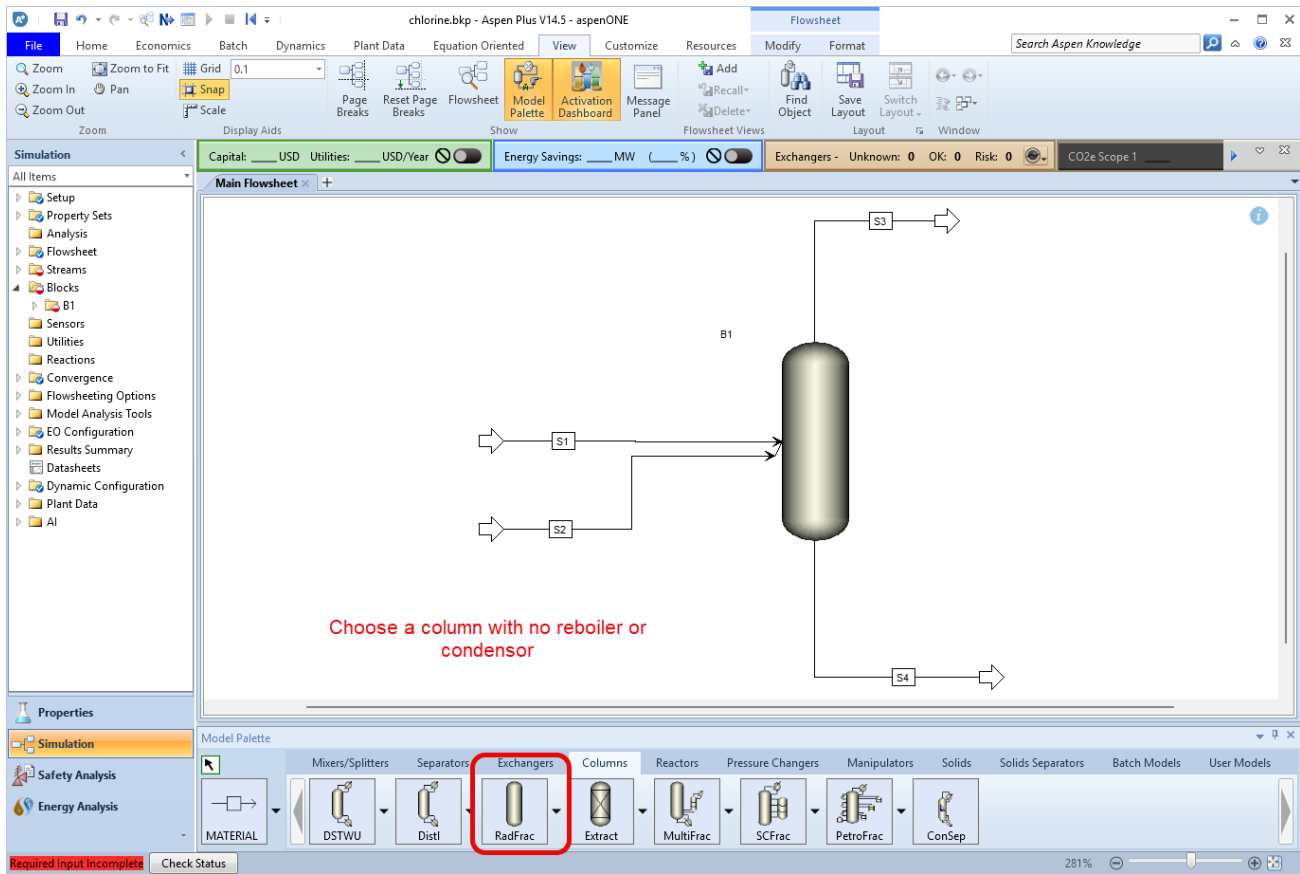


Figure 3-1

Caustic Feed Stream (S1)

Main Flowsheet × S1 (MATERIAL) × +

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

Component Attributes

Particle Size Distribution

Composition

Mole-Flow lbmol/hr

Component	Value
H2O	48.8
CO2	
CL2	
HClO	
HCL	
N2	
NAOH	2.57
HCLW1	
HCLW2	
HCLW3	
H2CO3	
NA2CO3	
NACO3W10	
NACO3W1	
NACO3W7	
NA2O	
Total	51.37

Feed Stream (S2)

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

Component Attributes

Particle Size Distribution

Composition

Mole-Flow lbmol/hr

Component	Value
H2O	2.27
CO2	23.59
CL2	2.27
HClO	
HCL	
N2	26.3
NAOH	
HCLW1	
HCLW2	
HCLW3	
H2CO3	
NA2CO3	
NACO3W10	
NACO3W1	
NACO3W7	
NA2O	
Total	54.43

RADFRAC (Block B1) configuration (5 stages)

The screenshot shows the configuration window for a RADFRAC block with 5 stages. The 'Configuration' tab is active. Under 'Setup options', the following settings are visible:

- Calculation type: Equilibrium
- Number of stages: 5 (with a 'Stage Wizard' button)
- Condenser: None
- Reboiler: None
- Valid phases: Vapor-Liquid
- Convergence: Standard

Under 'Operating specifications', there are several empty dropdown menus and a 'Free water reflux ratio' field set to 0, with a 'Feed Basis' button next to it.

RADFRAC (Block B1) streams

The screenshot shows the streams window for the RADFRAC block. The 'Streams' tab is active. It displays the following stream information:

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 [] atm
 Condenser pressure drop [] psi

Pressure drop for rest of column (optional)
 Stage pressure drop [] 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

Main Flowsheet x DS-1 - Input x +

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:

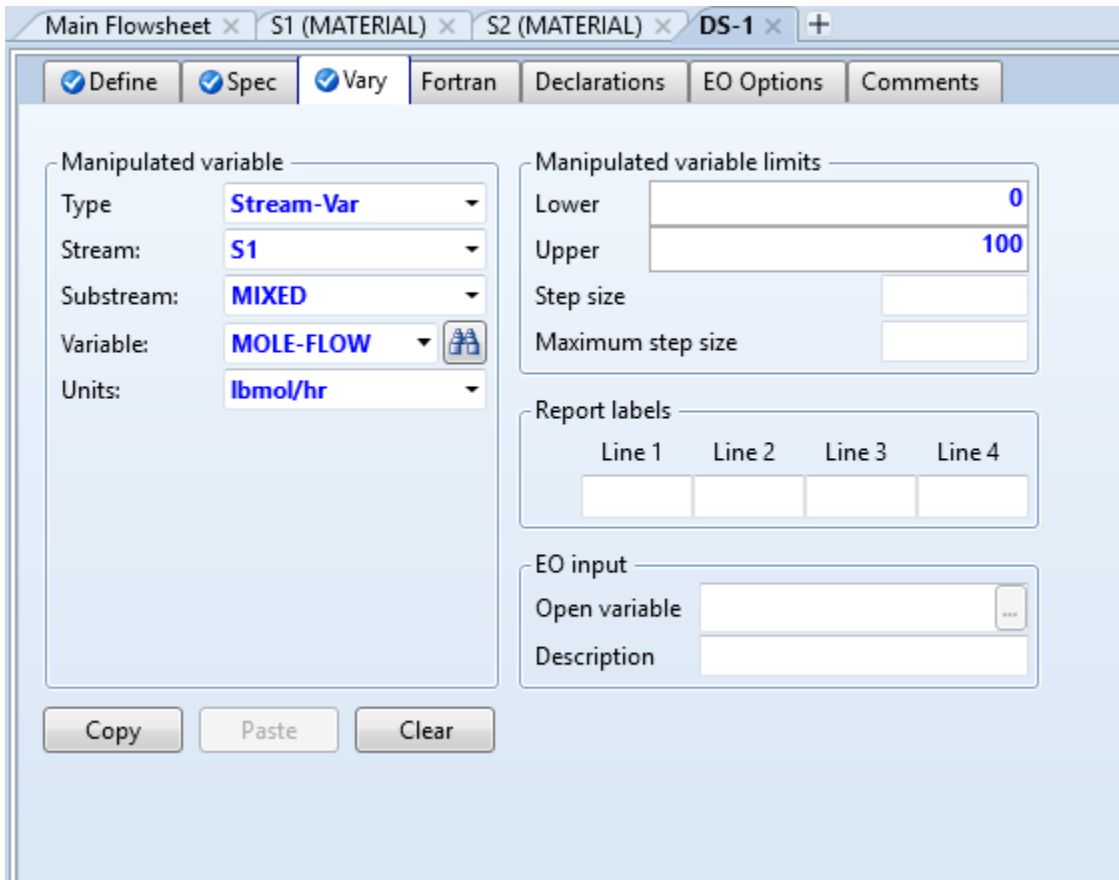
Description:

Main Flowsheet x DS-1 - Input x +

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

	Units	S1	S2	S3	S4
Description					
From				B1	B1
To		B1	B1		
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN
Maximum Relative Error					
Cost Flow	\$/hr				
MIXED Substream					
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Liquid Phase
Temperature	F	77	91.4	110.9184062	89.51948356
Pressure	psia	14.69594878	14.84290826	14.69594878	14.69594878
Molar Vapor Fraction		0	1	1	0
Molar Liquid Fraction		1	0	0	1
Molar Solid Fraction		0	0	0	0
Mass Vapor Fraction		0	1	1	0
Mass Liquid Fraction		1	0	0	1
Mass Solid Fraction		0	0	0	0
Molar Enthalpy	Btu/lbmol	-	-	-	-
		120910.6071	77606.16654	81473.38825	116925.4843
Mass Enthalpy	Btu/lb	-	-	-	-
		6641.881885	2136.843859	2379.848615	5733.410093
Molar Entropy	Btu/lbmol-R	-	-	-	-
		14.85892015	48.53681558	48.52375771	16.33121535
Mass Entropy	Btu/lb-R	-	-	-	-
		0.816232711	1.336434989	1.417385481	0.80079681
Molar Density	lbmol/cuft	-	-	-	-
		3.811204487	0.002516816	0.002405863	3.389175157
Mass Density	lb/cuft	-	-	-	-
		69.3801932	0.091406058	0.08236397	69.11784441
Enthalpy Flow	Btu/hr	-	-	-	-
		6375009.552	4224103.645	4426577.285	6172535.916
Average MW		-	-	-	-
		18.20426939	36.31812694	34.23469364	20.39370679
Mole Flows	lbmol/hr	-	-	-	-
		52.72498174	54.43	54.33157231	52.79033866
H2O	lbmol/hr	-	-	-	-
		47.70076477	2.269997668	4.330893326	45.8998837
CO2	lbmol/hr	-	-	-	-
		0	23.59	23.54990646	0.007019855
CL2	lbmol/hr	-	-	-	-
		0	2.269997668	0.04915845	0.001817761
HClO	lbmol/hr	-	-	-	-
		0	2.33E-06	0.101818683	1.857252763
HCL	lbmol/hr	-	-	-	-
		0	2.33E-06	5.60E-12	3.00E-14
N2	lbmol/hr	-	-	-	-
		0	26.3	26.2997954	0.000204605
NAOH	lbmol/hr	-	-	-	-
		2.92E-06	0	3.95E-42	2.14E-13
H2CO3	lbmol/hr	-	-	-	-
		0	0	0	0
NA2CO3	lbmol/hr	-	-	-	-
		0	0	0	0
NA2O	lbmol/hr	-	-	-	-
		0	0	0	0

NA3HCO32	lbmol/hr	0	0	0	0
NA5H3C34	lbmol/hr	0	0	0	0
NACL	lbmol/hr	0	0	0	0
NACLO	lbmol/hr	0	0	0	0
NAHCO3	lbmol/hr	0	0	0	0
OH-	lbmol/hr	2.512107027	0	0	9.22E-08
CLO-	lbmol/hr	0	0	0	0.259952344
CO3-2	lbmol/hr	0	0	0	6.01E-05
H3O+	lbmol/hr	2.53E-15	0	0	1.15E-07
HCO3-	lbmol/hr	0	0	0	0.033013538
NA+	lbmol/hr	2.512107027	0	0	2.512109948
NAOHCO-2	lbmol/hr	0	0	0	1.55E-13
CL-	lbmol/hr	0	0	0	2.219023789
Mole Fractions					
Mass Flows	lb/hr	959.8197714	1976.79565	1860.024733	1076.590688
Mass Fractions					
Volume Flow	cuft/hr	13.83420436	21626.52768	22582.99023	15.57616122
Vapor Phase					
Liquid Phase					
Molar Enthalpy	Btu/lbmol	120910.6071			116925.4843
Mass Enthalpy	Btu/lb	6641.881885			5733.410093
Molar Entropy	Btu/lbmol-R	14.85892015			16.33121535
Mass Entropy	Btu/lb-R	0.816232711			0.80079681
Molar Density	lbmol/cuft	3.811204487			3.389175157
Mass Density	lb/cuft	69.3801932			69.11784441
Enthalpy Flow	Btu/hr	6375009.552			6172535.916
Average MW		18.20426939			20.39370679
Mole Flows	lbmol/hr	52.72498174			52.79033866
Mole Fractions					
Mass Flows	lb/hr	959.8197714			1076.590688
Mass Fractions					
Volume Flow	cuft/hr	13.83420436			15.57616122
pH		14.35814337			6.571125775

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