OLI SYSTEMS, INC.

A Guide to Using the OLI Engine in Aspen Plus

Featuring Aspen Plus V14.x

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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 12.0.0.6 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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Contents

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 Venders, can get answers more quickly

Disadvantages of Aspen-OLI

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

Aspen-OLI Interface Layout

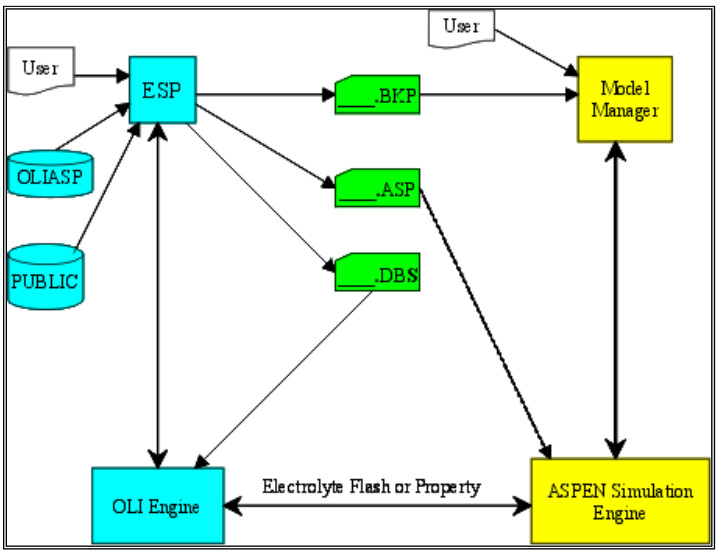


Figure 1-1 The layout of the Aspen OLI Interface

Aspen OLI Unit Operations

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

Aspen Property Set

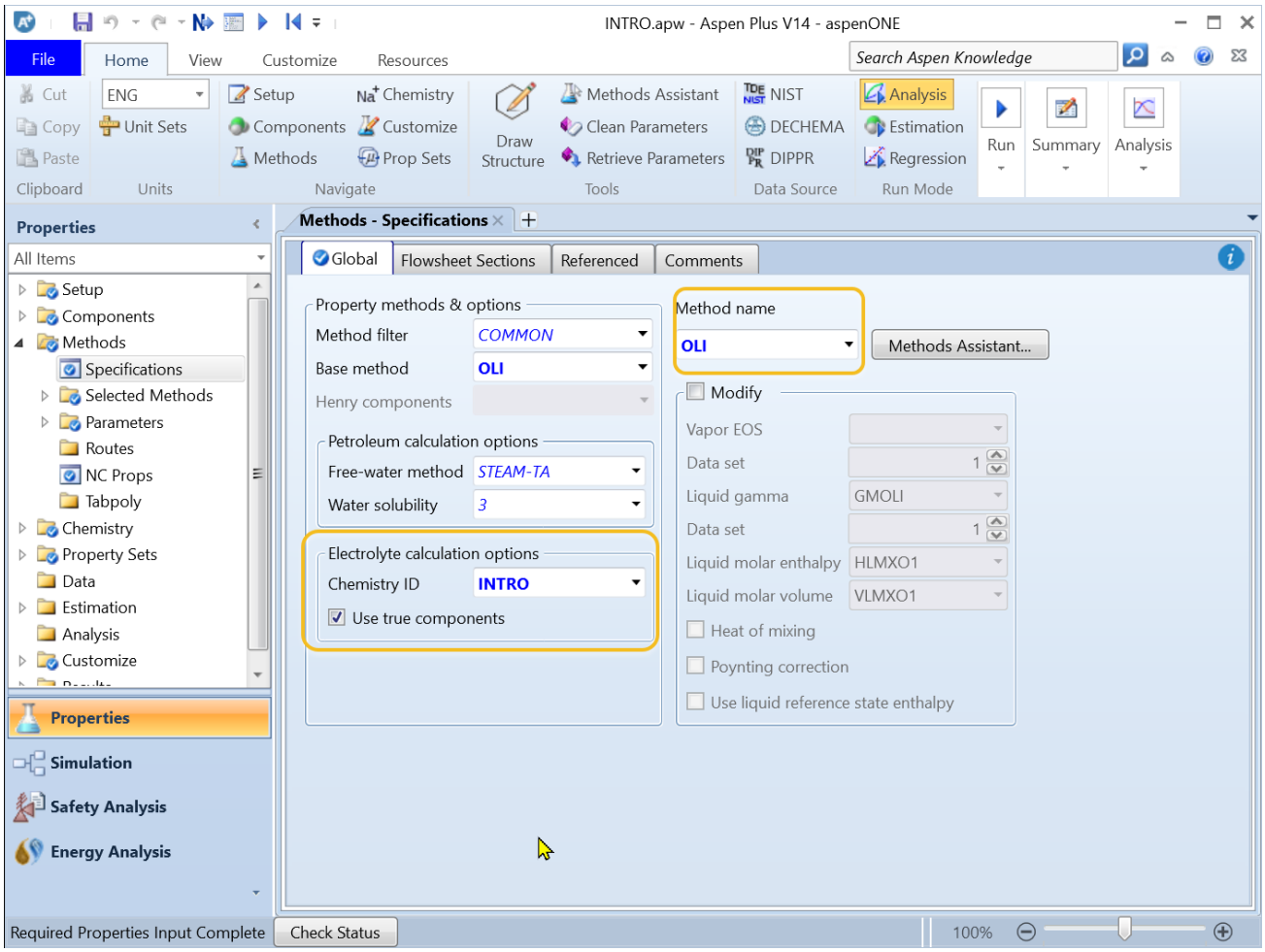


Figure 1-2 OLI Property Set, the boxed areas show that OLI is enabled.

Property	Route ID
PHIVMX	PHIVMXO1
PHILMX	PHILMXO1
HVMX	HVMXO1
HLMX	HLMXO1
GVMX	GVMXO1
GLMX	GLMXO1
SVMX	SVMXO1
SLMX	SLMXO1
VVMX	VVMXO1
VLMX	VLMXO1
MUVMX	MUVMX01
MULMX	MULMX01
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	HSMXO1
PHIL	PHIL00

Property	Route ID
MUVMXL	MUVMXLP1
MUVLP	MUVLP01
KVMXLP	KVMXLP01
KVLP	KVLP01
DHV	DHV00
DHL	DHL00
DHLPC	DHLPC00
DGV	DGV00
DGL	DGL00
PHILPC	PHILPC00
DSV	DSV00
KVPC	KVPC01

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 (FraChem[1])

New run command (RUNASP)

[1] This is also known as EFRACH

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.

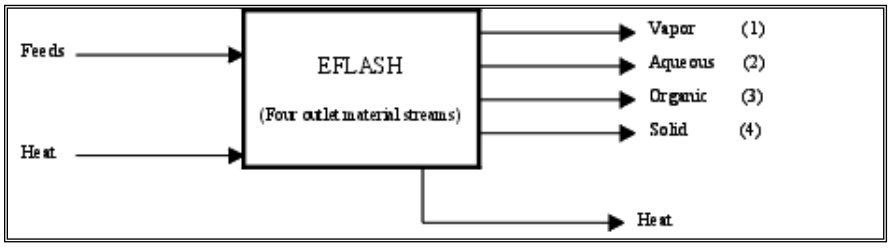


Figure 1-3 EFLASH unit operation

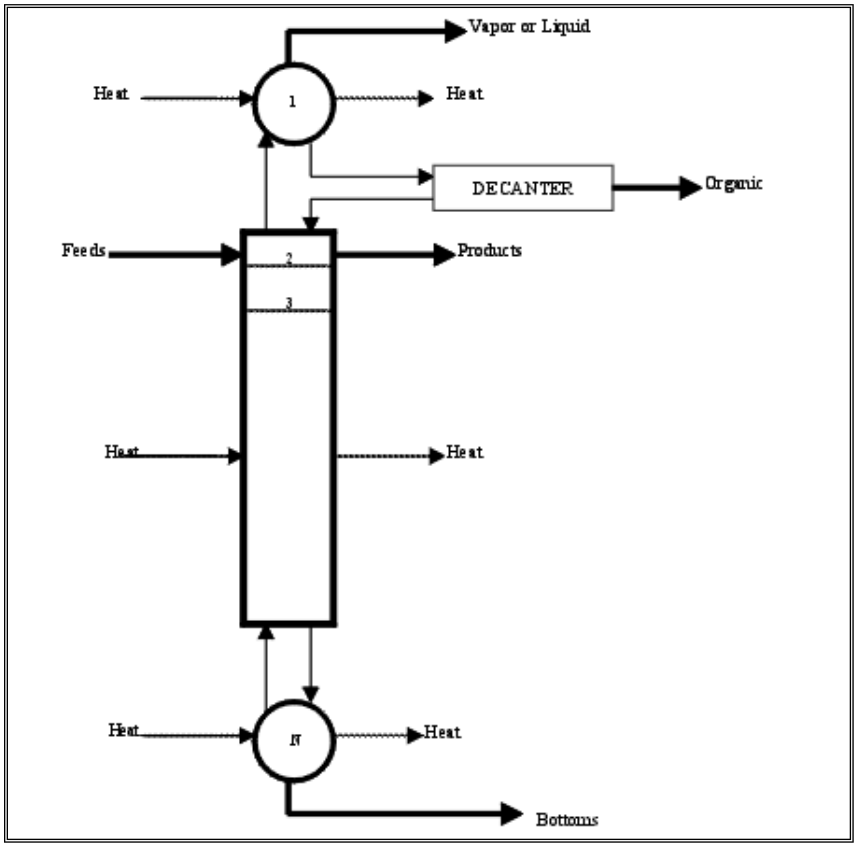


Figure 1-4 EFRACH Block

Chapter 2 ASPEN Neutralization Flowsheet

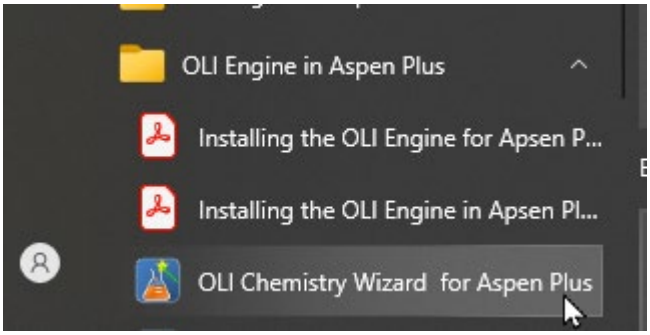
A Tour of the OLI-ASPEN Interface

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 Engine[2]. 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.

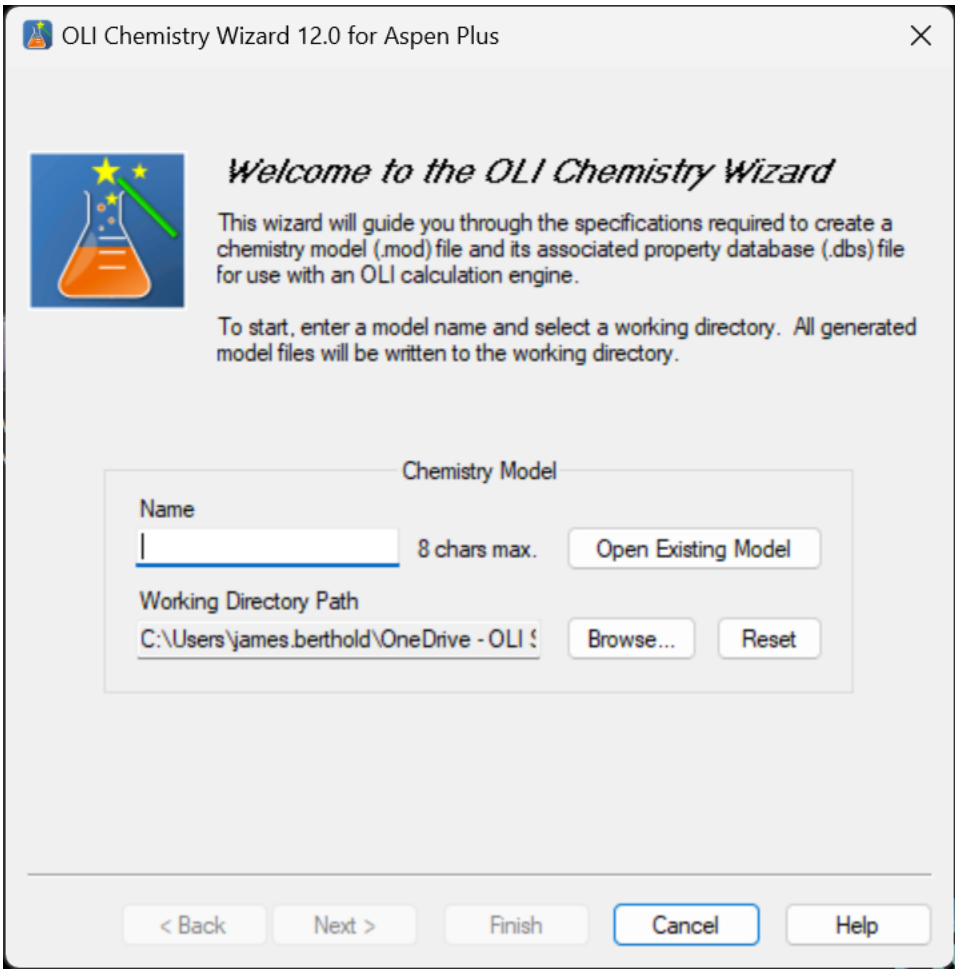
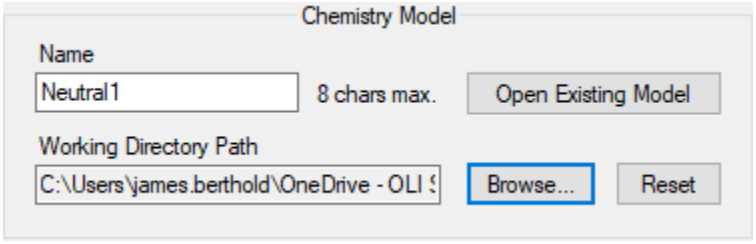
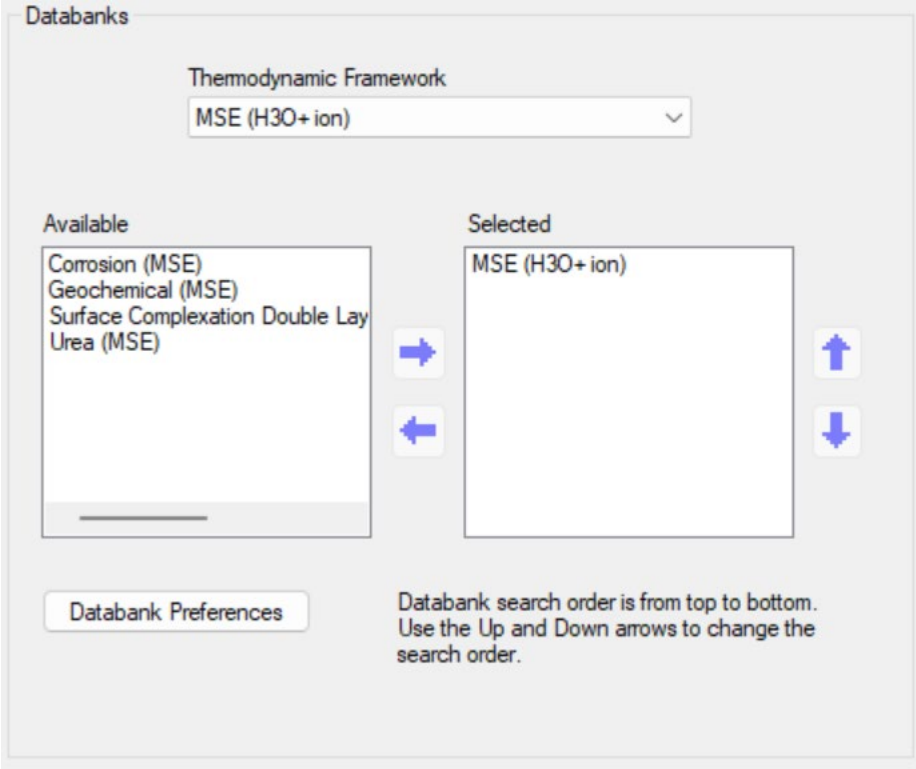


Figure 2-1 Specifying the model name and location



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 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

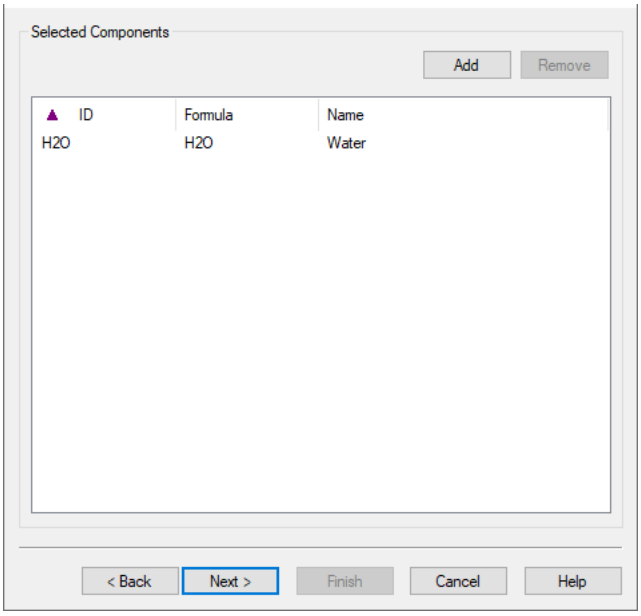


Figure 2-2 Adding components

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

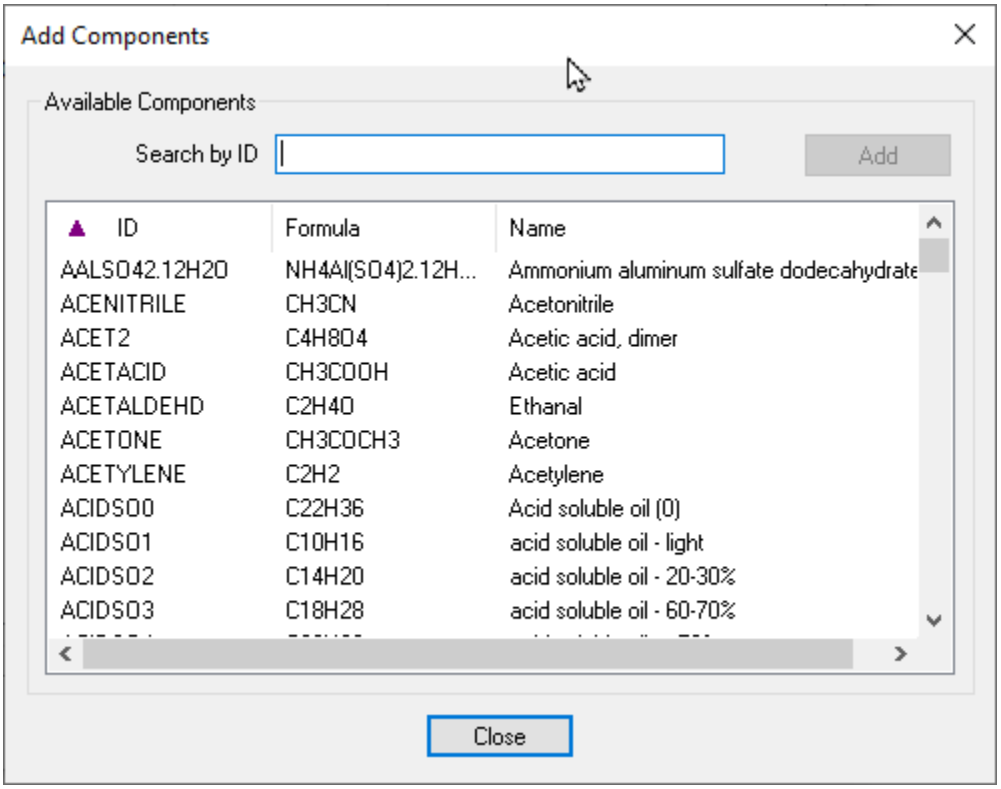


Figure 2-3 Select Components

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

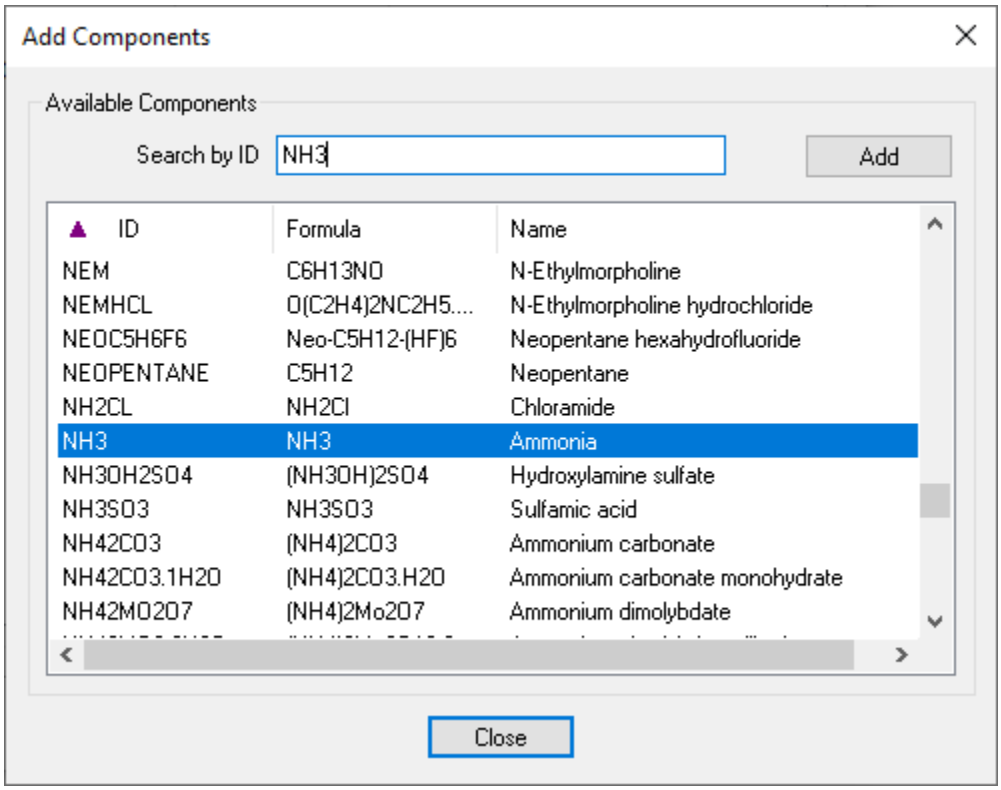


Figure 2-4 Adding NH3, ammonia

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.

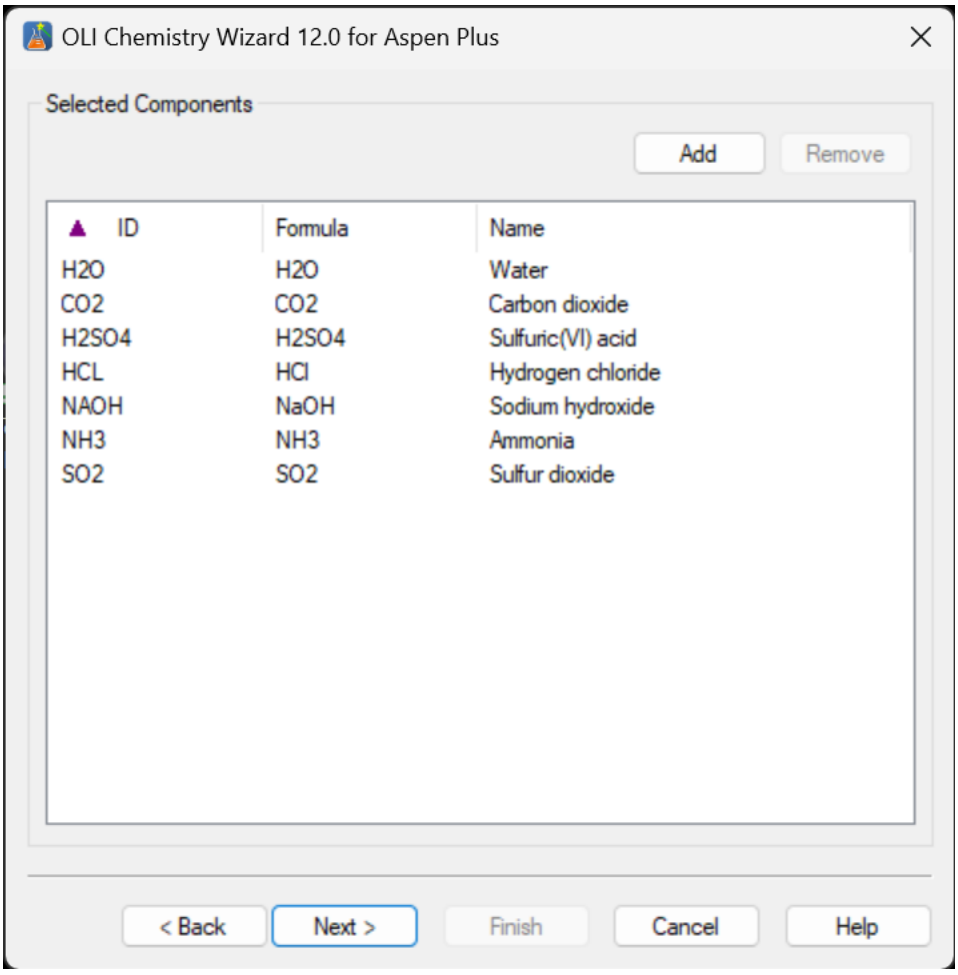


Figure 2-5 the added components

Click the ***Next>*** button.

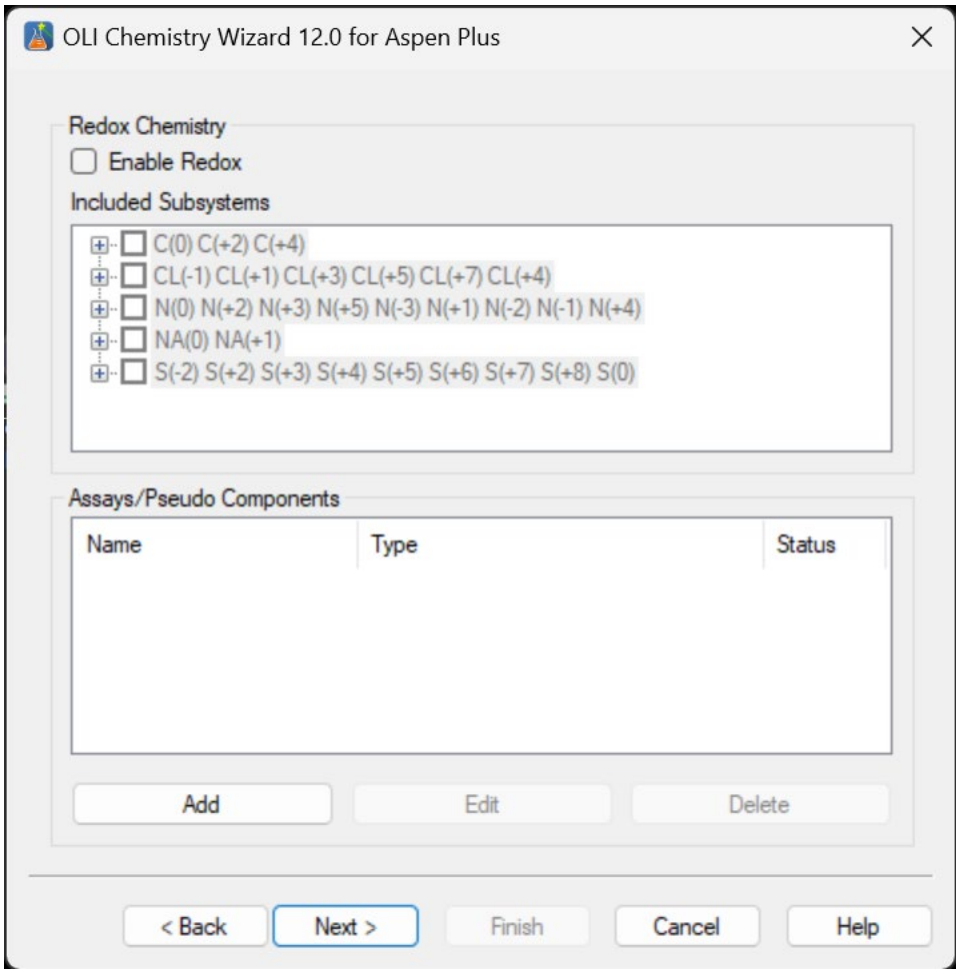


Figure 2-6 adding redox

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

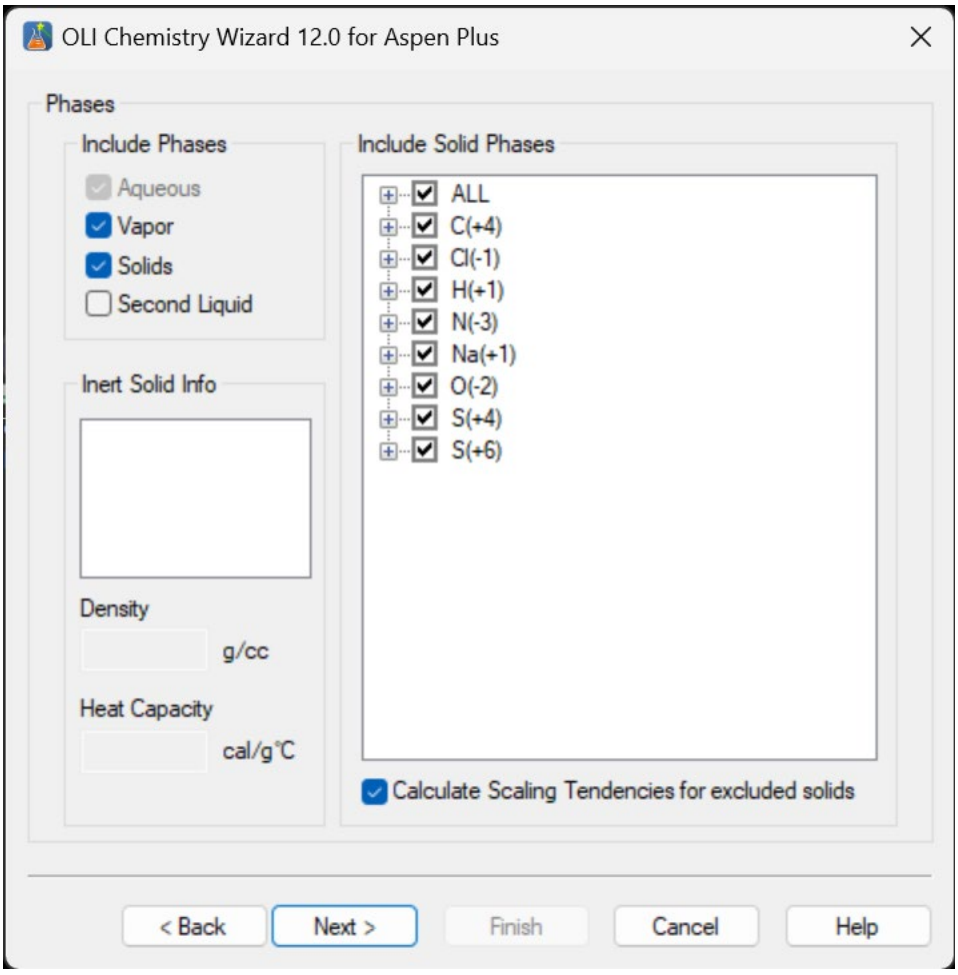


Figure 2-7 Selecting phases, including solids

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.

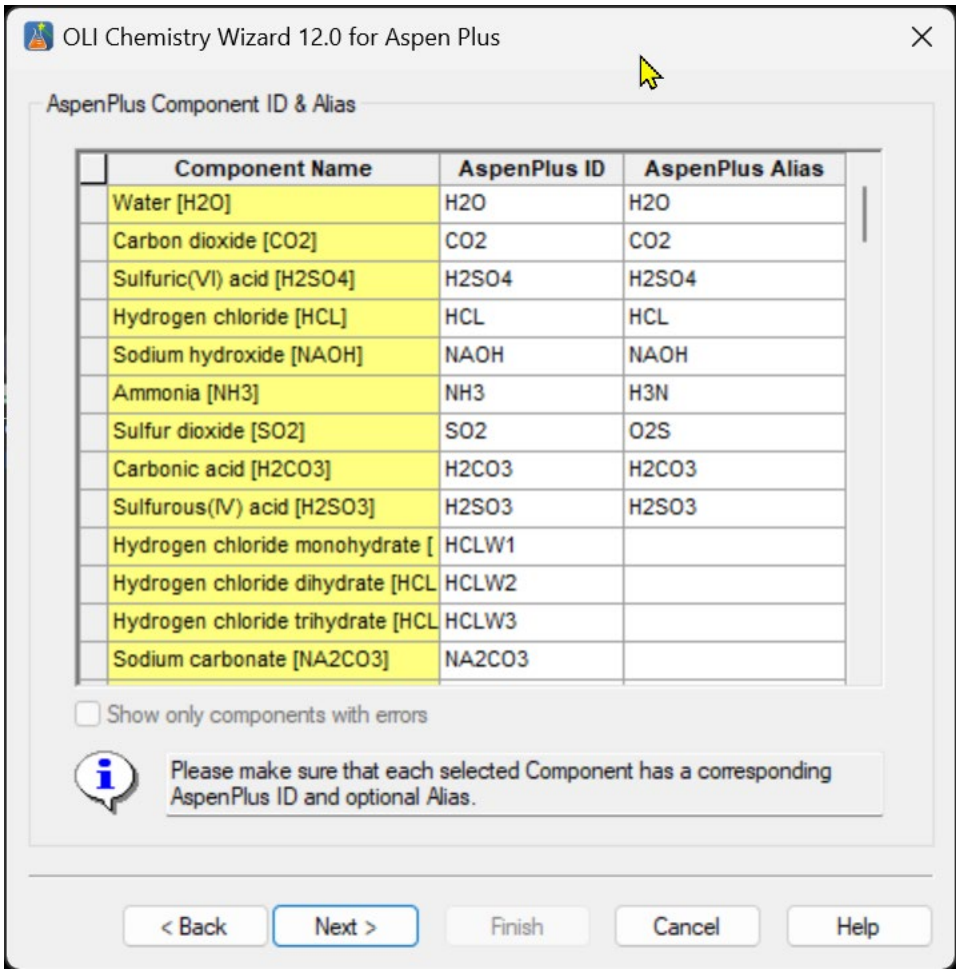


Figure 2-8 Aspen Alias names

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.

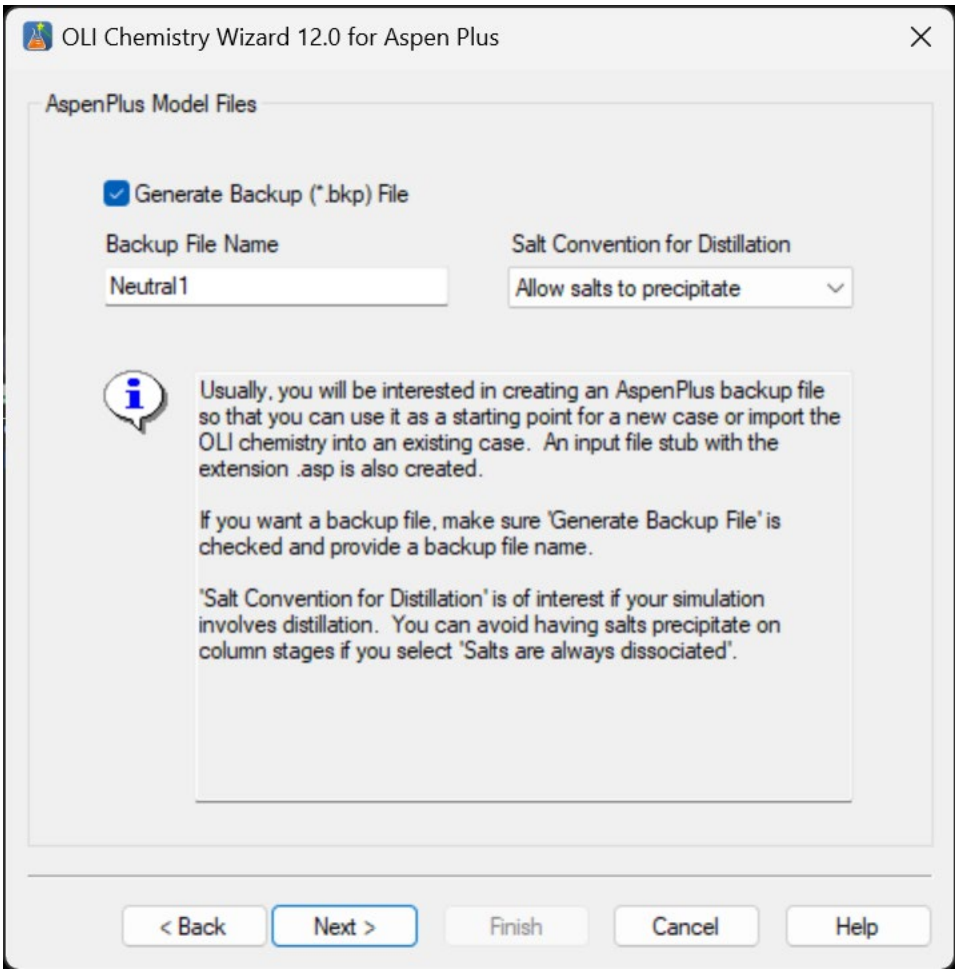


Figure 2-9 BKP file options

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.

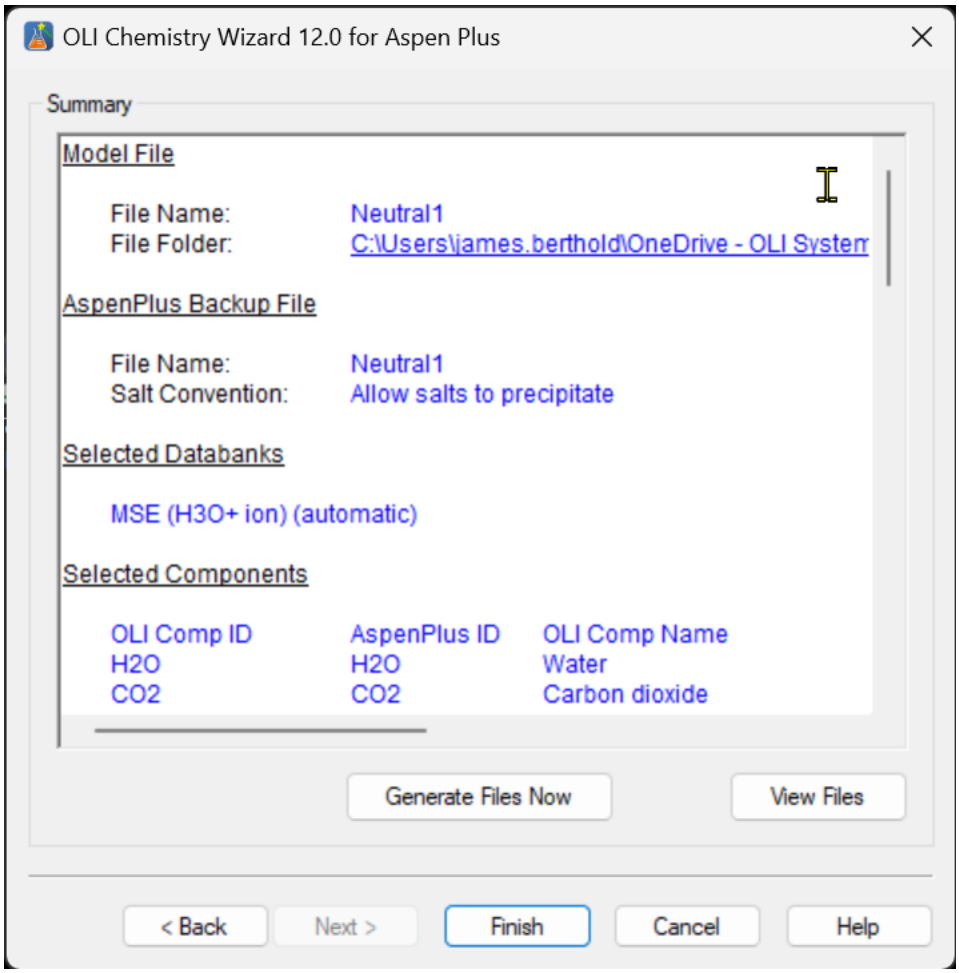


Figure 2-10 Almost done

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):

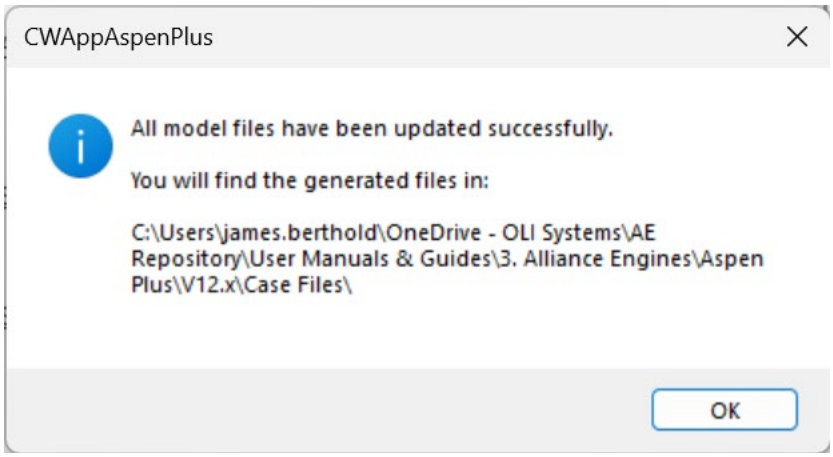


Figure 2-11 completed

Click the ***OK*** button.

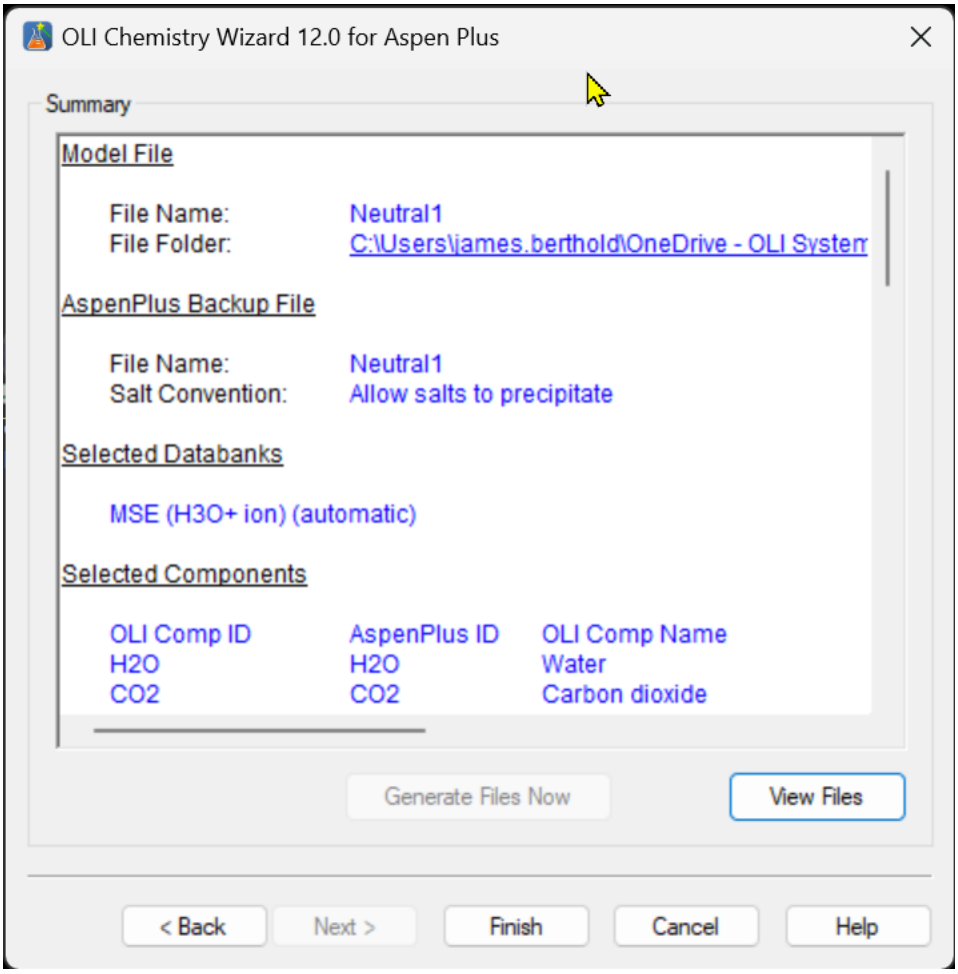


Figure 2-12 Done

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:

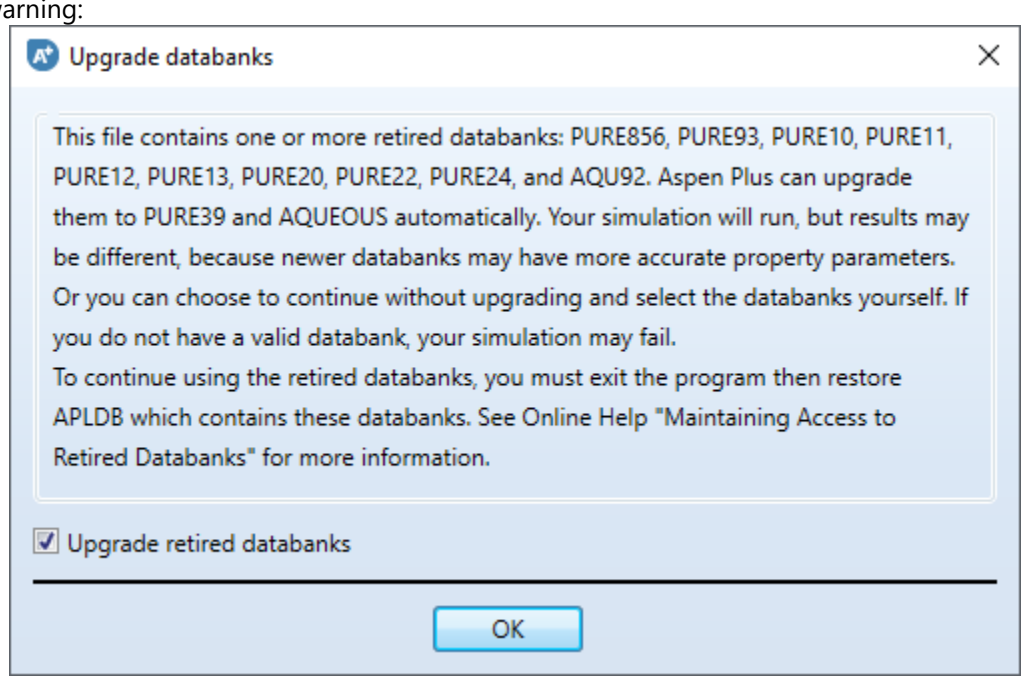


Figure 2-13 Compatibility warning

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.

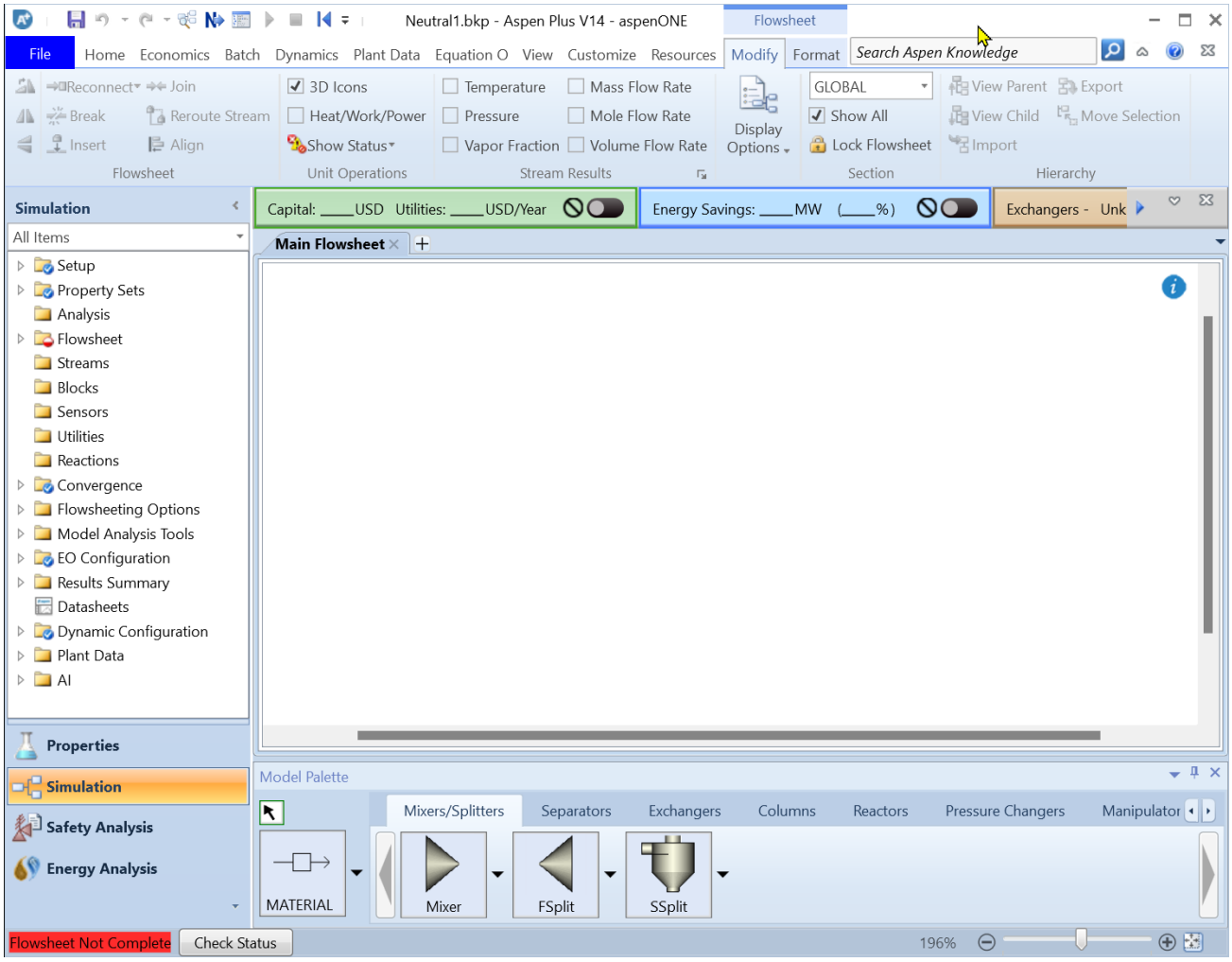


Figure 2-14 A blank flowsheet

We will create the following process:

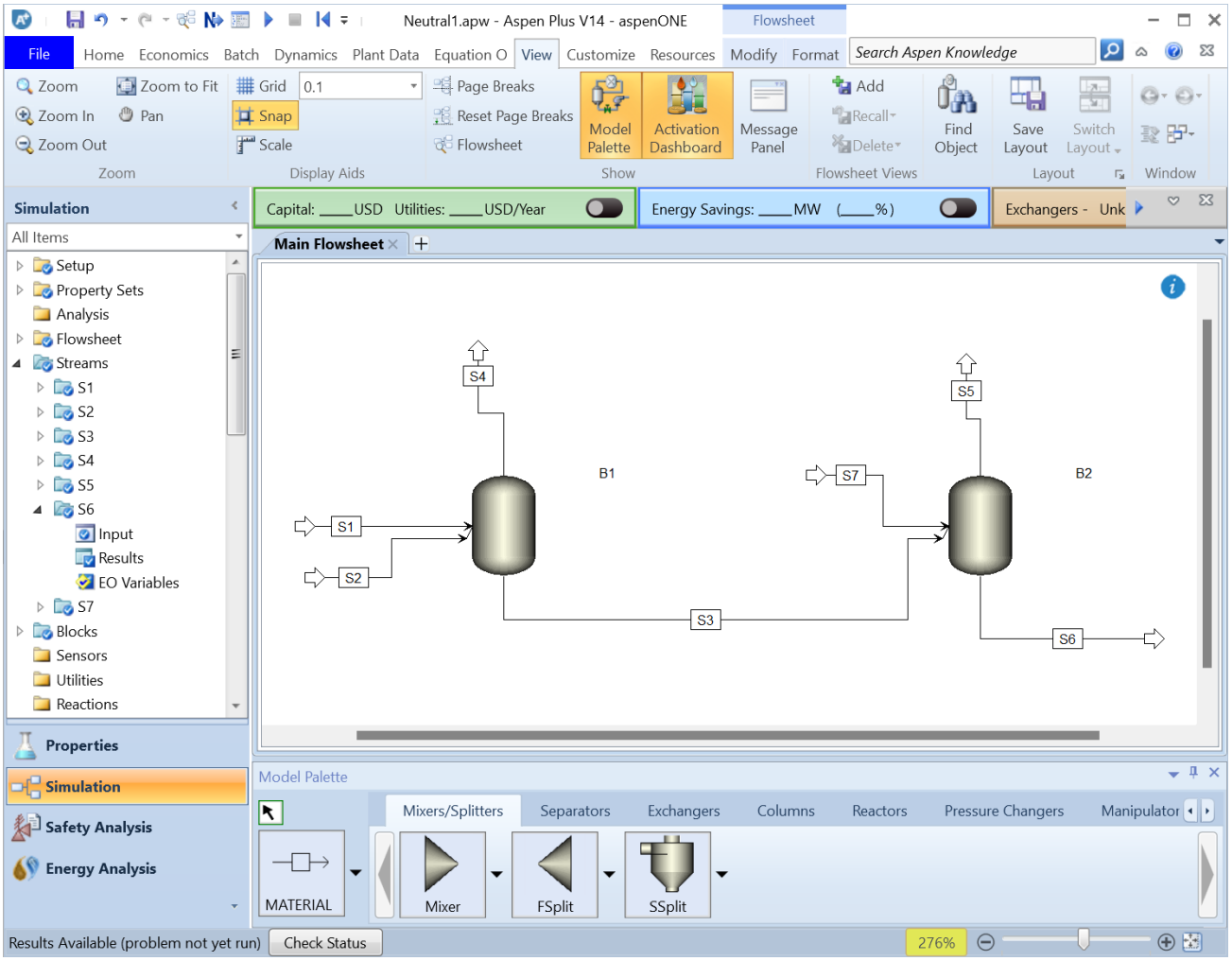


Figure 2-15 Neutral 1 Process

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 Specifications[4]

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

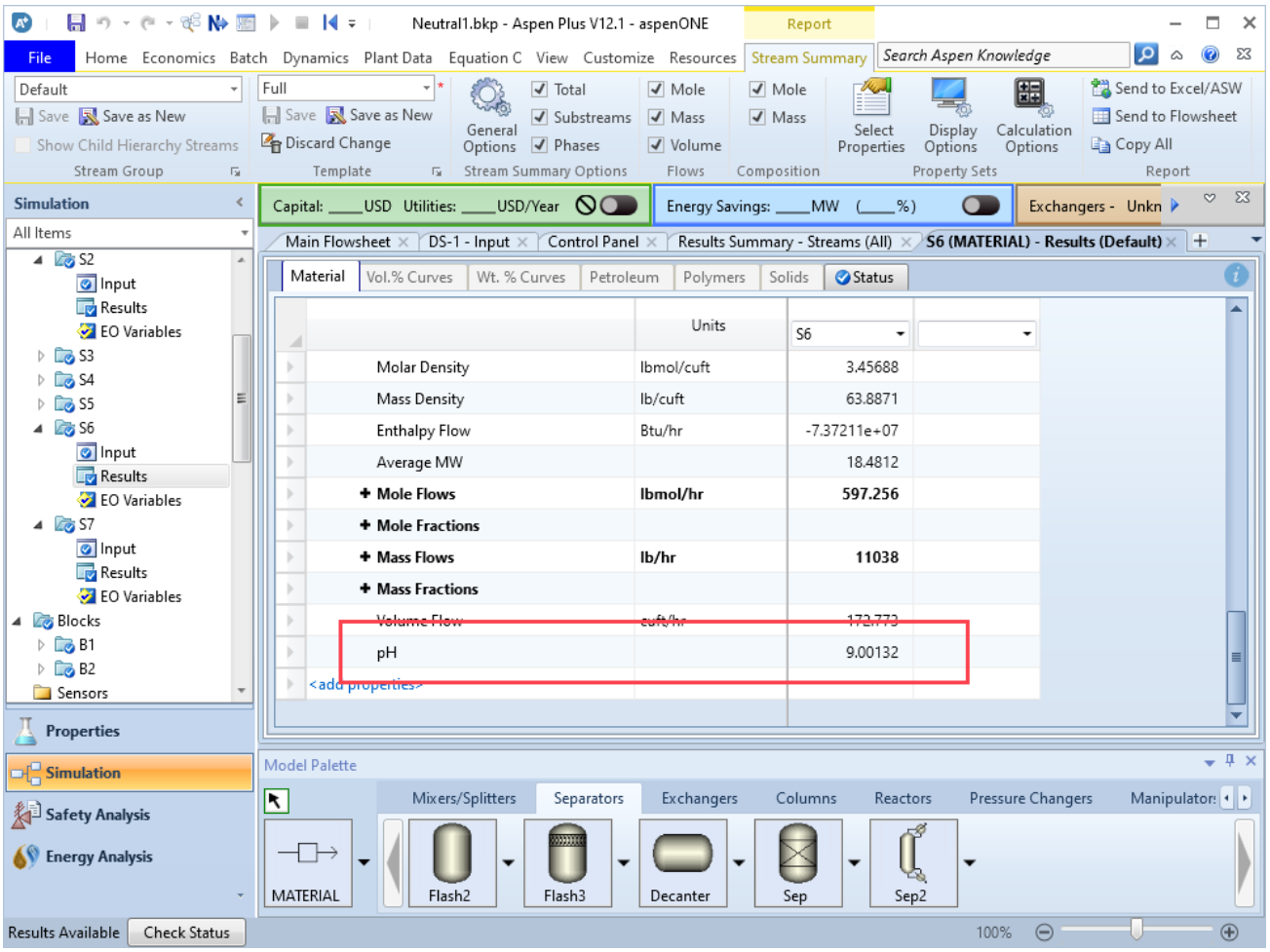
Table 2-4 Stream Results[5]

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

[5] Many zero rows have been eliminated from this report.

NH4OH	lbmol/hr	1.738548888	0	3.7603E-08	0	0	1.12560953	0
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.



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 Chlroine.BKP file just created.

Create the following flowsheet

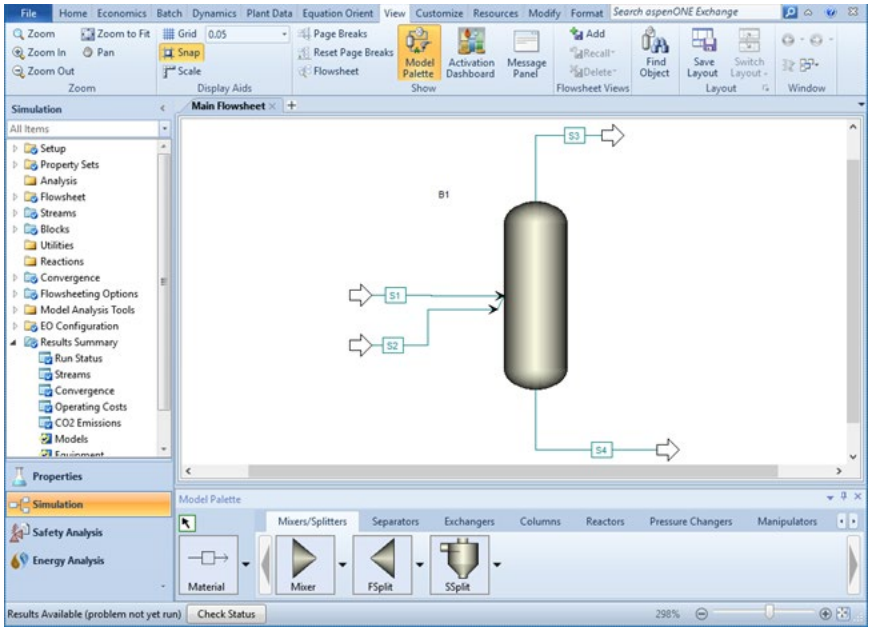
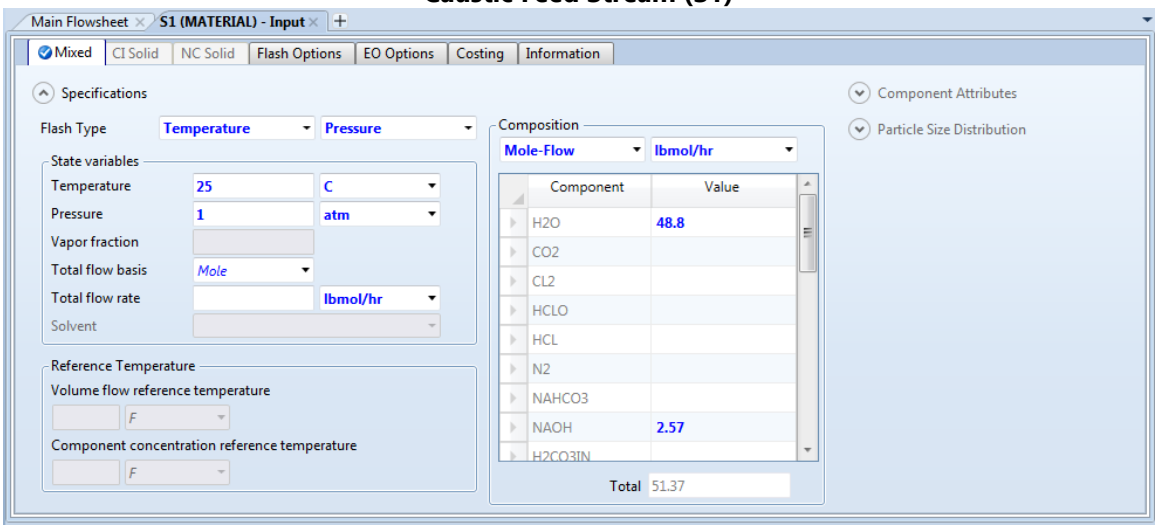
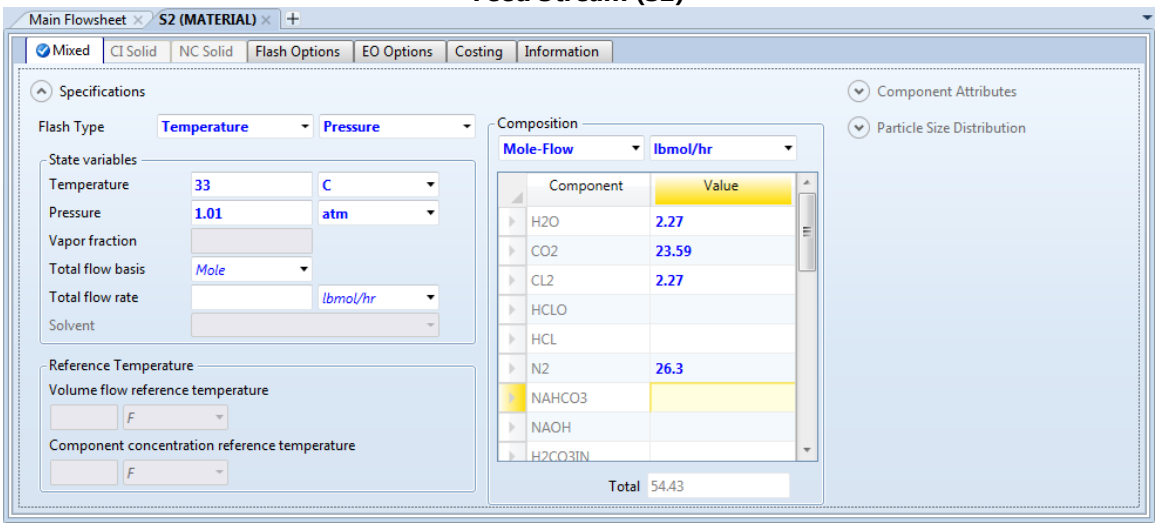


Figure 3-1

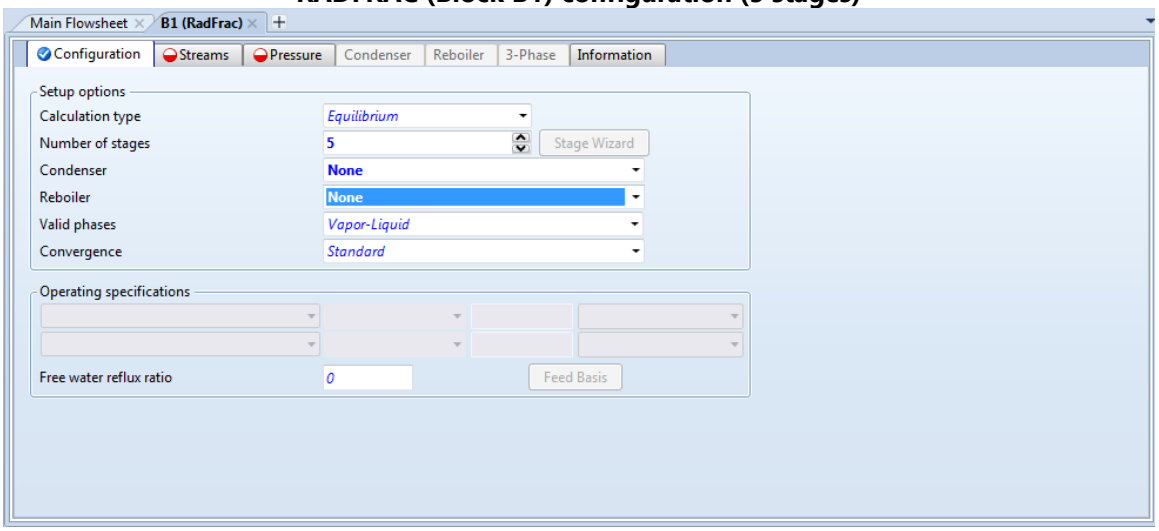
Caustic Feed Stream (S1)



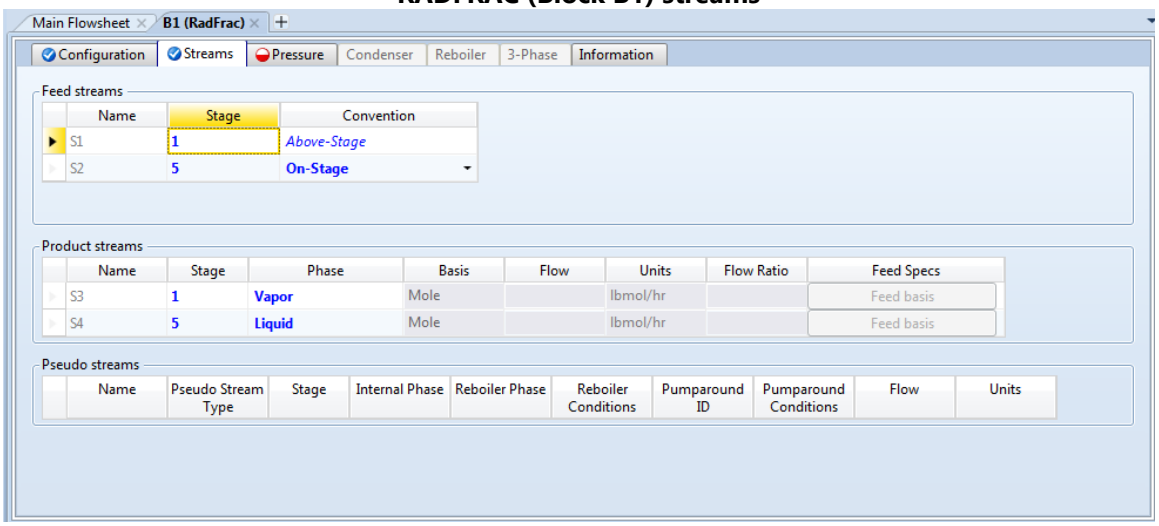
Feed Stream (S2)



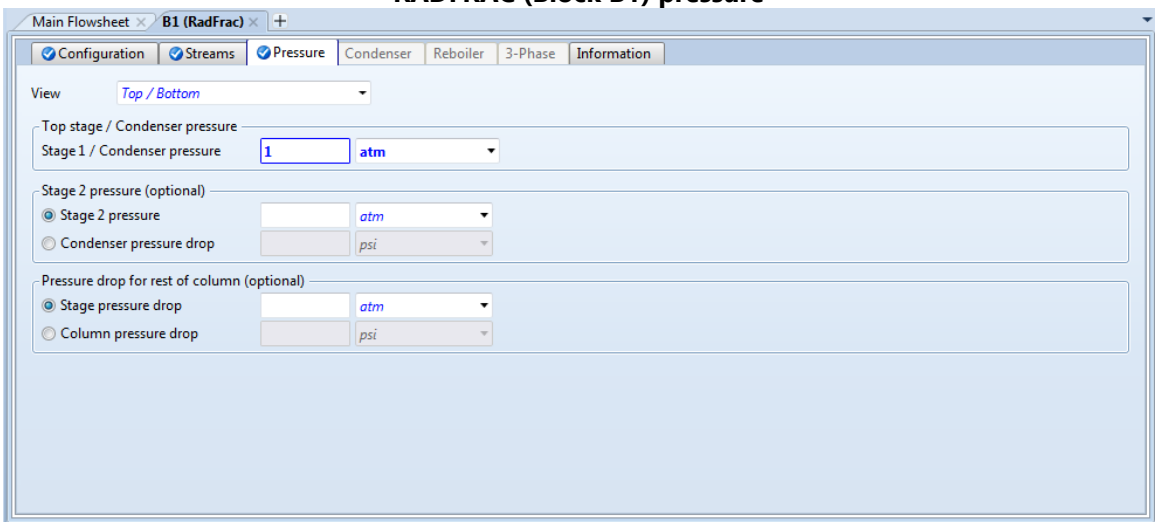
RADFRAC (Block B1) configuration (5 stages)



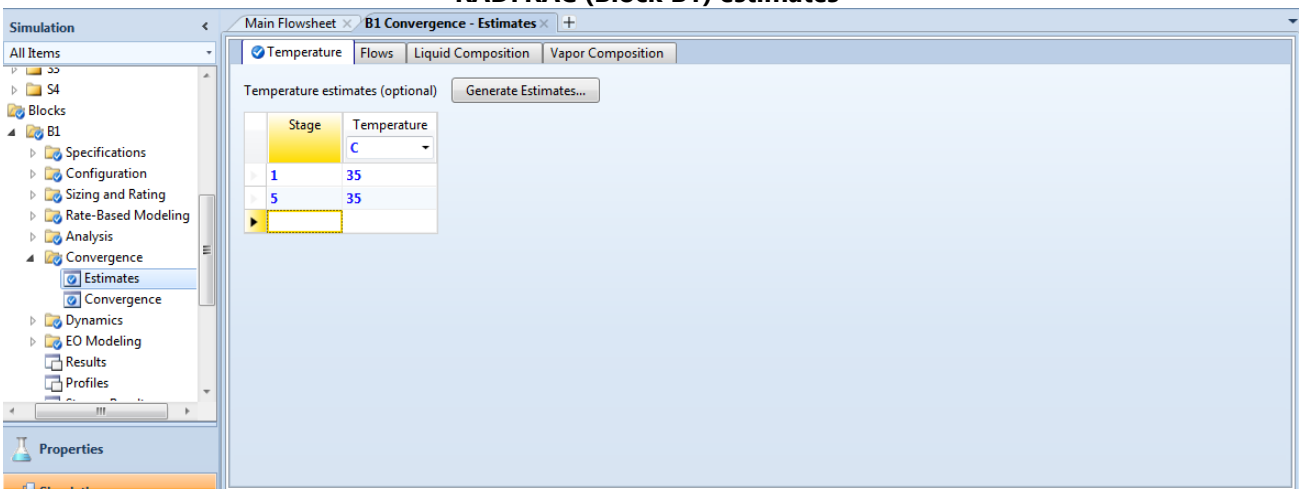
RADFRAC (Block B1) streams



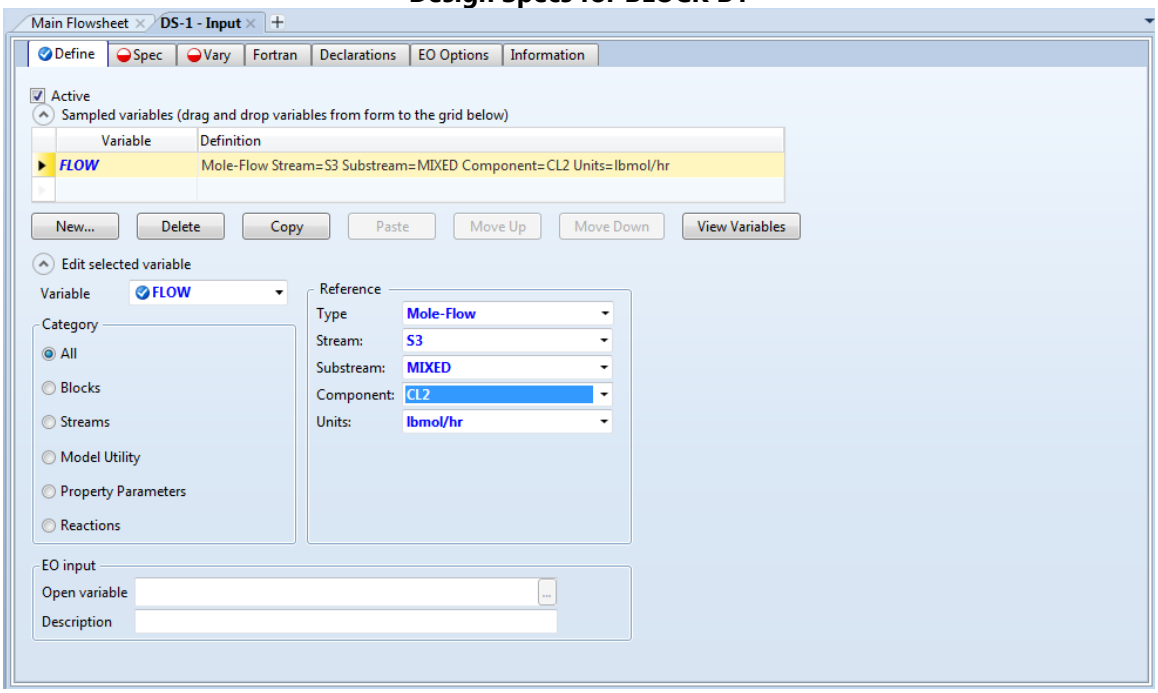
RADFRAC (Block B1) pressure

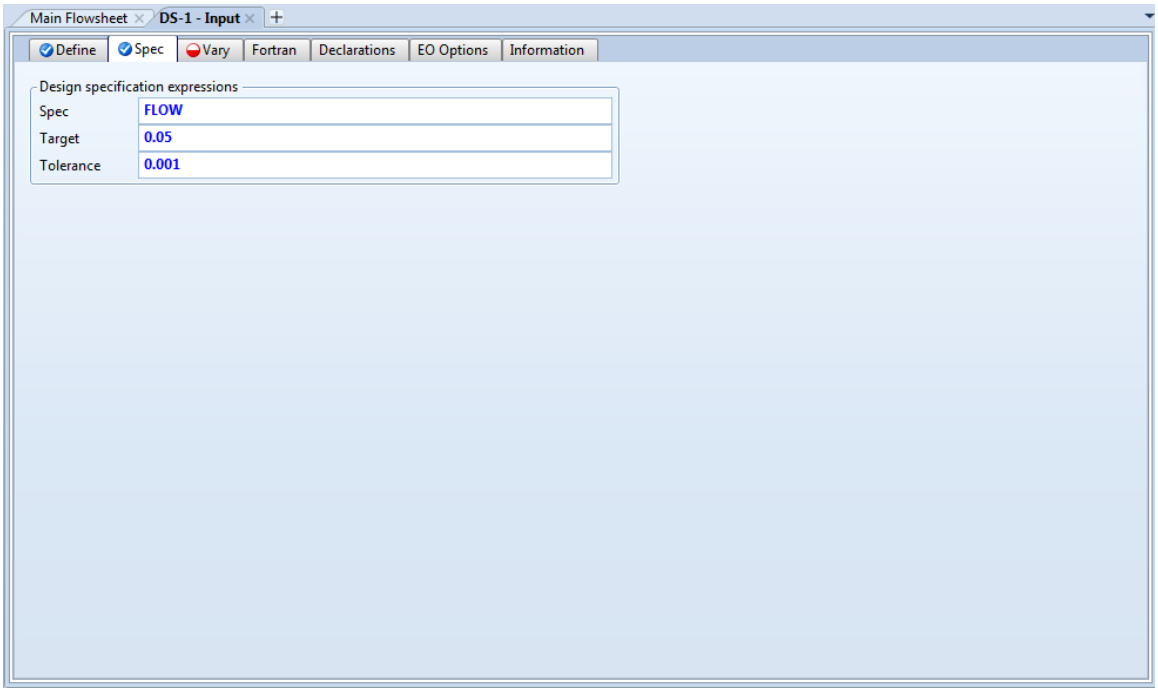


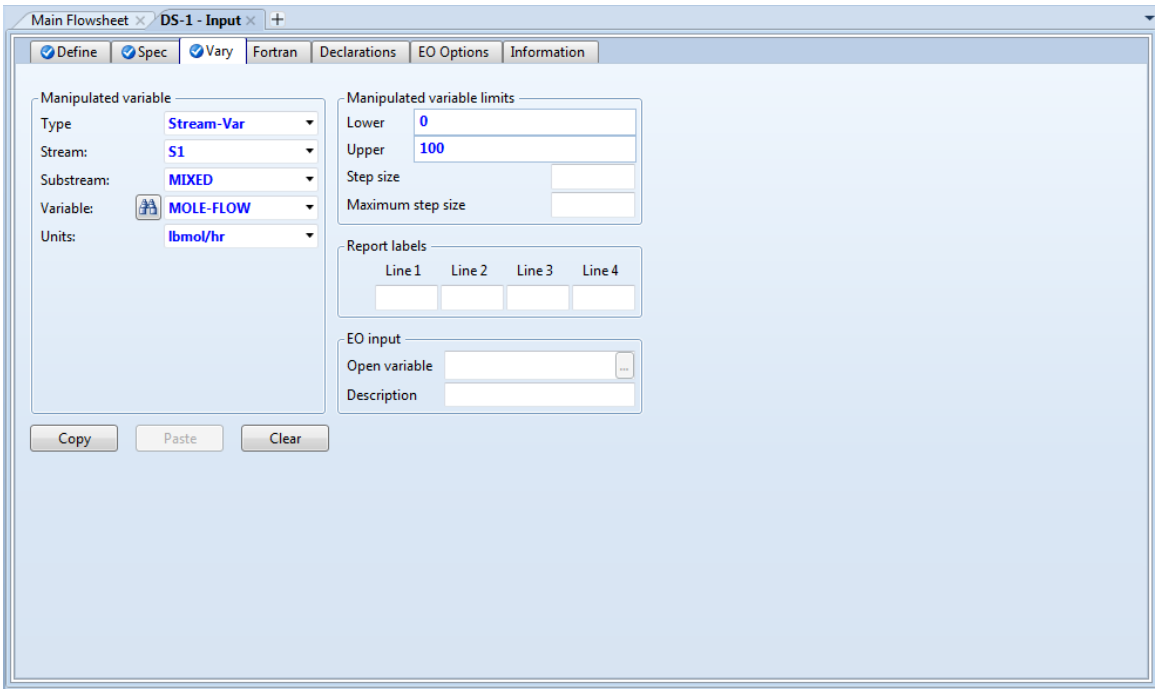
RADFRAC (Block B1) estimates



Design Specs for BLOCK B1







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	2.27	4.946512	53.29557
CO2	0	23.59	23.48042	6.66E-03
CL2	0	2.27	0.050656	9.90E-04
HCLO	0	0	0.128111	1.495381
HCL	0	0	7.55E-12	1.56E-13
N2	0	26.3	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	54.43	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	77	91.4	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)

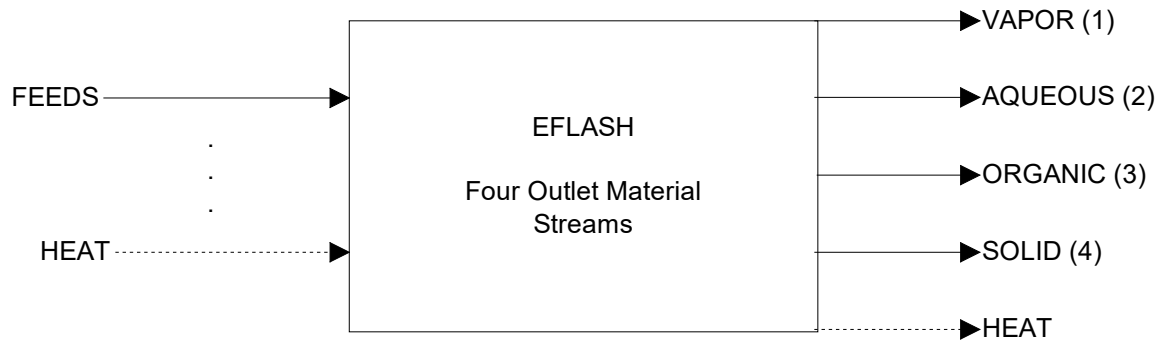


Figure 5-1 EFLASH diagram

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

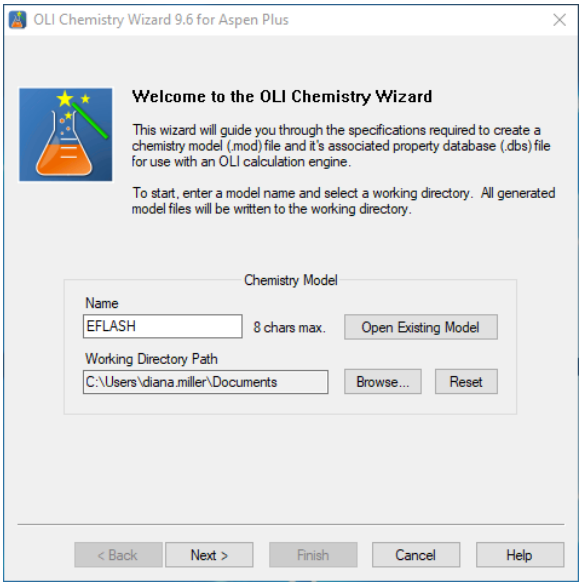
(1) - VAPOR
(2) - AQUEOUS & ORGANIC & SOLID

One Outlet Material Stream

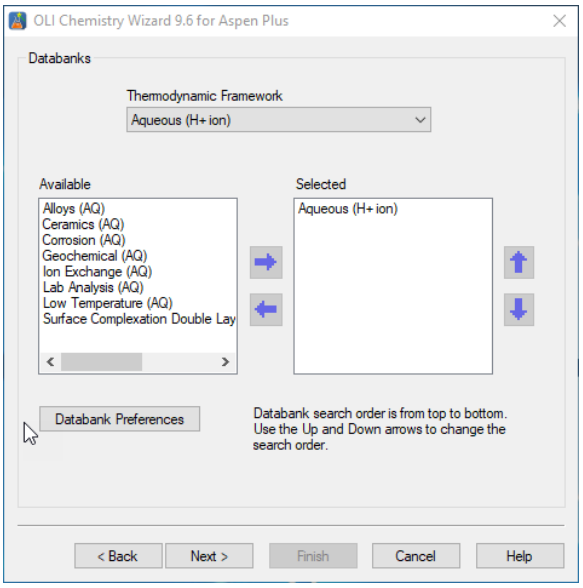
(1) - ALL PHASES

Example

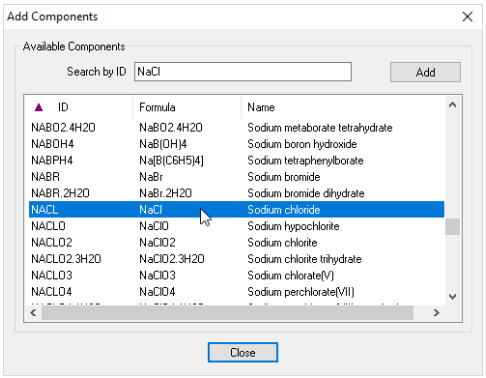
In this case we will create a chemistry model called EFLASH.

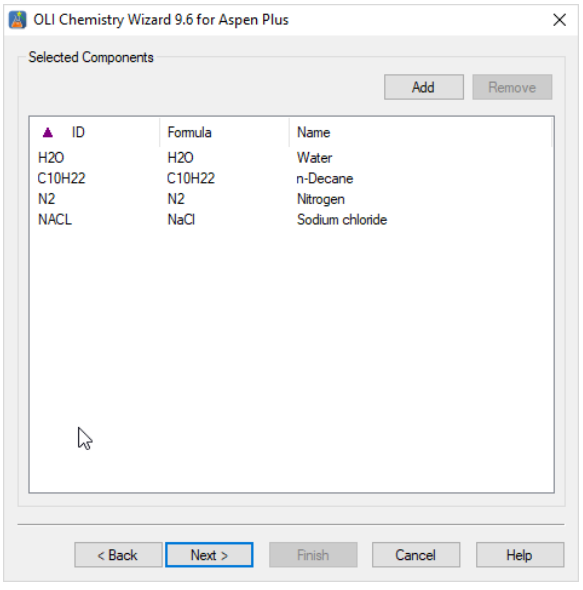


Select the Aqueous (H+ ion)

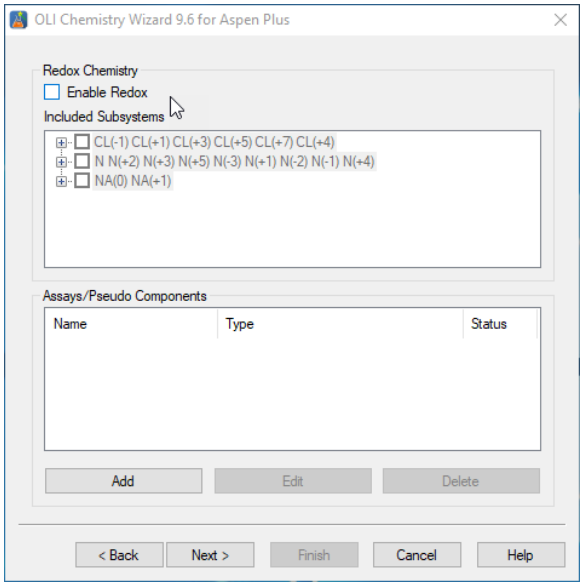


This model will contain H2O, NaCl, C10H22 and N2.

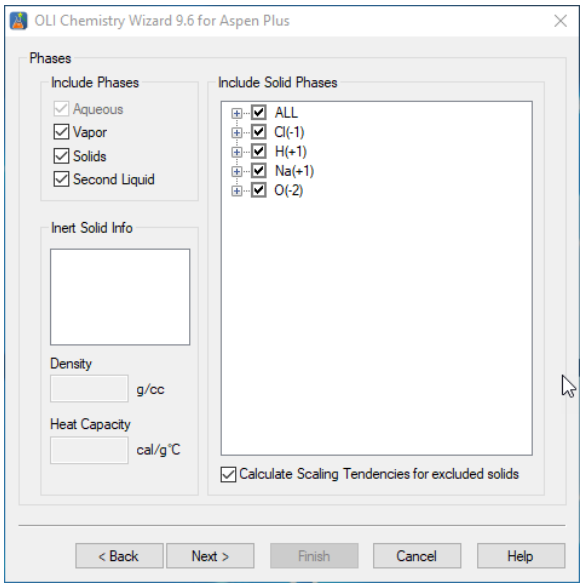




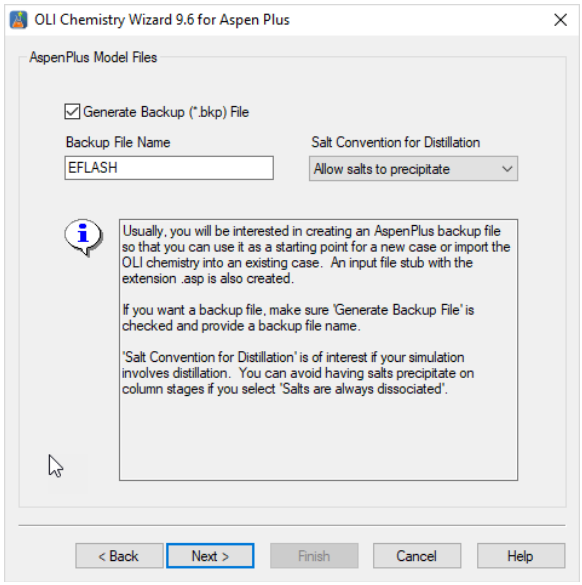
Do not Enable Redox reactions

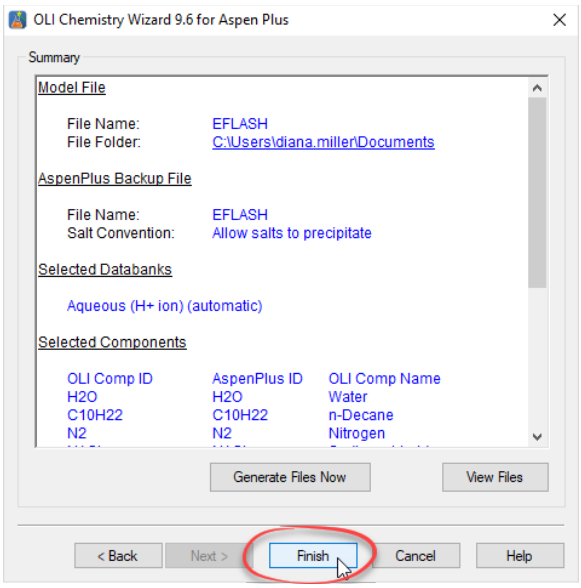


When prompted, select the second liquid (organic) phase as well as the aqueous, vapor and solid phases.



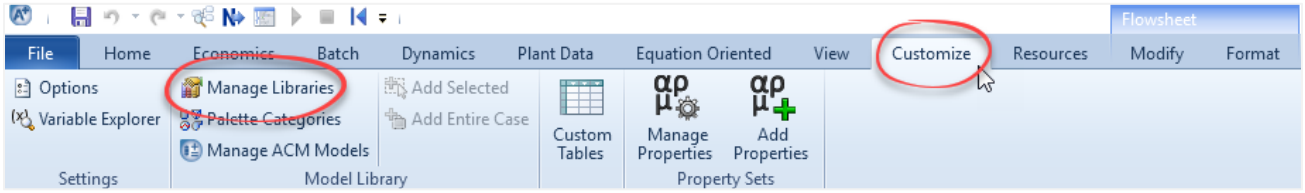
Generate the *.bkp file, and select finish.



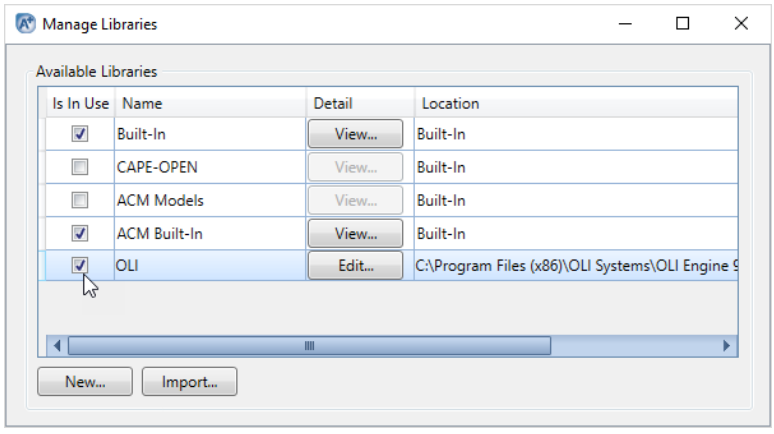


Start Aspen PLUS as you would normally and open the BKP file you just created using either the OLI Chemistry Wizard or OLI Chemistry Generator.

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).***



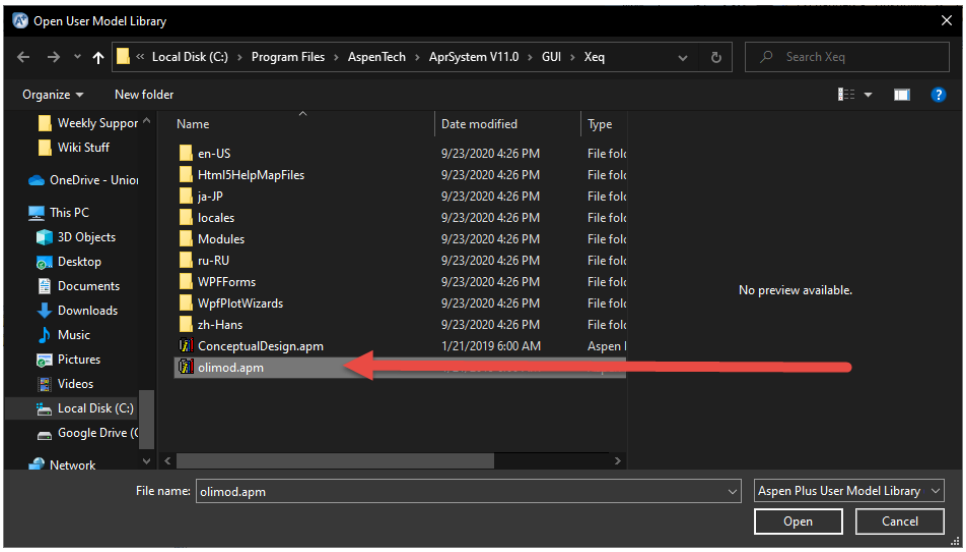
If the OLI library is not available, you will have to import it. Click the ***Import...*** button

Search for the following folder:

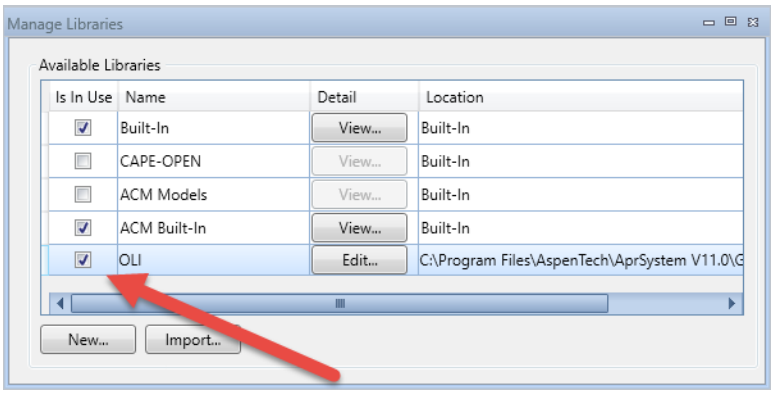
C:\Program Files\AspenTech\AprSystem **V11.0**\GUI\Xeq

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:

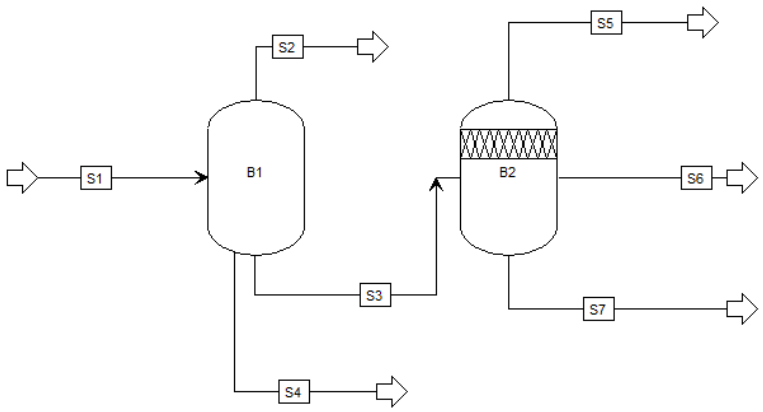


Once loaded, this library will always be available for this version on this computer.

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:

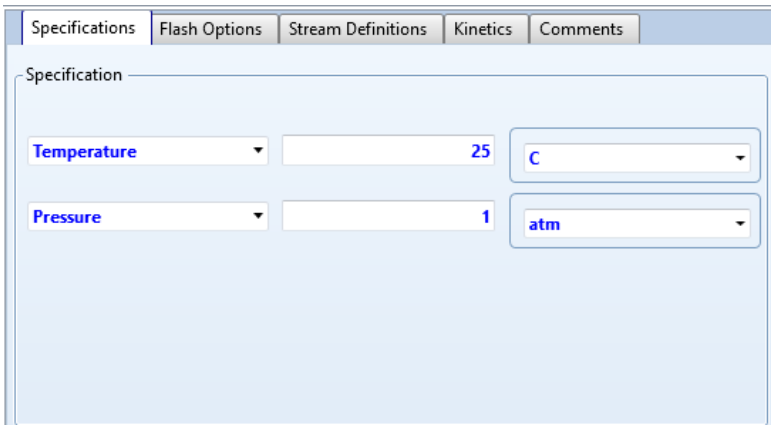


B1: EFlash4
B2: Flash3

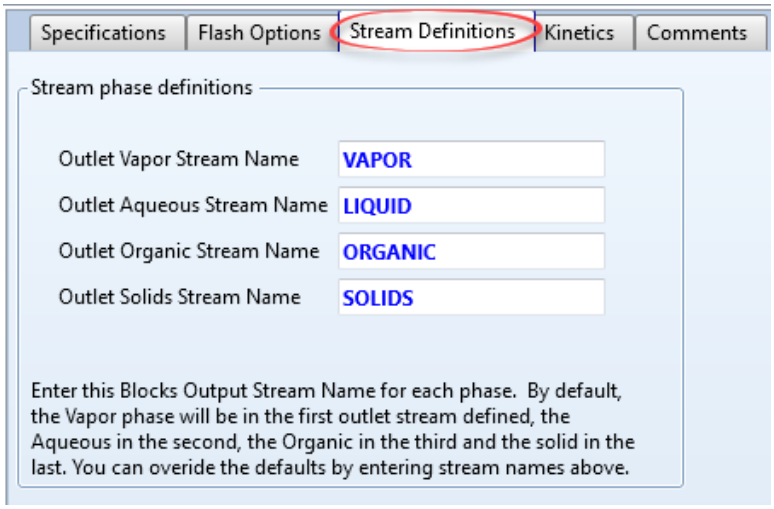
Enter the following composition for STREAM 1

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

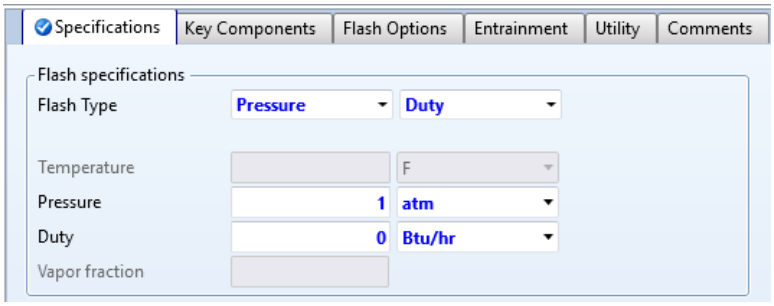
Double-click on block B1. Add the indicated temperature and pressure in the correct units.



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



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.



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..

```
FLOWSHEET
    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.

```
FLOWSHEET
   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 steam S1, aqueous and organic in stream S2 and solid in S3.

```
FLOWSHEET
   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

```
FLOWSHEET
   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)

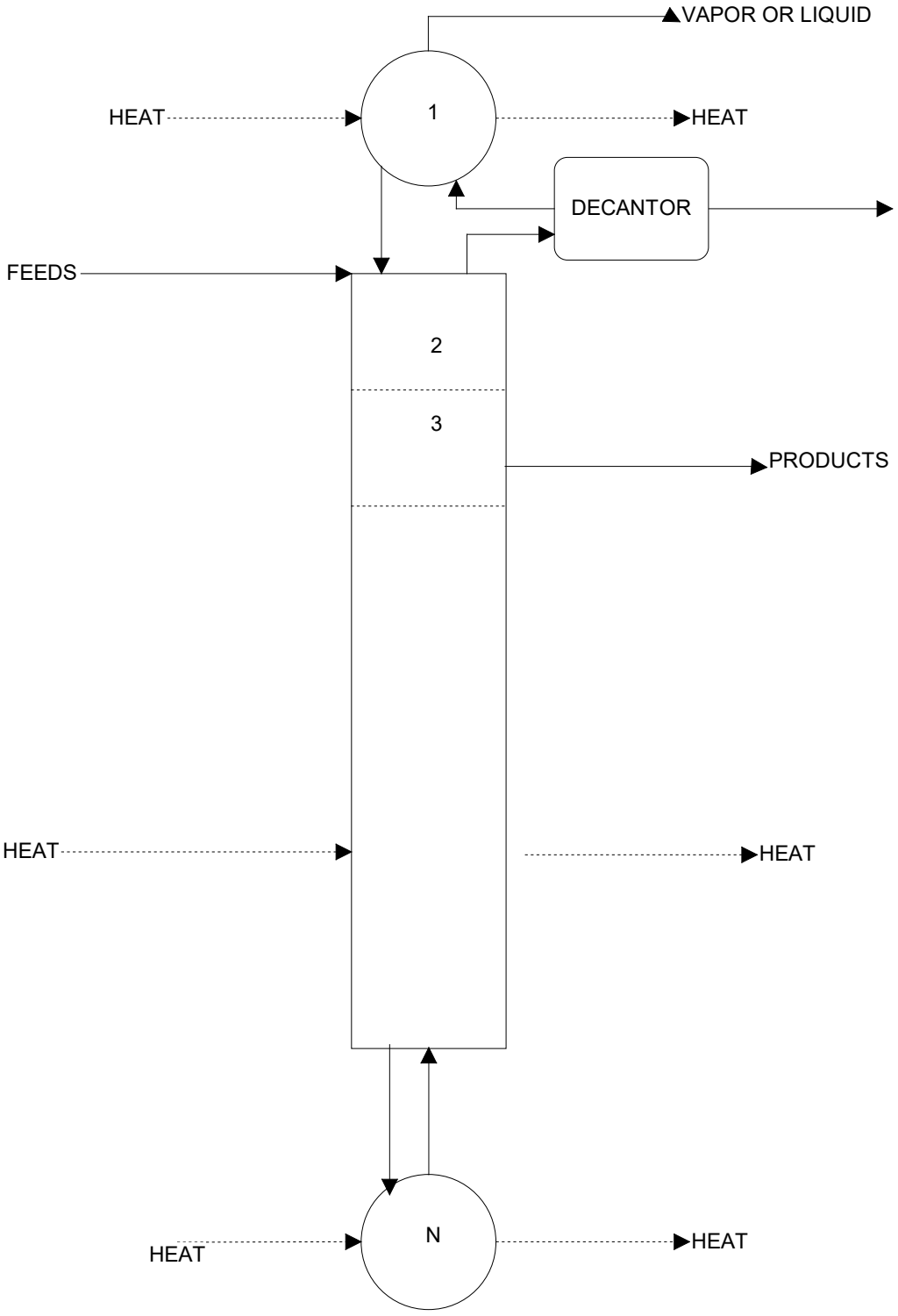


Figure 5-2 EFRACH diagram

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 *.bkp file.

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

Create the following flowsheet using the FraChem block.

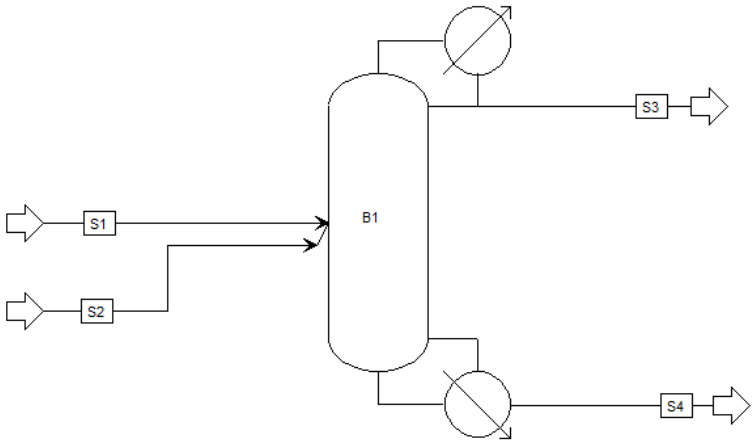
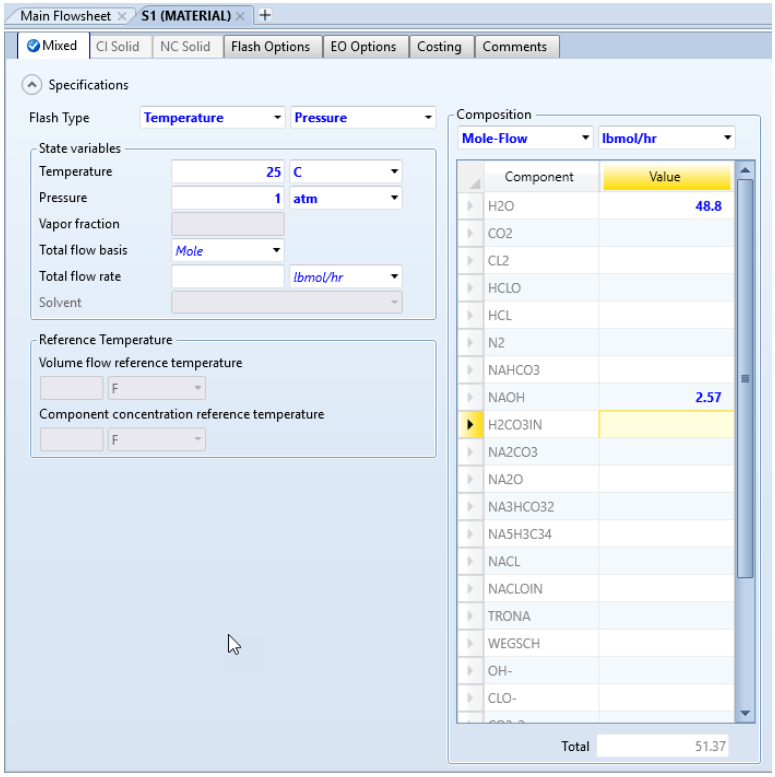
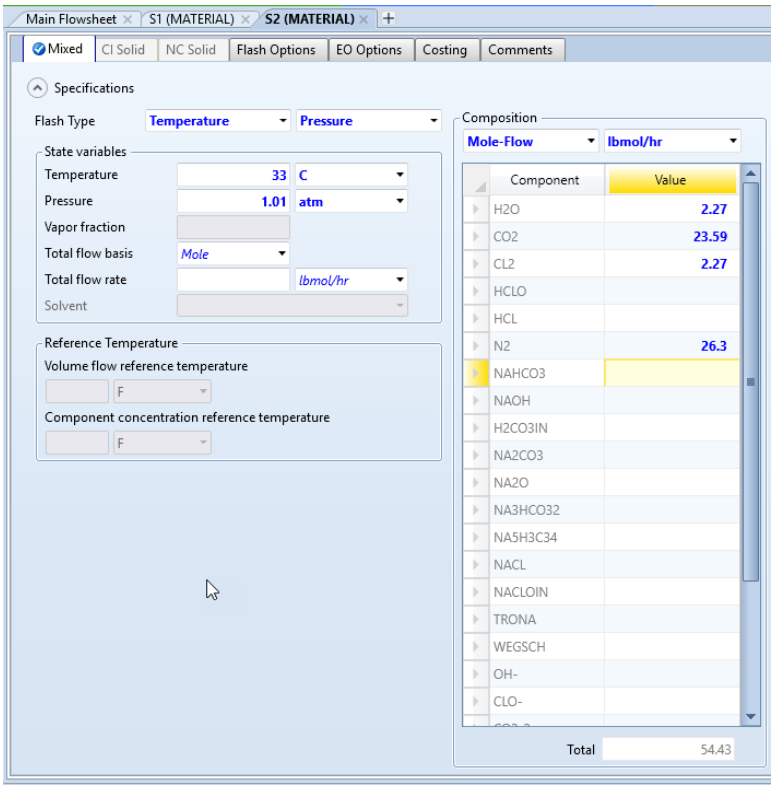


Figure 5-3 FraChem Diagram

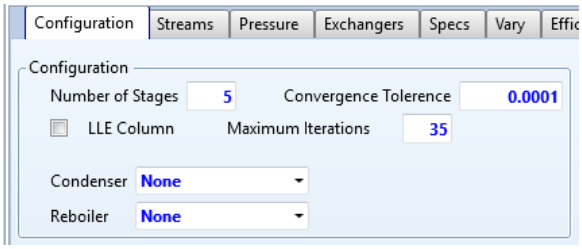
Enter the compositions for Streams 1 and 2.
The composition for Stream 1 is shown below:



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-
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:



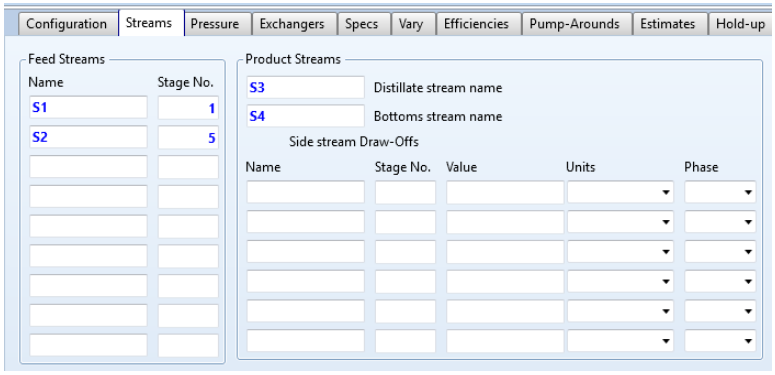
Now click on the ***Streams*** tab

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 1[6]. 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.

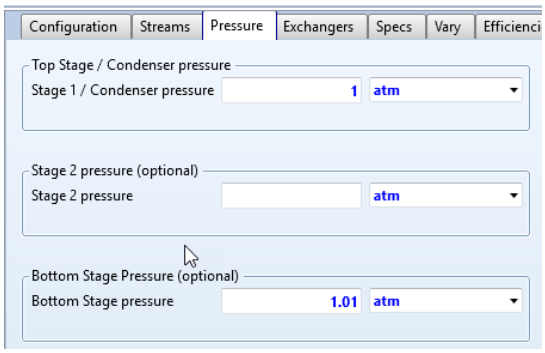
The vapor distillate stream is Stream 3 and the liquid bottoms are Stream 4. We are not using any side draws for this example.

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.

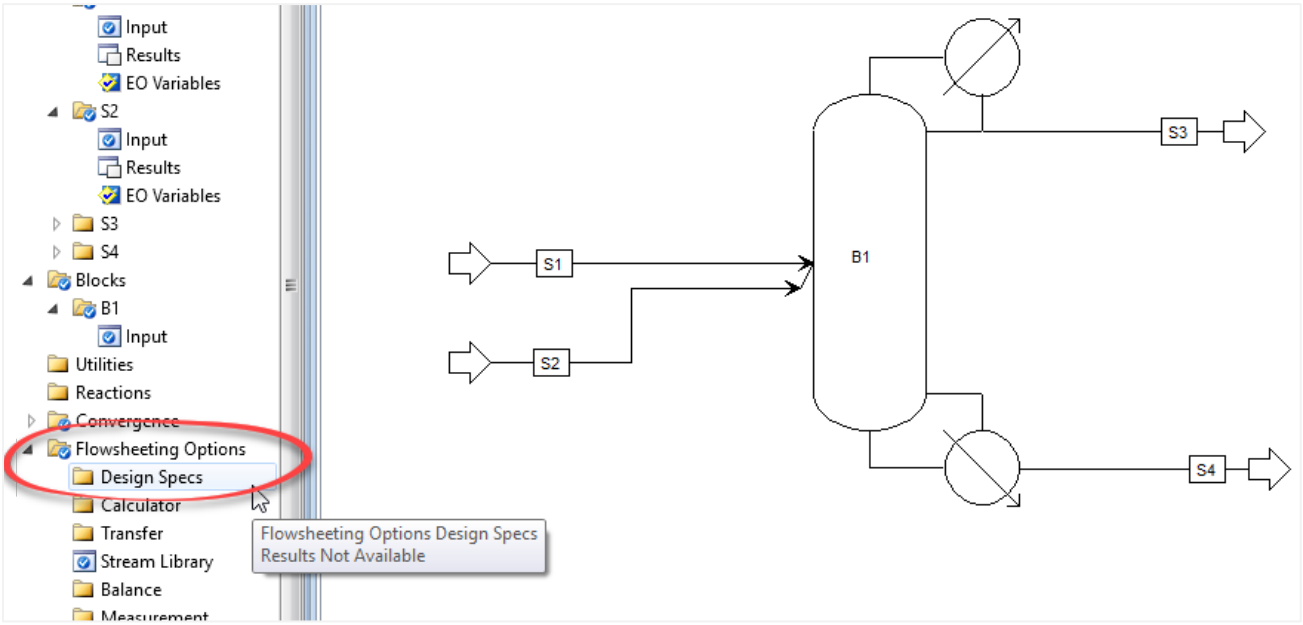


There are no exchangers or internal specifications for this unit.

Design Spec…

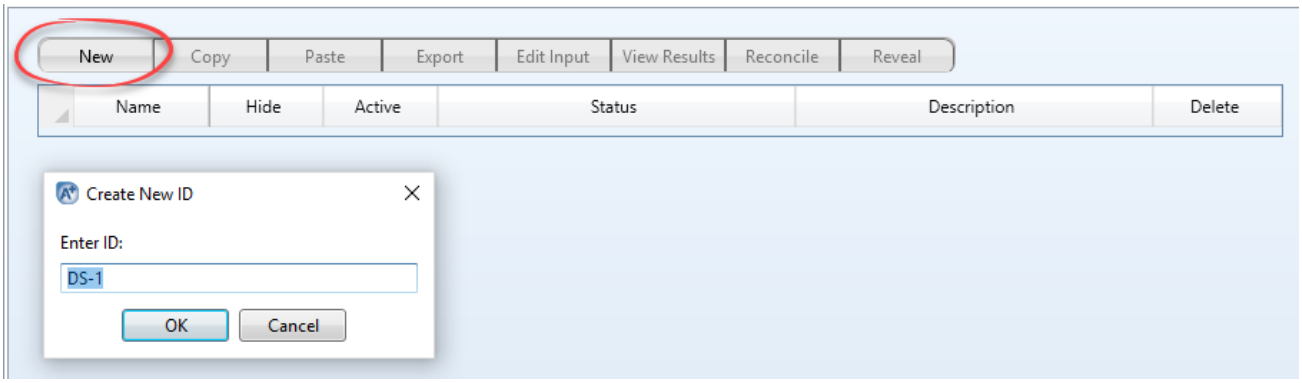
As with the example in Chapter 3, there is a design specification for this case. We will repeat the design specification here.

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.

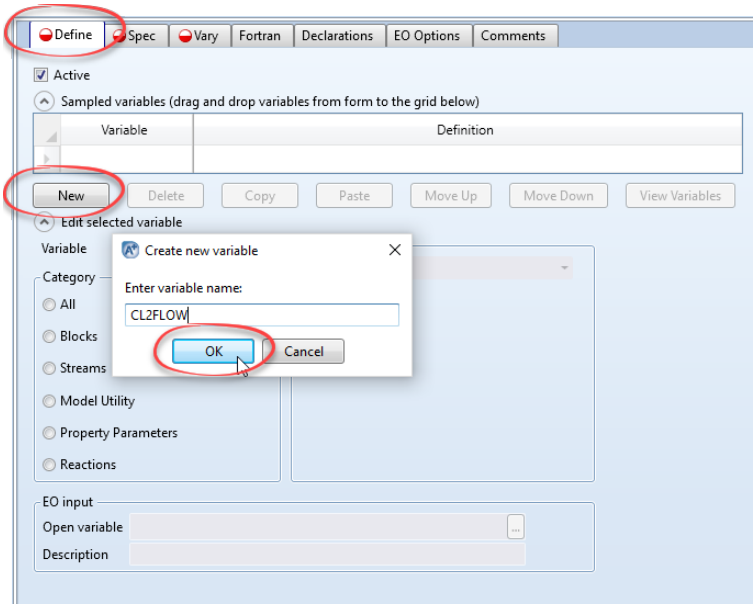
We will accept the default name DS-1. Click the **OK** button.



A new window is open.

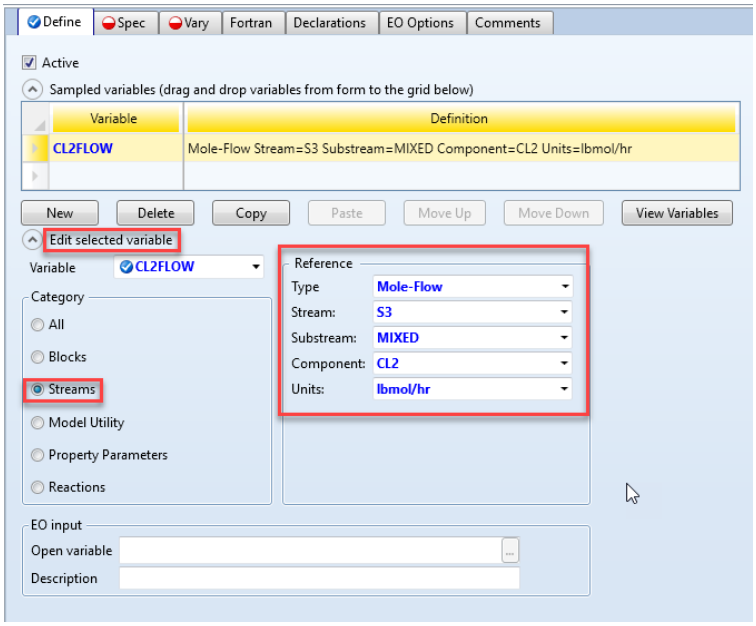
Now, we need to ***Define*** the variable for the specification.

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

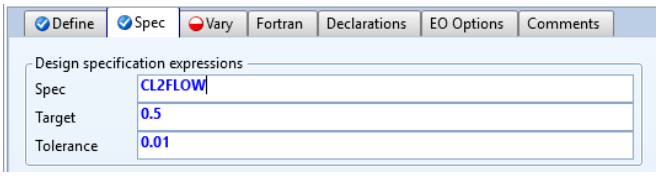


Now go to the ***Edit Selected Variable section***. The variable is part of the stream. The type is ***Mole-Flow*** and we are referring to Stream 3. The component is CL2.

Update this dialog as shown.



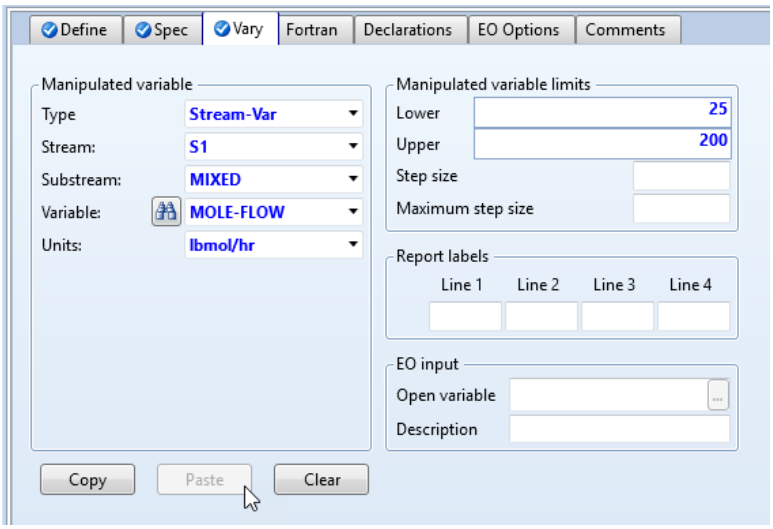
Next click the **Spec** tab. The spec variable is CL2FLOW at a value of 0.5 (in lbmol/hr). We will allow the variable to be between 0.49 and 0.51 lbmol/hr.



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.

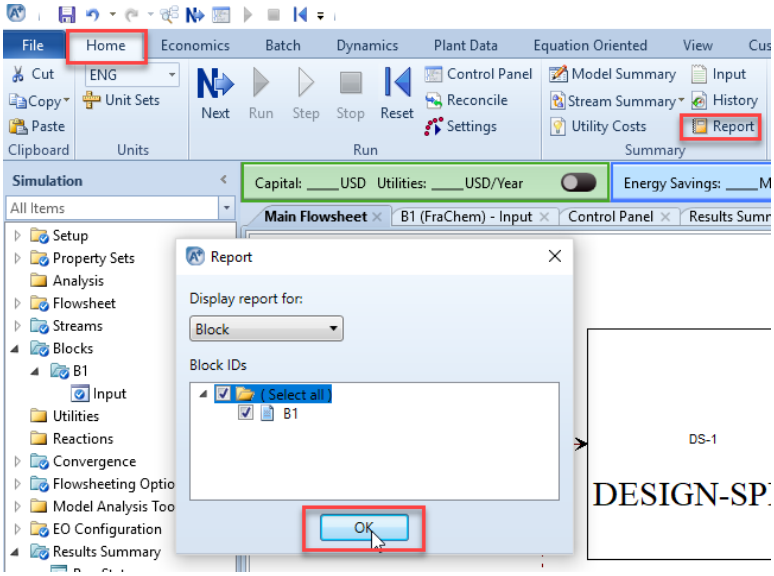
Please update the dialog as shown below.



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 ***Hom***e 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   Liquid Rate   Vapor Rate
       F             LBMOL/HR      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