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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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

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File	Home View	v Cu	stomize	R	esources					Search Aspen Kn	owledge	∞ 🔍	23 🕥
🕌 Cut	ENG -	📝 Setu	qı	Na ⁺ (Chemistry		掛 Methods	Assistant		Analysis			
🕒 Сору	🏪 Unit Sets	🌖 Con	nponen	ts 🔏 (Customize	Deres	🍫 Clean Par	ameters	🛞 DECHEMA	Estimation			
🖺 Paste		👗 Met	hods	(#) F	Prop Sets	Structure	🍫 Retrieve F	Parameters	PR DIPPR	🔏 Regression	Run Summary	Analysis	
Clipboard	Units		Na	vigate			Tools		Data Source	Run Mode			
Properties	s	*	Meth	ods - S	pecificatio	ons × 🕂							-
All Items		-	0	Global	Flowshee	t Sections	Referenced	Commen	ts				1
👂 詞 Setu	qı									<u> </u>			
🕨 📷 Com	nponents		Pro	perty r	nethods &	options —		Method	name				
🔺 🔯 Met	hods		Me	thod fi	ter	COMMON	· ·	OLI	•	Methods As	sistant		
S 🕥	Specifications		Bas	se meth	od	OLI	•			J			
Þ 🗔 S	Selected Methods		He	nry con	nponents		v	Mc	dify				
	Parameters		C P	etroleu	m calculatio	n options –		Vapor	EOS		-		
	Routes	=	F	ree-wat	er method	STEAM-TA	•	Data s	et		1		
	Tabnoly			Vatar or	Jubility	2		Liquid	gamma	GMOLI	-		
Image: Provide the second s	mistry		V	vater sc	nubility	3		Data s	et		1		
🕨 📷 Prop	perty Sets		E	lectroly	te calculatio	n options -		Liquid	molar onthalow				
📜 Data	a		C	hemist	y ID	INTRO	•						
👂 🚞 Estir	mation			/ Llse t	rue compo	nents		Liquid	molar volume	VLMXO1			
📜 Ana	lysis			030 0	rue compo	nemes		Hei	at of mixing				
👂 🔜 Cust	tomize	*						Poy	nting correction				
								Use	e liquid reference	state enthalpy			
Prope	erties								,				
⊐{ [©] Simul	lation												
Safet	y Analysis												
🎸 Energ	gy Analysis					D.	<u>.</u>						
		Ŧ											
Required Pr	roperties Input Co	mplete	Check	Status						10	0% Θ	-0	÷

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	HVMXO1	KVMXLP	KVMXLP01
HLMX	HLMXO1	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	HLOO		
GV	GV00		
GL	GL00		
SV	SV00		
SL	SLOO		
VV	00VV		
VL	VL01		
MUV	MUV01		
MUL	MUL01		
KV	KV01		
KL	KL01		
DV	DV01		
DL	DL01		
SIGL	SIGL01		
HSMX	HSMX01		

PHIL PHILOO

Property Mode	el Set OpCo	odes		Affecte	ed	
				Propert	ties	
				•		
PHIVMX	PHVMXOLI	1		PHIVM	K	
PHILMX	PHLMXOLI	1		PHILMX	X	
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	KVOSTLP	1		KVMX	KV	
KLMX	KL2SRVR	1		KLMX		
DVMX	DV1CEWL	1		DVMX		
DLMX	DL1WCA	1		DLMX		
SIGLMX	SIG2HSS	1	1	SIGLMX	K	
PHIV	ESIG0	1		PHIV	GL	SL
PHIL	PHILOLI	1		PHIL		
DHV	ESIGO	1		HV	HL	SL
PL	PLOXANT	1		HL	GL	SL
DHVL	DHVLWTSN	1		HL	SL	
DHLPC	DHLPC00	1		HL	SL	
DGV	ESIGO	1		GV		
PHILPC	PHILPC00	1		GL	SL	
DSV	ESIGO	1		SV		
VV	ESIGO	1		VV		
VL	VLORKT	1		VL		
MUL	MULOANDR	1		MUL		
KVPC	KVOSTPC	1		KV		
VV	esrk0	1		KV		
KL	KLOSR	1		KL		
DV	DVOCEWL	1		DV		
DL	DLOWCA	1		DL		
SIGL	SIGOHSS	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	PAG+ AG+ AG+
AGCL2ION	P AGCL2- AGCL2-2 AGCL2
AGSO4ION	P AGSO4- AGSO4- AGSO4-
ALION	P AL+3 AL+3 AL+++

P ALF2+ ALF2+

P ALF+2 ALF+2 ALF++

ALF2+

ALFION

ALF2ION

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 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 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.

칠 oli c	hemistr	y Wizard 12.0 for A	Aspen Plus		×
		Welcome to This wizard will gui chemistry model (r for use with an OL To start, enter a me model files will be w	to the OLIC de you through the nod) file and its ass I calculation engine odel name and sele written to the worki	Chemistry W e specifications requisociated property date. e. ect a working directing directing directory.	<i>Tizard</i> ired to create a stabase (.dbs) file ory. All generated
			Chemistry Model		
	Name				
	<u> </u>		8 chars max.	Open Existing M	lodel
	Worki	ng Directory Path			
	C:\Us	ers\james.berthold\C	neDrive - OLI (Browse	Reset
	< Ba	ack Next >	Finish	Cancel	Help

Figure 2-1 Specifying the model name and location

	- Chemistry Model	
Name		
Neutral1	8 chars max.	Open Existing Model
Working Directory Path		
C:\Users\james.berthold	\OneDrive - OLI {	Browse Reset

Click the *Next*> button to continue

MSE (H3O+ion)	ework	~	
Available	Selected		
Corrosion (MSE) Geochemical (MSE) Surface Complexation Double Lay Urea (MSE)	MSE (H3O+ io	n)	t t
Databank Preferences	Databank search orde Use the Up and Down search order.	er is from top to bottom a arrows to change the	1. B

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.

dd Components		N		
Available Components		43		
Search by ID			Add	
▲ ID	Formula	Name		^
AALS042.12H20	NH4AI(SO4)2.12H	Ammonium aluminum sulfate dodec	ahydrate:	
ACENITRILE	CH3CN	Acetonitrile		
ACET2	C4H8O4	Acetic acid, dimer		
ACETACID	CH3COOH	Acetic acid		
ACETALDEHD	C2H4O	Ethanal		
ACETONE	CH3COCH3	Acetone		
ACETYLENE	C2H2	Acetylene		
ACIDSO0	C22H36	Acid soluble oil (0)		
ACIDS01	C10H16	acid soluble oil - light		
ACIDS02	C14H20	acid soluble oil - 20-30%		
ACIDS03	C18H28	acid soluble oil - 60-70%		v
			>	

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).

 \times Add Components Available Components Search by ID NH3 Add Name ۸ ID Formula Δ NEM. C6H13NO N-Ethylmorpholine NEMHCL N-Ethylmorpholine hydrochloride O(C2H4)2NC2H5.... NEOC5H6F6 Neo-C5H12-(HF)6 Neopentane hexahydrofluoride NEOPENTANE C5H12 Neopentane NH2CL NH2CI Chloramide NH3 NH3 Ammonia NH30H2S04 Hydroxylamine sulfate (NH30H)2SO4 NH3SO3 NH3SO3 Sulfamic acid NH42CO3 (NH4)2CO3 Ammonium carbonate NH42C03.1H20 Ammonium carbonate monohydrate (NH4)2C03.H20 NH42M0207 (NH4)2Mo207 Ammonium dimolybdate < ъ Close

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.

👔 oli cł	nemistry Wiz	ard 12.0 for Aspen Pl	us			×
Selected	d Components					
				Add	Remove	
A I H2O CO2 H2SO4 HCL NAOH NH3 SO2	D 4	Formula H2O CO2 H2SO4 HCI NaOH NH3 SO2	Name Water Carbon dioxide Sulfuric(VI) acid Hydrogen chlor Sodium hydroxi Ammonia Sulfur dioxide	d ride ide		
	< Back	Next >	Finish	Cancel	Help	

Figure 2-5 the added components

Click the **Next>** button.

📓 OLI Chemistry Wiz	zard 12.0 for As	pen Plus		×
Redox Chemistry				
Enable Redox				
Included Subsyster	ns			
⊕ □ C(0) C(+2) ⊕ □ CL(-1) CL(-	C(+4) +1) CL(+3) CL(+5) N(+3) N(+5) N(-3 +1)) S(+3) S(+4) S(+3)) CL(+7) CL(+4) 3) N(+1) N(-2) N(-1) N 5) S(+6) S(+7) S(+8) S	(+4) 6(0)	
Assays/Pseudo Cor Name	mponents Type	e	Status	
Add		Edit	Delete	
< Back	Next >	Finish	Cancel He	elp

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.

Include Phases	Include Solid Phases
Aqueous Vapor Solids Second Liquid	
Density	
g/cc Heat Capacity cal/g°C	

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.

Component Name	AspenPlus ID	AspenPlus Allas
Water [H2O]	H20	H20
Carbon dioxide [CO2]	CO2	C02
Sulfuric(VI) acid [H2SO4]	H2SO4	H2SO4
lydrogen chloride [HCL]	HCL	HCL
Sodium hydroxide [NAOH]	NAOH	NAOH
Ammonia [NH3]	NH3	H3N
Sulfur dioxide [SO2]	S02	02S
arbonic acid [H2CO3]	H2CO3	H2CO3
Sulfurous(IV) acid [H2SO3]	H2SO3	H2SO3
ydrogen chloride monohydrate [HCLW1	
lydrogen chloride dihydrate [HCL	HCLW2	
lydrogen chloride trihydrate [HCL	HCLW3	
Sodium carbonate [NA2CO3]	NA2CO3	
varogen chloride dinydrate [HCL varogen chloride trihydrate [HCL odium carbonate [NA2CO3] ow only components with errors	HCLW2 HCLW3 NA2CO3	

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.

Backup	File Name	Salt Convention for Distillation
Neutral	1	Allow salts to precipitate $$
	If you want a backup file checked and provide a 'Salt Convention for Dist involves distillation. You column stages if you sel	e, make sure 'Generate Backup File' is backup file name. illation' is of interest if your simulation u can avoid having salts precipitate on ect 'Salts are always dissociated'.

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.

🔏 OLI Chemistry Wizard 12.0 for Aspen Plus						
Summary						
Model File			÷.			
File Name: File Folder:	Neutral1 <u>C:\Users\james</u>	.berthold\OneDrive	L - OLI System			
AspenPlus Backup File						
File Name: Salt Convention:	Neutral1 Allow salts to pr	ecipitate				
Selected Databanks						
MSE (H3O+ ion) (aut	omatic)					
Selected Components						
OLI Comp ID H2O CO2	AspenPlus ID H2O CO2	OLI Comp Name Water Carbon dioxide				
	Generate Files	Now	View Files			
< Back Ne	ext > Fini	sh Cancel	Help			

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.

OLI Chemistry Wizard 12.	0 for Aspen Plus		2
Summary			
Model File			
File Name: File Folder:	Neutral1 <u>C:\Users\jame</u> :	s.berthold\OneDrive - OLI Systen	
AspenPlus Backup File			1
File Name: Salt Convention:	Neutral1 Allow salts to p	recipitate	
Selected Databanks			
MSE (H3O+ ion) (aut	tomatic)		
Selected Components			
OLI Comp ID H2O CO2	AspenPlus ID H2O CO2	OLI Comp Name Water Carbon dioxide	
	Generate File	s Now View Files	
< Back N	ext > Fir	hish Cancel He	р
Figure 2-12	^o 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:

🐼 Upgrade databanks 🛛 🕹
This file contains one or more retired databanks: PURE856, PURE93, PURE10, PURE11, PURE12, PURE13, PURE20, PURE22, PURE24, and AQU92. Aspen Plus can upgrade them to PURE39 and AQUEOUS automatically. Your simulation will run, but results may be different, because newer databanks may have more accurate property parameters. Or you can choose to continue without upgrading and select the databanks yourself. If you do not have a valid databank, your simulation may fail. To continue using the retired databanks, you must exit the program then restore APLDB which contains these databanks. See Online Help "Maintaining Access to Retired Databanks" for more information.
✓ Upgrade retired databanks
ОК

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.

🐼 i 🔒 🔊 - (° - 🎨 🕪 🌆	▶ 🔳 🚺 ₹ Neu	ıtral1.bkp - Aspen P	lus V14 - asp	DenONE	Flows	heet		N	-	×
File Home Economics Batc	h Dynamics Plant Data	Equation O View	Customize	Resources	Modify	Format	Search Asp	en Knowledge	P 🛯 🛛	23
A →■Reconnect → ↓ Join	✓ 3D Icons	Temperature	🗌 Mass F	low Rate		GLOB	AL +	View Parent	🚯 Export	
🗥 💥 Break 🛛 🚹 Reroute Strea	am Heat/Work/Power	Pressure	🗌 Mole F	ow Rate		🖌 Sh	ow All	View Child	Move Selection	
🚽 👤 Insert 🛛 📮 Align	Show Status™	Vapor Fraction	Nolume	e Flow Rate	Display Options	, 🔒 Lo	ck Flowshee	t 😤 Import		
Flowsheet	Unit Operations	Stream	n Results	G.			Section	Hier	archy	
Simulation <	Capital:USD Utiliti	es:USD/Year	00	Energy Sa	vings:	_MW (_	%) (Exchange	ers - Unk 🕨 🔗	23
All Items 🔹	Main Flowsheet × +]								-
🕨 📷 Setup									-	
Property Sets									i	
a Analysis										
Flowsheet										
Streams										
Sensors										
Utilities										
Reactions										
Convergence										
Flowsheeting Options										
Model Analysis Tools										
EO Configuration										
Datasheets										
Dynamic Configuration										
Plant Data										
Þ 🚞 AI										
	Model Palette								•	μ×
	Miv	ers/Splitters	narators	Exchanger	colu	mns	Reactors	Pressure Changer	Manipulator	4.5
Safety Analysis					000		. louceors	sobure changers	manipulator	
🚯 Energy Analysis		> - <	-		•					
*	MATERIAL	Vixer FS	olit	SSplit						
Flowsheet Not Complete Check Sta	itus						1	96% Θ	•	*

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:

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 2-1 Stream Definitions

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	РН
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

			Ma	terial				
Stream Name	Units	S1	S2	S3	S4	S5	S6	S7
Description								
From				B1	B1	B2	B2	
То		B1	B1	B2				B2
						CON		
Stream Class Maximum Relative		CONVEN	CONVEN	CONVEN	CONVEN	VEN	CONVEN	CONVEN
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 Molar Liquid		0	0	0	1		0	0
Fraction		1	1	1	0		1	1
Molar Solid		0	0	0	0		0	0
Mass Vapor		0	0	0	U		0	0
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
			-	-	-		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
Н2О	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.

🔊 i 🔒 🤊 - 🤭 🥳 险 📓	🔄 🕨 🔳 🔰 🗧 👘 Neutral1.bkp - Aspen Plus V12.1 -	aspenONE P	Report		– 🗆 ×
File Home Economics Bat	tch Dynamics Plant Data Equation C View Custom	ize Resources Stream	n Summary Search	h Aspen Knowledge	🗵 🕥 a 🔍
Default 👻	Full 🔹 * 🏠 🗹 Total	✔ Mole ✔ Mo	ole 🧖		📸 Send to Excel/ASW
🗐 Save 🔣 Save as New	🔚 Save 🕵 Save as New 🖉 Substreams	✔ Mass ✔ Ma	iss of the		E Send to Flowsheet
Show Child Hierarchy Streams	General Options I Phases	✓ Volume	Properties	Options Options	🝙 Copy All
Stream Group 🕞	Template 🕞 Stream Summary Options	Flows Composi	ition P	roperty Sets	Report
Simulation <	Capital:USD Utilities:USD/Year 🛇 🔵	Energy Savings:	MW (%)	Exchange	ers - Unkn 🕨 🗢 🔀
All Items *	Main Flowsheet × DS-1 - Input × Control Pane	I × Results Summary	/ - Streams (All) 🗙	S6 (MATERIAL) - Result	ts (Default) × + 🔹
🔺 🔯 S2 🔺	Material Viel % Current With % Current Detroid	um Dahmara Sali	ide Ctatur		
💽 Input	Waterial Vol. // Curves Wit, // Curves Petrole	um Polymers Soli			
🖉 EO Variables —		Units	S6 •		
> 🕞 S3	Molar Density	lbmol/cuft	3 / 5688		
Þ 🐻 S4	Mars Density	lb (suft	62 0071		
> S5 =	Mass Density	ib/cuit	03.0071		
	Enthalpy Flow	Btu/hr	-/.3/211e+0/		
Results	Average MW		18.4812		
🧭 EO Variables	+ Mole Flows	lbmol/hr	597.256		
🔺 📷 S7	+ Mole Fractions				
🕑 Input	+ Mass Flows	lb/hr	11038		
Variables	Mass Fractions				
A 🔯 Blocks	Volume Flow	cuft/hr	172,773		
▷ 📷 B1	рН		9.00132		=
▶ 📷 B2	> sado propertiesz				
Sensors					Ţ
Properties		I			
	Model Palette				→ † ×
1 State to Annalyzia	Mixers/Splitters Separators	Exchangers Co	olumns Reacto	rs Pressure Changers	s Manipulator: 🔸 🕨
				ğ	
🚯 Energy Analysis		🔵 🗸 🗋	🔟 🖵 📙	-	
*	MATERIAL Flash2 Flash3	Decanter S	ep Sep	2	
Results Available Check Status			· · · ·	100% 🕞	•

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

Main Flowsheet × S1 (MATERIAL) - Input >	< +					•
Mixed CI Solid N	NC Solid Flash Opt	tions EO Options Cos	ting	Information			
Specifications							✓ Component Attributes
Flash Type Ten	nperature 🔹	Pressure -	Cor	mposition			 Particle Size Distribution
State variables			M	ole-Flow 🔻	lbmol/hr	•	
Temperature	25	С •		Component	Value	*	
Pressure	1	atm 🔹	•	H2O	48.8	_	
Vapor fraction			•	CO2		-	
Total flow basis	Mole 🔹		•	CL2			
Total flow rate		lbmol/hr 🔹	•	HCLO			
Solvent		-		HCL			
Reference Temperatur	re			N2			
Volume flow reference	e temperature		•	NAHCO3			
F	T			NAOH	2.57		
Component concentry	ation reference temp	erature		H2CO3IN		-	
F	-			Total	51.37		

Caustic Feed Stream (S1)

Feed Stream (S2)

Main Flowsheet ×/S2	$(MATERIAL) \times (+)$							
Mixed CI Solid	NC Solid Flash O	ptions EO	Options Cost	ing	Information			
 Specifications 								✓ Component Attributes
Flash Type To	emperature	 Pressure 	-	Con	nposition			Particle Size Distribution
- State variables				Mo	le-Flow •	lbmol/hr	•	
Temperature	33	С	•		Component	Value	*	
Pressure	1.01	atm	•		H2O	2.27		
Vapor fraction				•	CO2	23.59	-	
Total flow basis	Mole	•		•	CL2	2.27		
Total flow rate		lbmol/hr	-	•	HCLO			
Solvent			· ·	•	HCL			
Reference Temperat	ure			•	N2	26.3		
Volume flow referen	ice temperature			Þ	NAHCO3			
F T					NAOH			
Component concen	tration reference tem	perature			H2CO3IN		*	
F					Total	54.43		

RADFRAC (Block B1) configuration (5 stages)

Main Flowsheet × B1 (RadFrac) × +	
	Condenser Reboiler 3-Phase Information
Setup options	
Calculation type	Equilibrium 🔫
Number of stages	5 Stage Wizard
Condenser	None -
Reboiler	None 👻
Valid phases	Vapor-Liquid -
Convergence	Standard -
Operating specifications	
· · · · · · · · · · · · · · · · · · ·	· · · · · · · · · · · · · · · · · · ·
· · · · · · · · · · · · · · · · · · ·	• • •
Free water reflux ratio	0 Feed Basis

RADFRAC (Block B1) streams

Com	iguration	Streams 🎯	Pressure	Condenser R	eboiler 3-Pha	e Information	1			
ed str	reams —									
	Name	Stage		Convention						
S1		1	Above-Si	tage						
S2		5	On-Stag	e	-					
duc	Name	Stage	Phase	e E	Basis F	low U	nits Flow	/ Ratio	Feed Specs	
35		1	vapor	MOLE		ibmoi,			Feed basis	
S4		5	Liquid	Mole		Ibmol	/hr		Feed basis	
udo	streams -									
	Name	Pseudo Stre Type	am Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparound ID	Pumparound Conditions	Flow	Units

RADFRAC (Block B1) pressure

Configuration 🛛 🕜 Strea	ams 🕜 Pressure	Condenser	Reboiler	3-Phase	Information		
Top / Bottom		•					
op stage / Condenser pres	sure						
age 1 / Condenser pressur	e 1	atm	•				
age 2 pressure (optional) -							
Stage 2 pressure		atm	•				
Condenser pressure drop		psi	Ŧ				
ressure drop for rest of col	umn (optional) —						
) Stage pressure drop		atm	-				
		psi	Ŧ				

RADFRAC (Block B1) estimates



Design	Specs	for	BLOCK	B1

- --- - -

Main Flowsheet × DS-1 - Input × +	Declarations EO Options Information
Active Sampled variables (drag and drop varia Variable Definition FLOW Mole-Flow Strea	ables from form to the grid below) am=S3 Substream=MIXED Component=CL2 Units=Ibmol/hr
New Delete Copy	Paste Move Up Move Down View Variables
Variable © FLOW - - Category © All © Blocks © Streams © Model Utility © Property Parameters © Reactions	Reference Type Mole-Flow • Stream: S3 • Substream: MIXED • Component: C12 • Units: Ibmol/hr •
EO input Open variable Description	

Main Flowsheet ×	DS-1 - Input ×	÷
------------------	----------------	---

Spec 🝚 Vary Fortra	n Declarations	EO Options	Information						
tion expressions									
FLOW	FLOW								
0.05									
0.001									
	ipec Vary Fortrar tion expressions FLOW 0.05 0.001	ipec Vary Fortran Declarations tion expressions FLOW 0.05 0.001	ipec →Vary Fortran Declarations EO Options tion expressions FLOW 0.05 0.001	pec →Vary Fortran Declarations EO Options Information tion expressions FLOW 0.05 0.001					

Main Flowsheet $ imes / 1$	DS-1 - Input × +	
🔇 Define 🛛 🔇 Spec	: 🔗 Vary Fortran	Declarations EO Options Information
Manipulated variabl Type Stream: Substream: Variable:	e Stream-Var S1 MIXED MOLE-FLOW Ibmol/hr	Manipulated variable limits Lower 0 Upper 100 Step size Maximum step size Report labels Line 1 Line 2 Line 3 Line 4 EO input Open variable Description
Сору	Paste Clear	

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 Ibmol/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 Ibmol/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	7 7	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 Ibmol/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)





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.

📓 OLI Chemistry	Wizard 9.6 for Asp	en Plus		\times
	Welcome to th This wizard will guid chemistry model (m for use with an OLI To start, enter a mo model files will be w	e OLI Chemi le you through the od) file and it's as calculation enginu del name and sel ritten to the worki	stry Wizard e specifications required sociated property datab e. e. e. e. e. e. e. e. e. e. e. e. e.	l to create a ase (.dbs) file All generated
		Chemistry Model		
Name	21	0	On an Existing Made	
EFLA		8 chars max.	Open Existing Mode	1
Worki C:\Us	ng Directory Path ers\diana miller\Docu	ments	Browse Res	et
0.100			biomac	
< Ba	ack Next >	Finish	Cancel	Help

Select the Aqueous (H+ ion)

Databanks	Thermodynamic Fra Aqueous (H+ion)	mework		~	
Available Alloys (AQ) Ceramics (A) Geochemica Ion Exchang Lab Analysis Low Temper Surface Con	Q) Q) (AQ) (AQ) (AQ) ature (AQ) aplexation Double Lay	†	Selected Aqueous (H	+ ion)	1
Databank	Preferences	Datab Use th search	ank search or ne Up and Do n order.	der is from top to b wn arrows to chan	ge the

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

4

Available Lompone Search by	nts			
Search by				
	ID NaCl		Add	
	Formula	Name	^	
NAB02.4H20	NaB02.4H20	Sodium metaborate tetrahvdrate		
NABOH4	NaB(OH)4	Sodium horon hydroxide		
NABPH4	Na[B(C6H5)41	Sodium tetraphenvlborate		
NABB	NaBr	Sodium bromide		
NABR.2H2O	NaBr.2H2D	Sodium bromide dihydrate		
NACL	NaCl N	Sodium chloride		
NACLO	NaCIO 6	Sodium hypochlorite		
NACL02	NaCIO2	Sodium chlorite		
NACL02.3H20	NaCl02.3H20	Sodium chlorite trihydrate		
NACL03	NaCIO3	Sodium chlorate(∀)		
NACL04	NaCIO4	Sodium perchlorate(VII)	~	
<			>	
Chemistry Wiza	rd 9.6 for Aspen Pl	us		
Chemistry Wiza	rd 9.6 for Aspen Pl	us		
Chemistry Wizar	rd 9.6 for Aspen Pl	us Add	Ren	nove
Chemistry Wizar ted Components ID	rd 9.6 for Aspen Pl	us Add	Ren	nove
Chemistry Wiza ted Components	rd 9.6 for Aspen Pl Fomula	us Add Name Water	Ren	nove
Chemistry Wizar ted Components ID D	rd 9.6 for Aspen Pl Fomula H2O C10122	us Add Name Water	Ren	nove
Chemistry Wiza ted Components ID D H22	rd 9.6 for Aspen Pl Formula H2O C10H22	us Add Name Water n-Decane	Ren	nove
Chemistry Wiza ted Components ID)) HI22	rd 9.6 for Aspen PI Formula H2O C10H22 N2	us Add Name Water n-Decane Nitrogen	Ren	nove

< Back Next > Finish Cancel Help

Do not Enable Redox reactions

OLI Chemistry Wize	ard 9.6 for Asp	en Plus		>
Redox Chemistry Enable Redox Included Subsystem	_{1s} 🖓			
⊕- ☐ CL(-1) CL(- ⊕- ☐ N N(+2) N ⊕- ☐ NA(0) NA(-	+1) CL(+3) CL(+5 +3) N(+5) N(-3) +1)	i) CL(+7) CL(+4) N(+1) N(-2) N(-1) N(+4)		
Assays/Pseudo Cor	nponents Typ	e		Status
Add		Edit	Dele	ste

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

include i nases	Include Solid Phases	
Aqueous Vapor Solids Second Liquid	Image: Contract of the state of t	
Inert Solid Info		
Density g/cc Heat Capacity		
cal/g°C		

Generate the *.bkp file, and select finish.

_	2011/00		Model File			_
⊡ Gene Backup	rate Backup (*.bkp) File File Name	Salt Convention for Distillation	File Name: File Folder:	EFLASH <u>C:\Users\diana</u>	.miller\Documents	
EFLASH	1	Allow salts to precipitate $\qquad \qquad \lor$	AspenPlus Backup File			
٩	Usually, you will be interested so that you can use it as a sta OLI chemistry into an existing extension aso is also created	in creating an AspenPlus backup file ting point for a new case or import the case. An input file stub with the	File Name: Salt Convention: <u>Selected Databanks</u>	EFLASH Allow salts to p	recipitate	
	If you want a backup file, mak checked and provide a backu	e sure 'Generate Backup File' is p file name.	Aqueous (H+ ion) (automatic)		
	'Salt Convention for Distillation involves distillation. You can a column stages if you select 'Sa	' is of interest if your simulation avoid having salts precipitate on alts are always dissociated'.	OLI Comp ID H2O C10H22 N2	AspenPlus ID H2O C10H22 N2	OLI Comp Name Water n-Decane Nitrogen	
2				Generate Files	s Now	View Files

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*.

R.	9-6	- 🎨 🕪 🔤 🕨 🔳 🚺	₹ i					\frown		Flowsheet	
File	Home	Economics Batch	Dynamics	Plant Data	Equation O	riented	View	(Customize)	Resources	Modify	Format
🗈 Optio	ns (😭 Manage Libraries	📆 Add Selected	* * *	αp	αp		- has	2		
(🔌 Variab	ole Explorer	Palette Categories	👈 Add Entire Ca	se Custom	₩.Q: Manana	P					
		🕒 Manage ACM Models		Tables	Properties	Properties	5				
Set	tings	Model Lib	vary		Prope	rty Sets					

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)*.

Is In Use	Name	Detail	Location
-	Built-In	View	Built-In
	CAPE-OPEN	View	Built-In
	ACM Models	View	Built-In
-	ACM Built-In	View	Built-In
	OLI	Edit	C:\Program Files (x86)\OLI Systems\OLI Engine
3			

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.

🐼 Open User Model Libra	Ŋ			×
← → ∽ ↑ <mark> </mark> « L	.ocal Disk (C:) → Program Files → Asper	nTech > AprSystem V11.0 > GUI	> Xeq	
Organize 👻 New fol	der			III 🕶 🔟 😲
- Weekly Suppor ^	Name	Date modified	Туре	
📙 Wiki Stuff	en-US	9/23/2020 4:26 PM	File fold	
lange - OneDrive - Union	Html5HelpMapFiles	9/23/2020 4:26 PM	File fol:	
	📑 ja-JP	9/23/2020 4:26 PM	File fold	
💻 This PC	locales	9/23/2020 4:26 PM	File fold	
🧊 3D Objects	- Modules	9/23/2020 4:26 PM	File fold	
👧 Desktop	🔄 ru-RU	9/23/2020 4:26 PM	File fold	
🚔 Documents	WPFForms	9/23/2020 4:26 PM	File fold	No preview available
Downloads	WpfPlotWizards	9/23/2020 4:26 PM	File fold	No preview available.
h Music	rh-Hans	9/23/2020 4:26 PM	File fold	
Distures	1/1 ConceptualDesign.apm	1/21/2019 6:00 AM	Aspen I	
Pictures	🚺 olimod.apm 🛛 🗨			
Videos				
늘 Local Disk (C:)				
👝 Google Drive ((
A Network	<			
File	name [,] olimod anm			Aspen Plus User Model Library
	onnoadphr			
				Open Cancel

Then select the **<u>olimod.apm</u>** library

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

Is In Use	Name	Detail	Location
	Built-In	View	Built-In
	CAPE-OPEN	View	Built-In
	ACM Models	View	Built-In
	ACM Built-In	View	Built-In
	OLI	Edit	C:\Program Files\AspenTech\AprSystem V11.0\

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.

	Model Palette											
Safety Analysis		Mixers/Splitters	Separators	Exchangers	Columns	Reactors	Pressure Changers	Manipulators	Solids	Solids Separators	Batch Models	User Models OLI Models
•y Energy Analysis	Material	FraChem	Eflash4									
Flowsheet Not Complete Check S	tatus											

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	С
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.

Specifications	Flash Options	Stream Definitions	Kinetics	Comments
Specification —				
Temperature	•		25	C -
Pressure	•		1	
				aun

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

Specifications Flash Options	Stream Definitions Kinetics	s Comments
Stream phase definitions		
Outlet Vapor Stream Name	VAPOR	
Outlet Aqueous Stream Name	LIQUID	
Outlet Organic Stream Name	ORGANIC	
Outlet Solids Stream Name	SOLIDS	
Enter this Blocks Output Stream N the Vapor phase will be in the first Aqueous in the second, the Organ last. You can overide the defaults b	ame for each phase. By defau outlet stream defined, the ic in the third and the solid in t by entering stream names abov	lt, the ve.

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.

Specifications	Key Components	Flash Opti	ons Er	ntrainment	Utility	Comments
- Flash specificatior	15					
Flash Type	Pressure	- D	uty	-		
Temperature		F		~		
Pressure		1 at	m	•		
Duty		0 Bt	u/hr	-		
Vapor fraction						

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	S 3	S4	S5	S6	S7
	MIXED	VAPOR	LIQUID	SOLID	MISSING	LIQUID	LIQUID
Substream: MIXED							
Mole Flow Ibmol/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
MOLE	 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)
PHAS	 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.

📓 OLI Chemistry	y Wizard 9.5 for Aspen Plus	×
	Welcome to the OLI Chemistry Wizard This wizard will guide you through the specifications required to create a chemistry model (.mod) file and it's associated property database (.dbs) fil for use with an OLI calculation engine. To start, enter a model name and select a working directory. All generate model files will be written to the working directory.	e
Name EFRA Workii \\\GR/	Chemistry Model 8 chars max. Open Existing Model 1 g Directory Path ANITE\SupportCases\Technical Su Browse Reset	
< Ba	ack Next > Finish Cancel Help	

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:

Mixed CLSolid	NC Solid Elach Ont	ions EO Ontion	c Costin	a 1	Comments	
inited croolid	Ne Solid Hash Opt			a l	comments	
Specifications						
lash Type Te	mperature 🔹	Pressure	_ •	Con	nposition	
State variables				Mo	ole-Flow T lb	/mol/hr 🔻
Temperature	25	С	•		Component	Value
Pressure	1	atm	•	Þ	H2O	48.8
Vapor fraction				Þ	CO2	
Total flow basis	Mole •			Þ	CL2	
Total flow rate		lbmol/hr	·	÷.	HCLO	
Solvent			*	Þ	HCL	
Reference Temperatu	ire			Þ	N2	
Volume flow reference	e temperature			Þ	NAHCO3	
F	Ŧ			Þ	NAOH	2.57
Component concent	ration reference temp	erature		•	H2CO3IN	
F	·			₽	NA2CO3	
				Þ	NA2O	
				Þ	NA3HCO32	
				÷.	NA5H3C34	
				Þ	NACL	
				Þ	NACLOIN	
				•	TRONA	
	2			Þ	WEGSCH	
				Þ	OH-	
				Þ	CLO-	

Composition for Stream 2:

Mixed CI Solid	NC Solid Flash Opt	ions EO Option	ns Cost	ing	Comments	
Specifications						
lash Type Te	emperature 🔹	Pressure	-	Con	nposition	
State variables				Mo	ole-Flow •	lbmol/hr
Temperature	33	С	•		Component	Value
Pressure	1.01	atm	•		H2O	2.27
Vapor fraction					CO2	23.59
Total flow basis	Mole 🔹				CL2	2 27
Total flow rate		lbmol/hr	•		HCLO	LILI
Solvent			-		нсі	
Reference Temperati	ure				N2	26.3
Volume flow referen	ce temperature				NAHCO3	2015
F	-				NAOH	
Component concent	tration reference temp	erature			H2CO3IN	
F	Ŧ				NA2CO3	
					NA2O	
					NA3HCO32	
					NA5H3C34	
					NACL	
				•	NACLOIN	
				+	TRONA	
				-	WEGSCH	
				•	OH-	
				•	CLO-	

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:

Configuration	Streams	Pressure	Exchangers	Specs	Vary	Effic
Configuration –						
Number of S	tages	5 Con	vergence Toler	ence	0.00	01
📃 🛛 LLE Col	umn	Maximum It	erations	35		
Condenser	None	-				
Reboiler	None	•				

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.

Configur	ation	Streams	Pressure	Exchangers	Specs	Vary	Efficiencies	Pump-Arounds	Estimates	Hold-up
Feed Stre Name	ams —	Stag	e No.	Product Stream	s D	istillate st	ream name			
S2			5	S4 Side stre	B am Drav	ottoms st v-Offs	ream name			
				Name	S	tage No.	Value	Units	Ph	ase
									•	•
									•	-
									•	•
									•	•
									•	•
									•	•

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.

Configuration	Streams	Pressure	Exchangers	Specs	Vary	Efficienc
Top Stage / Con	denser pres	sure —				
Stage 1 / Conde	nser pressu	re	1	atm		-
Stage 2 pressure	(optional)					
Stage 2 pressure	:			atm		•
Bottom Stage Pi	ressure (opti	ional) —				
Bottom Stage p	ressure		1.01	atm		•
bottom stuge p						

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.

New	Сору Ра	iste Export	Edit Input View Results Recond	tile Reveal	
Name	Hide	Active	Status	Description	Delete
	, ,	~			
Enter ID:)	^			
DS-1					
ОК	Cancel				

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.

Denne	sher	Vary	rotan	Deciarations	- co options	Comments	
Active							
 Sampled 	variables	(drag and	drop variab	les from form to	o the grid belov	v)	
Va	riable				Defini	tion	
Þ.							
New	Del	ete	Сору	Paste	Move U	p Move	Down View Variable
▲ Edit select	ted varia	ble					
Variable	🕅 Cre	ate new var	iable		×		
Category —	Entory	ariable nam					*
O All	CL2EL		ic.				
O Blocks	CLEFE						
Streams	0	ОК		ancel			
O Madel Lit	lite						
	inty						
O Property	Paramete	rs					
Reaction:							
-EO input							
Open variab	e						
Description							

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.

🅑 Define	⊖ Spec	⊖ Vary	Fortran	Declarations	EO Options	Comments		
✓ Active								
\land Sample	ed variables	(drag and	drop varial	oles from form t	o the grid belov	/)		
4	Variable				Defini	tion		
CL2FL	ow	Mole	-Flow Strea	am=S3 Substrea	m=MIXED Com	ponent=CL2 Un	its=lbmol/hr	
•								
New	Del	ete	Сору	Paste	Move U	p Movel	Down View	Variables
 Edit sel 	ected varial	ble					_	
Variable	⊘CL2	FLOW	•	Reference -				
Category				Туре	Mole-Flow		•	
🔘 All				Stream:	\$3		-	
O Blocks				Substream:	MIXED		•	
Ctroom				Component:	UL2		-	
Juleann	2			onits.	101110ly11			
Model	Utility							
Propert	y Paramete	rs						
🔘 Reactio	ns							
-EO input -								
Open varia	able							
Descriptio	n							

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.

[🕜 Define 🔇	Spec	⊖ Vary	Fortran	Declarations	EO Options	Comments]
	Design specifi Spec Target Tolerance	cation e CL2FL 0.5 0.01	xpressions .OW					

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.

🕜 Define 🛛 🥝 Sp	ec 🥑 Vary Fortran	De	clarations EO Options Comments
Manipulated varia	ble		Manipulated variable limits
Stream:	Stream-var	•	Upper 200
Substream: Variable:	MIXED MOLE-FLOW	•	Step size Maximum step size
Units:	lbmol/hr	•	Report labels Line 1 Line 2 Line 3 Line 4
			EO input Open variable Description
Сору	Paste Clear		

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*.

₫ 🔒	• • • •	№ 题	▶ ≡ I4 =	i.					
File	Home Eco	nomics	Batch	Dynamics	Plant Data	Equation Or	iented	View	Cus
∦ Cut ⊡Copy▼	ENG 👻	Nevt	Run Sten		🔚 Control Pane 😪 Reconcile	l 📝 Mode	l Summary n Summary	📄 Inpu 🕶 🧑 Hist	ıt ory
🖺 Paste Clipboard	Units	INCAL	Kun Step	Run	💦 Settings	💡 Utility	Costs Summar	y 📴 Rep	ort
Simulatio	n	<	Capital:	USD Utilitie	es:USD/Year		Energy Sa	avings:	_м
All Items		-	Main Flov	vsheet × B1	(FraChem) - Inpu	t × Contro	$_{ m ol}$ Panel $ imes$	Results	Sumr
 Image: Setting Settin	up perty Sets Ilysis wsheet arms cks R1	Repo Display Block Block ID	report for:	•		×			
□ Utili □ Rea ▷ □ Cor ▷ □ Flov ▷ □ Mod	Input ities ctions wergence wsheeting Optio del Analysis Too		✓ (Select all ✓ ■ B1) 	DESIG	^{ds-1} GN-S	SP.
 EO Res 	Configuration ults Summary			OK		<u>.</u>			

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 CO2E1038.19LB/HRPRODUCT STREAMS CO2E1034.85LB/HRNET STREAMS CO2E PRODUCTION-3.34052LB/HRUTILITIES CO2E PRODUCTION0.00000LB/HRTOTAL CO2E PRODUCTION-3.34052LB/HR

Column Profile

 Stage Temperature
 Liquid
 Rate
 Vapor Rate

 F
 LBMOL/HR
 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)

					-			
Sta	age H2O	CO2	CL	2	HCLO	HCL		
1	0.88978	8.821431E	-05	2.6271	91E-06	1.556907E-02	2.025672E-15	5
2	0.88043	1.010818E	-04	1.2389	96E-05	2.428213E-02	3.022983E-15	5
3	0.87918	1.073444E	-04	1.54530	04E-05	2.527008E-02	2.765462E-15	5
4	0.87909	1.103697E	-04	1.63540	01E-05	2.525866E-02	2.637146E-15	5
5	0.88101	1.122432E	-04	1.6782	33E-05	2.323816E-02	2.871383E-15	5

Aqueous Composition (mole fractions)

Sta	ge N2	NAOF	H2	CO3	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)

Sta	ge NA3F	ICO32	NA5H3C	D34	NACL	NACLO	NAHCO3
1	0.0	0.0	0.0	0.0	7	7.093167E-04	
2	0.0	0.0	0.0	0.0	5	5.133475E-04	
3	0.0	0.0	0.0	0.0	5	5.547109E-04	
4	0.0	0.0	0.0	0.0	5	5.812645E-04	
5	0.0	0.0	0.0	0.0	5	5.613581E-04	

Aqueous Composition (mole fractions)

	-					
Stage TRONA			WEGSCHEIDER O	H-1 Cl	_0-1	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	2.720043E-06
3	0.0	0.0	1.273216E-09	1.019529E-	02 2	2.370144E-06
4	0.0	0.0	1.156253E-09	9.919940E-	03 2	2.312654E-06
5	0.0	0.0	1.064736E-09	8.513549E-	03 2	2.055105E-06

Aqueous Composition (mole fractions)

Sta	ge HCO3-1	H+1	NAC	203-1	NA	+1	CL-1		
1	1.906723E-03	1.911661E-()9 5	5.453994E	-06	4.69278	35E-02	3.0057281	E-02
2	1.104030E-03	3.216044E-0)9 ⁻	1.654501E	-06	4.7332	17E-02	3.539670	E-02
3	1.101185E-03	3.324143E-0)9 ⁻	1.558991E	-06	4.74348	32E-02	3.613205	E-02
4	1.118766E-03	3.322609E-0)9 ⁻	1.567946E	-06	4.7469	55E-02	3.642466	E-02
5	1.070891E-03	3.385240E-0)9 ⁻	1.405945E	-06	4.75293	31E-02	3.793936	E-02

Vapor Composition (mole fractions)

5	stag	e H2O	CO2	CL2	HCLO	HCL	
	1	7.593340E-02	2 0.42928	9.2883	394E-03	5.243251E-03	4.372068E-13
	2	5.027767E-02	2 0.43036	3.4898	392E-02	5.610078E-03	5.257991E-13
	3	4.284472E-02	2 0.43152	3.9517	23E-02	5.004990E-03	4.402945E-13
	4	4.019696E-02	2 0.43264	4.0155	503E-02	4.697222E-03	4.046567E-13
	5	3.945139E-02	2 0.43312	4.0407	731E-02	4.208825E-03	4.325753E-13

Vapor Composition (mole fractions)

Stage N2		NAOH	АОН Н2СОЗ		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			NA5H3C	034 N	IACL	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)

Sta	ge TR	ONA	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	