CHEMCAD SCDS Distillation Column

SUPERTEAM 2005

Experiment 300 ECH4404L

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Introduction

This is a basic tutorial for the creation of an SCDS column using CHEMCAD software version 5.5.0. The initial conditions are specified in the objectives for the Distillation Experiment in the Unit Operations Laboratory Manual (ECH4404L).

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- 1. Starting CHEMCAD
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Procedure

1. Starting CHEMCAD

- 1.1. Double click the CHEMCAD icon to run software.
- 1.2. To retrieve an existing file, click on "Open Job" in the "File" menu.
- 1.3. Select file, and click on "Open".
- 1.4. To create new file click on "New Job" in the "File" menu.
- 1.5. Name new file, "SCDS column" and click "Save".

2. Creating a Process Flow Diagram

- 2.1 The initial flow sheet will populate a selection table for various types of equipment. Equipment is listed in alphabetical order.
- 2.2 Moving curser through icons will allow for selection of the SCDS distillation column (7 down; 4 across)
- 2.3 Click on the SCDS Distillation column. This places the column on the flow sheet. Note: Right clicking on mouse will allow for additional selections of the flow arrangements for the SCDS column.
- 2.4 Now select the inlet (red) and outlet (blue) flow stream arrows.
- 2.5 Click the square labeled stream to connect the arrows to the inlet/outlets streams on column. An example process flow diagram is shown below:



SCDS Distillation Column

Figure 1 – SCDS Process Flow Diagram

3. Specification of Engineering Units

- 3.1 Click on "Format" and select "Engineering Units".
- 3.2 Click on SI units and modify as specified below in the red square:

	Units selection		Optio	ons and references	
Time	min	Liquid Density	lb/ft3	▼ Viscosity	cP 💌
Mass/Mole	mol	Vapor Density	lb/ft3	 Surf. Tension 	dyne/cm 💌
Temperature	C	Thickness	ft	✓ Solubility Par.	(cal/cc)**0.5
Pressure	atm	Diameter	ft	Dipole Moment	debyes 💌
Enthalpy	J	Length	ft	➡ Cake Resistance	ft/lb
Work	hp-hr	▼ Velocity	ft/sec	 Packing DP 	in water/ft
Liquid Volume	ft3	▼ Area	ft2	Currency	\$
Liquid Vol. Rate	ft3/hr	Heat Capacity	Btu/Ibmol-F	Currency factor	1
Crude Flow Rate	BPSD	Specific Heat	Btu/Ibmol	•	
Vapor Volume	ft3	Heat Trans. Coeff.	Btu/hr-ft2-F	ENGLISH	Save Profile
Vapor Vol. Rate	ft3/hr	Therm. Conduct.	Btu/hr-ft-F	•	Load Profile

Figure 2

3.3 Now click on the "Options and references" tab and choose "Mole fractions" for the component flow.

Vapor reference temperature	
	Vapor reference temperature =60F if temperature units are F or R =0C if temperature units are C or K C Custom

Figure 3

3.4 Click on "OK" to continue.

4. Specification of chemical components

- 4.1 Now click on the "Flow sheet" drop down menu and select "Simulation".
- 4.2 Click on "Thermophysical" and select "Component List".
- 4.3 Search for ethanol and list as the first component because it is more volatile. Click to add.
- 4.4 Search for n-propanol and click to add.
- 4.5 If initial search does not yield the desired chemical, click on next to continue the search. A sample diagram is given below.

134 Ethanol	141 Ethyl Formate	C3H602
146 N-Propanol	142 Methyl Acetate	C3H602
	142 Methyl Methanoate	C3H602
	143 Propanoic Acid	C3H602
	143 Propionic Acid	C3H602
	144 Dimethylformamide	C3H7N0
	145 Isopropanol	C3H80
	145 2-Propanol	C3H80
	145 Isopropyl Alcohol	C3H80
	146 1-Propanol	C3H80
	146 N-Propyl Alcohol	C3H80
	146 N-Propanol	СЗН80
Delete Clear Add	Insert Search for	Next

Figure 4

4.6 Once all components have been added, click "OK."

4.7 The following box shown below will appear. Maintain the default specifications and click "OK."

nermodynan	nics wizard	
The selection of thermo component class, data ange of the process, L as a guide only	dynamic models is ba: availibility as well as th Jse the suggestions of	sed on the le T/P operation the expert system
Please enter the temper	rature/pressure range	of the process:
Temperature Min	þ	с
Temperature Max	100	с
Pressure Min	1	atm
Pressure Max	10.2069	atm
	la a	_
Bip data threshhold	0.5	

Figure 5

4.8 Next a box showing the K-value options will appear. Select the "Wilson" option as shown below and click "OK."

alobal K. Value Uption	Global Phase Option:
Wilson	 Vapor/Liquid/Solid
JNIQUAC JNIQUAC / UNIFAC	C Vapor/Liquid/Liquid/Solid
JSRK	Water/Hydrocarbon Solubility:
Wilson	Miscible
/apor Phase Association:	C Immiscible
No Vapor Phase Association	Wilson model salt None>
Vapor Phase Association	No. of BIP sets
/apor Fugacity/Poynting Correction:	Default RIP set
Correction	
No Correction	Clear all local K models/BIPs
RK/PR Alpha function:	Set local K models/BIPs
Standard SRK/PR	C Set tray BIPs
Boston-Mathias extrapolation	Set Henry components

Figure 6

4.9 The next box that appears is shown below. Maintain the default settings and click "OK".

Fill Matri	ix by :	UNIFAC VLE	Comp List		Cancel	ОК
		L	Aij	Aji		
1 1		2	102.671	-40.8745		

Figure 7

5. Entering feed stream compositions

- 5.1 Double click on stream number "1".
- 5.2 For stream name enter "feed" and specify the following values for the temperature, pressure, total flow and mole fractions of ethanol and n-propanol.

Flash		Comp List	Cancel
Stream No.	1		
Stream Name	feed		
Temp C	50		
Pres atm	1		
Vapor Fraction	0		
Enthalpy J/min			
Total flow	3.5		
Total flow unit	mol/min		
Comp unit	mole frac		
Ethanol	0.5	2	
N-Propanol	0.5		

Figure 8

- 5.3 Click "Flash" button located in upper left corner.
- 5.4 Click "OK".

6. Entering SCDS Column Specifications

- 6.1 Double click on "SCDS column".
- 6.2 A screen showing the specifications for the column will appear. Under the tab labeled "General" specify the values as outlined within the red box below. For Subcooled delta T, enter 32.2 C. For the number of stages enter 6, and for the feed stage for stream 1 enter 2.

General	Specifications	8	Convergence	Cost E	stimation 1	Cost Estimation 2
		General	Model Parame	ters		ID: 1
Condenser type	0 Total or none	•				
Subcooled delta T	32.2	с	Simulation m	odel	Regular VLE mo	odel
Top pressure		atm	- For condens	er with de	cant:	
Cond press drop		atm .	Upper layer fra	iction to dec	ant (alpha)	
Colm press drop		atm	Lower layer fr	action to dec	cant (beta)	
Reflux pump press.		atm				
Bottom pump press.		atm	Check ne	re ror read	cive distillation	
No. of stages	6		Optional thre	ee phase c	control:	
Feed stages	10		Use local th	nree phase n	nodel	
Feed stage for stream	1 2		Three phase s	tage from		
	1-		Three phase s	tage to	1	
			Ambient Hea	at Transfer	· · · · ·	
			Heat transfer a	area/stage		ft2
			Heat transfer c	oeff. (U)		Btu/hr-ft2-F
			Ambient tempe	rature		С
						1

Figure 9

Note:

- 1. Actual number of stages is 6, consisting of 4 trays plus a condenser and a reboiler.
- 2. The "Subcooled delta T" is the temperature difference between the bubble point of the liquid on the top stage (i.e., the condenser) and the temperature of the reflux return stream. For example, suppose the distillate has a composition of $x_D =$ 0.716. The bubble point of this stream can be found using CHEMCAD to be 82.2 C. Suppose the reflux stream is at 50 C. Then the "Subcooled delta T" is 82.2 C -50 C = 32.2 C. [It is emphasized that this feature is different from the Subcooled temperature box in the TOWR module. In TOWR one just enters into the box the temperature of the reflux stream, or in this example 50 C.]

6.3 Under the tab labeled "Specifications" enter the following options, a diagram is given below.

General	Specifications	Converg	lence	Cost Estimal	tion 1	Cost Estima	tion 2
	Heat and	Material Ba	lance S	pecification	S	ID:	1
Condenser mode:		Specification		•			
1 Reflux ratio (R/D)	_	0.5					
Select reboiler mode:		Specification					
2 Reboiler duty, positive	_	78000	J/min				
			-0)ptional Tray Specifi	cation		
			,	diust the specification	on for	0 None	-
					511101		
			ι	intil the 0. Tray		Tray	
			V	/ariable 0 = Nor	ne		•
). Liauid	-	
			1	nase i			
			is	s equal to a specified	l value of		
			1				

Figure 10

- 6.4 For "Condenser mode", initiate drop down box and select "1 Reflux ratio (R/D)".
- 6.5 Tab to specifications and enter desired ratio "0.5".
- 6.6 For "Reboiler mode", initiate drop down box and select "2 Reboiler duty positive".
- 6.7 Tab to specifications and enter desired amount "78,000" J/min, which corresponds to 1300 W.
- 6.8 Click "OK" to continue.

7. Warnings

- 7.1 After clicking "OK" a CHEMCAD message box will display several warnings.
- 7.2 The figure below shows acceptable warnings. Disregard the warnings and click "Yes" to continue.

- CHEMCAD Message Box -	×
INPUT DATA CHECKING Warning: SCDS 1 No distillate estimation Warning: SCDS 1 No reflux rate estimation Warning: SCDS 1 No top T estimation Warning: SCDS 1 No bottom T estimation No. of errors = 0, No. of warnings = 4 Warnings found in input data	
✓ Do you wish to continue ? Yes	×

Figure 11

7.3 Should an error or additional warnings be displayed; this will need to be addressed on a separate basis.

8. Running Simulation

- 8.1 Click on the "R" in the upper left corner to run the simulation.
- 8.2 After it has finished, each stream number may be clicked on to view the final compositions.

9. Results

- 9.1 Double click on Stream 2 and type "Distillate" for the stream name.
- 9.2 Double click on Stream 3 and type "Bottoms" for the stream name.
- 9.3 To set the units of each stream for the results, click on the "Results" tab at top, and choose "Set Flow Units". Choose mole fractions for the flow units.

- View	Flow Rate Unit -	×
Unit S	election	
0	Mole	
0	Mass	
0	Std. Liquid Vol.	
0	Std. Vapor Vol.	
•	Mole Fractions	
0	Mass Fractions	
0	Std. Liquid Vol. Fractions	
0	Std. Vapor Vol. Fractions	
0	Mole %	
0	Mass %	
0	Std. Liquid Vol. %	
0	Std. Vapor Vol. %	
0	Mole ppm	
0	Mass ppm	
0	Std. Liquid Vol ppm	
0	Std. Vapor Vol. ppm	
	Cancel OK	

Figure 12

- 9.4 Click "OK" to continue.
- 9.5 To generate a report of various types of results, click on "Results" on the top menu bar, follow the drop down to the preferred selection A diagram is given below:



Figure 13

9.6 The results are generated in a word pad document. Results for the "Stream Compositions" are displayed below:

👿 scds_column0 - WordPad				
File Edit View Insert Format H	lelp			
	B 🖪 🗠 💀			
Courier New 💽 10	•	• B /	' <u>u</u> 🔊 🖹 🛓	≣ <u>⊨</u>
<u></u>	· 2 · · ·] · ·	• 3 • • • • • • • •	4 • • • • • • • • • • •	
CHEMCAD 5.5.0				Page 1
Job Name: scds column	Date: 12/0'	7/2005 Time:	05:08:30	
Stream No.	1	2	3	
Stream Name	feed	distillate	bottoms	
Temp C	50.0000*	49.9813	87.1463	
Pres atm	1.0000*	1.0000	1.0000	
Enth J/min -	1.0033E+006	-2.6666E+005	-7.2188E+005	
Vapor mole fraction	0.00000	0.00000	0.00000	
Total gmol/min	3.5000	0.9475	2.5525	
Total g/min	185.7888	47.4302	138.3586	
Total std L ft3/hr	0.4895	0.1255	0.3641	
Total std V scfh	166.22	45.00	121.22	
Component mole fractio	ns			
Ethanol	0.500000	0.715726	0.419918	
N-Propanol	0.500000	0.284274	0.580082	

Figure 14

9.7 When requesting the remaining types of results, make sure to specify the unit operation number for the corresponding results. Results for the "Unit Op's" are displayed below:



Figure 15

9.8 Results for the "Tower Profiles" are displayed below:

📕 scds_	column2 -	WordPad					
File Edit	: View In:	sert Format	Help				
		A X		ъ			
Courier N	lew	1	0 🖌	• [B / U 🔎	E E E	E
<u>.</u>	i į i i i	1	••• ? • • • • ! •	· · 3 · · · 1	••••	* * * 5 * * *	<u>i</u>
CHEM	CAD 5.5.	0					Page 1
Job 1	Name: so	ds column	Date: 12	/07/2005 T:	ime: 05:20::	12	
Unit	tume .	5CD5 11	nit name:	From # 1			
onre	суре .	3003 0		гар и т			
			* Net Fi	Lows *			
	Temp	Pres	Liquid	Vapor	Feeds	Product	Duties
Stg	С	atm	gmol/min	gmol/min	gmol/min	gmol/min	J/min
1	50.0	1.00	0.47			0.95 - 6	5.325E+004
2	84.9	1.00	4.50	1.42	3.50		
3	84.9	1.00	4.50	1.95			
4	85.1	1.00	4.50	1.95			
5	85.7	1.00	4.48	1.94			
6	87.1	1.00		1.93		2.55	7.8E+004
Mole	Reflux	ratio	0.500				

Figure 16

9.9 Results for the "Tray Compositions" are displayed below:

CHEMCAD 5.5.0			
Page 1			
1030 1			
Job Name: scds column	n Date: 12/07/20	05 Time: 05:24:	24
Unit type : SCDS	Jnit name: Eqp	p # 1	
Stage # 1	49.98 C	1.00 atm	
	V Mole frac	L Mole frac	Y/X
Ethanol	0.0000	0.71573	0.0000
N-Propanol	0.00000	0.28427	0.0000
Total gmol/min	0.0000	0.4738	
Stage # 2	84.89 C	1.00 atm	
	V Mole frac	L Mole frac	Y/X
Ethanol	0.71573	0.54656	1.30951
N-Propanol	0.28427	0.45344	0.62693
Total gmol/min	1.4213	4.5018	
Stage # 3	84.94 C	1.00 atm	
	V Mole frac	L Mole frac	Y/X
Ethanol	0.71238	0.54242	1.31334
N-Propanol	0.28762	0.45758	0.62856
Total gmol/min	1.9494	4.4999	
Stage # 4	85.14 C	1.00 atm	
	V Mole frac	L Mole frac	Y/X
Ethanol	0.70298	0.53087	1.32419
N-Propanol	0.29702	0.46913	0.63314
Total gmol/min	1.9475	4.4955	
Stage # 5	85.69 C	1.00 atm	
	V Mole frac	L Mole frac	Y/X
Ethanol	0.67663	0.49941	1.35485
N-Propanol	0.32337	0.50059	0.64598
Total qmol/min	1.9430	4.4837	
Stage # 6	87.15 C	1.00 atm	
	V Mole frac	L Mole frac	Y/X
Ethanol	0.60448	0.41992	1.43951
N-Propanol	0.39552	0.58008	0.68184
Total gmol/min	1.9313	2.5525	

Figure 17

9.10Results for the "Tray Properties" are displayed below:

CHEMCAD	5.5.0					
Page 1						
Job Name	: scds	column	Date: 12/0	7/2005 T	ime: 05:26:	15
Unit typ	e : SCI	OS Uni	t name:	Eqp # 1		
LIQUID			Actual	Actual		Thermal
tension		Average	vol rate	density	viscosity	conduct.
Stg	g/min	mol wt	ft3/hr	lb/ft3	CP	Btu/hr-ft-F
1	24	50.06	0.07	47.95	0.7918	0.091
20.451	236	52.43	0.68	45.98	0.4678	0.085
3	236	52.49	0.68	45.98	0.4681	0.085
4	237	52.65	0.68	45.98	0.4685	0.085
5	238	53.09	0.68	45.98	0.4695	0.085
6 17 750	138	54.21	0.40	45.97	0.4711	0.084
1/./30						
Stg		Liq H				
1	1 2 2	J/min				
1	-1.33	33e+005				
2	-1.20	17-+006				
3	-1.20	15-:006				
4 5	-1.20	015e+006				
5	-1.2	880+005				
0	-/.21	.0007005				
VAPOR		Average	Actual vol rate	Actual density	viscosity	Thermal conduct.
Compr.						
Stg	g/min	mol wt	ft3/hr	lb/ft3	cP	Btu/hr-ft-F
factor						
1	0	0.00	0	0.0000	0.0000	0.000
0.000						
2 0,978	71	50.06	86	0.1088	0.0102	0.012
3	98	50.10	119	0.1089	0.0102	0.012
4	98	50.24	119	0.1091	0.0102	0.012
5	98	50.60	118	0.1098	0.0101	0.012
6	100	51.62	118	0.1115	0.0101	0.012
0.9//						

Stg	Vap H
	J/min
1	0
2	-3.3674e+005
3	-4.6196e+005
4	-4.6182e+005
5	-4.6161e+005
6	-4.6114e+005

Figure 18