CHEMCAD TOWR Distillation Column

SUPERTEAM 2005

Experiment 300 ECH4404L

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Introduction

The purpose of this module is to introduce the basics of distillation on CHEMCAD version 5.5. The simulation is based on experiment 300 in the Unit Operations Laboratory.

Basic Setup



First you start by pasting the representative symbols from the palette on the blank workspace and you connect them as shown in the figure above.

🔄 File	Edit	View	Format	Mode	ThermoPhysical	Specifications	Run	Results	Plot	Output :
		X	e c	8	Databank	•		🗉 Si	mulati	ion 🔽
					Component Li:	st				
•					Electrolytes					
ł					Pick Solids	I				
[Particle Size D					
					Distillation Cur					
					K-Value Wizar	d				
					K- Values	I				
					Enthalpy	I				
					Transport Pro	perties				
					Edit BIP's					

Figure #2

Step number 2 is to select the components. As seen in the picture above go to *ThermoPhysical* in the menu options and the click on *Component List*.

In our case we will use Ethanol and Propanol. **Note:** Ethanol should be chosen first because it is the more volatile species.

👺 - Component Selection -		×
Selected Components	Component Databank	
134 Ethanol	141 Ethyl Formate	СЗН602 🔺
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 L	isert Search for	Next
Copy components from another job		Cancel OK

Figure #3

For a proper and smooth simulation it is best if you state the appropriate units. From the menu, select *Format* and then click on *Engineering Units*.



Figure #4

Units selection				Options and references			
Time	min	-	Liquid Density	kg/m3	•	Viscosity	Pa-sec 💌
Mass/Mole	mol	•	Vapor Density	kg/m3	-	Surf. Tension	N/m 💌
Temperature	С	•	Thickness	m	-	Solubility Par.	(J/m3)**0.5 💌
Pressure	atm	•	Diameter	m	•	Dipole Moment	C.m 💌
Enthalpy	J	•	Length	m	-	Cake Resistance	m/kg 💌
Work	kW-h	•	Velocity	m/sec	•	Packing DP	mm water/m 💌
Liquid Volume	m3	•	Area	m2	•	Currency	\$
Liquid Vol. Rate	m3/h	•	Heat Capacity	J/kmol-K	-	Currency factor	1
Crude Flow Rate	m3/h	•	Specific Heat	J/kmol	•		
Vapor Volume	m3	•	Heat Trans. Coeff.	W/m2-K	-	SI	Save Profile
Vapor Vol. Bate	m3/h	•	Therm. Conduct.	W/m-K	•		Load Profile

Figure #5

For convenience, we shall change the component flow units from mol/time to mol fractions. This can be done by clicking the *Options and references* tab while in the Engineering Units Selection screen.

		-
Units selection Stream Flow Units Total Flow Default mole/mass Component Flow Default mole/mass Stream Edit Default mole/mass Hole fractions Hass fractions Line, vol fractions Line, vo	Options and references Vapor reference temperature C Default G Default C Custom O Custom O Custom O Default O Custom O Custom O Custom O Default O Custom O Custom O Default O Default O Custom O Default O	
Liq. vol. fractions -Atmospheric pressure reference Default = 14.696 psia (1.01325 bar) Custom		

Figure #6

Before starting the simulation you have to set the correct K-values calculation. To see the K-value wizard select *ThermoPhysical* from the menu and then select the *K-value wizard* option. From the list of models select the *Wilson* model.



Figure #7

t Mode	e ThermoPhysical Specifications Run Results Plot	Output Sizing Tools Window Help
	 K Value Options - Global K Value Option Wilson Ethane/Ethylene, Propane/Propylene: Regular SRK/PR Bips Special SRK/PR Bips Vapor Phase Association: No Vapor Phase Association Vapor Phase Association Vapor Phase Association Vapor Phase Association Standard SRK/PR Boston-Mathias extrapolation 	Global Phase Option: Vapor/Liquid/Solid Vapor/Liquid/Solid Water/Hydrocarbon Solubility: Miscible Miscible Wilson model salt No. of BIP sets Default BIP set Clear all local K models/BIPs Set local K models/BIPs Set tray BIPs Set tray BIPs Set Henry components
	Help Options in gray are not applicable	for this k value option Cancel OK

The starting feed is 50 $^{\circ}$ C and 3.5 mol/min, 0.5 mol fraction and 0.5 mol fraction ethanol and propanol respectively.

Flash Comp List Cancel O Stream No. 1 Stream Name Feed Temp C 50 Pres atm 1 Vapor Fraction 0 Enthaley. Junin -997682)К
Stream No. 1 Stream Name Feed Temp C 50 Pres atm 1 Vapor Fraction 0 Forthalky/min -997682	
Stream Name Feed Temp C 50 Pres atm 1 Vapor Fraction 0 Enthalow Junin -997682	
Temp C 50 Pres atm 1 Vapor Fraction 0 Enthalpy J/min -997682	
Pres atm 1 /apor Fraction 0 Inthalpy J/min -997682	
/apor Fraction 0	
inthalpy J/min -997682	
otal flow 3.5	
otal flow unit mol/min	
Comp unit weight frac	
ithanol 0.5	
I-Propanol 0.5	

Figure #9

Tower Configuration

To modify the specs of the column double click on the tower and sub menu would appear.

General

General	Specifications	Convergence	Cost Estimation 1	Cost Estimation 2
	- possibulions		to an	
	Gen	erai wodel Parame	ters	ID: 1
Condenser type	0 Total or no condenser	 Ambient 	heat transfer	
Subcooled temp.	50 C	Heat tran	sfer area/stage	m2
Top pressure	atm	Heat tran	sfer coeff. (U)	W/m2-K
Cond press drop	atm	Ambient t	emperature	С
Colm press drop	atm			
Reflux pump pout	atm			
Bottom pump pout	atm			
No. of stages	6			
Feed stages:				
Feed tray for stream	1 2			
Help				Cancel OK



- Set the condenser to total or no condenser, option number 0.

Note: The condenser for the Unit Operations Laboratory is a total condenser.

- Set sub-cooled temperature to 50 °C.

Note: This temperature corresponds to the measured temperature of the reflux stream.

- Set number of stages to 6 and the Feed tray for stream to stage 2.

Note: Six stages in Chemcad is equivalent to four trays, one reboiler, and one condenser.

Note: Setting the feed tray to stage two is equivalent to the top of the column. The location will depend on the actual feed location of the unit being simulated.

		1	1	1	
General	Specifications	Convergence	Cost Estimation 1	Cost Estimation 2	
	Heat and I	Material Balance Sp	ecifications	ID: 1	
Condenser/Rebo	oiler Specifications				
Condenser mode:		Specification			
1 Reflux ratio (R/D)		0.5			
Select reboiler mode:		Specification			
2 Reboiler duty, positive	· ·	78000 J/min			
Halp				Carried OK	

Figure #11

The next set of specifications, set the condenser mode to option number 1 Reflux ratio and set the ratio to 0.500, for the reboiler mode select option number 2 Reboiler duty positive and set it to 78000 J/min which is equivalent to 1300 W (the effective heat duty of the reboiler in the lab).

After you finished with the steps described above you are set to run the simulation. From the menu go to *Run* and select the option *Run All*.



Figure #12

Next, it is necessary to obtain the data from the simulation. This is done by going to stream compositions from the Results menu. After clicking on *Stream Compositions* followed by *All Streams*, a window showing the compositions for each stream will appear.

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CHEMCAD 5.5.0 Job Name: hgfuly Date:	12/08/200	5 Time: 17:54	:43	Page 1
Stream No.	1	2	3	
Stream Name	Feed	Distillate	Bottoms	
Temp C	50.0000*	50.0000	87.1440	
Pres atm	1.0000*	1.0000	1.0000	
Enth J/min -1.0	033E+006	-2.6659E+005	-7.2192E+005	
Vapor mole fraction	0.00000	0.00000	0.00000	
Total gmol/min	3.5000	0.9473	2.5527	
Total g/min	185.7888	47.4153	138.3734	
Total std L m3/h	0.0139	0.0036	0.0103	
Total std V m3/h Component mole fractions	4.71	1.27	3.43	
Ethanol	0.500000	0.715834	0.419909	
N-Propanol	0.500000	0.284166	0.580091	
For Help, press F1				NUM //

Figure #13

Next, you need to get the table which has the Unit Op's summary. This is found under the results menu by clicking on Unit Op's.

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CHEMCAD 5.5.0
Page 1
Job Name: hgfuly Date: 12/08/2005 Time: 18:06:23
Towr Rigorous Distillation Summary
Turnin V. d
Equip. No. I
No of stars
let feed etame
Condenser mode 1
Condenser spec. 0.5000
Subcooled temp C 50.0000
Reboiler mode 2
Reboiler spec. 78000.0000
Calc cond duty J/min -63206.8086
Calc rebr duty J/min 78010.8359
Calc Reflux ratio 0.5000
Calc Reflux mole 0.4736
(gmol/min)
Calc Reflux mass 23.7076
(g/min)
For Help, press F1

Figure #14

Another result that is desired is the tower profile. This is also found under the results menu by clicking on *Tower Profiles*.

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CHEMCAD 5.5.0 Page 1									
Job	Name: h	gfuly Da	te: 12/08/20)05 Time: 3	18:07:52				
Unit	Unit type : TOWR Unit name: Egp # 1								
			* Net Fl	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 -	-6.321E+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	7.801E+004		
Mole	Reflux	ratio	0.500						
For Help, j	press F1						NUM //		

Figure #15

The last two tables of results that are desired are the tray compositions and tray properties. These are found under the results menu by clicking on *Tray Compositions* or *Tray Properties*.



Figure #16 – Tray Compositions

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File Edit	View Insert	Format He	lp				
	. .	M X I		•			
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1							_
Job Na	me: hgful	y Date.	: 12/08/20	D5 Time:	18:10:14		
Unit t	уре : ТОЖ	R Uni	t name:	Eggp # 1			
LIOUID)		Actual	Actual		Thermal	Surface
		Average	vol rate	density	viscosity	conduct.	tension
Stg	g/min	mol wt	m3/h	kg/m3	Pa-sec	₩/m-K	N/m
1	24	50.06	0.00	768.02	0.0008	0.158	0.020
2	236	52.43	0.02	736.61	0.0005	0.148	0.018
3	236	52.49	0.02	736.60	0.0005	0.147	0.018
4	237	52.65	0.02	736.59	0.0005	0.147	0.018
5	238	53.09	0.02	736.55	0.0005	0.147	0.018
6	138	54.21	0.01	736.35	0.0005	0.146	0.018
Sta		Lig H					
July		J/min					
1	-1.33	29e+005					
2	-1.26	09e+006					
3	-1.26	14e+006					
4	-1.26	16e+006					
5	-1.26	08e+006					
6	-7.21	96e+005					
VAPOR		_	Actual	Actual		Thermal	_
		Average	vol rate	density	viscosity	conduct.	Compr.
Stg	g/min	mol wt	m3/h	kg/m3	Pa-sec	₩/m-K	factor
	0	U.UU 50.00	0	0.0000	0.0000	0.000	0.000
2	/1	30.06	2	1.7432	0.0000	0.021	0.978 💌

Figure #17 – Tray Properties