

## **ChemSep Tutorial: Extraction**

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Here we consider the modeling of an extraction column using *ChemSep*. This tutorial is derived from Exercise 10.43 in *Separation Process* Principles (2<sup>nd</sup> Edition) by J.D. Seader and E.J. Henley (Wiley, 2006).

## **Tutorial 1: Setting up a Simple Extractor**

Ethyl Acetate is to be used as the solvent in an extraction process to recover acetic acid from a binary liquid mixture that is predominantly water. The exercise calls for us to determine the number of equilibrium stages needed to recover 99.5% of the acetic acid in the feed. In Exercise 10.43 Seader and Henley refer back to Figure 8.1 (on page 296) where a flowsheet for the entire extraction process is shown (with considerable accompanying discussion). The component flow rates into and from the extraction column to be used in this example are taken from Figure 8.1 and summarized in Table 1.

Stream	Feed	Solvent	Extract	Raffinate
Stage Pressure (psia) Light phase fraction Temperature (oF)	1 15 0 100	10 15 1 100	1 15 1 100	10 15 0 100
<b>Mass Flows (lb/h)</b> Ethyl Acetate Water Acetic Acid	23,600 6,660	68,600 2,500	67,112 6,660 6,649	1,488 19,440 11

Table 1: Extractor Stream Flows: Feed Specifications and Products

We begin by clicking on the Components Panel and selecting the components that are listed in Table 1 (the components should be selected in the order in which they appear in Table 1).

Selected components in simulation:							
Component(s):	Identifier	L#	File	Loc.			
Add 🧼	Ethyl acetate	1313	c:\chemsep\pcd\a	87			
	Water	1921	c:\chemsep\pcd\a	14			
4.0	Acetic acid	1252	c:\chemsep\pcd\a	48			
Remove							

Next, select the **Operation** tab and choose **Equilibrium Column**. Complete the specification of the column configuration as shown in the screen shot below:

🕂 ChemSep v6.17		
File Edit Solve Analysi	is Databanks Tools Help	
🕒 🚅 🖬 🕨 🥭 🗇		
Title Components	✓ Operation Select Type of Simulation	
🕀 🗙 Properties	O Flash	
<b>×</b> Feeds	Equilibrium column	
Units		
- Solve options	Column Configuration	
- Paths	Operation: Simple Extractor	
		Тор
	Condenser: None	
	Reboiler: None	Feed1 1
	Number of stages (e.g. 10) 10	
	Feed stage(s) (e.g. 5,7) 1,10	
	Sidestream stage(s) (e.g. 2,9)	
	Pumparound(s) (e.g. 6>8, 3>1)	Feed2 10 10
		Bottom
		→
Changed Not converg	Jed	

The next step is to select the appropriate thermodynamic models. The property models selection and and the interaction parameters are shown in the screen shot below:

Select Thermodynamic	ic Models				
-					
K-Value	Liquid-Liquid	Show ent	halpy/exergy	settings:	
Equation of state	<b></b>				
Activity coefficient	NRTL				
Vapour pressure	Y				
Enthalpy	None				
Enter Thermodynamic	: Model Parameters (when req	uired)			
NRTL	▼ NRTL	Units K		•	Temperature dependent
		A-ii	A-ii	A-ii	
Reset	Thul an eteter Attales				
	Ethyl acetate - Water	166.360	1190.10	0.200000	
🗁 Load	Ethyl acetate - Acetic acid		-702.570	0.200000	
	Water - Acetic acid	-302.630	-1.68300	0.200000	
Save				Record int	eraction parameters in this matrix

Seader and Henley provide parameters for the NRTL activity coefficient model.\*

\*The units for the parameters are not provided so we have guessed that the first two parameters on each row are in K (simply because that is the unit used most often for reporting liquid-liquid parameters. When we solve this problem we will find that this choice was correct – an incorrect choice would lead to ridiculous answers or no solution at all.

The next step is to provide the details of the two feeds. Click on the **Feeds** line and complete the feeds panel so that it appears as it does in the screen shot below:

Feed Stream(s) Specific	ations —			
Insert	Remo	ve	Mass flows	•
Feed:	1		2	]
Name	Fe	eed	Solvent	
Stage	1		10	
Two-phase feed	S	olit	Split-below	
State	L	& T	L & T	
Pressure (psia)				
Light fraction (-)	0.	000000	1.00000	
Temperature (F)	10	00.000	100.000	
Flowrates (lb/h):				
Ethyl acetate	0.	000000	68600.0	
Water	23	3600.1	2500.00	
Acetic acid	66	659.90	0.000000	
Total flowrate	30	0260.0	71100.0	

It is important to note that a few things here. First. we have entered the feed flows in mass units (because the problem specification by Seader and Henley provided the stream data in mass units). Second, the default names of the feed streams have been changed. Finally, and very importantly, the second feed has been set to *Split-below* so that ChemSep recognizes that this feed is to the very bottom of the column.

For liquid-liquid systems we must choose the light phase fraction (rather than the vapor fraction that could be specified for gas/vapor-liquid systems). The feed to the top of the column (stage 1) *must* have a light phase fraction of zero (in order to force it to flow down the column) and the feed to the bottom of the column must have a light phase of one (in order to force it to flow up the column).

The column pressure is set to 15 psia:

Column pressure	Constant pressure	•
Top pressure	15.0000	(psia)

The column specifications are completed by setting the heat losses to zero and the default efficiency to one. There are no *Column Spefications* as such, we do however, rename the *Top* and *Bottom* product streams as *Extract* and *Raffinate* respectively.

Prior to solving the problem it is wise to check the **Solve Options** panel, the upper part of which should look like this:

Numerics Options Initialization	Automatic	•	Newton step limits:	Flow	1.00000	0
Method	Newton's method	•		Temperature	18.0000	(oF)
Accuracy	1.0000E-06			Composition	1.00000	0
Number of Iterat	ions 30			Flux	1.00000	Θ

The next step is to save the file (using the **File** menu – note that the file name will appear on the blue bar at the top of the ChemSep window).

Click on the green arrow head icon to start the calculations. This will bring up the solve window:

Acetic acid				
etermining fee	d conditions			
enerating initia	I flow profiles			
	l composition profiles			
nit 30 mil	liseconds			
tarting Newtor	is method			
	rminate execution			
Iteration	Error			
				1
0	2.9522E+00			
1	4.9982E-01			
2	5.6653E-01			
2 3	7.7288E-01			
4	1.6873E-01			
4 5 6 7	1.9717E-02			
6	1.8620E-04			
7	2.4728E-08			
Convergence of	btained in 7 iterations			
	nilliseconds			
ixMem driver d	one			
Process ended				
				Ī
C .				
<u> </u>				

Click on **Done** to close the window and bring up the results panel.

<u> ChemSep - Seader10_4</u> 3	3.sep					_ 🗆 🗵
<u>File Edit Solve Analysis [</u>	<u>)</u> atabanks <u>T</u> ools <u>H</u> elp					
🗅 🚅 🕞 🕨 🍣 🍝	XUTE					
Title T	ables Graphs Rating					
	Tables					
Properties Thermodynamic:	Select table: Streams	<b>-</b>	XL Edit	Сору	Font Print	
Physical properti						
	Stream	Feed	Solvent	Extract	Raffinate	
V Feeds	Scream	Feeu	Sorvenc	Extract	Karrinate	
🖃 🗸 Specifications	Stage	1	10	15 0000	10	
	Pressure (psia) Light phase fraction (-)	14.6959 0.000000	14.6959 1.00000	15.0000 0.000000	15.0000 0.000000	
	Temperature (oF)	100.000	100.000	99.9678	100.002	
	Mole flows (lbmol/h)					
Efficiencies	Ethyl acetate	0.000000	778.608	761.788	16.8194	
Column specifica	Water Acetic acid	1310.02 110.902	138.773 0.000000	370.041 110.899	1078.75 0.00335030	
∃ -√ Results		110.902	0.000000	110.099	0.00000000	
Tables	Total molar flow	1420.92	917.380	1242.73	1095.58	
Graphs Rating	Mole fractions (-)					
Units	Ethyl acetate	0.000000	0.848729	0.612997	0.0153521	
- Solve options	Water Acetic acid	0.921951 0.0780491	0.151271 0.000000	0.297765 0.0892380	0.984645 3.0580E-06	
Paths		2.07.00491	0.000000	5.0002000	5.25022 20	
	Mass flows (lb/h) Ethyl acetate	0.000000	68600.0	67118.1	1481.89	
	Water	23600.0	2500.00	6666.30	19433.8	
	Acetic acid	6659.99	0.000000	6659.79	0.201195	
	Total mass flow	30260.0	71100.0	80444.2	20915.8	
						<b>_</b>
	<u>र</u>					
Saved Converged 7 iter	ations C:\ChemSep_\Sep_Files\S	StandardTest\LLX\S	eader10_43.sep			

If we compare the mass flows shown here with those in Table 1 we will see that we have recovered more than the 99.5% of the acetic acid present in the Feed stream. We leave it as an exercise for readers to determine how many stages are, in fact, necessary to recover 98.5%.