

ChemSep Tutorial: Extraction

Ross Taylor and Harry Kooijman

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

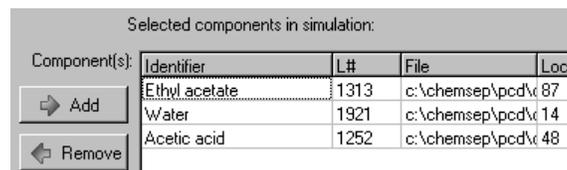
Tutorial 1: Setting up a Simple Extractor

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.

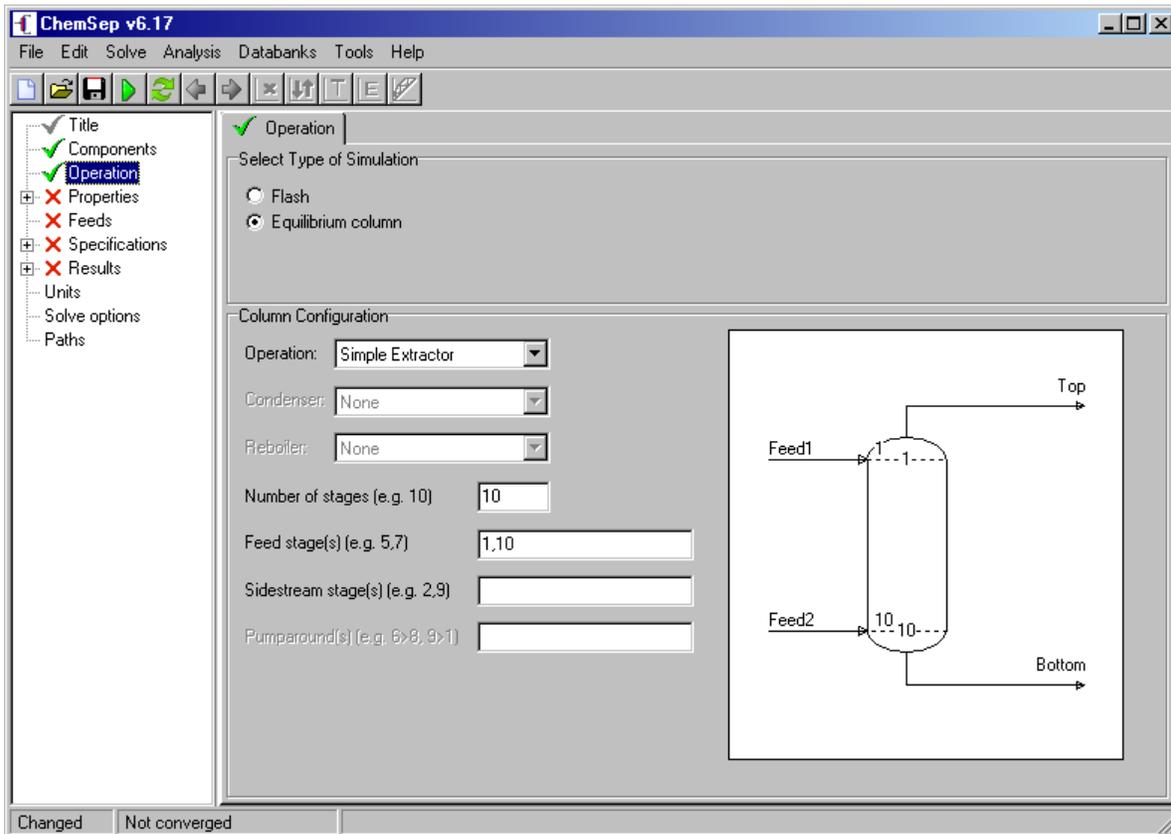
Table 1: Extractor Stream Flows: Feed Specifications and Products

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

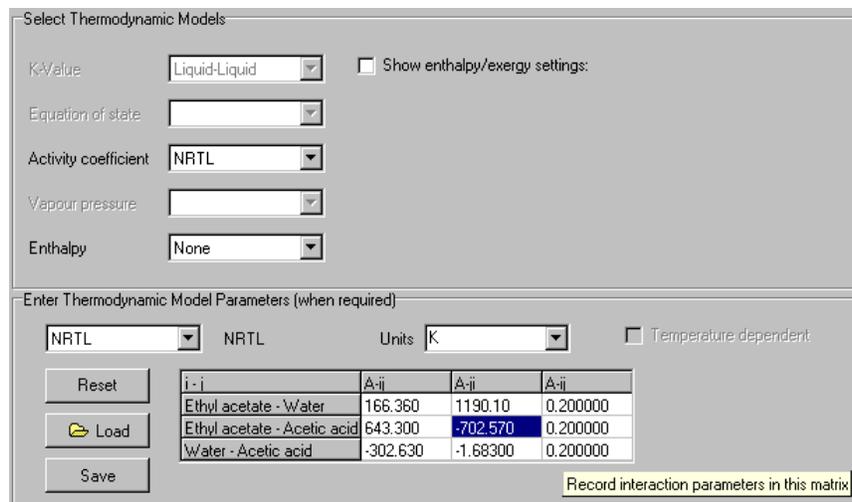
We begin by clicking on the Components Panel and selecting the components that are listed in Table 1 (the components should be selected in the order in which they appear in Table 1).



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



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



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) Specifications

Insert Remove Mass flows

Feed:	1	2
Name	Feed	Solvent
Stage	1	10
Two-phase feed	Split	Split-below
State	L & T	L & T
Pressure (psia)		
Light fraction (-)	0.000000	1.000000
Temperature (F)	100.000	100.000
Flowrates (lb/h):		
Ethyl acetate	0.000000	68600.0
Water	23600.1	2500.00
Acetic acid	6659.90	0.000000
Total flowrate	30260.0	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 Specifications* 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 (-)

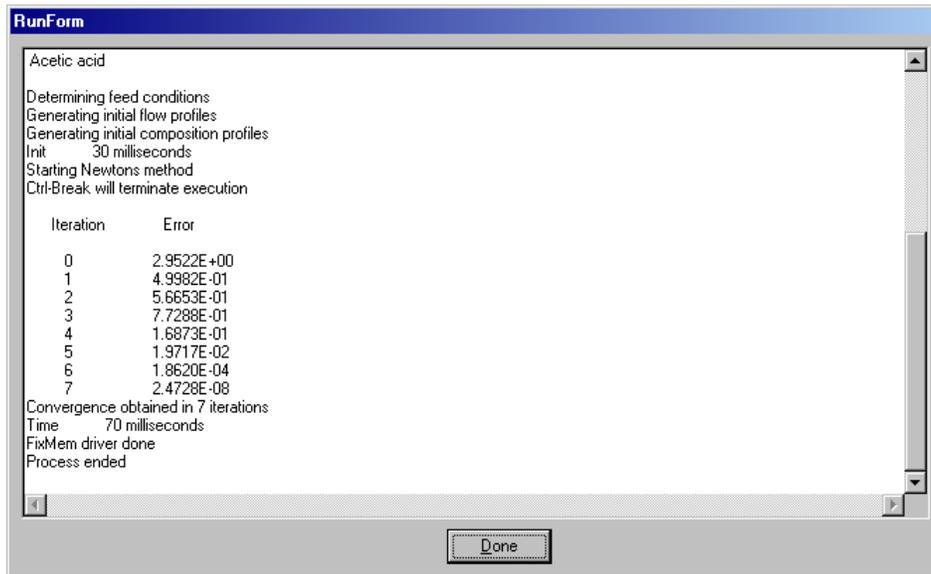
Method Newton's method Temperature 18.0000 (oF)

Accuracy 1.0000E-06 Composition 1.00000 (-)

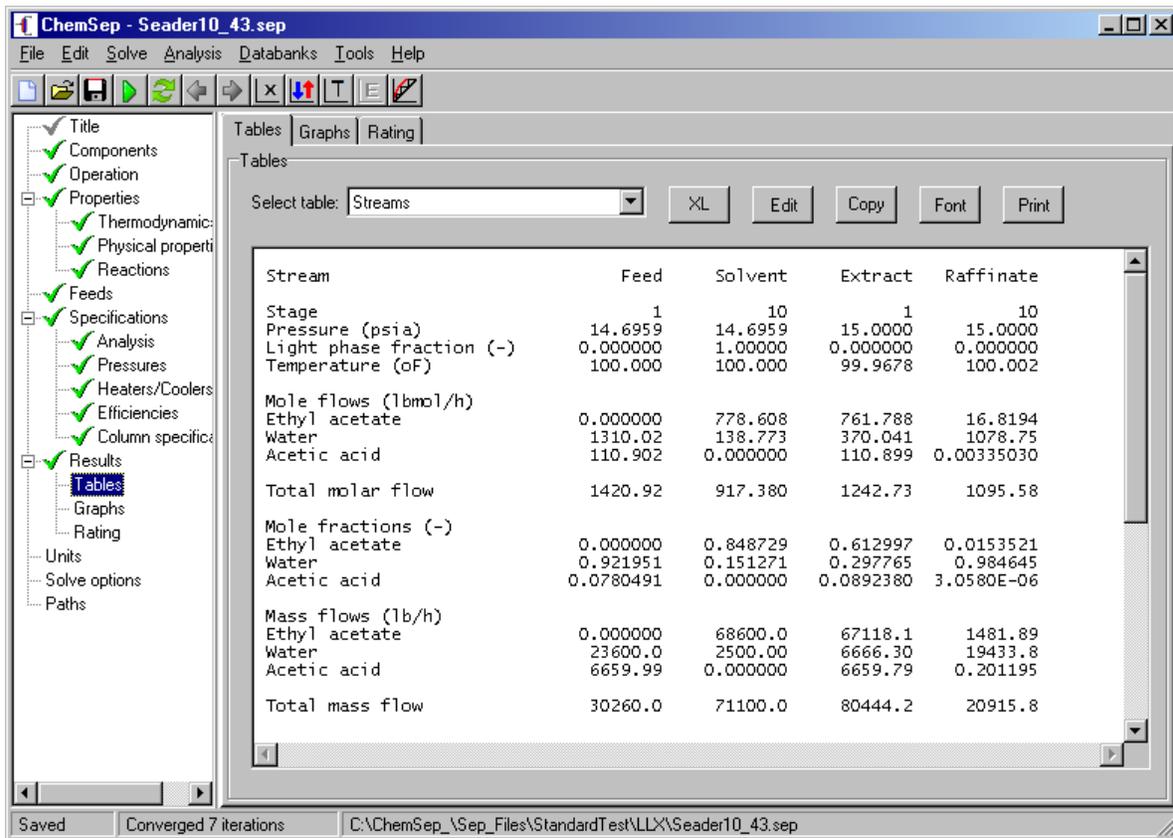
Number of Iterations 30 Flux 1.00000 (-)

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:



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



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%.