

Quick guide for using ChemSep to solve solvent extraction problems in general (and problem 6 of Problem Set 6 in particular)

1. Select the proper components in the components node. Select the components in the order of ethyl acetate, water, acetic acid (from top to bottom) in the components list to facilitate later debugging of your ChemSep program for problem 6.

2. Select "simple extraction" in the operation node. Also specify in this node that there are two feeds, with one ("Feed1") being at the top plate of the column (this is the real aqueous feed, also termed here the heavy phase), and the other ("Feed2") being at the bottom plate of the column (this is the organic solvent "separating agent", also termed here the light phase).

3. In the properties node, select "liquid-liquid (gamma)", then select "NRTL", and then leave the binary interaction parameters as the symbol *. ChemSep will then use the UNIFAC model to estimate these parameters.

4. In the feeds node, for the "two phase feed" entry, you need to select "split" for Feed1 (the aqueous phase going down the column) and "split-below" for the Feed2 (the organic phase going up the column). The simulation will not run unless you make these choices. "Split-below" tells ChemSep that this option applies to Feed2 that enters at the bottom of the column. Even though this **problem** involves a single phase feed at the top and bottom, in which case you might think your selection wouldn't matter here, in fact your selection does matter. Also, for the "light fraction" entry in the feed node, you need to enter 0 for Feed1 (there is no light phase present in this feed), and you need to enter 1 for Feed2 (this feed is entirely composed of the light phase). Also, the "L&T" entry in the feed node denotes you are entering the amount of light phase and the temperature to specify the feeds. This option can't be changed.

5. Enter the proper values in the specifications node. The choices here should be obvious.

6. In general this problem should converge readily although you may want to reduce somewhat the maximum allowable Newton step sizes in the options node to facilitate convergence. If you have trouble with the converge, then you probably didn't follow the instructions given above. Note that when you are solving this problem, you may get various warnings that some correlations are out of range etc. Just press the ignore or ok button when you see these warnings and continue until you get convergence.

7. When making plots or tables of your results, note that in some menus the aqueous liquid phase traveling down the column is denoted as the "liquid phase" having a molar flow rate of L and molar compositions denoted as x . Similarly, the organic liquid-phase traveling up the column is denoted in some menus as the "vapor phase" having a flow rate of V and molar compositions denoted as y . Note also that the phase diagram feature of ChemSep does not work for this particular system, so you will need to manually plot points on a triangular diagram to visualize the equilibrium predictions as described in the statement to problem 6.