Multicomponent Distillation Example Problem

A liquid feed stream at 2 atm and 298 K produced from mixing together a stream from a catalytic reforming unit and a stream from a toluene trans-alkylation unit contains benzene, toluene, *o*-xylene, *m*-xylene, and *p*-xylene at mole fractions of 0.34, 0.33, 0.11, 0.11, and 0.11, respectively. It is desired to produce purified components from this feed stream according to the process flow diagram shown in Fig. 1. Note that the most valuable component of this feed mixture is *p*-xylene, which is employed to make polyethylene terephthalate. This polymer is used to make plastic bottles for soft drinks, among many other applications, and is denoted as PET or PETE (or just the number "1" inside the recycling symbol) on plastic bottles meant for recycling.

Each distillation column shown in Fig, 1 operates with the purity and recovery specifications indicated in Table 1. Note that in the proposed BTX purification process shown, the toluene column is operated with a relatively low recovery of toluene, in which case a recycle stream is needed as shown that mixes with the bottom product of the benzene column. Furthermore, a xylene purification unit which employs a zeolite adsorption bed is able to return essentially all the toluene and *o*-xylene in the distillate produced by the third column to a mixer located upstream from the second column, as shown in Fig. 1. It is proposed that the process shown in Fig. 1 is highly tolerant of column fouling at a low capital cost compared to alternative designs that are possible.

The pressure is 1 atm in all the columns, and each of the columns incorporates a partial reboiler and a partial condenser. The stage efficiencies on each plate of each column and for the reboilers and condensers are estimated to be 0.8. For convenience, you may assume a flow rate basis of 1 mole/s for the BTX feed when solving this problem. Note that the third column in Fig. 1 is a so-called "xylene splitter." These types of columns operate at the very upper limit of what can be accomplished in a single distillation column and are some of the tallest distillation columns built worldwide. A recent installation of a xylene splitter is described at the following link: http://www.fibre2fashion.com/news/textile-news/newsdetails.aspx?news_id=120879

Propose an approximate optimal design for each column in this process where the combined capital and operating costs are minimized. Your optimal design should specify the total number of plates in the column, the location of the feed plate, the vapor flow from the reboiler, the reflux liquid flow, and the flows of the two products leaving the column. For your design you can use the standard "rule of thumb" that the optimal operating reflux ratio is 1.25 times the minimum reflux ratio. You may use the Fenske-Underwood-Gilliland ("FUG") shortcut method to produce an approximate optimal design, but your reported results should be for an actual column simulation near this approximate optimal design point. Also, for the optimal design conditions for each column, make graphs of the mole fractions in the vapor and liquid phases versus the plate number, the total molar flows in the vapor and liquid streams versus the plate number, and the temperature versus the plate number inside the distillation column. Briefly explain the observed trends in your graphs. In addition, using the common plate spacing of 3 feet between plates, determine the height of each of the three columns in Fig. 1 and briefly comment on whether these heights are reasonable. Make sure you also describe any additional assumptions not specified above used in your calculations. You may use COCO/ChemSep or Aspen to perform your calculations.

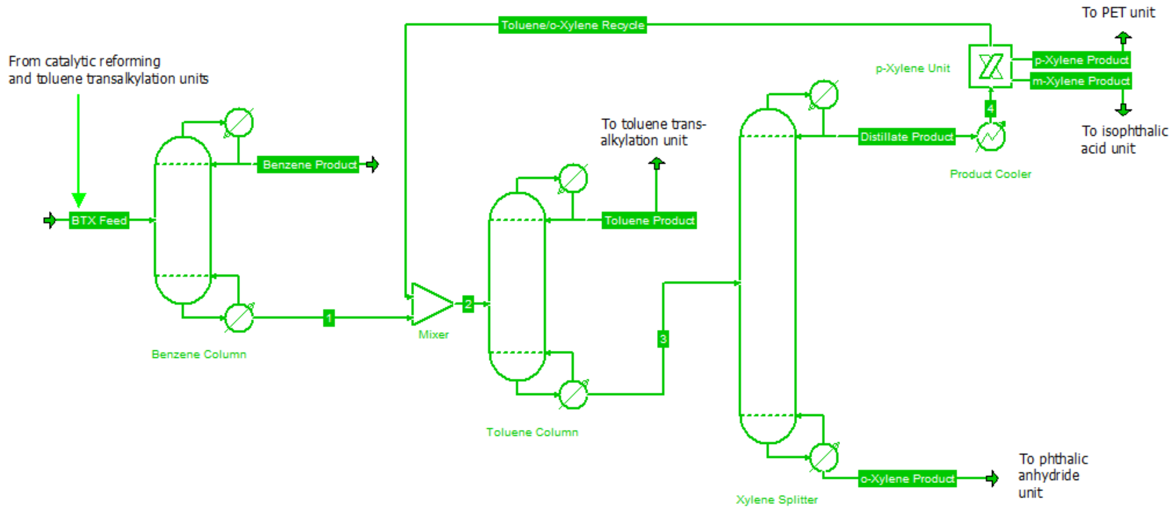

Figure 1. Process flow diagram for BTX distillation sequence (simplified version).

Column	Specification	Rough starting guess for column design (if needed)
Benzene column	98% recovery of benzene at 98% purity	Column has 36 plates with feed at plate 18
Toluene column	85% recovery of toluene at 95% purity	Column has 72 plates with feed at plate 36
Xylene splitter	90% recovery of o-xylene at 95% purity	Column has 136 plates with feed at plate 68

Table 1. Column specifications

Comments and Hints:

1. The simulation of this system converges fairly easily if you select the predictive Soave Redlich Kwong (the predictive SRK) equation of state for the vapor and the UNIFAC model for the liquid when using ChemSep. You may also need to reduce the maximum permitted step size in the Newton search method by a factor of 5 for all the search variables. You can do this by using the "Solve Options" sub-node in the ChemSep node tree. If you do this, you should also increase correspondingly the maximum number of iterations allowed in this same sub-node. Another good practice is to calculate each unit individually using the "calculate this unit" option in COFE before you try to solve the entire flow sheet. If you still have trouble converging, another useful method is to perform a simulation individually for each unit for the case where the vapor is an ideal gas and the liquid is an ideal mixture, which generally will converge easily. Then, in the Solve Options sub-node, select "old results" in the initialization feature, and then change the vapor and liquid phase equilibrium model back to the nonideal choices mentioned above. In this case ChemSep will use the solution for the ideal case as the starting guess for the nonideal case, which often facilitates convergence for the latter case. Also, the recycle stream should be initialized at reasonable values for the mole fractions, and the temperature of this stream should be such that it is a subcooled or saturated liquid. If you select starting conditions for the recycle stream corresponding to a superheated liquid (so that it will flash into separate vapor and liquid phases) an error will occur when using COFE.

2. If you have trouble accounting for the recycle stream, or if you are using only ChemSep to solve this problem instead of the full COFE environment so that you are not able to account for the recycle stream, you can ignore this stream for only a minor grade penalty.