Aromatics Column

In his book *Random Packings and Packed Towers, Design and Applications* R. Strigle (Gulf, 1987) describes a heavy naphta reformer aromatics column separating the toluene and lighter components from the xylenes and heavier aromatics. The column is 6 ft 6 inches in diameter and contains 60 valve trays (of a type unspecified) that are 20 inches apart. The column is being considered for refitting with packing. The feed consists of benzene through C-10 aromatics and the column operates at a top pressure of 21.4 psia.

The feed is superheated and undergoes a 12-weight % flash on entry to the column. Strigle states that the distillate flow is 18,580 lb/hr containing 0.40 wt % xylenes, the bottoms flow is 43,170 lb/hr with 0.25 wt % toluene, and the reflux flow is 70,600 lb/hr.

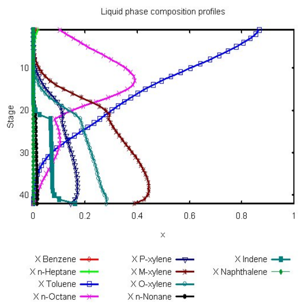
Strigle reports that the column is equivalent to 42 theoretical stages. The feed location is not specified but when discussing the packed column revamp Strigle states that the rectifying section has 25 theoretical stages and the stripping section has 22. This is more than the 42 stages mentioned above but we have used the ratio of 25/47 to determine where the relative feed location in all of our calculations with this system.

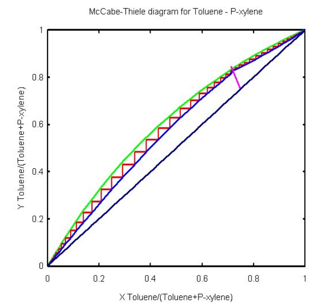
With this information we are able to conduct a preliminary simulation based on the equilibrium stage model in ChemSep. We assumed constant pressure operation (at the top pressure of 21.4 psia specified by Strigle). Thermodynamic properties were calculated from the Peng-Robinson equation of state. For simplicity the feed pressure was assumed to be the same as the column pressure and the feed vapor fraction was specified to be 12 mole percent rather than 12 wt % that Strigle reports (This was done in order to avoid carrying out a number of simulations to find the correct vapor fraction in molar units because at present ChemSep does not permit the user to specify the feed vapor fraction in weight units). Specifying the bottoms flow rate in lb/hr and the reflux ratio (calculated from the reflux and distillate flows given above) completed the column specifications. The feed and product flows from this calculation are shown below. Numbers shown as 0 are less than 0.001 lb/hr.

Feed specifications and product compositions

Component wt%	Feed	Distillate	Bottoms
Benzene	0.3	1	0
n-Heptane	0.6	2	0
Toluene	25.5	84.6	0.1
n-Octane	4.2	12.4	0.7
p-Xylene	9.9	0	14.2
m-Xylene	26.7	0	38.2
o-Xylene	19.2	0	27.5
n-Nonane	1.3	0	1.9
Indene	12.0	0	17.2
Naphthalene	0.3	0	0.4
Total mass flow (lb/h)	61750	18580	43170

The liquid composition profiles are shown below.





(a) Liquid mole fractions profiles equilibrium column (b) The McCabe-Thiele diagram between the key components Toluene

We now model the column as it really was: with 60 valve trays. We know only that the column was 6.5 ft in diameter. Design specifications and options used here are summarized in the table below. All other details of the trays were left for ChemSep to determine using its built in design procedure.

The material balance from this simulation is very similar to those obtained from the equilibrium stage calculation (as, for this kind of system, they should be). The only difference is that the n-Octane percentage is 12.3 instead of 12.4 mole%.

The tray design produced by ChemSep is summarized below (recall that Strigle provided no details of the tray design so ChemSep was allowed to design them as part of the simulation). The composition profiles also don't look very different from their equilibrium stage counterparts (again, we should be surprised if there was a significant difference).

Valve tray models and computed layout

Mass transfer coefficient	AIChE	Tray spacing (ft)	2
Liquid phase resistance	Included	Number of flow passes	2
Vapour flow model	Plug	Liquid flow path length (ft)	2.23
Liquid flow model	Plug	Tray spacing (ft)	1.7
Pressure drop	Estimated	Active area (%total)	76
Entrainment	None	Total hole area (%active)	15
Column diameter (ft)	6.5	Downcomer area (%total)	12
		Hole diameter (”)	0.0156
		Hole pitch (”)	0.03842
		Weir type	Segmental
		Weir length (ft)	11.325
		Weir height (”)	2
		Downcomer clearance (”)	1.5
		Deck thickness (”)	0.1
K closed (-)	2.76004	K open (-)	0.401854
Eddy loss coefficient (-)	4.26509	Weight ratio valve (-)	4.23228
Valve density (lb/ft3)	25751.3	Valve thickness (ft)	0.00984252

The fact that the trays do not operate at equilibrium is emphasized in the plot that shows the Murphree efficiencies. The average efficiency in the rectifying section is found to be around 65% and approximately 80% in the stripping section.

The trayed column easily meets both product specifications and is also well balanced: the top product contained 0.51 mole% C4's and the bottoms 0.48 mole% C3's. From the tray efficiency plot we see that the tray efficiencies are around

90 %, which is normal for this kind of operation. Inspecting the fraction of flooding profile we observe that the bottom section is limiting the capacity of the column as it peaks at tray 20 (from the top). Turndown is a factor 2.7 for the trays in the rectifying section versus about 1.9 for the trays in the stripping section. This can be improved by using different tray layouts in the rectifying and stripping section. Observe that combining the two sections caused the design method to come with a tray layout with a maximum of 83% of flood. But the actual column is only 5 ft in diameter, not 5.37 ft! This implies that at this reflux ratio the stripping section would be flooding ($83\% * 5.37^2/5^2 = 96\%$) and can explain why Strigle used a low tray efficiency of just $14/22 = 64\%$. When the reflux ratio is lowered down to 0.92 the 5ft double pass sieve tray *can* operate at around 90% of flood (stripping section) and tray efficiencies remain high at 90+% resulting in 1.94 mole% C3 in the bottoms and 0.67 mole% C4 in the distillate.

Strigle refits his column with #40 IMTP packing which is not available in ChemSep and we have selected an alternative.

If we pack the 102ft tall tower with 35mm NORPAC packing, ChemSep estimates that a column only just over 6 feet in diameter is needed while delivering a slightly improved separation.

Our column, however, is 6.5 ft in diameter. So the next step is to specify the actual diameter. The simulation clearly shows that the column now is underperforming as there are a great many warnings that the packing in insufficiently wet. It does, however, converge to give a column with a significantly improved separation.

This allows us to (again following Strigle) cut the reflux ratio from 3.8 to 3.2 with still a significant improvement in performance over the original tray column design.

Clearly, therefore, we can increase column throughput should we wish to do so. Strigle, in fact, proposes to increase the feed flow rate by 30%. We can do this easily in ChemSep by double clicking on the total flow cell in the feed flow panel (to make sure the contents of the cell are not highlighted) and typing *1.3 after the number that is in that cell. Click out of the cell and the calculation is done and the new flow rate recorded. It is important also to change the desired bottoms mass flow rate by 30% as well. ChemSep converges this new design quite easily with no warnings indicating the hydrodynamic design is satisfactory.

The stream table for this final design is the same as before except that the Toluene mole fraction of the distillate is 84.7 instead of 84.6 mole%.

Conclusion

We have used *ChemSep*^{TM} to determine if an existing tray column can be refitted with #50 IMTP packing. This design exercise was posed in *Random Packings and Packed Towers, Design and Applications* by R. Strigle. Although not all details of the exercise are in agreement with Strigle we find that a packed column can meet the purity specifications but that it provides no capacity advantage over a convential double pass sieve tray.

We have used ChemSep to determine if an existing tray column can be refit with packing and provide an increase in capacity. The design exercise was posed in Random Packings and Packed Towers: Design and Applications by R. Strigle (Gulf, 1987). Although not all details of the exercise are in exact agreement with Strigle (due to a lack of information in most cases) we find, in agreement with him, that it is possible to equip the tower with packing, gain an improvement in separation and increase capacity by (at least) 30%.