The DeRosier Problem Revisited

We consider here a design problem posed by Doherty and Malone (Conceptual Design of Distillation Systems, McGraw-Hill, 2001). They call this example the DeRosier Problem after the student who first developed a successful design. Design a distillation column to separate a feed of 20 mol/s methanol, 10 mol/s isopropanol, and 20 mol/s water. The bottom product is to contain no more than 0.5 mol% methanol and the distillate is to contain at least 99 mol% methanol but no more than 50 ppm water.

As a first step we attempt to design the column using the equilibrium stage model. Following Doherty and Malone, the NRTL model was used for the activity coefficients and the Antoine equation for the vapour pressures. Doherty and Malone estimate the minimum reflux as 5; we used a value 50% higher in this example and specified the bottoms product rate at 30 mol/s; this choice provides a consistent basis for the comparison of different models. The number of stages and the location of the feed were varied until a column configuration was obtained that met the desired product purity: 80 total stages (including total condenser and partial reboiler) with the feed to stage 16.

Efficiencies of alcohol-water and alcohol-alcohol systems obtained experimentally in sieve tray columns vary from 60% to 100% (Chapter 14 in *Perry's Chemical Engnrs. Handbook*, 7th Edition). After specifying an average efficiency of 80% we find that 99 total stages with the feed to stage 21 were needed to get the distillate below 50 ppm water.
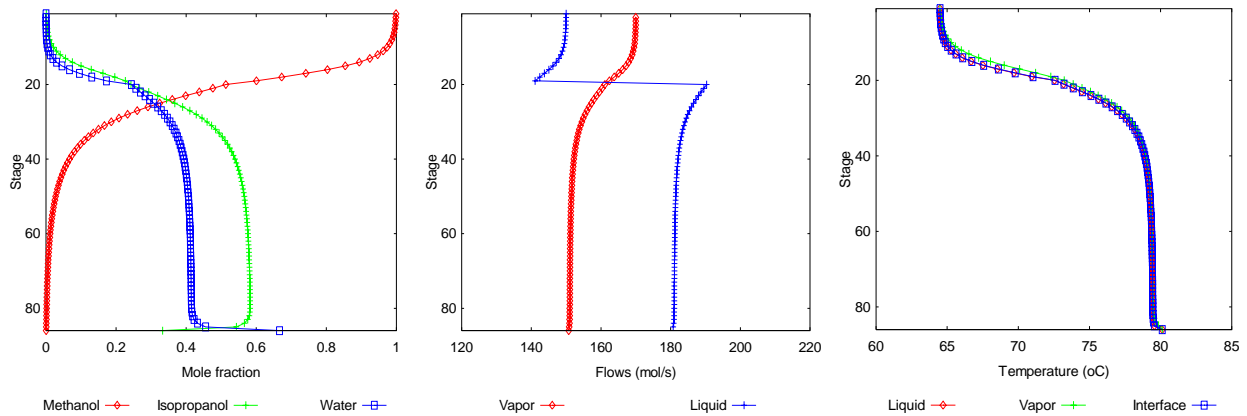
If we use the nonequilibrium model to design a sieve tray column we found that a column with 84 trays (plus condenser and reboiler) and with the feed to tray 21 (stage 22) will produce an overhead product of the desired purity. The reflux ratio and bottoms flows were maintained at the values employed for the equilibrium stage design. The AIChE method was used for estimating the mass transfer coefficient – interfacial area products, and the vapour and liquid phases were assumed to be in plug flow. The pressure was assumed constant in the column (an assumption that would need be relaxed at a later stage of the design exercise). The computer simulation also provided a preliminary tray design; that for the trays above the feed is summarized in the table below.

Column diameter (m)	1.76
Total tray area (m^2)	2.43
Number of flow passes	2
Tray spacing (m)	0.6
Liquid flow path length (m)	0.75
Active area (%total)	91.4
Total hole area (%active)	14
Downcomer area (%total)	4.3
Hole diameter (mm)	5

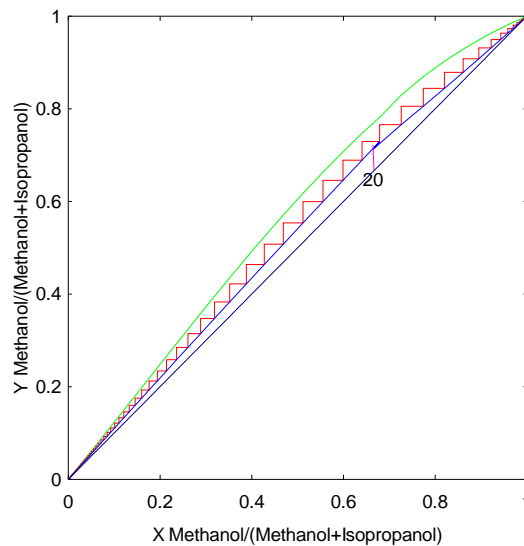| Hole pitch (mm) | 12 |
Weir type	Segmental
Combined weir length (m)	1.55
Weir height (mm)	50

To converge the nonequilibrium model at the specified reflux ratio it was necessary first to solve the problem at a much lower reflux ratio ($R = 2$) and then increase R in steps until the desired value of 7.5 was reached.

The liquid composition, flow, and temperature profiles are shown below. In this particular system the vapour and liquid temperatures estimated by the rate-based model are quite close (as often is the case in distillation operations).
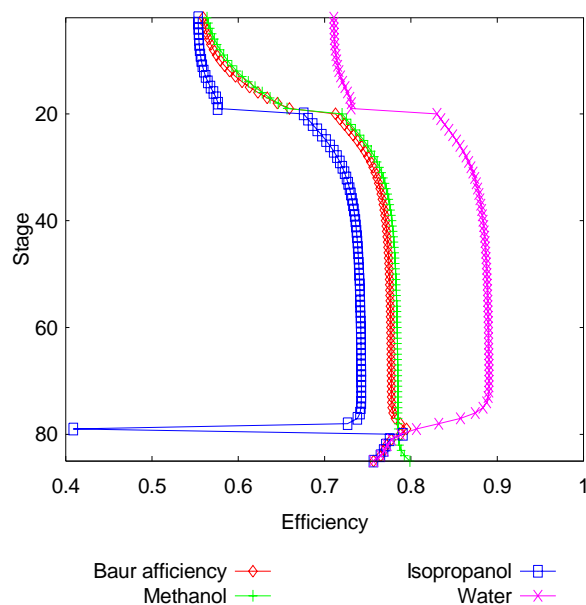

Composition, flow and temperature profiles in nonideal distillation process.

The McCabe-Thiele diagram for this column is shown below. Note that in this case the triangles the represent the stages do not touch the equilibrium line.

McCabe-Thiele diagram for nonideal distillation column.

The length of the horizontal section of each triangle in the McCabe-Thiele diagram is a measure of the efficiency of that tray. The component Murphree efficiencies calculated from the simulation results and as well as the average Baur efficiency are shown below. The efficiency of methanol in the stripping section is seen to be around 80%, that of isopropanol to be approximately 75%, while that of water is close to 90% in the bulk of the column before falling off on the bottom few trays. All component efficiencies are found to be lower in the rectifying section. The average efficiency is close to the Murphree efficiency of methanol and varies from 60% in the top of the column to 78%. Thus, the constant value of 80% used above appears to be appropriate, and yet, the column designed with the constant efficiency model required no less than 99 stages (97 trays)!

Component Murphree and Baur average efficiency for nonideal distillation.

With 84 trays as opposed to 78 equilibrium stages (not counting condenser and reboiler in either case) we find an overall efficiency of 93%, a figure that is quite at odds with the values of the individual component efficiencies seen in the figure above. How, then, is it possible that the nonequilibrium model suggests that the column needs only 6 trays more than the number of equilibrium stages. It is, in fact, because the efficiency of water is so much higher than that of the alcohols that leads to a column design that can produce high purity methanol while producing the 50 ppm methanol bottom product in so few extra stages. It should be noted that nonequilibrium models will not always lead to a design with fewer trays than might be suggested by a constant efficiency model; it is just as likely for the mass transfer rate-based model to predict that more stages will be needed – it all depends on the differences between the component efficiencies.

Individual component efficiencies can only vary as much as they do in this example when the diffusion coefficients of the three binary pairs that exist in this system differ significantly. For ideal or nearly ideal systems all models lead to essentially the same results. This example demonstrates the importance of mass transfer models for nonideal systems, especially when trace components are a concern. For further discussion of this example see Doherty and Malone (op. cit.) and Baur et al. [*AIChE J*. **51**, 854 (2005)]. It is worth noting that there exists extensive

experimental evidence for mass transfer effects for this system, and it is known that nonequilibrium models accurately describe the behaviour of this system, whereas equilibrium models (and equal efficiency models) sometime predict completely erroneous product compositions [Pelkonen et al., *Ind. Engng. Chem. Res.,* **36**, 5392 (1997), *Chem. Eng. Process*, **40**, 235 (2001), Baur et al., *Trans. I. Chem. E.*, **77**, 561 (1999)].