CHEG 325-010 Spring 2020 Final Project Assignment - Part 2

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Distilling a mixture of n-heptane (1) and ethylbenzene (2) has its industrial applications, especially separating aromatic hydrocarbon (ethylbenzene) from aliphatic compounds (n-heptane) in the petrochemical industry [1]. It is due to the high demand of aromatic compounds by the chemical industry, such as to produce paints and wood stains for arts and crafts finish [2]. Moreover, there are strict legal restrictions on the content of aromatics in gasoline, in order to ensure the safety of all consumers [1]. To determine the appropriate number of stages and reflux ratio to distillate a mixture fed at $x_{F,1}$ of 0.55 as saturated liquid, two different methods were performed; McCabe-Thiele and short cut distillation column (DSTWU) analysis.

For McCabe-Thiele analysis, the x-y plot from Wilson model's regression fitting was used. The minimum number of stages, N_{min} required was 6 as shown in Figure 1, with an infinite reflux ratio, R^{∞}, where the rectification (C) and stripping (S) operating line overlapped the y = x line. The molar ratio of 1 at distillate, x_{D1} and bottom, x_{B1} were 0.95 and 0.061 respectively. A horizontal line from x_{D1} at y = x line was drawn until it touched the y-x curve, continued with a vertical line until it reached back the y = x line. Multiple of these steps were performed until it immediately passed through $x_{B,1}$. The number of 'square hoops' represented the number of stages. With the obvious C and S line, the vertical lines instead were drawn until it reached these lines, before and after $x_{F,1}$ respectively. For a saturated liquid feed, a vertical line (q line) was drawn from the feed line after passing through the y = x line [3]. For N^{∞} condition, a pinch point at the y-x curve, from the intersection of S, C, and q line was identified, resulting in an R_{min} of 0.8199, by interpolating the C-line's intercept to be 0.522, and equating it to intercept equation in Eq. 1 to find R_{min}, as shown in Figure 2. With R = $1.2R_{min}$, with the same steps, R = 0.9839 with N = 14, where the feed should enter at the 7^{th} stage, since it's where the 'square hoops' started to transit from C to S line, illustrated in Figure 3. This analysis only took into account binary mixture and neglected other thermodynamic effects on it [4]. Plus, it assumed that liquid and vapor always reached its equilibrium at each tray in the column [4].

DSTWU analysis is performed in ASPEN, by setting up the simulation and applying the same constraints as mentioned previously. It was found that N_{min} = 5.57 and R_{min} = 0.7970. For R = $1.2R_{min}$, R = 0.9564 with N = 13.11, where the feed should enter at 7^{th} stage. The assumption made in this analysis was that the relative volatilities of the pure component in the mixture and its molar overflow (L and D) remained constant [5].

In real distillation columns, these assumptions would not hold anymore. A mixture is not always binary and it is hard to reach equilibrium at all trays in the column. Besides, the molar overflow might not be constant too. It is more reliable to choose DSTWU methods than McCabe-Thiele analysis, as the latter one employs interpolation of data plots which creates uncertainty in final values. From Table 1, there's an inverse relationship between the reflux ratio and number of stages, where decreasing one of them will increase the other. From an economic perspective, cutting down the operational cost by reducing the reflux ratio will increase the capital cost, since more stages are required. However, a substantially reduced reflux ratio reduced the amount of product circulating in the column, where only a small diameter of column is needed [6]. Overall, the capital cost will decrease with a great amount. As a rule of thumb, it is suggested to operate at 20 % or higher than R_{min} to optimize the equipment and operating costs [6].

[6] $C\ line : y_{i+1} = \frac{x_D}{1+R} + \frac{R}{1+R}x_i,\ intercept = \frac{x_D}{1+R},\ slope = \frac{R}{1+R}$ (Eq. 1)

Table 1: Theoretical number of stages from DSTWU analysis

Number of Stages	Reflux Ratio
11	1.11514
12	1.00556
13	0.96004
14	0.93324
15	0.91489

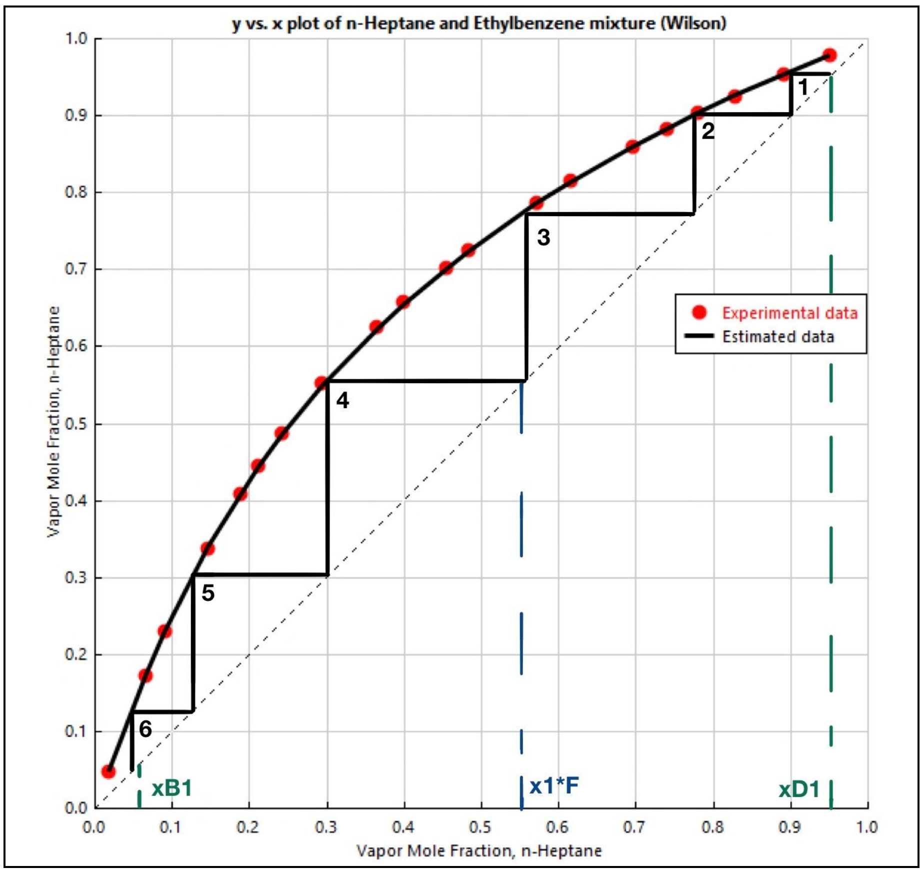

Figure 1: McCabe-Thiele Analysis with the condition N_{min} with respect to R^{∞}

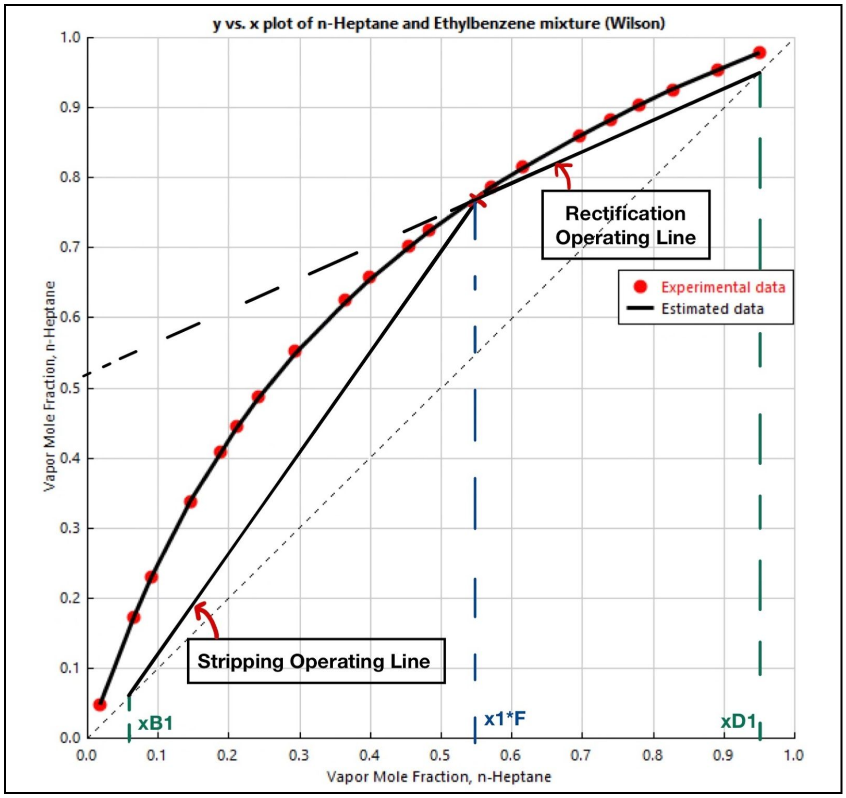

Figure 2: McCabe-Thiele Analysis with the condition R_{min} with respect to N^{∞}

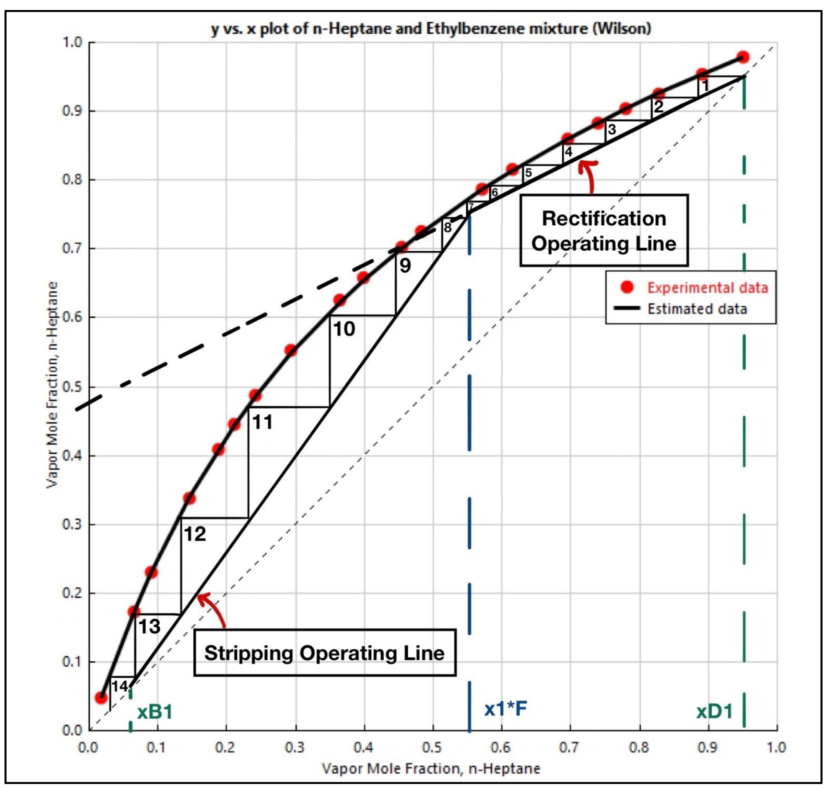

Figure 3: Mc-Cabe Thiele Analysis with $R = 1.2R_{min}$

REFERENCES

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