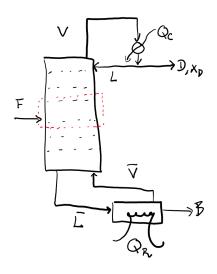
1)

a.



$$P=101.325~\mathrm{kPa}$$

$$x_B = 0.10$$

$$x_D = 0.96$$

$$x_F = 0.72$$

$$F = 250 \text{ mol/hr}$$

$$R = 4:1$$

Assume: CMO

Solve: The material balances around the entire column are,

$$F = D + B$$
,

$$x_F F = x_D D + x_B B,$$

from which we find,

$$\frac{D}{F} = \frac{x_F - x_B}{x_D - x_B}.$$

Thus,

$$D = (250 \text{ mol/hr}) \left(\frac{0.72 - 0.10}{0.96 - 0.10} \right) = 180 \text{ mol/hr},$$

and,

$$B = F - D = 70 \text{ mol/hr}.$$

b.

$$LK = i = n - \text{heptane}, HK = j = \text{toluene}.$$

c.

The detailed McCabe-Thiele results are presented in the appendix, they are essentially the same results as in HW 8, problem 2, but with a different reflux ratio.

The Fenske equation is given as,

$$N_{min} = \frac{\ln\left(\left[\frac{x_{N+1,i}}{x_{1,i}}\right]\left[\frac{x_{1,j}}{x_{N+1,j}}\right]\right)}{\ln\left(\alpha_{ij}\right)},$$

where,

$$\alpha_{ij} = \sqrt{(\alpha_{ij})_1 (\alpha_{ij})_{N+1}} = \sqrt{(\alpha_{ij})_B (\alpha_{ij})_D}.$$

The relative volatility at a stage, k, may be calculated from the equilbrium data,

$$(\alpha_{ij})_k = \frac{(y_i/x_i)_k}{(y_j/x_j)_k} = \frac{(y/x)_k}{([1-y]/[1-x])_k},$$

where the second equality only holds for binary mixtures. A plot of x_{LK} against α_{ij} is shown in the following.

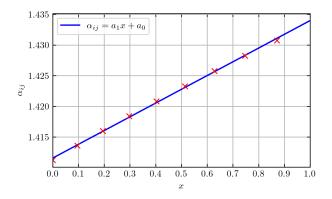


Figure 1: Relative volatility for n-heptane-toluene mixture, $(a_1, a_0) = (0.0224, 1.412)$ with estimated $R^2 = 0.999$. Observe that the α_{ij} is not exactly linear, but it is a good approximation.

From this, the bottoms and distillate relative volatilities may be estimated as $(\alpha_{ij})_D = 1.433$ and $(\alpha_{ij})_B = 1.414$, from which we calculate,

$$\alpha_{ij} = \sqrt{(1.414)(1.433)} = 1.423.$$

Thus, N_{min} may be calculated,

$$N_{min} = \frac{\ln\left(\left[\frac{0.96}{0.10}\right]\left[\frac{0.90}{0.04}\right]\right)}{\ln(1.423)} = 15.23,$$

meaning at least $N_{min} = 16$ stages are required. This agrees exactly with the McCabe-Thiele analysis which is likely because the change in relative volatility is small. The ratio of the top to bottom relative volatility $(\alpha_{ij})_B/(\alpha_{ij})_D = 0.987$ which is slightly above 1%, and much less than the 15% rule of thumb. Therefore, we should expect the Fenske and McCabe-Thiele results to be close.

d.

The Underwood equations are given as,

$$\sum_{i=1}^{N_c} \frac{(\alpha_{ij})_{\infty} x_{F,i}}{(\alpha_{ij})_{\infty} - \theta} = 1 - q,$$

$$\sum_{i=1}^{N_c} \frac{(\alpha_{ij})_{\infty} x_{D,i}}{(\alpha_{ij})_{\infty} - \theta} = 1 + R_{min},$$

for some θ ('s) satisfying $1 < \theta < \alpha_{ij}$. For the saturated liquid, q = 1, meaning the RHS of the first equation becomes 0. Additionally, from Figure 1, $(\alpha_{12})_{\infty} = (\alpha_{12})_F = 1.428^{-1}$ and by definition, $(\alpha_{22})_{\infty} = 1.0$. Therefore, we have the root finding problem,

$$f(\theta) = \frac{(1.428)(0.72)}{1.428 - \theta} + \frac{(1.0)(0.28)}{1.0 - \theta} = 0.$$

This is a 'nice' function for root finding since,

$$f'(\theta) = \sum_{i=1}^{N_c} \frac{(\alpha_{ij})_{\infty} x_{F,i}}{((\alpha_{ij})_{\infty} - \theta)^2},$$

is always positive. Thus, applying Newton's method is straightforward,

$$\theta_{k+1} = \theta_k - \frac{f(\theta_k)}{f'(\theta_k)},$$

since it will converge (fast); all that is needed is a good guess, which may be found by plotting $f(\theta)^2$.

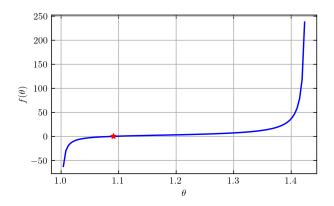


Figure 2: Graphical solution to the Underwood equation

 $^{{}^{1}}$ If $(\alpha_{12})_{F}$ is not known, the previously calculated mean value, α_{ij} may be used. By the assumptions of the Fenske equation, the α_{ij} , does not vary significantly, so using the mean value will only introduce small errors. Using α_{ij} , the resulting $R_{min} = 2.67$, which is still an acceptable number compared to M-T.

²It's also possible just to guess the roots based on the α_{ij} values. Observe that $f(\theta)$ will blow up at any α_{ij} 's between $\alpha_{LK,HK}$ and $\alpha_{HK,HK} = 1$, so any guesses between the sandwich relative volatilities are likely to converge.

Using this, Newton's method gives $\theta = 1.091$. R_{min} may now be calculated from this,

$$R_{min} = \frac{(1.428)(0.96)}{1.428 - \theta} + \frac{(1.0)(0.04)}{1.0 - \theta} - 1$$
$$= \frac{(1.428)(0.96)}{1.428 - 1.091} + \frac{(1.0)(0.04)}{1.0 - 1.091} - 1$$
$$= 2.64.$$

Thus, for the saturated liquid feed, $R_{min} = 2.64$. McCabe-Thiele gives $R_{min} = 2.63$ which, is *very* close to the Underwood result, again this is likely due to the system being relatively ideal and only small variations in α_{ij} along with CMO being valid.

e.

The Gilliland correlation is given as,

$$Y = 1 - \exp\left(\left[\frac{1 + 54.4X}{11 + 117.2X}\right] \left[\frac{X - 1}{X^{0.5}}\right]\right),\,$$

where,

$$X = \frac{R - R_{min}}{R + 1}$$
 , $Y = \frac{N - N_{min}}{N + 1}$.

Often, we may take $R = 1.3R_{min}$ if not given further information, but since we know R = 4, we may calculate X directly,

$$X = \frac{4 - 2.64}{4 + 1} = 0.272,$$

from which we find, Y = 0.402. Thus, we may solve for N,

$$N = \frac{Y + N_{min}}{1 - Y} = \frac{0.402 + 15.23}{1 - 0.402} = 26.14,$$

meaning N = 26 + 1 stages are required. The Kirkbride equation may now be used to estimate the feed location, N_F ,

$$\frac{N_R}{N_S} = \left[\left(\frac{x_{HK,F}}{x_{LK,F}} \right) \left(\frac{x_{LK,B}}{x_{HK,D}} \right)^2 \left(\frac{B}{D} \right) \right]^{0.206},$$

giving,

$$\frac{N_R}{N_S} = \left[\left(\frac{0.28}{0.72} \right) \left(\frac{0.10}{0.04} \right)^2 \left(\frac{180}{70} \right) \right]^{0.206} = 0.988.$$

Since,

$$N = N_R + N_S + 1,$$

we have,

$$\frac{N-1}{N_S} = \frac{N_R}{N_S} + 1 = 1.988,$$

and since $N=26.14\sim 27$, this gives, $N_S=12.65\sim 13$, meaning, $N_R=N-N_S-1=12.49\sim 13$, and thus, $N_F=N_R+1=14$. This varies slightly from the McCabe-Thiele result of $N_F=12$, however, the number of stages is also 1 greater than McCabe-Thiele. Regardless, the Kirkbride correlation is still a good enough estimate to find that the feed is nearly halfway through the column.

f.

The minimum number of stages remains the same regardless of the feed conditions, therefore, from problem c., $N_{min} = 16$.

g.

The general setup of the Underwood equations remains the same as in part d., the only difference is the root finding function since q = 0 for the saturated vapor. This gives,

$$f(\theta) = \frac{(1.428)(0.72)}{1.428 - \theta} + \frac{(1.0)(0.28)}{1.0 - \theta} - 1 + 0 = 0.$$

Graphically, this is shown in the following figure.

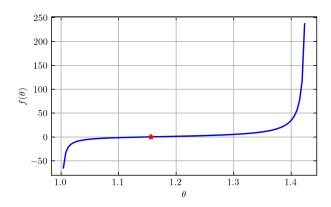


Figure 3: Graphical solution to the Underwood equation

Using this as an estimate, Newton's method gives $\theta = 1.156$. R_{min} may now be calculated from this,

$$R_{min} = \frac{(1.428)(0.96)}{1.428 - \theta} + \frac{(1.0)(0.04)}{1.0 - \theta} - 1$$
$$= \frac{(1.428)(0.96)}{1.428 - 1.156} + \frac{(1.0)(0.04)}{1.0 - 1.156} - 1$$
$$= 3.117.$$

Thus, for the saturated vapor feed, $R_{min} = 3.12$. McCabe-Thiele gives $R_{min} = 3.11$, which is again very similar to the Underwood result for the same reasons listed in part d.

h.

Calculating X for the Gilliland correlation,

$$X = \frac{4 - 3.12}{4 + 1} = 0.177,$$

from which we find, Y = 0.481. Thus, we may solve for N,

$$N = \frac{Y + N_{min}}{1 - Y} = \frac{0.481 + 15.23}{1 - 0.481} = 30.25,$$

meaning N = 30 + 1 stages are required. The Kirkbride equation may now be used to estimate the feed location, N_F ,

$$\frac{N_R}{N_S} = \left[\left(\frac{0.28}{0.72} \right) \left(\frac{0.10}{0.04} \right)^2 \left(\frac{180}{70} \right) \right]^{0.206} = 0.988.$$

Since,

$$N = N_R + N_S + 1,$$

we have,

$$\frac{N-1}{N_S} = \frac{N_R}{N_S} + 1 = 1.988,$$

and since $N=30.25\sim31$, this gives, $N_S=14.71\sim15$, meaning, $N_R=N-N_S-1=14.54\sim15$, and thus, $N_F=N_R+1=16$. This varies slightly from the McCabe-Thiele result of $N_F=15$, however, the number of stages is also 2 greater than McCabe-Thiele. Regardless, Kirkbride the correlation is still a good enough estimate the feed within 1-2 stages.

2)

a.

$$Z_{i}$$
 Q_{c}
 Q_{c

(1) Benzene, (2) Toluene, (3) Cumene
$$x_{F,1}=0.30,\ x_{F,2}=0.40,\ x_{F,3}=0.30$$

$$d_1=0.99f_1$$

$$b_2=0.92f_2$$

$$\alpha_{12}=2.25,\ \alpha_{32}=0.21$$

$$q=0$$

$$F=100\ \mathrm{mol/hr}$$

Assume: CMO, constant α_{ij} 's

Solve:

Let be nzene be the light key and toluene be the heavy key. The material balance for a component, i, is given by,

$$f_i = d_i + b_i.$$

For the light key, $d_1 = 0.99 f_1 = 29.7 \text{ mol/hr}$, meaning $b_1 = 0.01 f_1 = 0.3 \text{ mol/hr}$. Similarly, for the heavy key, $b_2 = 0.92 f_2 = 36.8 \text{ mol/hr}$, giving $d_2 = 0.08 f_2 = 3.2 \text{ mol/hr}$. The Fenske equation in terms of flow rates is then given as,

$$N_{min} = \frac{\ln\left(\left[\frac{d_1}{d_2}\right]\left[\frac{b_2}{b_1}\right]\right)}{\ln\left(\alpha_{12}\right)}$$

$$= \frac{\ln\left(\left[\frac{29.7}{3.2}\right]\left[\frac{36.8}{0.3}\right]\right)}{\ln\left(2.25\right)}$$

$$= 8.68.$$

Therefore, $N_{min} = 8 + 1$ stages are required at total reflux. To estimate the composition of cumene in the bottoms, consider a rearranged form of the Fenske equation,

$$\frac{d_i}{b_i} = \frac{f_i - b_i}{b_i} = \frac{d_2}{b_2} \alpha_{i2}^{N_{min}},$$

or solving for b_i ,

$$b_i = \frac{f_i}{1 + (d_2/b_2)\alpha_{i2}^{N_{min}}}.$$

Therefore, using i = 3 for cumene,

$$b_3 = \frac{30 \text{ mol/hr}}{1 + (3.2/36.8)(0.21)^{8.68}} = 29.99... \text{ mol/hr}.$$

The distillate flow of cumene is about 3.4×10^{-6} mol/hr, therefore, <u>practically 100% of the cumene</u> is recovered in the bottoms. For the Underwood equation, it is useful to calculate $x_{D,i} = d_i/D$. Summing over i yields D = 32.9 mol/hr, giving,

$$(x_1, x_2, x_3)_D = (0.9027, 0.0973, \sim 0).$$

Similarly, for the bottoms, B = 67.1 mol/hr, giving,

$$(x_1, x_2, x_3)_B = (0.0045, 0.5484, 0.4471).$$

b.

Using q = 0, the given α_{ij} 's, and the $x_{F,i}$, we may set up the Underwood root finding function,

$$f(\theta) = \frac{(2.25)(0.30)}{2.25 - \theta} + \frac{(1.0)(0.40)}{1.0 - \theta} + \frac{(0.21)(0.30)}{0.21 - \theta} - 1 + 0 = 0.$$

Plotting for the initial guess.

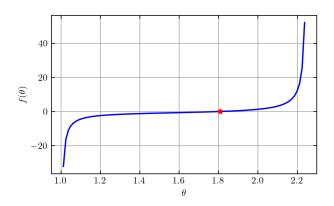


Figure 4: Graphical solution to the Underwood equation

With this, Newton's method gives $\theta = 1.8098$. R_{min} may now be calculated with this ³,

$$R_{min} = \frac{(2.25)(0.9027)}{2.25 - \theta} + \frac{(1.0)(0.0973)}{1.0 - \theta} + \frac{(0.21)(1.04 \times 10^{-7})}{0.21 - \theta} - 1$$

$$= \frac{(2.25)(0.9027)}{2.25 - 1.8098} + \frac{(1.0)(0.0973)}{1.0 - 1.8098} + \frac{(0.21)(1.04 \times 10^{-7})}{0.21 - 1.8098} - 1$$

$$= 3.494.$$

Thus, for the saturated vapor feed, $R_{min} = 3.49$

c.

Since $R = 1.25R_{min}$, we have R = 4.368, meaning we can calculate X for the Gilliland correlation,

$$X = \frac{4.368 - 3.94}{4.368 + 1} = 0.101,$$

from which we find, Y = 0.552. Thus, we may solve for N,

$$N = \frac{Y + N_{min}}{1 - Y} = \frac{0.552 + 8.68}{1 - 0.552} = 20.62,$$

meaning N = 20 + 1 stages are required.

 $^{^{3}}$ I included the cumene distillate composition in the R_{min} calculation out of curiosity. Unsurprisingly, it doesn't appreciably change the answer whether it is included or not.

d.

The Kirkbride equation may now be used to estimate the feed location, N_F ,

$$\frac{N_R}{N_S} = \left[\left(\frac{0.28}{0.72} \right) \left(\frac{0.0045}{0.0973} \right)^2 \left(\frac{67.1}{32.9} \right) \right]^{0.206} = 0.345.$$

Since,

$$N = N_R + N_S + 1,$$

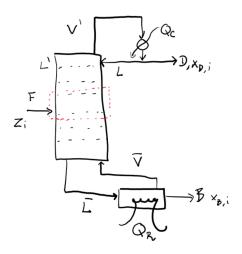
we have,

$$\frac{N-1}{N_S} = \frac{N_R}{N_S} + 1 = 1.345,$$

and since $N=20.62\sim 21$, this gives, $N_S=14.59\sim 15$, meaning, $N_R=N-N_S-1=5.04\sim 5$, and thus, $N_F=N_R+1=6$.

3)

a.



- (1) Ethylbenzene, (2) p Xylene,
- (3) o Xylene, (4) Cumene

$$(x_1, x_2, x_3, x_4)_F = (0.06, 0.40, 0.30, 0.24)$$

$$d_2 = 0.99f_2$$

$$b_3 = 0.96 f_3$$

$$\alpha_{13} = 1.25, \ \alpha_{23} = 1.15$$

$$\alpha_{33} = 1.00, \ \alpha_{43} = 0.68$$

$$q = 1$$

$$F = 80 \text{ mol/hr}$$

Assume: CMO, constant α_{ij} 's

Solve:

Let p-xylene be the light key and o-xylene be the heavy key. The feed flow rates are given by,

$$f_i = (f_1, f_2, f_3, f_4) = x_{F,i}F = (4.8, 32, 24, 19.2) \text{ mol/hr}.$$

The material balance for a component, i, is then given by,

$$f_i = d_i + b_i$$
.

For the light key, $d_2 = 0.99 f_2 = 31.68 \text{ mol/hr}$, meaning $b_2 = 0.01 f_2 = 0.32 \text{ mol/hr}$. Similarly, for the heavy key, $b_3 = 0.96 f_3 = 23.04 \text{ mol/hr}$, giving $d_3 = 0.04 f_3 = 0.96 \text{ mol/hr}$. The Fenske equation in terms of flow rates is then given as,

$$N_{min} = \frac{\ln\left(\left[\frac{d_2}{d_3}\right]\left[\frac{b_3}{b_2}\right]\right)}{\ln\left(\alpha_{23}\right)}$$
$$= \frac{\ln\left(\left[\frac{31.68}{0.96}\right]\left[\frac{23.04}{0.32}\right]\right)}{\ln\left(1.15\right)}$$
$$= 55.62$$

Therefore, $N_{min} = 55 + 1$ stages are required at total reflux. To estimate the composition of light and heavy non-keys in the bottoms, consider a rearranged form of the Fenske equation,

$$b_i = \frac{f_i}{1 + (d_3/b_3)\alpha_{i3}^{N_{min}}}.$$

Therefore, using i = 1 for ethylbenzene,

$$b_1 = \frac{4.8 \text{ mol/hr}}{1 + (0.96/32)(1.25)^{55.62}} = 4.69 \times 10^{-4} \text{ mol/hr}.$$

The distillate flow of ethylbenzene is about $d_1 = 4.80 \text{ mol/hr}$, therefore, <u>nearly all of the ethylbenzene</u> is recovered in the distillate. A similar calculation for cumene yields,

$$b_4 = \frac{19.2 \text{ mol/hr}}{1 + (0.96/32)(0.68)^{55.62}} = 19.2... \text{ mol/hr}.$$

The distillate flow of cumene is on the order of 4×10^{-10} mol/hr, therefore, <u>practically 100%</u> of the cumene is recovered in the bottoms. For the Underwood equation, it is useful to calculate $x_{D,i} = d_i/D$. Summing over i yields D = 37.44 mol/hr, giving,

$$(x_1, x_2, x_3, x_4)_D = (0.1282, 0.8462, 0.0256, 0.0000).$$

Similarly, for the bottoms, B = 42.56 mol/hr, giving the light key mole fraction,

$$x_{B,2} = 0.00752.$$

b.

Using q = 1, the given α_{ij} 's, and the $x_{F,i}$, we may set up the Underwood root finding function,

$$f(\theta) = \frac{(1.25)(0.06)}{1.25 - \theta} + \frac{(1.15)(0.40)}{1.15 - \theta} + \frac{(1.0)(0.30)}{1.0 - \theta} + \frac{(0.68)(0.24)}{0.68 - \theta} - 1 + 1 = 0.$$

Plotting for the initial guess.

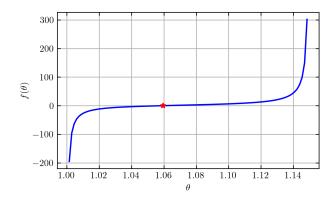


Figure 5: Graphical solution to the Underwood equation

With this, Newton's method gives $\theta = 1.059$. R_{min} may now be calculated with this,

$$R_{min} = \frac{(1.25)(0.1282)}{1.25 - \theta} + \frac{(1.15)(0.8462)}{1.15 - \theta} + \frac{(1.0)(0.0.0256)}{1.0 - \theta} + 0 - 1$$

$$= \frac{(1.25)(0.1282)}{1.25 - 1.059} + \frac{(1.15)(0.8462)}{1.15 - 1.059} + \frac{(1.0)(0.0.0256)}{1.0 - 1.059} - 1$$

$$= 10.16.$$

Thus, for the saturated vapor feed, $R_{min} = 10.16$

c.

Since $R = 3R_{min}$, we have R = 30.48, meaning we can calculate X for the Gilliland correlation,

$$X = \frac{30.48 - 10.16}{30.48 + 1} = 0.645,$$

from which we find, Y = 0.168. Thus, we may solve for N,

$$N = \frac{Y + N_{min}}{1 - Y} = \frac{0.168 + 55.62}{1 - 0.168} = 67.05,$$

meaning N = 67 + 1 stages are required.

d.

The Kirkbride equation may now be used to estimate the feed location, N_F ,

$$\frac{N_R}{N_S} = \left[\left(\frac{0.30}{0.40} \right) \left(\frac{0.00752}{0.0256} \right)^2 \left(\frac{42.56}{37.44} \right) \right]^{0.206} = 0.584.$$

Since,

$$N = N_R + N_S + 1,$$

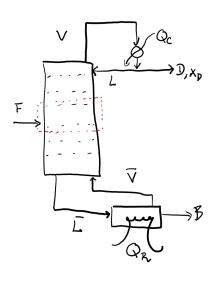
we have,

$$\frac{N-1}{N_S} = \frac{N_R}{N_S} + 1 = 1.584,$$

and since $N=67.05\sim 68$, this gives, $N_S=41.70\sim 42$, meaning, $N_R=N-N_S-1=24.34\sim 25$, and thus, $N_F=N_R+1=26$.

Appendix

a.



$$P = 101.325 \text{ kPa}$$

 $x_B = 0.10$
 $x_D = 0.96$
 $x_F = 0.72$
 $F = 250 \text{ mol/hr}$
 $R = 4.0: 1.0$

Assume: CMO

Solve: The material balances around the entire column give,

$$D = (250 \text{ mol/hr}) \left(\frac{0.72 - 0.10}{0.96 - 0.10} \right) = 180 \text{ mol/hr},$$

and,

$$B = F - D = 70 \text{ mol/hr}.$$

b.

Fitting the equilibrium data to a 5th order polynomial with a fixed intercept yields,

$$(a_5, a_4, a_3, a_2, a_1) = (0.1844, -0.4951, 0.5804, -0.6996, 1.430),$$

with an estimated $R^2 = 1.000$.

Additionally, the rectifying line is given by,

$$y = \left(\frac{R}{R+1}\right)x + \frac{x_D}{R+1},$$

where for R=4,

$$\frac{R}{R+1} = \frac{4}{5} = 0.80,$$

and,

$$\frac{x_D}{R+1} = \frac{0.96}{4+1} = 0.192.$$

By observing the narrow equilibrium line in the following figure, we notice that this system will be much harder to separate. Therefore, to practically perform a graphical solution, we must break the plot into multiple sections. To this end, it is convenient to get the explicit equation for the stripping line, this may be done by using the point $(x_B, x_B) = (0.10, 0.10)$ and the q-line intersection, $(x_q, y_q) = (0.72, 0.768)$, from which we may calculate the slope and intercept,

$$\frac{\bar{L}}{\bar{V}} = 1.077, \quad -\frac{B}{\bar{V}}x_B = -0.0077.$$

Plotting these curves and stepping yields the following figures.

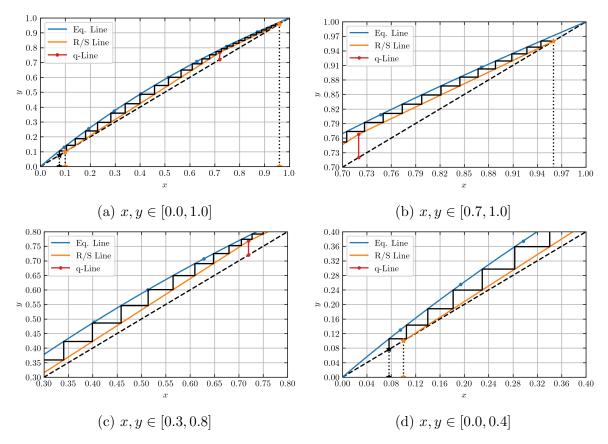


Figure 6: McCabe-Thiele diagrams for n-heptane-toluene distillation with R=18 and saturated liquid feed

Thus, we may (carefully) count that the feed stage should be at $N_F = 12$ and the total number of stages is N = 25 + 1 for R = 4.

c. & f.

We may find the R_{min} values by generating pinch points between the q-line and equilibrium curves.

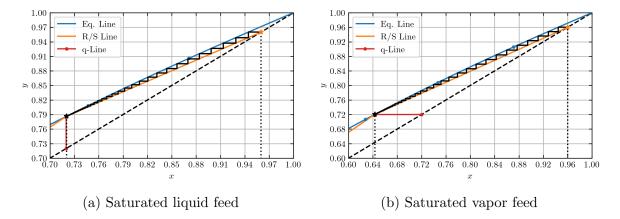


Figure 7: McCabe-Thiele diagrams for n-heptane-toluene distillation with R_{min}

For the saturated liquid feed,

$$\frac{R_{min}}{R_{min} + 1} = \frac{x_D - y(x_F)}{x_D - x_F} = \frac{0.96 - 0.786}{0.96 - 0.72} = 0.724,$$

$$\implies \boxed{R_{min} = 2.63}.$$

For the saturated vapor feed,

$$\frac{R_{min}}{R_{min} + 1} = \frac{x_D - x_F}{x_D - x_q} = \frac{0.96 - 0.72}{0.96 - 0.643} = 0.757,$$

$$\implies \boxed{R_{min} = 3.11}.$$

The stages from total reflux remains the same for both the saturated vapor and liquid. This is simply found by stepping down the y = x line.

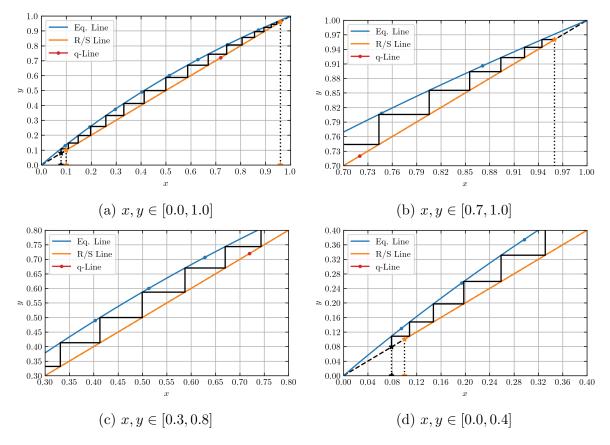


Figure 8: McCabe-Thiele diagrams for n-heptane-toluene distillation with total reflux

Thus,
$$N_{min} = 15 + 1$$

e.

For a saturated vapor feed with R=4, the slopes and intercepts of the rectifying and stripping lines are given by,

$$\frac{R}{R+1} = 0.80, \quad \frac{x_D}{R+1} = 0.192,$$

$$\frac{\bar{L}}{\bar{V}} = 1.107, \quad -\frac{B}{\bar{V}}x_B = -0.011.$$

Which yields the following plots.

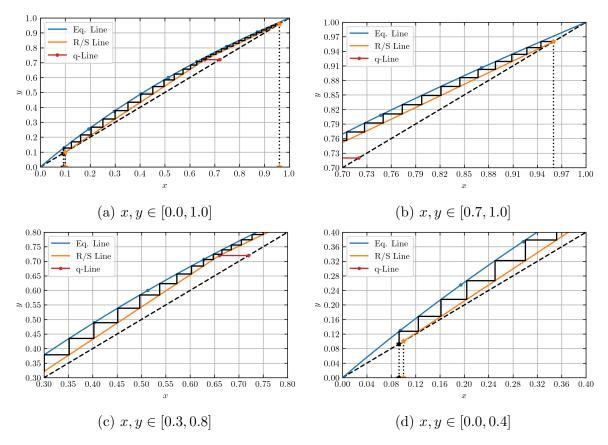


Figure 9: McCabe-Thiele diagrams for n-heptane-toluene distillation with R=6 and saturated vapor feed

Therefore, the feed stage should be at $N_F = 15$ and the total number of stages is N = 28 + 1 for N = 4.