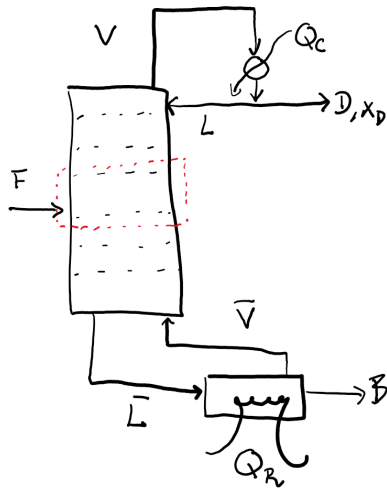# 1)

a.

$$P = 101.325 \text{ kPa}$$
$$x_B = 0.10$$
$$x_D = 0.70$$
$$x_F = 0.40$$
$$F = 500 \text{ mol/hr}$$
$$R = 3 : 1$$

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,

$$\boxed{D = (500 \text{ mol/hr}) \left(\frac{0.40 - 0.10}{0.70 - 0.10} \right) = 250 \text{ mol/hr}},$$

and,

$$\boxed{B = F - D = 250 \text{ mol/hr}}.$$

b.

For an arbitrary stage in the rectifying section, the material balances around the top of the column imply,

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

whose intercept is given by,

$$\frac{x_D}{R+1} = \frac{0.70}{3+1} = 0.175.$$

Since the distillate vapor is totally condensed, we know $y_1 = x_D$ must lie on the rectifying line. Therefore, we now know two points, $(0, 0.175)$ and $(0.70, 0.70)$, and the curve may be drawn on an xy diagram. The equation for the stripping line is,

$$y = \frac{\bar{L}}{\bar{V}}x - \frac{B}{\bar{V}}x_B.$$

Plugging in $x = x_B$ and using $\bar{V} = \bar{L} - B$ implies that the point (x_B, x_B) lies on the stripping line. The second point comes from the intersection with the q-line whose equation is given by,

$$y = -\frac{q}{1-q}x + \frac{x_F}{1-q}.$$

Since the the feed is a saturated liquid, we have $q = 1$, meaning the q-line has an infinite slope and must pass through x_F. Two points of the stripping curve are now known and the line may be drawn on the xy diagram.

The equilibrium line may be estimated by fitting a polynomial to the data. 5th and 6th order polynomials were used to prevent overfitting and the intercept was set to 0. That is,

$$y(x) = a_6 x^6 + a_5 x^5 + a_4 x^4 + a_3 x^3 + a_2 x^2 + a_1 x,$$

for some constants $(a_6, a_5, a_4, a_3, a_2, a_1)$. Additionally, for the non-ideal solution, only the first 13 data points up to $(x, y) = (0.98, 0.76)$ were used since the later data points prevent a good fit and are not required for this problem. Using scipy's optimize.curve_fit function in Python, this gives for the non-ideal solution,

$$(a_5, a_4, a_3, a_2, a_1) = (3.407, -10.90, 14.05, -9.744, 4.193),$$
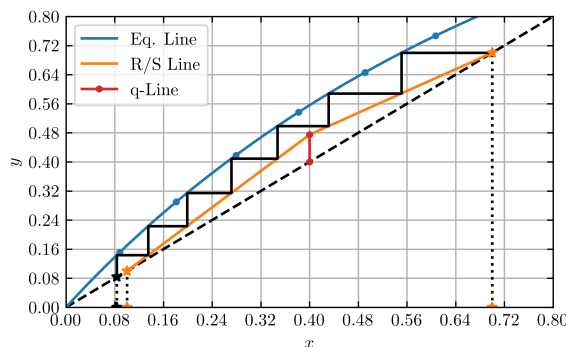
with estimated $R^2 = 0.999$. Likewise, for the ideal solution,

$$(a_6, a_5, a_4, a_3, a_2, a_1) = (-9.015, 32.39, -47.60, 37.62, -17.95, 5.562),$$

with estimated $R^2 = 1.000$. By starting at (x_D, x_D) and stepping off the equilibrium and rectifying/stripping lines, the number of stages may be determined.
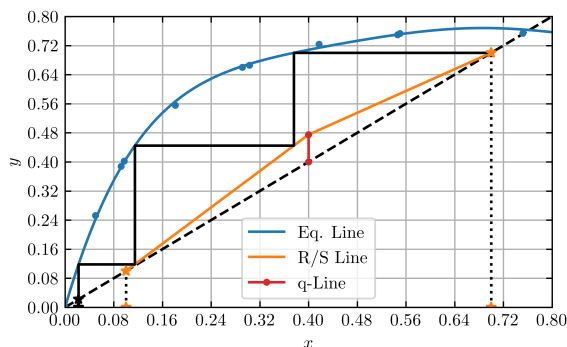
(a) Non-ideal   (b) Ideal

Figure 1: McCabe-Thiele diagrams for water-n-butantol distillation with $R = 3$ and saturated liquid feed

Thus, for the non-ideal data, the feed should be at stage $\boxed{N_F = 1}$ and the total number of stages is $\boxed{N = 2 + 1}$.

For the ideal data, the feed should be at stage $\boxed{N_F = 3}$ and the total number of stages is $\boxed{N = 6 + 1}$.

The non-ideal solution is *much* easier to separate for the given distillate composition and has a very 'wide' equilibrium curve compared to the ideal solution. However, if a more pure product is desired, the non-ideal solution is much harder to separate due to the formation of an azeotrope.
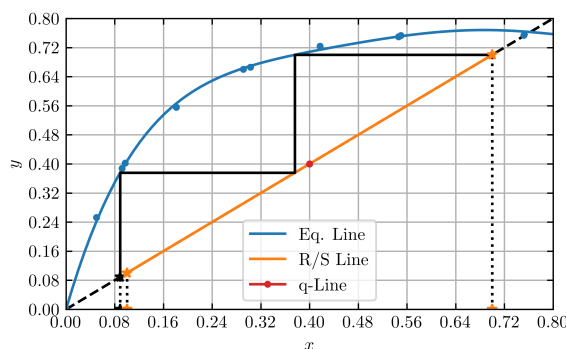
c.

The minimum reflux ratio, R_{min}, is given by generating a pinch point and having the q-line touch the equilibrium curve. The slope of the resulting rectifying line may be used to find R_{min}. However, for the non-ideal solution, the equilibrium curve is so wide that this generates a negative slope and R_{min}, which is unphysical, thus, we may take $\boxed{R_{min} = 0}$. This implies that for the given distillate composition, the separation is possible for any R value [1].

Total reflux occurs when the column operates without a feed (also implying no outputs). The q-line simply becomes a point at (x_F, x_F) and the rectifying and stripping lines degenerate into the same curve. The minimum number of stages, N_{min}, may be found by stepping off the diagram in this case.
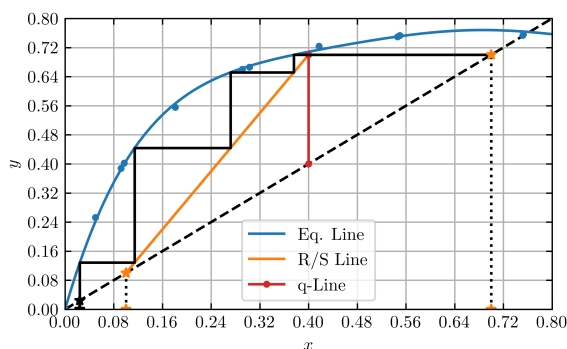
(a) $R_{min} = 0$, saturated liquid feed   (b) Total reflux

Figure 2: McCabe-Thiele diagrams for non-ideal water-n-butantol distillation with R_{min} and total reflux

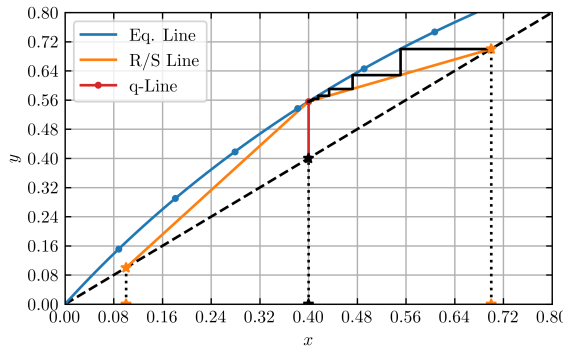Therefore, $\boxed{N_{min} = 1 + 1}$ for the non-ideal solution.

---

[1]This result may be more of a reflection of the polynomial used to fit the data. However, I tried this for multiple polynomial orders and selecting different data points to fit and always arrived at this result.
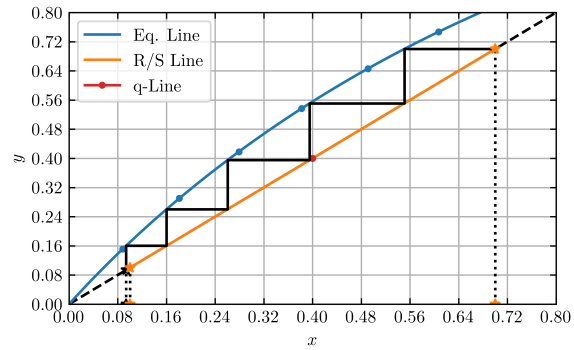
The ideal solution is more straightforward,

$$\frac{R_{min}}{R_{min} + 1} = \frac{x_D - y(x_F)}{x_D - x_F} = \frac{0.70 - 0.556}{0.70 - 0.40} = 0.481.$$

Solving for R_{min},

$$\boxed{R_{min} = 0.925}.$$
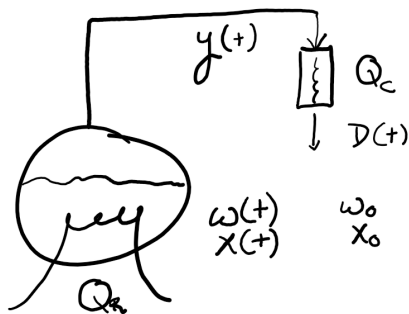

(a) R_{min}, saturated liquid feed

(b) Total reflux

Figure 3: McCabe-Thiele diagrams for ideal water-n-butantol distillation with R_{min} and total reflux

Therefore, $\boxed{N_{min} = 4 + 1}$ for the ideal solution.

2)

a.

$P = 101.325$ kPa

$x_0 = 0.40$

$w/w_0 = 0.25$

Assume:

Solve:

We may perform an unsteady material balance for the overall mixture and the more volatile component. In rate form,

$$-\frac{dw}{dt} = D, \quad -\frac{d(xw)}{dt} = yD,$$

or in differential form,
$$-dw = D\,dt, \quad -x\,dw - w\,dx = y\,D\,dt.$$

Plugging in $D\,dt = -dw$ into the second relation,

$$-x\,dw - w\,dx = -y\,dw,$$

which gives upon rearrangement,

$$\frac{dx}{y - x} = \frac{dw}{w}.$$

The initial conditions are given as x_0 and w_0, thus, we may integrate from the initial state to an arbitrary final state to find,

$$\ln\left(\frac{w}{w_0}\right) = \int_{x_0}^{x} \frac{dx}{y - x}.$$

We wish to evaluate the above using numerical integration on the equilibrium data. Simpson's rule would give fairly accurate results, but since we only wish for a first estimate, we will use the midpoint rule,

$$\int_{x_0}^{x} \frac{dx}{y - x} \approx \sum_i \left(\frac{f_i + f_{i-1}}{2}\right) \Delta x_i,$$

where $f_i = 1/(y_i - x_i)$ and $\Delta x_i = x_i - x_{i-1}$. The above formula may be automated in Excel. In the following table, A_i denotes the approximated area (integral) over the Δx_i interval. A left sided integral was used for the last interval since f is badly behaved at $(x, y) = (0, 0)$.

Table 1: Numerical Integration of the Rayleigh Equation for Batch Distillation

T (ºC)	x	y	A_i	ΣA_i
79.8	0.400	0.624	-	-
80.3	0.350	0.602	-0.211	-0.211
80.8	0.300	0.579	-0.189	-0.399
81.6	0.250	0.554	-0.172	-0.571
82.5	0.200	0.525	-0.159	-0.730
83.8	0.150	0.489	-0.151	-0.881
86.0	0.100	0.435	-0.148	-1.030
87.4	0.080	0.404	-0.061	-1.090
89.2	0.060	0.361	-0.064	-1.154
91.7	0.040	0.300	-0.072	-1.226
93.3	0.030	0.258	-0.041	-1.267
95.1	0.020	0.206	-0.049	-1.316
97.2	0.010	0.137	-0.066	-1.382
100.1	0.000	0.000	-0.079	-1.461

The remaining liquid composition may be estimated by finding the x value corresponding to the closest integral value to $\ln(w/w_0)$. Since $\ln(w/w_0) = -1.386$, we find $\boxed{x = 0.01}$ [2]. To find the distillate composition, we perform an integral balance for the overall process,

$$w_0 - w = D,$$

$$x_0 w_0 - xw = yD,$$

where D is the total distillate collected and y is its composition. Solving for y yields,
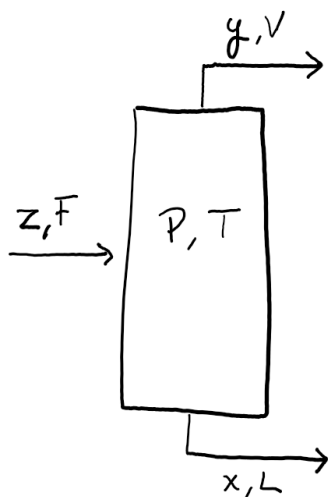
$$y = \frac{x_0 w_0 - xw}{w_0 - w} = \frac{x_0 - x(w/w_0)}{1 - (w/w_0)}.$$

Numerically,

$$\boxed{y = \frac{0.4 - (0.01)(0.25)}{1 - 0.25} = 0.53}.$$

3)

a.

$P = 101.325$ kPa
$z = 0.70$
$L = 40$ mol/hr
$V = 60$ mol/hr
$F = 100$ mol/hr

Assume: Ideal mixture (Raoult's law)

Solve:

The component balance gives,
$$zF = yV + xL,$$

or,
$$y = -\frac{L}{V}x + \frac{F}{V}z.$$

---

[2]It's possible to do linear interpolation between the last two integral values, but the error introduced by interpolation is likely worse that just taking $x = 0.01$, which is *very* close.

x and y values are further constrained by the equilibrium relation. Thus, a solution may be found at the intersection of the material balance and equilibrium curves.

Using scipy's optimize.curve_fit function in Python, the equilibrium curve may be estimated by a fixed intercept polynomial, giving,

$$(a_6, a_5, a_4, a_3, a_2, a_1) = (-9.015, 32.39, -47.60, 37.62, -17.95, 5.562),$$

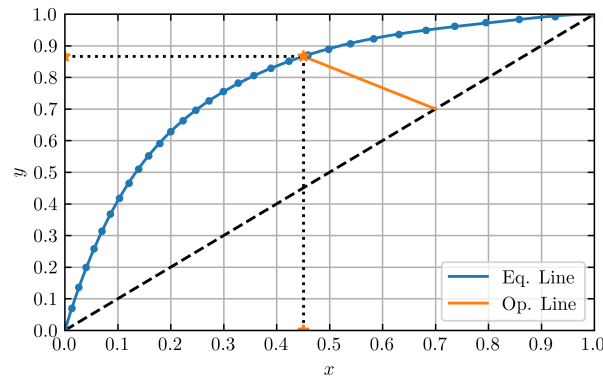with estimated $R^2 = 1.000$. This yields the following figure.

Figure 4: xy plot for flash distillation of n-pentane - n-heptane mixture

Therefore,

$$\boxed{x = 0.451},$$

$$\boxed{y = 0.866}.$$

Sanity check:

$$yV + xL = [(0.866)(60) + (0.451)(40)] \text{ mol/hr} = 70 \text{ mol/hr}.$$