

Exercise 2 – Multi component separation processes

Section A

1. a) Given that the minimum temperature approach of the heat exchange is 10 °C and the condensing process stream is at 132.5 °C, a temperature of 122.5 °C was assumed for the feed. Equation 1 (Antoine equation) was used in order to calculate saturated vapour pressures P_{sat} , for a dew point vapour feed of thermal quality $q = 0$. A dew point calculation was conducted as shown in equation 2 and the feed and column pressure were estimated at 0.497 bar. In equation 2, z_i denotes the feed mole fraction of component i .

$$\log_{10}(P_i^{sat}) = A_i - \frac{B_i}{T+C_i} \quad (1)$$

$$P_{feed} = P_{drum} = \frac{1}{\sum_{i=1}^3 \frac{z_i}{P_i^{sat}}} = \frac{1}{\frac{0.33}{1.95} + \frac{0.33}{1.11} + \frac{0.34}{0.22}} = 0.497 \text{ bar} \quad (2)$$

b) The required column pressure can be achieved by use of a vacuum booster integrated with an initial vacuum pump or steam jet ejector. For the required feed and outlet specifications, a dry vacuum pump such as a vacuum booster is recommended. Vacuum boosters offer high volumetric speeds at low pressures as opposed to vane and ring pumps of similar power. This system works by pulling a vacuum on the top of the distillation column. Steam jet ejectors can also be employed to generate the distillation unit's vacuum environment. Steam ejectors take advantage of the Bernoulli and continuity equations. The ejectors generate low pressure regions due to their variable area and the motive fluid used in the process is steam. When low pressure regions form, the process fluid which in this case is the n-heptane (n-C₇), n-octane (n-C₈) and n-decane (n-C₁₀) mixture, is introduced into the steam jet via an open suction valve. Steam jet ejectors are simple, reliable and relatively inexpensive. No source of power is required other than the motive gas which is steam in this case. For the purposes of sustaining a vacuum environment and removing overhead vapours in a distillation column, venturi-type steam ejectors can be employed (<http://www.venturipumps.com/ejector.htm>).

Vacuum distillation has a lot of advantages in downstream processing operations. On the other hand, it also has a couple of disadvantages. Some of the advantages include use of lower process temperatures and more economical heating media such as saturated steam against hot oil. Vacuum distillation allows processing of thermally sensitive substances, necessitates use of fewer stages than atmospheric distillation due to higher relative volatilities being achieved, and lowers the reflux ratio R . The risk of cracking of process stream components is greatly reduced because of reductions in boiling points. Sub-atmospheric operation is usually employed in order to recover residue from the bottoms of atmospheric distillation units. With vacuum distillation, each stage provides a purer product. Moreover, much shorter towers are employed in vacuum as opposed to atmospheric distillation so as to minimise pressure differentials from top to bottom. In addition, vacuum distillation can be used so as to separate

azeotropic mixtures. It alters the position of the azeotropic point for special mixtures thus allowing efficient separation at lower pressures. Vacuum distillation also reduces energy consumption as a result of reductions in boiling points.

Disadvantages of vacuum distillation include the construction of more complicated equipment and larger vessel diameters. Low vapour pressures tend to limit the flow rate of vapour and as a result, reduce the capacity for equipment of any given size. Larger column diameters are required in order to provide larger areas and reduce vapour superficial velocities. Moreover, a costlier cooling source may be required for condensation due to a lower condensation temperature. The possibility of product contamination by air and other atmospheric components is also increased (Thakore & Batt, Introduction to Process Engineering and Design, McGraw-Hill, 2007, pp 383-384).

2. Specifications state 95% recovery of n-C₁₀ in bottoms, 100% and 90% recovery of n-C₇ and n-C₈ respectively in distillate. n-C₈ was chosen as light key (LK) and n-C₁₀ as heavy key (HK). n-C₇ is lighter than the light key (LLK). For calculation purposes, it was assumed that none of the LLK ends up in the residue. Table 1 shows that the molar percentage of LK in the residue was calculated at 9.3% and that of the HK in the distillate was calculated at 2.6%.

Table 1: Molar flows and mole fractions of n-C₇, n-C₈ and n-C₁₀ in feed, distillate and bottoms

Component <i>i</i>	n-C ₇ (LLK)	n-C ₈ (LK)	n-C ₁₀ (HK)
<i>F_i</i> / kmol hr ⁻¹	33	33	34
<i>z_i</i>	0.33	0.33	0.34
<i>D_i</i> / kmol hr ⁻¹	33	29.7	1.7
<i>B_i</i> / kmol hr ⁻¹	0	3.3	32.3
<i>X_{D,i}</i>	0.512	0.461	0.026
<i>X_{B,i}</i>	0	0.093	0.907

3. Equation 3 was employed in order to estimate the temperature of the condenser. A bubble point calculation was performed for the outflow from the condenser to yield $T_{condenser} = 359.0$ K. For the partial reboiler, the outflow is expected to be of thermal quality $0 < q < 1$. As a result, both bubble and dew point calculations were conducted using equations 4 and 5 respectively to yield $411.2 < T_{reboiler} < 418.7$. For subsequent calculations, the bottoms bubble point estimate of 411.2 K was selected for $T_{reboiler}$. $T_{reboiler} = 411.2$ K because the bottoms stream consists of a bubble point liquid (the residue).

$$\frac{\sum_{i=1}^3 \frac{P_i^{sat} * X_{D,i}}{P}}{P} = \frac{\sum_{i=1}^3 X_{D,i} * 10^{\frac{A_i - T_{condenser} + B_i}{C_i}}}{P} = 1 \Rightarrow T_{condenser} = 359.0 \text{ K} \quad (3)$$

$$\frac{\sum_{i=1}^3 \frac{P_i^{sat} * X_{B,i}}{P}}{P} = \frac{\sum_{i=1}^3 X_{B,i} * 10^{\frac{A_i - \frac{B_i}{T_{bubble,B} + C_i}}{10}}}{P} = 1 \Rightarrow T_{bubble,B} = 411.2 \text{ K} \quad (4)$$

$$\sum_{i=1}^3 \frac{X_{B,i}}{P_i^{sat}} * P = \sum_{i=1}^3 \frac{X_{B,i}}{10^{\frac{A_i - \frac{B_i}{T_{dew,B} + C_i}}{10}}} * P = 1 \Rightarrow T_{dew,B} = 418.7 \text{ K} \quad (5)$$

For the purposes of subsequent calculations, let i be the LK, j be the HK and k be the LLK. The parameters a_{ij} , a_{jj} and a_{kj} are the volatilities of the LK, HK and LLK respectively relative to the HK. Raoult's law was assumed given that the 3 components in the mixture are homologues and that no ionic or hydrogen bond interactions are present. The relevant pressure is also sufficiently low for Raoult's to be applicable. Equation 6 was therefore used in order to estimate volatilities of components relative to the HK. Table 2 shows the relative volatility values and their geometric averages. Equation 7 (Fenske's equation) was then employed in order to estimate the minimum number of ideal equilibrium stages $N_m = 3.08$ (Part IIA Chemical Engineering, 2019, Separation Processes 2, handout #3, pp 4-6).

For the LK, P_{sat} was estimated at 0.31 and 1.78 bar at the top and bottom of the distillation column respectively. Furthermore, P_{sat} for the LLK was estimated at 0.69 and 2.85 bar at the top and bottom of the column respectively.

$$\alpha_{ij} = \frac{P_i^{sat}/P}{P_j^{sat}/P} = \frac{P_i^{sat}}{P_j^{sat}} \quad (6)$$

Table 2: Relative volatilities of components at top and bottom of column including their geometric averages

Relevant calculation	Top at 359 Kelvin	Bottom at 411.2 Kelvin	Geometric average
a_{ij}	5.80	4.85	5.31
a_{kj}	13.05	7.78	10.07

$$N_m = \frac{\ln \left[\frac{X_{D,i} / X_{D,j}}{X_{B,i} / X_{B,j}} \right]}{\ln \left[(\alpha_{ij})_{\text{geometric average}} \right]} = \frac{\ln \left[\frac{0.461/0.026}{0.093/0.907} \right]}{\ln [5.31]} = 3.08 \quad (7)$$

Equation 8 (Underwood's equation) was employed so as to calculate the parameter θ for subsequent use in equation 9, where the minimum reflux ratio was estimated at $R_m = 0.709$. In equations 8 and 9, a_i represents the volatility of any of the three components relative to the HK. Underwood's

analysis was applicable in this case because specifications indicate high LK recovery of 90% in the distillate and high HK recovery of 95% in the bottoms stream. In addition, the LLK's relative volatility doesn't lie close to those of the other two component keys. For the analysis, two pinches in the distillation column were assumed as well as constant molar overflows and constant relative volatilities in regions between these pinches. θ was estimated at 2.87 which lies in the required range of $1 < \theta < 5.3$. The value of the operating reflux ratio was estimated at 0.85 using $1.2R_m$. Economic considerations dictate that $R = 1.2R_m$ corresponds to a sensible R value estimate (Part IIA Chemical Engineering, 2019, Separation Processes 2, handout #3, pp 6-8).

$$\sum_{i=1}^3 \frac{\alpha_i * z_i}{\alpha_i - \theta} = 1 - q = \frac{10.07 * 0.33}{10.07 - \theta} + \frac{5.31 * 0.33}{5.31 - \theta} + \frac{0.34}{1 - \theta} = 1 \Rightarrow \theta = 2.87 \quad (8)$$

$$R_m + 1 = \sum_{i=1}^3 \frac{\alpha_i * X_{D,i}}{\alpha_i - \theta} = \frac{10.07 * 0.512}{10.07 - \theta} + \frac{5.31 * 0.461}{5.31 - \theta} + \frac{0.026}{1 - \theta} \Rightarrow R_m = 0.709 \quad (9)$$

Gilliland's empirical graphical correlation was employed in order to estimate the actual number of stages N . Gilliland's correlation is suitable because, 3 components are involved and the pressure, R_m and N_m are within the appropriate range. In addition, approximately ideal thermodynamics were assumed since the components in the mixture are homologues. The coefficient for use in Gilliland's correlation was estimated at 0.0766 using equation 10 (Part IIA Chemical Engineering, 2019, Separation Processes 2, handout #3, pp 9).

$$\frac{R - R_m}{R + 1} = \frac{0.85 - 0.709}{0.85 + 1} = 0.0766 \quad (10)$$

From the empirical graph correlation and by use of the estimated coefficient value of 0.0766, $(N - N_m) / (N + 1) = 0.56$. As a result, $N = 8.27$. The operating number of stages is therefore 9.

Kirkbride's empirical correlation shown in equation 11 was employed in order to relate the number of stages in the rectifying section N_R to the number of stages in the stripping section N_S .

$$\log \left[\frac{N_R}{N_S} \right] = 0.206 * \log \left[\frac{B}{D} * \frac{z_{HK}}{z_{LK}} * \frac{X_{B,LK}}{X_{D,HK}} \right] = 0.206 * \log \left[\frac{35.6}{64.4} * \frac{0.34}{0.33} * \frac{0.093}{0.907} \right] \Rightarrow N_R = 1.5 * N_S \quad (11)$$

$N_R = 3.31$ and $N_S = 4.96$ and as a result, the actual number of stages in the rectifying section is 4 and that in the stripping section is 5. The feed should be positioned between stages 4 and 5 counting from the top of the column, provided that the total condenser is stage 1 (or between column trays 3 and 4).

4. The short-cut distillation column tool with the Antoine thermodynamic package in UniSim was used in order to estimate essential parameter values tabulated in table 3. The optimal feed stage was estimated at 6.06, counting from the top of the column. The optimal feed position should therefore be between column trays 6 and 7 counting from top or between stages 7 and 8, provided that stage 1 is the total condenser.

Table 3: Values of R_m , R , N_m , N and condenser and reboiler temperatures estimated using the short cut distillation column tool in UniSim

R_m	0.76
R	0.91
N_m	3.46
N	10.10
$T_{condenser} / K$	360.0
$T_{reboiler} / K$	412.4

Section B

5. Equation 12 is a heat balance for component i over a single plate j . V_j and L_j denote overall vapour and liquid molar outflows respectively from stage j . Furthermore, $C_{pg\ i,j}$ and $C_{pl\ i,j}$ denote gas and liquid phase molar heat capacities respectively for component i outflows from stage j . In addition, T_j , T_{j+1} and T_{j-1} denote the temperatures of stages j , $j+1$ and $j-1$ respectively. T_o is a reference temperature used in calculations, taken as absolute zero in kelvin.

$$V_{j+1} * y_{i,j+1} * C_{pg\ i,j+1} (T_{j+1} - T_o) - L_j * x_{i,j} * C_{pl\ i,j} (T_j - T_o) = V_j * y_{i,j} * C_{pg\ i,j} (T_j - T_o) - L_{j-1} * x_{i,j-1} * C_{pl\ i,j-1} (T_{j-1} - T_o) \quad (12)$$

Equation 12 was derived by assuming that the stage is adiabatic. Good lagging will ensure that heat losses over stage j are negligible. In addition, zero shaft work was assumed, and kinetic and potential energy terms were neglected. Steady state operation was also assumed thus neglecting any accumulation terms. The heat of solution was also assumed to be minimal and this was indeed a good approximation since the components involved are homologues. Isobaric operation across stage j was also assumed, but this approximation may not hold under the vacuum conditions encountered in the distillation column. Moreover, constant molar overflow was not assumed. The plate modelled in deriving equation 12 was assumed to be far from the feed entry stage and any exit streams. The steady state assumption neglecting any radical changes in vapour flows or liquid flows due to side streams, was therefore valid. Furthermore, $C_{pg\ i,j}$, $C_{pg\ i,j+1}$, $C_{pl\ i,j}$ and $C_{pl\ i,j-1}$ were assumed to be independent of temperature but dependent on the composition of i in the relevant phase (Coulson & Richardson, Chemical Engineering: Particle Technology & Separation Processes, ELSEVIER, vol. 2, 5th edition, pp 562-563).

6. a) Equation 14 was derived for the total condenser (stage 1), by performing a component i molar balance over the stage. Equation 14 is a special case of equation 13. In equation 13, $K_{i,j}$ is the volatility of component i leaving stage j . In equation 14, R is the reflux ratio and d_i is the distillate flowrate of component i .

$$A_{i,j-1} * v_{i,j-1} + v_{i,j+1} - v_{i,j}(1 + A_{i,j}) = 0 \Rightarrow A_{i,j} = \frac{L_j}{K_{i,j}V_j} \quad \& \quad v_{i,j} = V_j y_{i,j} \quad (13)$$

$$v_{i,2} - d_i(1 + R) = 0 \quad (14)$$

b) In deriving equation 15, the feed entry position from question 4 was used which was between stages 7 and 8, counting the total condenser as stage 1. In equation 15, F denotes the overall feed molar flowrate and z_i denotes the feed molar ratio of component i . In ideal column operation z_i from equation 15 should be equal to $y_{i,8}$, where $y_{i,8}$ denotes the mole fraction of component i in the vapour flow emerging from stage 8.

$$F * z_i + A_{i,6} * v_{i,6} + v_{i,8} - v_{i,7}(1 + A_{i,7}) = 0 \quad (15)$$

7. For a distillation column with a total condenser, a partial reboiler and 10 stages in total (10 stages include total condenser as stage 1 and partial reboiler as stage 10), the matrix \mathbf{M}_i shown on the left-hand side of equation 16 was constructed.

$$\begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 - A_{i,2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{i,2} & -1 - A_{i,3} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_{i,3} & -1 - A_{i,4} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & A_{i,4} & -1 - A_{i,5} & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{i,5} & -1 - A_{i,6} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & A_{i,6} & -1 - A_{i,7} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{i,7} & -1 - A_{i,8} & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{i,8} & -1 - A_{i,9} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & A_{i,9} & -1 & 1 \end{bmatrix} \begin{bmatrix} v_{i,2} \\ v_{i,3} \\ v_{i,4} \\ v_{i,5} \\ v_{i,6} \\ v_{i,7} \\ v_{i,8} \\ v_{i,9} \\ v_{i,10} \end{bmatrix} = - \begin{bmatrix} (1 + R)d_i \\ Rd_i \\ 0 \\ 0 \\ Fz_i \\ 0 \\ 0 \\ 0 \\ 0 \\ d_i - Fz_i \end{bmatrix} \quad (16)$$

The vapour feed of $q = 0$ was assumed to enter the column between stages 5 and 6. The vector of molar flows \mathbf{v}_i for component i is shown on the left-hand side of equation 16, to the right of \mathbf{M}_i . In \mathbf{v}_i , $v_{i,1}$ was taken as zero and therefore not included since, there's no vapour outflow from a

total condenser. In addition, the vector $-f_i$ describing the feed flows of component i , is shown on the right-hand side of equation 16. For vector f_i in equation 16, $(d_i - F_{zi})$ denotes the bottoms stream's molar flow of component i , where F_{zi} is the feed molar flowrate of component i . Moreover, in f_i , Rd_i denotes the liquid flowrate from the total condenser back into the distillation column.

Section C

8. a) Table 4 lists the rough temperature estimates for each stage of the distillation column. The temperature estimates were made by assuming linear temperature variation from the point of feed entry all the way up to the total condenser. Linear temperature variation was also assumed from the point of feed entry (between stages 3 and 4 counting the condenser as stage 1) all the way down to the partial reboiler.

Table 4: Estimates of temperatures on each stage of the distillation column by use of the linear temperature variation approximation

Stage	T / K
1 (Total condenser)	360.0
2	377.9
3	395.7
4	398.1
5	400.5
6	402.9
7	405.2
8	407.6
9	410.0
10 (Partial reboiler)	412.4

Equation 17 is a sample calculation performed using linear interpolation, in order to estimate the temperature on stage 5. In equation 17, T_5 denotes the temperature estimate for stage 5. The heat exchanger used to treat the feed was assumed to operate at 132.5 °C with respect to the process fluid.

$$T_5 = 412.4 - \left(\frac{10-4}{10-3} \right) (412.4 - 395.7) = 398.1 K \quad (17)$$

b) Vapour V and liquid L molar flowrates on each of stages 1-10 were estimated by using the constant molar overflow assumption, to begin with. An R of 0.91 was assumed, which was estimated in section a using the UniSim short-cut distillation column tool with the Antoine thermodynamic package. V for the total condenser was taken as zero, since there is no vapour outflow. The distillate flowrate of 64.12 kmol hr⁻¹ from question

4 (short-cut distillation tool answer) was used. Moreover, the bottoms flowrate of 35.88 kmol hr⁻¹ was calculated by performing an overall molar balance over the column. The remaining stream flowrates were then estimated using the constant molar overflow approximation.

Table 5: Estimates of vapour and liquid flowrates on each stage of the distillation column by use of the constant molar overflow approximation

Stage	$V / \text{kmol hr}^{-1}$	$L / \text{kmol hr}^{-1}$
1 (Total condenser)	0	122.47
2	122.47	58.35
3	122.47	58.35
4	22.47	58.35
5	22.47	58.35
6	22.47	58.35
7	22.47	58.35
8	22.47	58.35
9	22.47	58.35
10 (Partial reboiler)	22.47	58.35

9. a) Using the initial conditions generated in question 4 (short-cut distillation tool answers), 6 iterations were carried out before achieving convergence for the distillation column. The initial condition data used in order to achieve convergence after 6 iterations, was derived from results for a column of different geometry. By changing the initial conditions to those estimated using the short-cut manual methods in question 3 (for example using an R of 0.85 instead of 0.91), the number of iterations performed in order to achieve convergence didn't change. Changing the feed entry position from stages 3 & 4 to stages 4 & 5 but using the same R of 0.91, resulted in the requirement of more iterations (7) prior to convergence. Use of an R of 0.86 with feed entry position between stages 3 & 4 initially led to divergence.

On the other hand, use of $R=0.86$ and a feed entry position between stages 5 & 6 led to faster convergence in only 5 iteration attempts. In addition, use of $R=0.78$ and feed entry position between stages 5 & 6 led to even faster convergence in only 4 iteration steps. On all occasions, the overall mass balance over the column was not satisfied, despite the fact that convergence was being achieved. In addition, specifications were not being met.

Overall, the accuracy of the initial condition data derived from a column of different geometry doesn't greatly affect the number of iterations required to converge the distillation column. This is a sensible observation since, initial conditions evaluated by performing calculations on a distillation column that is geometrically different shouldn't greatly affect the speed of convergence.

b)

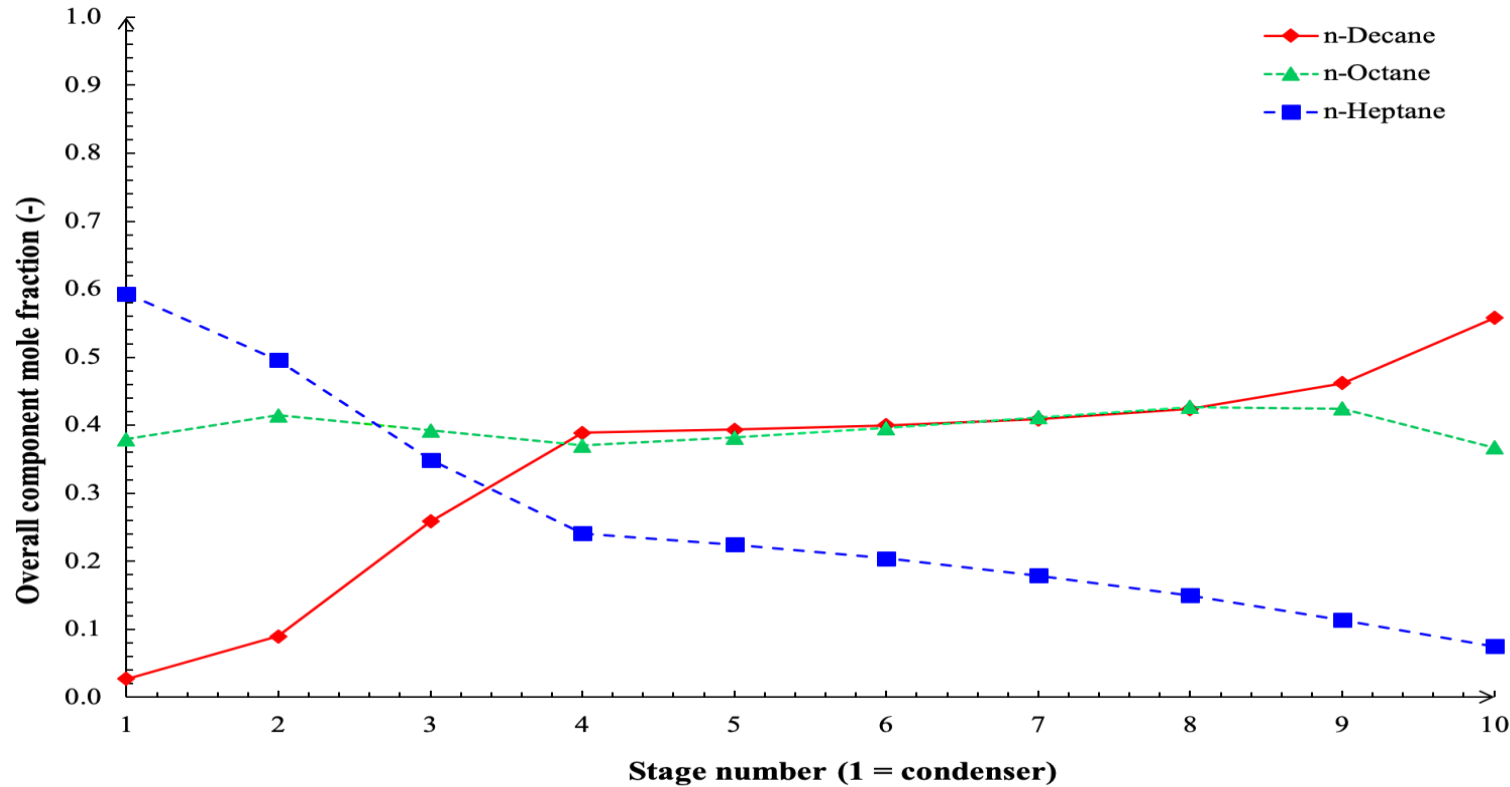


Figure 1: Plot of overall component mole fractions as function of stage number for the converged distillation column using $R=0.91$

Figure 1 shows a plot of the overall component mole fractions as a function of stage number for the converged column with feed entry position between stages 3 & 4 and $R=0.91$ using initial estimates for $T_{condenser}$ and $T_{reboiler}$ from question 4. The plot is indicative of the fact that mole fraction specification of n-C₇ in the distillate is more than being met. This implies that the distillate rate is lower than the value that specification would necessitate. Furthermore, n-C₁₀ mole fraction in bottoms is much less than the value required in order to meet specification demands (approximately 0.88). Figure 1 is also indicative of an inconsistency in overall column molar balance. The bottoms and distillate flowrates add up to a value greater than 100 kmol hr⁻¹. In addition, R seems to be higher than the value required so as to meet specification. This is consistent with the fact that the distillate flowrate is less than the value required so as to meet specification demands.

Figure 1 is also indicative of the fact that the LLK distributes across the column. In optimal distillation column operation for the separation of a mixture of hydrocarbons, LLKs and higher than the high keys (HHKs) should not distribute across the column.

The most intermediate species, n-C₈ in this case, passes through maxima according to figure 1. Nevertheless, the feed position used to generate figure 1 seems to be incorrect. For all three keys, the composition does not change significantly below the feed position (between stages 3 & 4). On the contrary, the composition changes abruptly above the feed position. This implies that the feed should be positioned lower down the column (Part IIA Chemical Engineering, 2019, Separation Processes 2, handout #4, pp 6-10).

c) In order to meet the LK and HK specifications, I would position the feed between stages 4 & 5 instead of stages 3 & 4. In addition, I would lower the reflux ratio to $R=0.57$. Changing R to 0.57 still allows convergence of the distillation column but also satisfies the overall molar balance in a better manner. There's only a 0.67% error in the overall mass balance calculation, which is good enough. By changing the feed position and R , the LLK won't distribute as much over the distillation column. A drawback of the suggested changes is the fact that, low vapour flowrates will be encountered at the bottom of the column. As a result, the residence time in bottom column trays for efficient transfer between the phases will increase. On the other hand, the suggested reduced R will decrease operating costs. Moreover, the recommended changes will reduce overall LLK distribution across the column and will lead to successfully achieving the n-C₇ specification of 100% recovery in the distillate (only a 0.005% error).

Furthermore, I would increase the number of stages in the distillation column to 14 as opposed to 10, including the condenser and partial reboiler. One of the reasons for specifications in part b of question 9 not being met was the fact that the number of stages in the suggested design were sub-optimal. A drawback of increasing the number of plates in the column would be an increase in capital costs as a result of the extra plates. On the other hand, this could also lead to a decrease in R thus further reducing pumping, turbine and operating costs in general. There's a thin line between operating and capital cost optimisation. More careful consideration of this issue will lead to identification of the most appropriate changes in design that will lead to total cost minimisation.

Section D

10. Using the information obtained from the UniSim short cut model in question 4, a rigorous distillation column was specified and converged to the LK and HK specifications. The LK specification of 90% recovery in the distillate was met with a 0.44% error. In addition, the HK specification of 95% in the residue was met with a 0.26% error.

Figure 2 is a plot of component mole fraction against stage number using $R=1.03$ for a distillation column with 13 stages in total (including the reboiler and total condenser). The feed stage for this distillation column is stage 6 (counting from the top of the column). Using $R=0.91$ initially

led to a 7% error in specifications. The specification demands were not being met. As a result, R was increased to 1.03 which is 1.36 times the value of R_m from question 4. This value is consistent with what is dictated by process economics ($R=1.2-1.4R_m$).

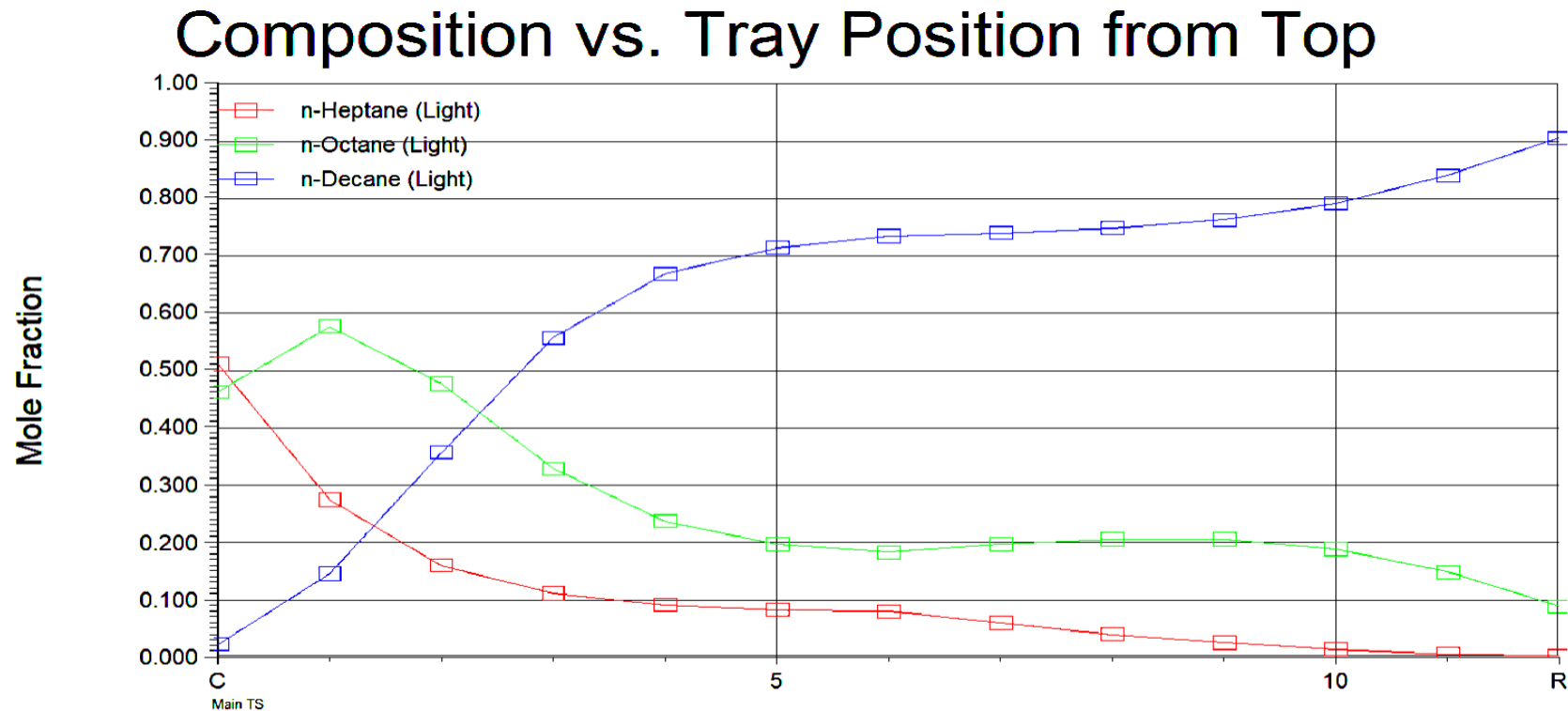


Figure 2: Plot of overall component mole fractions as function of stage number for the converged rigorous distillation column using $R=1.03$

Information that would be important to a process designer includes actual number of stages N (including condenser and reboiler), R , temperatures and heat duties of condenser and reboiler, feed conditions, column pressure, product specifications, feed and product tray nozzle sizing, internal column tray nozzle sizing, tray diameter, tray packed volume, tray packed space, weir height, weir length as well as condenser and reboiler diameters and heights. For the converged rigorous distillation column, the information that would be provided to a process designer is tabulated in table 6. The process designer would also be provided with the HK specification of 95% recovery in the residue, the LK specification of 100% recovery in the distillate, the distillate and residue molar flowrates of 64.12 and 35.88 kmol hr⁻¹ respectively, $q=0$ for the feed, the feed molar

flowrate of 100 kmol hr⁻¹ and its molar composition and temperature of 122.5 °C including the minimum temperature approach of 10 °C for the heat exchanger.

Table 6: Information important to a process designer with regard to converged rigorous distillation unit in question 10

<i>N</i>	13
<i>R</i>	1.03
Condenser diameter / m	1.193
Condenser height / m	1.789
Reboiler diameter / m	1.193
Reboiler height / m	1.789
<i>T</i>_{condenser} / °C	86.8
<i>T</i>_{reboiler} / °C	140.1
Condenser heat duty / GJ hr⁻¹	4.814
Reboiler heat duty / GJ hr⁻¹	0.780
<i>P</i>_{column} / bar	0.497
Feed tray nozzle diameter / m	0.375
Product tray nozzle diameter/ m	0.500
Internal nozzle diameter by tray/ m	0.0030
Tray diameter / m	1.5
Tray packed volume / m³	0.8836
Tray packed space / m	0.5
Weir length / m	1.2
Weir height / m	0.508

11. a) The distillation column from question 10 can't operate if the operating pressure is increased to 3 bar. For the same number of actual stages $N=13$ (including total condenser and partial reboiler) and same feed stage (6) the UniSim rigorous solver tool leads to divergence when trying to solve the distillation column.

For operation with pressure increased to 3 bar, the inlet feed would have to change in temperature. The heat exchanger duty required for the inlet feed so as to achieve this would also have to change. A new dew point calculation for the inlet feed reveals that the feed temperature would have to be at 187.8 °C. Key changes that will facilitate operation of a distillation system at 3 bar as well as achieve specification demands include an

increase in number of actual stages to a total of 15 (including total condenser and partial reboiler), a reflux ratio of 1.3 and a new feed entry position between stages 6 and 7 counting from top. The new temperatures for the total condenser and partial reboiler required are 152.8 and 213.2 °C respectively. In addition, the new duties for the total condenser and partial reboiler are 4.679 and 1.291 GJ hr⁻¹ respectively. The specification for LK recovery in the distillate (90%) was met according to the UniSim solved column with an error of 1.1% and that of the HK in the residue (95%) was met with an error of 1%.

Table 7 summarises the temperatures and vapour V and liquid L molar flowrates for each of the 15 stages of the modified distillation column for operation at 3 bar. According to table 7, the condenser liquid flowrate is 83.4 kmol hr⁻¹ which is higher than the value of 70.2 kmol hr⁻¹ reported for the distillation column operating at 0.497 bar. Furthermore, the reboiler vapour flowrate of 34.4 kmol hr⁻¹ is higher than the value reported for the distillation column operating at 0.497 bar.

Table 7: Temperatures and vapour and liquid molar flowrates on each distillation column stage for operation at 3 bar

Stage	$T / ^\circ\text{C}$	$V / \text{kmol hr}^{-1}$	$L / \text{kmol hr}^{-1}$
1 (Total condenser)	152.8	0	83.4
2	161.0	147.5	76.8
3	169.0	140.9	70.8
4	176.7	134.9	66.8
5	182.9	130.9	64.9
6	186.9	129.0	64.1
7	189.2	128.2	65.9
8	191.1	30.0	66.5
9	193.0	30.6	67.1
10	194.9	31.3	67.7
11	197.0	31.8	68.2
12	199.6	32.3	68.6
13	203.1	32.7	69.2
14	207.8	33.4	70.3
15 (Partial reboiler)	213.2	34.4	35.9

b) An increase in column pressure would lead to the requirement of a greater degree of process control systems on the distillation column. Additional pressure, temperature and level controls would have to be installed on both ends of the distillation unit (reboiler and condenser) and a

more thermotolerant material would have to be employed when constructing the distillation column (for example grade 304 stainless steel). In addition, thicker pipe walls would have to be constructed as far as the distillation column's structural integrity is concerned. Furthermore, by increasing the pressure to 3 bar more stages will be required for the distillation unit. As a result, the unit will be larger in height and more solid foundations and a reasonable aspect ratio would be required. Structural supports would also have to be put in place just in case.