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Analysis of the effect of feed composition and thermal conditions on distillation plant performance using a computer model

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This paper presents the effect of feed composition, \( x_F \), and feed thermal conditions on benzene-toluene distillation plant performance. An interactive computer model was developed to simulate the process using vapor-liquid equilibrium (VLE) data, mass and energy balances and McCabe-Thiele method. The feed thermal conditions studied were vaporized feed (VF), feed at its boiling point (FBP) and subcooled liquid (SCL) feed. The feed composition was varied between 0.20 and 0.45 kmol/kmol. The process was simulated at fixed feed flow rate (1000 kmol/h), reflux ratio (\( R = 4.0 \)) and distillate and bottoms compositions (95 and 5%, respectively). The minimum reflux ratio, theoretical and actual number of stages, reboiler duty and steam mass flow rate, and boil-up ratio changed with increasing \( x_F \) according to fourth-order polynomial functions. The condenser duty and cooling water flow rate increased linearly with \( x_F \). The effect of increasing \( x_F \) on the stripping section operating line (SOL) is reported separately for different feed thermal conditions. While all \( q \)-lines for VF passed at \((x_B, x_D)\) with decreasing slope; the \( q \)-lines for FBP were vertical and those for SCL feed were parallel. Graphical presentations of \( q \)-lines and SOLs for increasing \( x_F \) were developed in this study.

Key words: Distillation plant performance, feed composition, feed thermal conditions, number of stages, reboiler duty, condenser duty, boil-up ratio, mass and energy balances, vapor liquid equilibrium.

INTRODUCTION

Binary distillation is defined as a process in which a liquid or vapor mixture of two substances is separated into its component fractions of desired purity, by the simultaneous application and removal of heat. Historically, distillation has long been used to produce alcoholic beverages (batch distillation). In the 16th century, it was established that separation by distillation could be improved by multiple vapor-liquid contacting or stages (Lone and Rather, 2015). Therefore, in the 20th century, multiple-stage distillation became the most widely used industrial method for separating liquid mixtures (Lone and Rather, 2015).

Distillation is the most widely used separation method in the chemical and petrochemical industries (Luyben,
Binary distillation is an equilibrium-limited separation which uses heat as separating agent, in which process two or more relatively volatile liquids that vaporize at different temperatures are separated into almost pure streams. Thus, distillation separates components of a liquid mixture based on their differing boiling points. When the feed species' boiling points are significantly different, distillation can easily separate the feed into almost pure product streams of each component. The distillation process can be carried out in a batch (Barolo and Guarise, 1996; Salomone et al., 1997; Jana et al., 2013; Asiedu et al., 2014) or continuous mode (Khan et al., 2012; Jana et al., 2013; Asiedu et al., 2014; Patil and Patil, 2016). It is known that batch distillation column uses more energy than continuous column (Thurton et al., 2003); however, the former is convenient to operate. Other techniques developed for separation of binary mixtures include liquid-liquid extraction or solvent extraction, based on differences in solubility (Jawad and Sahib, 2018) and evaporation (for concentrating a solution removing the most volatile component), ion exchange and chromatography (Bhusure and Mali, 2015) and supercritical CO₂ extraction (Gustinelli et al., 2018).

The applications of distillation are in alcoholic beverage production and in the petroleum industry (for production of refinery gas, petrol, naphtha, kerosene and diesel, residue of which is used as fuel for ships, lubricants and road surface). Most significant uses of the distillation process have been in the petroleum industry where crude oil is separated into different fractions, light hydrocarbons (C₅’s to C₁₀’s) and aromatic chemicals. However, to date, the studies using computer modeling are still developing. New observations impart more insight into understanding of the parameters, performance factors, and other relationships useful in designing, operating and training of new engineers in the chemical and process industry. Because it is difficult to sample and analyze the column internal liquid traffic composition in most of the distillation columns that are commercially operated, process simulation modelling has been widely utilized to predict internal liquid composition and determine the optimum feed location in the actual industrial design. Modeling of distillation columns helps in predicting various performance parameters for a given separation (Kurkarni, 2017), such as number of stages, reboiler and condenser duties, etc. The models may vary from McCabe-Thiele binary distillation with constant or variable reflux, to short-cut or approximate methods (Diwekar and Madhavan, 1991; Sundaram and Evans, 1993; Barolo and Guarise, 1996; Salomone et al., 1997; Narvaez-Garcia et al., 2014), to rigorous methods used in the past. This study focuses on modeling of the distillation process to assess the effect of feed composition and thermal conditions, and can be regarded as a feed optimization. This method is convenient and does not require additional costs for field measurements and laboratory analysis (Manzo et al., 2012; Kulkarni, 2017; Sharmila and Mangaiyarkarasi, 2014). In this study, mass and energy balance equations, together with McCabe-Thiele diagram were used to create the mathematical model, details of which are given later.

A distillation plant can receive feeds of different characteristics (composition and phase or thermal properties). Such variations in the feed have strong impact on the distillation plant performance, including number of stages required, energy consumption and behavior of the stripping and rectifying sections of the column. In this study, mathematical modeling has been used to study such changes as the feed composition and feed thermal conditions were changed, results of which are presented in tabular and graphical forms.

The thermal condition of the feed affects the column internal flows of vapors and liquids. If the feed is below its bubble point, heat is needed to raise its temperature. This heat is obtained from condensing vapor rising through the column. Hence, the liquid flow moving down the column increases by the entire amount of the feed plus the vaporized material. If the feed enters as superheated vapor it will vaporize some of the liquid to equalize the enthalpy. In this case, the liquid flow down the column decreases and the vapor flow upwards increases by the entire amount of the feed plus the vaporized material. If the feed is saturated (liquid or vapor), no additional heat must be added or subtracted, and the feed adds directly to the liquid or vapor flow.

The basic mathematical formulations for distillation start with separation of binary mixtures (where a light key component (LKC) is separated from a heavy key component (HKC)). In advanced modeling, however, more than two components are involved in such separation systems (called multi-component distillation) (Diwekar and Madhavan, 1991; Bernot et al., 1993; Narvaez-Garcia et al., 2014). The separation in a distillation process is governed by a difference in the composition of a liquid and vapor phases, usually characterized by a difference in actual vapor pressures, or volatilities, of the liquid-phase components. The separation possibility is established based on the relative volatility, α, between the two components. When α is low, distillation becomes very energy intensive and necessitates high equipment cost as it requires large number of stages. To show the effect of feed composition and feed thermal conditions, other parameters were fixed such as distillate composition, x_D; bottoms composition, x_W; reflux ratio, R; and plant capacity, expressed in terms of molar flow rate of the feed, F.

The analysis presented in this paper is based on the mass balance relationships (for molar flow rates of the distillate and bottoms), loci of the point of intersection between the operating lines and the q-line on the y-x
diagram, minimum reflux, number of stages required, energy balances (made across reboiler and condenser to establish steam and cooling water requirements), boil-up ratio, etc., as \( x_F \) was increased from 0.2 to 0.45 kmol/kmol. The performance of a given distillation column depends on many factors, for example, thermal condition of the feed, internal liquid and vapor flow rates, tray design (Popoola et al., 2012; Patil and Patil, 2016), etc. The performance indices were separated in three classes: distillation parameters, energy saving (Nakaiwa et al., 2000; Soave and Feliu, 2002; Pribic et al., 2006) and money (costs and revenues). Literature shows that the state of the feed and its composition affects the operating lines and hence the number of stages required for a given separation (Luyben, 2005). It also affects the location of feed tray, which demarcates the top rectifying section from the bottom stripping section (Wankat, 2014, 2015). Two scenarios must be well correlated, that is, the design and operation of the distillation column, when the two deviates from each other, the desired separation cannot be attained. Usually, as \( x_F \) changes, the feed location is also changed accordingly to attain the desired separation. Thus, the column is made to allow for multiple feed points to choose from, especially when the raw materials of varying composition and varying components are to be used.

The feed to be separated may enter at any point in the column, although the optimal feed tray location should be determined and used (Wankat, 2014, 2015). While more than one stream may be fed to the system, and more than one product may be drawn, in this study, the feed composition was varied as fed to a single feed plate.

### Trayed versus packed distillation columns

Distillation can also be conducted in a packed column, analysis of which, differ from that of trayed column, presented in this study (as shown in Figure 1). The packed column design features include Packing Height (Number of equilibrium stages \( \times \) height equivalent to a theoretical plate, HETP). The HETP is typically a function of gas flow rate (m/s), packing type and the binary mixture characteristics.

A trayed distillation column is normally divided into a series of stages to allow multiple liquid-vapor contacting leading to a cascade of equilibrium stages. Each tray in a distillation column is designed to promote contact between the vapor and liquid. This study focuses on trayed columns. Based on agreed conventions, stages are preferably numbered from the top increasing downwards. During stage analysis, flows and compositions take the number of the stage they leave.

### Feed-plate considerations

In this paper, three feed thermal conditions were studied, that is, FBP, VF and SCL (expressed as the thermal conditions of the feed). Depending on the feed composition and thermal conditions, there is a variation in the amounts of both LKC and HKC in the vapor and liquid flows. While \( x_D \) and \( x_B \) can be selected independently, the reflux ratio, \( R \), and vapor flow rate in the column, \( V \), are related by the feed thermal conditions. The distribution of vapor and liquid flows at the feed plate for different thermal conditions of the feed are presented in Table 1.

A partially vaporized feed allows complete control over condenser and reboiler duties. One can manipulate the feed quality according to the requirements by minimizing the exchanger duties. A saturated liquid feed can be regarded as a sub-cooled liquid minus the sensible heat of a sub cooled liquid. It also condenses the vapors coming from the bottom, but not as significant as a sub-cooled liquid. A sub-cooled feed at the feed tray, on the other hand, allows the vapors coming from the bottom to condense at the feed tray. This in-turn increases the liquid load on the stripping section and increase the reboiler duty. For SCL feed, the reboiler must supply the sensible heat of the liquid as well as latent heat of vaporization.

A large concentration of the LKC in the feed (based on the range studied) corresponds to moderate reflux ratios (Luyben, 2005). A small concentration of the LKC in the feed means large reflux ratios because the distillate flow rate is small. Changes in the feed flow rate and the feed composition are the most important disturbances that will enter the column under control based on reflux ratio (Roffel et al., 2003).

By definition, an ideal stage is one where the vapor and liquid leave the stage in equilibrium. Consequently, the vapor composition functionally depends on the liquid composition, which forms the basis of modeling using VLE data. When no azeotropes are present, both top and bottom products may be obtained in any desired purity if enough stages are provided (analysis of which is reported for both theoretical and actual number of stages) and enough reflux is available. In practice, there are limits to the number of stages and to the amount of reflux. Theoretical limits on performance are imposed by total reflux (minimum stages) and minimum reflux (infinite number of ideal stages). This study was conducted between these two limits.

The growing application of distillation and increase in capacity of distillation plants results in the increase in energy consumption since it uses heat in thermodynamically inefficient way (Olujic et al., 2003; Patil and Patil, 2016). Thus, high energy consumption is practically the only weakness of distillation, necessitating thorough investigation during plant design and operation.

Techniques for increasing the energy efficiency of a distillation column exist (Li et al., 2008; Patil and Patil, 2016) including vapor recompression (Pribic et al., 2006), internal heat integration in distillation column (Nakaiwa et al., 2000; Jansens et al., 2001), changing feed thermal conditions and feeding mechanisms (Soave and Feliu,
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Packed tower design features

Trayed tower design features

Figure 1. Comparison between packed and trayed distillation columns designs.

2002; Soave et al., 2006; Wankat, 2007, 2014, 2015) and heat integration with external processes within the plant (Manzo et al., 2012; Patil and Patil, 2016). The most critical energy consumption areas are in the condenser and reboiler, located at the top and bottom sections of the column, respectively. The heat exchanged in these units is also referred to as duties.

There are two main categories of condensers, differentiated by the extent of condensation. In a total condenser, the entire vapor leaving the top of the column is condensed. Consequently, the composition of the vapor leaving the top tray \( y_t \) is the same as that of the liquid distillate product and reflux, \( x_D \). In a partial condenser, on the other hand, the vapor is only partially liquefied. The liquid produced is returned to the column as liquid, and a vapor product stream is removed. The compositions of these three streams (\( V_1, D \), and reflux) are therefore different. Normally, \( D \) (with composition \( y_D \)) is in equilibrium with reflux (composition \( x_D \)). In this study, both partial and total condenser duties were studied. A partial condenser functions as an equilibrium separation stage, so that columns with a partial condenser effectively have an extra ideal stage.

Most reboilers are partial reboilers, that is, they only vaporize part of the liquid in the column base allowing the vapors to flow upwards while the remaining liquid forms the bottoms stream. Partial reboilers also provide an ideal separation stage. Reboilers take several forms: they may
be thermosiphon types (that rely on the thermal effects on density to draw liquid through the heat exchanger), forced circulation types that use a pump to force liquid through, or stab-in types (that come through the side of the column into the liquid reservoir). In large, complex columns, side-stream reboilers can be used. These draw liquid off a tray, heat it, and then return the vapor-liquid mixture to the same or nearby trays.

Zhu et al. (2001) carried out rigorous mass and energy balances for modelling of the reboiler and condenser systems. Because of heat duties in these two units, use of heat integrated columns within the plant was suggested (Manzo et al., 2012). The feed flow rate can be can be limited due to capacity of reboiler, when the liquid cannot be vaporized as required (Popoola et al., 2012). Strategies used for minimizing energy in continuous distillation such as vapor recompression and heat integration are of great importance (Khan et al., 2012; Jana et al., 2013; Asiedu et al., 2014).

**MATERIALS AND METHODS**

**Process description**

This study was based on separation of benzene-toluene mixture, with benzene as an LKC. The layout of a distillation column is as shown in Figure 2. A single feed enters the column and two products are produced: a distillate containing more of the light or most volatile component is withdrawn from the top at a molar flow rate \(D\), and composition of the LKC, \(x_A\), and the bottoms containing more of the HKC is removed from the bottom at a molar flow rate \(B\), and composition of the LKC, \(x_B\). Heat (in the case shown, steam) for evaporation of the liquid is supplied to the reboiler, and heat is again removed (in this case, through cooling water) at the top in the condenser. The nomenclature used in this paper is as shown in Figure 1, where \(V\) is the vapor molar flow rate, \(F\) is the molar feed flow rate, \(RD\) is the reflux flow rate. The distillate flow rate denoted as \(D\). The \(m_w\) and \(m_s\) are cooling water and steam flow rates and are denoted as \(m_{cw}\) and \(m_{steam}\), respectively, in kg/h. In order to maintain constant separation in the distillation column, it should be well instrumented and controlled comprising of temperature, pressure flow and level controllers. The treatment of instrumentation and control techniques are, however, not covered in this paper.

A feed mixture of two components (in this case benzene and toluene), was separated into two, that is, overhead distillate with composition \(x_D\) and bottoms with composition \(x_B\) whose composition differ from that of the feed, \(x_F\). The bottoms product is almost always a liquid, but distillate in this model was either a saturated liquid reflux and liquid distillate at a bubble-point temperature (total condenser) or both vapor and liquid (partial condenser). At the bottom of the column, a partial re-boiler was used to produce vapor boil up with boil-up ratio \(v_B = V/B\) and a liquid bottoms product \(B\). The partial reboiler function as additional theoretically stage. The distillation is a very energy-intensive technique, especially when the relative volatility, between the components being separated is low \((\alpha < 1.5)\). The operation and design factors that influenced by the change in feed composition and conditions, which forms the basis of this study include: number of stages (theoretical and actual), condenser and reboiler duties, cooling water and steam mass flow rates and boil-up ratio.

The feed enters the column at a feed stage denoted as \(f\). At the feed-stage pressure, the feed thermal conditions studied were SCL, VF and FBP the overall mole fraction with respect to the LKC, denoted. The problems addressed in this study include solving mass and energy balances equations across a distillation column with condenser and operating at atmospheric pressure with a fixed reflux ratio, to separate and purify a binary mixture of benzene and toluene fed at a rate of 1000 kmol/h, and needing molar composition of benzene in the distillate of 0.97 kmol/kmol or better.

**Model setup and fixed variables**

Due to complexity of variables in the distillation column operations and the corresponding larger number of equations, some variables were fixed whose specifications are shown in Table 2. The minimum number of stages was fixed at 6.0, based on which the actual number of stages, \(N_{act}\) and the ratio, \(N_{act}/N_{min}\), were determined.

**Mathematical relations used in modeling the distillation of binary mixtures**

In this study, a computer model was created using a series of equations consecutively solving VLE relationships, mass balance equations across the whole column and across different sections, analytical implementation of the McCabe Thiele diagram due to changing \(x_F\) and feed thermal conditions and q-line data, heat balance equations to determine condenser and reboiler duties (cooling water and steam requirements), as shown in Equations 1 to 34. The numerical methods used were mainly algebraic solution for the complete \(y-x\) diagram to determine points of intersection (for q-line, SOL, ROL, VLE, \(y\)-intercepts) and solving the operating line equations to establish the theoretical number of stages by
comparing the values of $x$ and $y$ stage by stage. Using a computer model it was possible to solve all this set of equations within short time, allowing the researchers to change conditions several times, which could require several days for manual calculations. All computations were carried out simultaneously wherever changes in $x_F$ or feed thermal conditions were made, results of which were organized and presented using graphs and in tabular form.

**Equilibrium and mass balance relationships**

The fundamental equations used in the model are summarized as the following.

The equilibrium curve based on constant relative volatility is given as per Equation 1:

$$y = \frac{ax}{1+x(a-1)}$$

Equation 1

The material and energy balance equations were developed as:

Overall mole balance:

$$F = D + B$$

Equation 2

Light key mole balance:

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

Equation 3

or, based on the distillate flow rate and composition,

$$D.x_D = F.x_F - B.x_B$$

Equation 4

Combining Equations 2 and 3 gives:

$$D = F \left(\frac{x_F - x_B}{x_D - x_B}\right)$$

Equation 5

where $x_B < x_F < x_D$.

Taking a mole balance around the column excluding the condenser gives:

$$F + L = V_1 + B$$

Equation 6

while light key component balance for this section gives (assuming total condenser):

$$F.x_F + L.x_D = V_1.x_D + B.x_B$$

Equation 7

The mole balance around the condenser gives:

$$V_1 = L + D$$

Equation 8
The McCabe-Thiele method for analysis of distillation process uses graphical method with the following important lines: VLE curve, reference line at 45°, ROL, SOL and q-line (describing the feed thermal conditions). Assuming a subsystem cutting the column above the feed plate and taking mole balance for the stripping part yields:

\[ F + L = V + B \]  

while an LKC balance gives:

\[ F \cdot x_F + L \cdot x = V \cdot y + B \cdot x_B \]  

Equation 10 leads to ROL equation as per Equation 11:

\[ y = \left( \frac{1}{y_i} \right) x + \left( \frac{y_F - y_B}{v} \right) x_D \]  

Combining Equations 12 and 5 simplifies to:

\[ y = \left( \frac{1}{y_i} \right) x + \left( \frac{D}{v} \right) x_D \]  

where \( L \) and \( V \) are the liquid and vapor total molar flow rates, which are assumed to be constant from one stage to another. From the definition of the reflux ratio, \( R = L/D \) or \( L/(L+D) \), and \( V = L + D \), the ROL equation becomes,

\[ y = \left( \frac{R}{R+1} \right) x + \left( \frac{1}{R+1} \right) x_D \]  

Based on Equations 13 and 14, when \( x = 0 \), the y-intercept, \( y_i \), is related to the minimum reflux ratio, \( R_{min} \), as per Equation 15:

\[ R_{min} = \left( \frac{D}{y_i} \right) - 1 \]  

Based on mole balance across a system boundary excluding the feed plate (stripping section):

\[ L = V + B \]  

while an LKC balance gives in this section gives:

\[ L \cdot x = V \cdot y + B \cdot x_B \]  

Combining Equations 15 and 16 gives the SOL equation as per Equation 17:

\[ y = \left( \frac{1}{y_i} \right) x + \left( \frac{B}{y_i} \right) x_B \]  

Based on Equation 17 and defining the boil-up ratio as \( V/B \), then the slope of the SOL can be changed to \( (V_B+1)/B \), and the SOL equation changes to:

\[ y = \left( \frac{V_B+1}{V_B} \right) x + \left( \frac{1}{V_B} \right) x_B \]  

Once the number of stages is determined by stepping towards the point of intersection (POL) from \( x_B \) and \( x_D \), that is \( N_{min} \), the actual number of theoretical stages was determined from Equation 19:

\[ N_{min} = N_{ac} + 1 \]  

which accounts for the reboiler being considered as an additional equilibrium stage. The actual number of stages was then determined based on the Murphree efficiency, \( E_m \), as per Equation 20 for either gas phase or liquid phase:

\[ E_m = \frac{20}{y_B - y_{SCL}} \cdot \frac{y_B - y_{SCL} - 1}{y_S - y_{SCL}} \]  

Considering the fact that the states are not 100% efficient, the actual number of stages was determined by dividing the theoretical number of stages by \( E_m \).

**Feed thermal conditions and q-line equation**

In the McCabe-Thiele method of distillation column design, the thermal condition of the feed, \( q \), is defined as the ratio of the heat required to fully vaporize the feed into saturated vapor, \( (H_v - H_f) \), and the latent heat of vaporization of the feed mixture, \( (H_v - H_f) \), The feed quality can be varied from superheated vapor condition (that is, \( q < 0 \)) to SCL condition (that is, \( q > 1 \)). Defining \( V' \), the vapor flow rate in the stripping section = \( V + (q-1)F \), and also \( q \) as the fraction of liquid in the feed, the operating line for a feed tray considering the \( F \) moles/h of feed, with fraction \( q \) of liquid, the liquid flow = \( qF \) moles/h and vapor flow = \( (1-q)F \) moles/h. The feed section operating line (FSOL), also called q-line, is given by Equation 21:

\[ y = \frac{q}{(1+q)} x + \frac{1}{(1-q)} x_F \]  

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Formula or symbol</th>
<th>Range or fixed values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed composition range</td>
<td>( x_F )</td>
<td>0.2 - 0.45 mol/mol</td>
</tr>
<tr>
<td>Distillate composition</td>
<td>( x_D )</td>
<td>0.95 mol/mol</td>
</tr>
<tr>
<td>Bottoms composition</td>
<td>( x_B )</td>
<td>0.05 mol/mol</td>
</tr>
<tr>
<td>Feed flow rate</td>
<td>( F )</td>
<td>1000 kmol/h</td>
</tr>
<tr>
<td>Reflux ratio</td>
<td>( R )</td>
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</tr>
<tr>
<td>Slope of the ROL</td>
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</tr>
<tr>
<td>Y intercept for ROL, ( y_i )</td>
<td>( \frac{x_D}{R+1} )</td>
<td>0.19</td>
</tr>
<tr>
<td>Minimum of number of stages</td>
<td>( N_{min} )</td>
<td>6</td>
</tr>
</tbody>
</table>

**Table 2.** Model set-up and fixed variables for studying the effects of feed composition on the distillation column performance.
For a given feed thermal condition, $x_F$ and $q$ are fixed; therefore, the $q$-line is a straight line with slope -$\Delta q/(1-q)$ and intercept $x_F/(1-q)$. The formulas for determination of the values of $q$ are different for different feed thermal conditions. For SCF, the value of $q$ is given as per Equation 22:

$$q = 1 + \frac{C_T(T_{km} - T_F)}{\Delta H_{B}^s}$$  \hspace{1cm} (22)

For the feed entering the column as VF, the value of $q$ is given as per Equation 23:

$$q = \frac{(F - T_F)}{F}$$ \hspace{1cm} (23)

where $D/F = V_r/F$ is the distillate-to-feed ratio. For the feed entering as bubble or boiling point (FBP), the value of $q = 1.0$.

Condenser and reboiler duties based on energy balances

An energy balance for an entire column gives:

$$F \cdot h_f + Q_h = D \cdot h_D + B \cdot h_B + Q_C + Q_{\text{loss}}$$ \hspace{1cm} (24)

For insulated distillation column, $Q_{\text{loss}}$ is negligible and can be ignored. For a total condenser, the condenser duty can be approximated as per Equation 25:

$$Q_C = D(R+1) \Delta H_{B}^v$$ \hspace{1cm} (25)

where $\Delta H_{B}^v$ is the average molar heat of vaporization of the two components being separated. For partial condenser, only the distillate is condensed, so that Equation 26 becomes:

$$Q_C = D \Delta H_{B}^v$$ \hspace{1cm} (26)

If the inlet and outlet temperatures of the cooling water ($T_{\text{in}}, T_{\text{out}}$) are known, then the condenser duty can also be expressed as per Equation 27:

$$Q_C = \dot{m}_{cw} c_{pw} (T_{\text{out}} - T_{\text{in}})$$ \hspace{1cm} (27)

The cooling water rate mass flow rate, $m_{cw}$, for the condenser is, therefore:

$$m_{cw} = \frac{Q_C}{c_{pw}(T_{\text{out}} - T_{\text{in}})}$$ \hspace{1cm} (28)

where $Q_C$ = condenser duty/rate of heat transfer, $T_{\text{out}}, T_{\text{in}}$ are the temperature of cooling water out of and into condenser, respectively. The cooling water flow rate can also be expressed in terms of heat released in condensing the vapors comprising of the LKC and HKC, with latent heats of $\Delta H_1$ and $\Delta H_2$, respectively, as per Equation 29:

$$\dot{m}_{\text{water}} = \frac{\nu [\lambda_1 x_D + \lambda_2 (1-x_D)]}{c_{pH2O}(T_{\text{out}} - T_{\text{in}})}$$ \hspace{1cm} (29)

For partial reboiler, the rate of heat transfer from the steam to the solution being separated is given as per Equation 30:

$$Q_R = B V_{\text{so}} \Delta H_{B}^v$$ \hspace{1cm} (30)

When the feed is at the bubble point and a total condenser is used, using the relationship that $V_R = (L + D - V)B$, that is, $BV_R = L + D = D(R+1)$, then, comparing Equation 26 with Equation 29, $Q_C = Q_R$. When the feed is partially vaporized and total condenser is used, the heat required by the reboiler is less than the condenser duty and is given by Equation 31:

$$Q_R = Q_C (1 - \frac{v_F}{D(R+1)})$$ \hspace{1cm} (31)

The heat transfer in the reboiler, can also be expressed based on the latent heat of condensation released by the steam (flowing at $m_s$ in kg/h), as per Equation 32:

$$Q_R = m_s \Delta H_{B}^s$$ \hspace{1cm} (32)

If saturated steam is used as heating medium for the reboiler, the steam mass flow rate (kg/h) required is given by an energy balance, as per Equation 33:

$$m_s = \frac{m_{s} \Delta H_{B}^{s}}{\Delta H_{B}^{v}}$$ \hspace{1cm} (33)

where $Q_R$ is the reboiler duty or rate of heat transfer, $m_s$ is molecular weight of steam and $\Delta H_{B}^{v}$ = molar enthalpy of vaporization of the steam, as per Equation 34:

$$\dot{m}_{\text{steam}} = \frac{v [\lambda_1 x_D + \lambda_2 (1-x_D)]}{\dot{c}_p \text{water}}$$ \hspace{1cm} (34)

To emphasize on the energy requirements for the reboiler during separation to produce the distillate and bottoms, the specific energy consumption is defined as per Equations 35, 36 and 37:

$$\text{Specific energy for distillate} = \frac{D}{Q_R} \frac{\text{kmol}}{\text{kw} \cdot \text{h}}$$ \hspace{1cm} (35)

$$\text{Specific energy for bottoms} = \frac{B}{Q_R} \frac{\text{kmol}}{\text{kw} \cdot \text{h}}$$ \hspace{1cm} (36)

$$\text{Specific steam consumption} = \frac{m_s}{Q_R} \frac{\text{kmol}}{\text{kg}}$$ \hspace{1cm} (37)

Higher values of specific energy indicate a good performance of the separation process, that is, more product generated per unit of energy consumed.

RESULTS AND DISCUSSION

Mass balance relationships

Material balance relationships allows the conceptualization of flows into and out from distillation process, for operational and economic benefits. Such equations allow the designer to size the column, the vendor selling the product to set the supply and demand volumes (including raw materials and product material analysis). In this study, the balances were conducted while changing $x_F$. Figure 3 shows the mass balance relationship between $D, B, F$, and $V$ as $x_F$ varied. The mass balance relationships do not depend on feed thermal conditions. The feed flow rate was fixed at 1000
kmol/h, to study the effect of increasing $x_F$ in the selected range. While $V$ increased faster with increasing $x_F$ (from 800 to 2200 kmol/h), $D$ increased from 150 to 480 kmol/h. The bottoms flow rate, on the other hand, decreased from 800 to 520 kmol/h as $x_F$ changed from 0.2 to 0.45.

The fact that $V$ exceeds $F$ for $x_F > 0.225$, can be explained based on the fact that during startup of the process, materials to be distilled are fed into the column initially in order to establish steady state conditions, after which the feed flow rate is maintained constant and distillate and bottoms are then continuously withdrawn. That is, the total material circulating in the system (column, condenser and reboiler) is far above feed flow rate at steady state. Thus, to achieve production at a set capacity, there must be a dead amount of material fed to the process before distillate and bottoms can be withdrawn at rates given by mass balance equations.

Application of McCabe-Thiele method for analysis of VLE for different scenarios

Determination of minimum number of stages

The minimum number of stages is traced between the $y = x$ and the equilibrium curve depending on $x_F$ and $x_D$. Given that $x_D$ was fixed at 0.95, the minimum number of stages depend only on $x_F$, and the characteristics of the equilibrium curve, that is, $y = x$. Thus, increasing $x_F$ from 0.2 to 0.45 decreases the minimum number of stages based on McCabe-Thiele diagram. Practically, increasing $x_F$ increases chance of obtaining higher distillate throughout put although the duties both condenser and reboiler increases.

Determination of minimum reflux ratio

The minimum reflux ratio, $R_{\text{min}}$, is determined when the point of intersection between ROL and SOL is located on the equilibrium curve, where also the $q$-line passes. To determine $R_{\text{min}}$, $x_F$, $x_D$, and $q$ must be known. While the slope of the $q$-line depends on feed thermal conditions, the $R_{\text{min}}$ is based on the corresponding point of intersection between ROL and $y$-axis, $y_i$ or $y$-intercept, as per Equation 14. Figure 4 shows the graphical method for determination of $R_{\text{min}}$ based on the three feed thermal conditions (VF, FBP and SCL). The key parameters are the $y$-intercepts, which were observed to be 0.28, 0.32 and 0.41, leading to values of $R_{\text{min}}$ values equal to 2.39, 1.97 and 1.32, respectively. Thus, at a fixed feed composition of $x_F = 0.3$, $R_{\text{min}}$ varied with feed thermal conditions.

Determination of number of equilibrium stages for various feed thermal conditions

When the SOL and ROL meet below the VLE and above the $y = x$ line, the point of intersection determines the $q$-line equation and number of equilibrium stages are traced
between the VLE and the operating lines as shown in Figure 5.

**Effect of feed composition on minimum reflux ratio, $R_{\text{min}}$**

Reflux ratio is the ratio of liquid returned to the column to that drawn from the process after condensation of vapors leaving the top (denoted as $V$), that is, $L/D$, where $V = L + D$. In this study, the effect of increasing $x_F$ on the ratio $R/R_{\text{min}}$ was studied for fixed values of $R = 4.0$, $x_D = 0.95$ and $x_B = 0.05$, also for three feed thermal conditions (VF, FBP and SCL). This is based on the fact that changing $x_F$ has an effect on the location of the point of intersection of the two operating lines and the $q$-line, thus affecting $R_{\text{min}}$. For a fixed reflux ratio, $R/R_{\text{min}}$ can indicate the changes taking place as a result of moving the point of intersection towards the RHS as shown in Figure 6.

Results show that increasing $x_F$ increases the ratio $R/R_{\text{min}}$ showing that $R_{\text{min}}$ decreases as $x_F$ increases towards $x_D$. This was observed for all feed thermal conditions. Moreover, higher values of $R/R_{\text{min}}$ were observed for SCF followed by FBP, while VF shows lowest values of $R/R_{\text{min}}$. Increasing $x_F$, therefore, implies that separation becomes easy and high amount of distillate is obtained, since less liquid is refluxed back to the column. The lower values of $R/R_{\text{min}}$ for VF indicate that the latter allows easy separation of the components leading to higher molar flow rate of distillate, $D$, compared to FBP and SCF.

**Effect of feed composition on the number of stages required to effect separation**

Based on the method presented in Figure 5, the data on theoretical number of stages for VF, FBP and SCL feed thermal conditions was collected for increasing values of
Figure 5. Variation of minimum number of stages, minimum reflux ratio and equilibrium number of stages with feed thermal conditions (VF, FBP, and SF) at a fixed feed composition $x_F = 0.3$.

$x_F$, as presented in Figure 6. The actual number of stages was also determined based on estimated tray efficiency. Theoretical stages are those determined between the equilibrium curve and the SOL and ROL, which assumes that a complete equilibrium is achieved across stages during the distillation which assures 100% efficiency in the process. On the contrary, the actual conditions inside the distillation are slightly away from the equilibrium scenario represented by operating lines due to insufficient time of contact, and insufficient degree of mixing. To achieve the required degree of separation required, more trays will have to be added to compensate for the lack of perfect separation. The adjustment is based on tray efficiency, determined in this study using Murphree efficiency, which is a measure of the closeness to equilibrium on a plate or stage within a fractional distillation column (Equation 20).

With fixed $x_D$ and $R$, increasing $x_F$ leads to lower number of stages required to achieve such a separation as shown in Figure 7. This is because, increasing $x_F$ brings a mixture with high concentration of a light component, thus reaching $x_D$ in rather fewer stages. The increase in $N_{\text{theo}}$ follows a fourth order polynomial function for all feed thermal conditions as approximated using equations with $R^2 = 0.995 - 0.998$. For $x_F \geq 0.35$, the number of theoretical and actual stages remains the same for VF and FBP, before which the number of both theoretical and actual stages are highest for VF. Both
Manyele

Figure 6. Effect of varying feed composition on minimum of reflux ratio for different feed thermal conditions ($R = 4.0$).

Theoretical and actual numbers of stages were lowest for SCF in the whole range of $x_F$. The RHS of the $y$-axis shows in Figure 7 the actual number of stages as $x_F$ was increased from 0.20 to 0.45, profile of which are similar to those of theoretical number of stages. While the theoretical number of stages increased from 7.9 to 14.5, the actual number of stages ranged between 8.5 and 17.0, being higher than the latter for all the three thermal conditions for the feed.

This difference in $N_{th}$ and $N_{act}$ highlights the fact that stages in the distillation column cannot attain 100% efficiency, and hence the actual number of plates is higher than the theoretical number of plates or trays determined from McCabe-Thiele diagram. Therefore, the actual number of stages can also be determined by dividing the theoretical number of stages by the tray efficiency. There are several different measures of tray efficiency with each measure highlighting different performance issues. The three main tray efficiency metrics are overall tray efficiency, Murphree vapor efficiency and Baur efficiency.

Moreover, if the distillation column uses a partial condenser and reboiler (both of which acting as trays), then the theoretical number of stages increases by 2. Meanwhile, if the condenser condenses all the vapors (total condenser) it cannot be regarded as a theoretical stage and only a reboiler can be counted, increasing the total number of theoretical stages by 1. For an existing column, the number of trays is fixed inside the column plus 2 or 1 stage depending on condenser type. Thus, modeling work is important before actual design and installation (Kulkami, 2017).

Based on results presented in Figure 7, one may assume that the number of stages/trays maybe increased without limitations. In fact, there is a limitation on number of plates and cannot be increased at a certain point. There are, however, limitations in terms of equipment cost, structural requirements, feed composition and sometimes space, while $x_F$ is also determined by upstream process conditions or raw materials.

Effect of changing feed composition on energy requirements

Partial and total condenser duties for varying feed composition

The condenser duty, $Q_c$, for both total and partial condensers, increases linearly with $x_F$ as shown in Figure 8. The $Q_c$ increases with $x_F$ because more vapors are generated at higher $x_F$ necessitating high heat removal rate during condensation of vapors. Regardless of the feed thermal conditions, only one linear equation was obtained since $Q_c$ does not depend on feed thermal conditions since only vapors reach the condenser. The duty for total condenser is, however, higher than that of a partial condenser for the whole range of $x_F$ also regardless of feed thermal conditions. This is because the partial condenser only condenses part of the vapors while the total condenser changes all the vapors into liquid form necessitating extraction of large amount of heat for the latter. Use of a total condenser requires that the available cooling water is at a very low temperature sufficient to condense all the vapors exiting at the top of the column.

Analysis of the condenser duty in relation to the distillate produced indicated that the kmol distillate per
Figure 7. Effect of varying feed composition on the theoretical and actual number of stages

Figure 8. Effect of varying feed composition on the total and partial condenser duties.

kWh of heat energy removed was 0.02 and 0.025 kmol/kWh for total and partial condensers, respectively. This indicates that more distillate is produced per unit of energy consumed for total condenser than partial condenser. The cooling water requirements in the condenser for varying feed composition, follows the similar trend as the condenser duties shown in Figure 8. Given the values of condenser duty requirements, $Q_{tc}$ and $Q_{pc}$ in kW, the cooling water requirements can be established. The cooling water requirements in relation to $x_F$, $Q_{tc}$ and $Q_{pc}$ were observed to be linear, expressed using a combined mathematical equation, shown in
Equations 38 and 39:

\[
\begin{align*}
    m_{\text{ef}} &= \begin{cases} 
        2379 x_F - 119.95 \\ 0.0431 Q_{\text{ff}} \\ 0.0836 Q_{\text{rp}}
    \end{cases} \\
    Q_{\text{pc}} &= \frac{0.0431}{0.0836} Q_{\text{ff}} = 0.8 Q_{\text{ff}}
\end{align*}
\]  

Reboiler duty for different feed thermal conditions and composition

Figure 9 shows the variation of reboiler duty with \( x_F \) for the three feed thermal conditions. Increasing \( x_F \) increases reboiler duty for all feed thermal conditions. Increasing \( x_F \) should generally result into lower \( Q_{\text{ff}} \) since the vapors of HKC could be easily generated. However, due to fixed conditions of \( R \), \( x_D \), \( x_B \) and \( F \), the observed scenario was an increase in \( Q_{\text{ff}} \). The VF shows the lowest reboiler duty followed by FBP, while the SCL had highest reboiler duty. This is because, for VF, most of the feed joins the upward flow of vapors and do not reach the bottom, while SCL leads to most of the liquid flowing downwards to the reboiler, increasing heat requirements to create vapors, as a result, the reboiler duty for SCL is highest compared to VF and FBP.

Figure 9 shows further that there is a highly non-linear relationship between reboiler duty, \( Q_{\text{ff}} \) and \( x_F \), as a principal operating condition used in this study. This is an indication that not only \( x_F \) but also other parameters affect \( Q_{\text{ff}} \), such as \( R \), \( x_D \), \( x_B \) and \( F \), which require separate simulation studies. Thus, if there is a possibility of utilizing a hot process stream to exchange heat with the feed at any composition within the plant, such opportunities should be utilized to save energy requirements in the reboiler during distillation process. Similarly, since the reboiler utilizes steam for heating the liquid to its boiling point, the variation of \( x_F \) with steam requirements (kg steam/h) follows similar trend, as shown in Figure 9, whereby, steam flow rate increases with \( x_F \) for all three feed thermal conditions. Most reboilers will be operated using high pressure condensing steam (at higher boil-up) to save area requirements in the reboiler heat exchanger. Higher \( x_F \) means more LKC that need to be boiled off since \( x_B \) is fixed and hence higher \( Q_{\text{ff}} \). Challenging issues in the reboilers operation include: bottoms are mixture having substantial boiling ranges; for the purpose of liquid recirculation, the reboiler and connecting piping must be considered as a unit adding another iterative loop in design procedures necessitating use of modeling packages. Another challenge is the dead volume of mixture that need to be filled in the reboiler and the column bottom to the required hydrodynamic setup before the steady state conditions can be attained in the column, and ready for product and bottoms withdrawal at a design flow rate. This causes also an increase in reboiler duty.

Detailed analysis of the reboiler duty included the distillate generation rate in relation to the energy consumed in the reboiler at varying feed composition measured as kmol distillate produced per kWh of energy consumed in the reboiler. Figure 10 summarizes the
results for three feed thermal conditions. The kmol/kWh data for VF and FBP changed very slightly with $x_F$, average values of which were 0.0253 and 0.0199 kmol/kWh, respectively. For SCL feed however, the kmol distillate produced per kWh spent in the reboiler was the lowest and increased with $x_F$, as shown in Figure 10. Lower kmol/kWh indicates that more energy is spent in the reboiler while least amount of distillate is generated as product. For all feed thermal conditions, the variation of reboiler duty with $x_F$ followed a fourth-order polynomial function with $R^2 = 0.9945, 1.0$ and 0.9998 for SCL feed, FBP and VF, respectively.

**Effect of feed composition on the steam flow rate**

While reboilers are an integral part of the production process, they are regarded as a part of steam system although located far away from boiler and closer to the distillation plants. Figure 11 shows the effect of increasing $x_F$ on steam mass flow rate, $m_s$, for the three different feed thermal conditions. The steam mass flow rate was observed to increase with $x_F$ for all feed thermal conditions. The same reasons can be stated similar to the observation presented in Figure 9.

The SCL feed has highest required steam flow rate at any given feed composition, which increases faster with $x_F$ compared to other feed thermal conditions. The lowest steam requirement was observed for VF, for which the reboiler only heats the down-flowing refluxed liquid from the top. At entry into the feed plate the feed for VF join the up-flowing vapors and none of the feed flows downwards into stripping section. The required steam flow rate change widely as $x_F$ increases, for instance, for SCL feed, the $m_s$ increased from 10,000 to 28,000 kg/h indicating that steam flow rate is highly sensitive to the feed composition, especially for SCL. In this study, the steam flow ranged from 10,000 to 62,000 kg/h which indicates a larger consumption depending on feed thermal conditions and feed composition. The SCL feed shows highest steam consumption into the reboiler compared to FBP and VF, for the whole range of feed composition studied. Results show further that the relationship between steam flow rate and feed composition follows fourth order polynomial function depending on the feed thermal conditions.

Further analysis involved relating the reboiler duty with the bottoms flow rate as a ratio of kmol bottoms per kWh consumed and also per kg steam used, defined in this study as specific energy consumption and specific steam consumption, respectively, as expressed in Equations 36 and 37. Figure 12 shows the variation of kmol bottoms per kWh of reboiler duty and also per kg steam consumed in the reboiler, as a function of $x_F$. Results show that, initially both specific energy and kmol/kg steam decreased faster with $x_F$, approaching a common value for $x_F$ beyond 0.4 kmol/kmol. Increasing the feed composition decreases both the kmol/kWh of energy and kmol/kg steam consumed as indicated by the two vertical axes, respectively. This is because at higher $x_F$, the bottoms flow rate, $B$, decreases (as shown in Figure 4) lowering the specific wand and steam consumption. Both kmol/kWh and kmol/kg steam were highest for vaporized feed, and lowest for SCL. For subcooled liquid feed, however, more energy is used in the reboiler, lowering the specific energy and also the specific steam consumption. This again necessitates use of bottoms to pre-heat the feed to the distillation column, as an option for energy conservation.
Effect of feed composition on the boil-up ratio

Figure 13 shows the effect of increasing $x_F$ on the boiling rate at the bottom of the column. The boil-up ratio, $V_B$, increases with $x_F$ for all feed thermal conditions. The SCL feed shows highest boil-up ratio than VF and FBP for all values of $x_F$. The increase in $V_B$ as $x_F$ increases can be attributed to the fact that at higher concentration of LKC, more vapors will be generated at a given QR, since the mixture will have lower latent heat of vaporization.

The higher $V_B$ for SCL feed can be attributed to the fact that since most of the feed flows down to the reboiler cooling and condensing part of vapors flowing upwards in the stripping section, more vapors must be generated in
Figure 13. Effect of varying feed composition on the boil-up ratio.

At the feed plate, changes in $x_F$ for different feed thermal conditions also affect the column performance, based on the dependence of $q$ on $x_F$. In this study, a thorough analysis was conducted on the variation of $q$, slope of $q$-line, $q/(q-1)$, and its y-intercept, $x_F/(q-1)$. Table 5 shows the variations of $q$, $q/(q-1)$ and $x_F/(q-1)$ for different feed thermal conditions as $x_F$ was varied. Increasing $x_F$ lowers the value of $q$ for VF from 0.833 to 0.556 while $q$ remains constant for FBP ($q = 1$) and SCL feed ($q = 1.53$). The slope of the $q$-line, on the other hand, increases for VF (from -5.0 to -1.25) and remains undefined for FBP and constant at 2.9 for SCL feed. The y-intercept of the $q$-line changes slightly for VF (from -1.200 to -1.013), remaining undefined for FBP and increasing from 0.38 to 0.854 for SCL feed.

The reboiler to maintain a constant molar flow of vapors across the whole column. This in turn puts a high demand on reboiler duty and steam mass flow rate. The relationship between $V_B$ and $x_F$ for all feed thermal conditions follows a fourth-order polynomial function with good fit ($R^2 = 1$), similar to other parameters (Figures 7 and 9) as summarized in Table 3. For SCL feed, $V_B/\min$, $Q_R$, $m_s$ and $V_B$ were highest while the number of stages was lowest, different from VF. For FBP, all parameters were in between VF and SCL, since this feed thermal condition comprise the properties of both VF and SCL. In short, increasing $x_F$ increases $V_B/\min$, $Q_R$, $m_s$ and $V_B$, while the number of stages decreases ($N_{th}$ and $N_{actual}$). This implies that increasing $x_F$ lowers the number of stages required to effect separation by distillation.

**Model results for detailed analysis of the stripping section**

**Variations in the OLE for stripping section due to changes in feed composition**

In the bottom section, the operating line equation is affected strongly by changes in both feed thermal conditions and composition. As per Equation 19, the key variables of SOL equation are slope and intercept, that is, $(V_B/\min)/V_B$ and $x_F/V_B$, both of which are functions of the boil-up ratio $V_B$ which in turn varies with $x_F$ as shown in Figure 13. Thus, any changes in $x_F$ will affect the SOL characteristics. Table 4 summarizes the data from the variation of $V_B$ with $x_F$ and also for three different feed thermal conditions. For all values of $x_F$, $V_B$ values were highest for SCL and lowest for VF. Increasing $x_F$ increases $V_B$ and lowers both $(V_B/\min)/V_B$ and $x_F/V_B$, which in turn affects the required number of stages based on McCabe-Thiele method and affects operating parameters such as $Q_R$, $Q_c$ and $D$. While $V_B$ increases with $x_F$ for all feed thermal conditions, $(V_B/\min)/V_B$ and $x_F/V_B$ decreases with $x_F$.

At the feed plate, changes in $x_F$ for different feed thermal conditions also affect the column performance, based on the dependence of $q$ on $x_F$. In this study, a thorough analysis was conducted on the variation of $q$, slope of $q$-line, $q/(q-1)$, and its y-intercept, $x_F/(q-1)$. Table 5 shows the variations of $q$, $q/(q-1)$ and $x_F/(q-1)$ for different feed thermal conditions as $x_F$ was varied. Increasing $x_F$ lowers the value of $q$ for VF from 0.833 to 0.556 while $q$ remains constant for FBP ($q = 1$) and SCL feed ($q = 1.53$). The slope of the $q$-line, on the other hand, increases for VF (from -5.0 to -1.25) and remains undefined for FBP and constant at 2.9 for SCL feed. The y-intercept of the $q$-line changes slightly for VF (from -1.200 to -1.013), remaining undefined for FBP and increasing from 0.38 to 0.854 for SCL feed.
The fact that the q-line for VF shows a wide range of variation with $x_F$ (as per Table 5), necessitates further analysis. Figure 14 presents the changes in the loci of the point of intersection PoI between ROL, SOL and the q-line as the $x_F$ was increased from 0.2 to 0.45. The plot reveals two important features of the SOL, and q-lines. All the SOLs meet at the point $(x_B, x_D)$ on the $y = x$ line while the q-lines meet at a point $(x_0, x_D)$. The two points add on the control gives by fixed $x_B$ and $x_D$ values in the modal as $x_F$ increases. For vaporized feed, increasing $x_F$ lowers the $y$-intercept, while the point of intersection between line and the two operating lines moves towards $x_D$. While all stripping section operating lines pass through $(x_D, x_D)$, all q-lines, on the other hand, pass, through $(x_B, x_D)$. Increasing $x_F$ also increases the $y$-intercept of the stripping section operating line and lowers its slope.

It was also noted that for vaporized feed, the value of $x$ at the point of intersection of the three lines, PoI, is lower than $x_F$ for all cases presented in Figure 14. The change in slope and $y$-intercept as $x_F$ increases is faster for q-lines than for stripping section operating lines. Increasing $x_F$ changes the point of intersection towards $x_D$ along the rectifying section operating line, indicating that the number of stages in the rectifying section decreases, while those in the stripping section increases. This implies that the feed plate location moves upwards along the distillation column, a scenario observed for all feed thermal conditions. For vaporized feed, FBP and SOL, there are no changes in the ROL, since none of the equation parameters is affected, that is $R$ and $x_D$, as per Equation 7.

### Effect of increasing feed composition on q-lines and SOL for vaporized feed

Table 3. Summary on the effect of increasing feed composition on distillation process performance variables for different feed thermal conditions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SCF</th>
<th>VF</th>
<th>FBP</th>
<th>Increasing $x_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R/R_{min}$</td>
<td>Highest</td>
<td>Lowest</td>
<td>-</td>
<td>Increases</td>
</tr>
<tr>
<td>$N_l$</td>
<td>Lowest</td>
<td>Highest</td>
<td>-</td>
<td>Decreases</td>
</tr>
<tr>
<td>$N_{th}/N_{min}$</td>
<td>Lowest</td>
<td>Highest</td>
<td>-</td>
<td>Decreases</td>
</tr>
<tr>
<td>$N_{actual}$</td>
<td>Lowest</td>
<td>Highest</td>
<td>-</td>
<td>Decreases</td>
</tr>
<tr>
<td>$Q_R$</td>
<td>Highest</td>
<td>Lowest</td>
<td>-</td>
<td>Increases</td>
</tr>
<tr>
<td>$m_s$</td>
<td>Highest</td>
<td>Lowest</td>
<td>-</td>
<td>Increases</td>
</tr>
<tr>
<td>$V_B$</td>
<td>Highest</td>
<td>Lowest</td>
<td>-</td>
<td>Increases</td>
</tr>
</tbody>
</table>

Table 4. Variations in the stripping section operating line equation for increasing feed composition and changing feed thermal conditions.

<table>
<thead>
<tr>
<th>$x_F$</th>
<th>$V_B$</th>
<th>$(V_B + 1)/V_B$</th>
<th>$x_B$ / $V_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>VF</td>
<td>FBP</td>
<td>SCL</td>
</tr>
<tr>
<td>0.20</td>
<td>0.80</td>
<td>1.00</td>
<td>2.00</td>
</tr>
<tr>
<td>0.25</td>
<td>1.14</td>
<td>1.44</td>
<td>2.63</td>
</tr>
<tr>
<td>0.30</td>
<td>1.50</td>
<td>1.92</td>
<td>3.6</td>
</tr>
<tr>
<td>0.35</td>
<td>1.97</td>
<td>2.50</td>
<td>4.25</td>
</tr>
<tr>
<td>0.40</td>
<td>2.50</td>
<td>3.18</td>
<td>5.57</td>
</tr>
<tr>
<td>0.45</td>
<td>3.18</td>
<td>4.04</td>
<td>7.03</td>
</tr>
</tbody>
</table>

### Effect of increasing feed composition on q-lines and SOL for feed at its bubble point

Figure 15 shows the effect of increasing $x_F$ on q-lines and SOLs, for FBP. For a feed at its bubble point, the q-lines are vertical, passing through $x_F$ to the PoI of the operating lines. The q-lines have no $y$-intercept, and meet the two operating lines at the same value of $x = x_F$. Figure 15 shows six q-lines and six stripping section operating lines to indicate the effect of increasing $x_F$ on the distillation column performance in terms of feed plate location, number of stages in each section required to attain a distillate of composition $x_D = 0.95$. All the SOL passes at $(x_B, x_D)$ similar to VF, with all PoIs coinciding with the corresponding $x_F$ on horizontal axis. There will be a change in number of stages for each value of $x_F$, since the q-lines assume a different location and also a new feed location is obtained.

Increasing $x_F$, therefore, increases the number of stages in the stripping section and lowers the number of stages in the rectifying section. At higher $x_F$ therefore the liquid in the feed travels many stages down to reach reboiler while
the vapor in the feed travels shorter distance toward the exit to the condenser with short length for vapors, heat exchange with refluxed liquid is minimal which increases the condenser duty. With increases in the number of stages or height of the stripping section, the vapors leaving the reboiler are therefore stripped of the HKC, allowing more of the MVC to travel upward to the condenser. Higher \( x_F \) leads to large changes in both \( x \) and \( y \) hence lowering the number of stages. This implies that distillation becomes more effective.

**Effect of increasing \( x_F \) on \( q \)-lines and SOL for a SCL**

Figure 16 shows the effect the increasing \( x_F \) for subcooled liquid feed on the distillation column performance. All \( q \)-lines are parallel and meet the \( y = x \) line at the corresponding value of \( x_F \), but the PoI is
Figure 15. Loci of SOL and q lines for increasing composition of feed at its boiling point.

Figure 16. Loci of SOL and q lines for increasing composition for sub cooled liquid feed.
Table 6. Loci of Point of Intersection between SOL, ROL and \( q \)-line.

<table>
<thead>
<tr>
<th>( x_F )</th>
<th>VF</th>
<th>FBP</th>
<th>SCL</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.20</td>
<td>0.33</td>
<td>0.35</td>
<td>0.34</td>
</tr>
<tr>
<td>0.25</td>
<td>0.36</td>
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<td>0.39</td>
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<td>0.40</td>
<td>0.48</td>
<td>0.52</td>
<td>0.52</td>
</tr>
<tr>
<td>0.45</td>
<td>0.51</td>
<td>0.55</td>
<td>0.55</td>
</tr>
</tbody>
</table>

Table 7. Summary on the observed effect of feed composition and feed thermal conditions on distillation process performance.

<table>
<thead>
<tr>
<th>Key parameters for distillation process</th>
<th>Increasing ( x_F )</th>
<th>Affected by feed thermal conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass balances</td>
<td>( D ) Increases</td>
<td>Independent</td>
</tr>
<tr>
<td></td>
<td>( B ) Decreases</td>
<td>Independent</td>
</tr>
<tr>
<td></td>
<td>( V ) Increases</td>
<td>Independent</td>
</tr>
<tr>
<td>Minimum reflux, ( R_{min} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Theoretical number of stages, ( N_{theo} )</td>
<td>Decreases</td>
<td>Dependent</td>
</tr>
<tr>
<td>Actual number of stages, ( N_{actual} )</td>
<td>Decreases</td>
<td>Dependent</td>
</tr>
<tr>
<td>( N_{theo}/N_{min} )</td>
<td>Decreases</td>
<td>Dependent</td>
</tr>
<tr>
<td>Condenser duty</td>
<td>Partial condenser, ( Q_{pc} ) Increases</td>
<td>Independent</td>
</tr>
<tr>
<td></td>
<td>Total condenser, ( Q_{tc} ) Increases</td>
<td>Independent</td>
</tr>
<tr>
<td>Reboiler duty, ( Q_R )</td>
<td>Increases</td>
<td>Dependent</td>
</tr>
<tr>
<td>Steam requirements in the reboiler, ( m_s )</td>
<td>Increases</td>
<td>Dependent</td>
</tr>
<tr>
<td>Absorption factor, ( A )</td>
<td>For light key, ( A_{benzene} ) Decreases</td>
<td>Dependent</td>
</tr>
<tr>
<td></td>
<td>For heavy key, ( A_{toluene} ) Independent</td>
<td>Independent</td>
</tr>
<tr>
<td>Boil-up ratio, ( V_B )</td>
<td>Increases</td>
<td>Dependent</td>
</tr>
<tr>
<td>( q )-lines</td>
<td>Moves to the right</td>
<td>Independent</td>
</tr>
<tr>
<td>Stripping operating line, SOL</td>
<td>Moves to the right</td>
<td>Independent</td>
</tr>
<tr>
<td>Rectifying operating line, ROL</td>
<td>Moves to the right</td>
<td>Independent</td>
</tr>
<tr>
<td>Pol between SOL, ROP and ( q )-line</td>
<td>Moves to the right</td>
<td>Dependent</td>
</tr>
</tbody>
</table>

slightly at higher value of \( x \), that is, to the right of \( x_F \) or towards \( x_D \). Still increasing \( x_F \) increases the number of stages in the stripping section and reduces the number of stages in the rectifying section for SCL feed, similar to VF and FBP. Different from VP and FBP, the change in the number of stages in the rectifying section is faster for SCL, since the \( q \)-lines slope towards \( x_D \). In the same way, the condenser duty increases with \( x_F \). It should be noted that increase with \( x_F \) and do not depend on feed thermal conditions.

In general, the effect of changing feed composition affects the SOL and \( q \)-lines for vaporized feed, feed at its bubble point and also for sub-cooled feed. This was exhibited by having the same rectifying section operating line for the three feed thermal conditions. Since does not affect the ROL equation. Only the \( q \)-lines and the SOL were changing with \( x_F \).

Table 5 shows the vertical movement of the PoI between SOL, ROL and \( q \)-line as \( x_F \) was increased from 0.2 to 0.45 for different feed thermal condition. Based also on Figures 13 to 15, it can be stated that by increasing \( x_F \), the Pol between SOL and \( q \)-lines (which coincide with ROL), moves upwards along \( y \)-axis. Thus, the values presented in Table 6 are those of \( y \) at the Pol. Any combination of \( x_F \) and these values gives the coordinates of the Pol in the form of \((x, y)\). For example, at \( x_F = 0.4 \) kmol/kmol, the corresponding Pol can be presented as \((0.4, 0.48), (0.4, 0.52)\) and \((0.4, 0.52)\) for VF, FBP and SCL feed, respectively. In the whole range of \( x_F \), the points of intersection are higher for SCL feed, than for VF and FBP.

Table 7 summarizes the effect of \( x_F \) and feed thermal conditions on distillation process performance. The data shows whether increasing \( x_F \) increases or lowers or has no effect on the performance parameter and also the effect of feed thermal conditions on the distillation plant
performance parameters. Presented in Table 7 is an overall picture of the simulation results for distillation process due to changes in \( x_F \). Starting with simple mass balances across the column, increasing \( x_F \) increases distillate or product flow rate, \( D \). This implies that with a solution of higher LKC concentration, more distillate will be produced. Also, the vapor flow rate towards the condenser will be higher. According to Table 7, the required number of stages will be lower at higher \( x_F \), compared to lower feed composition. Due to fixed conditions of \( x_D \), \( x_B \) and \( R \), the \( Q_c \) and \( Q_b \) were observed to increase with \( x_F \). The slope of the SOL increased with increasing \( x_F \) with the lines slanting towards the right at higher \( x_F \), all which passes at \((x_F, x_B)\).

Table 8 summarizes the effect of increasing \( x_F \) on the number of stages in the stripping and rectifying sections and feed plate location, duties for total and partial condensers, reboiler duty, cooling water flow rate and steam mass flow rate for VF, FBP and SCL.

As shown also in Figure 7, the number of stages decreased with increasing \( x_F \). It is interesting to note that FBP and SCL have the lowest number of stages required for both stripping and rectifying sections, despite the extra energy input required to change the thermal conditions of the VF prior to introducing it into the feed plate. The feed plate is also located further down for lower \( x_F \). For SCL and FBP, on the other hand, the feed plate location is higher up compared to VF. The condenser and reboiler duties and the corresponding cooling water and steam mass flow rate, increased with increasing \( x_F \), as discussed in Figures 7, 8 and 10. It can be seen further that the cooling water requirements is excessively higher necessitating installation of cooling tower (to lower the inlet cooling water temperature) and high cooling water recirculation rate.

Figure 17 summarizes the variation of the number of stages, feed plate location and column height (for a stage height of 0.5 m) with the feed composition, for vaporized feed. Tray Spacing is normally large if froth is expected, also to allow space for crawling (normally between 0.3 and 0.6 m). The highest number of stages was observed at \( x_F = 0.2 \), and the lowest were at \( x_F = 0.40 \) and 0.45 kmol/kmol. While the number of stages were the same for \( x_F = 0.25 \) and 0.30, and also for \( x_F = 0.40 \) and 0.45, that is, 10 and 8 stages, respectively, the major difference was on the feed plate location. At \( x_F = 0.2 \) and 0.25, the feed plates were at 7 and 6th plates, respectively. Such a location determines the height for rectification and stripping sections. There was no difference in feed plate location for \( x_F = 0.40 \) and 0.45, as shown in both Table 7 and Figure 17, respectively, differences of which were observed in the condenser and reboiler duties, and between cooling water and steam flow rates.

**Conclusion**

The adopted methodology, which uses a computer model designed to solve mass and energy balance equations, allowed an intensive computations and simplified simulation of a rather complex system of binary distillation. By having equations in the computer, changes in feed conditions and other operating parameters as inputs were computed in very short time (involving 37
### Table 8. Effect of increasing feed composition on number of stages, condenser and reboiler duties.

<table>
<thead>
<tr>
<th>Feed condition</th>
<th>$x_F$</th>
<th>$N_{str}$</th>
<th>$N_{rect}$</th>
<th>$N_{feed}$</th>
<th>Number of stages</th>
<th>Condenser and reboiler duty (kW)</th>
<th>Cooling water and steam flow rates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$Q_C$</td>
<td>$Q_R$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Total condenser</td>
<td>Partial condenser</td>
</tr>
<tr>
<td>VF</td>
<td>0.20</td>
<td>6</td>
<td>8</td>
<td>9</td>
<td>8,350</td>
<td>6,680</td>
<td>6,658</td>
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<tr>
<td></td>
<td>0.25</td>
<td>4</td>
<td>6</td>
<td>7</td>
<td>11,133</td>
<td>8,906</td>
<td>8,868</td>
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<tr>
<td></td>
<td>0.30</td>
<td>5</td>
<td>5</td>
<td>6</td>
<td>13,916</td>
<td>11,133</td>
<td>10,854</td>
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<tr>
<td></td>
<td>0.35</td>
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<td>5</td>
<td>6</td>
<td>16,699</td>
<td>13,359</td>
<td>13,171</td>
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<td>5</td>
<td>19,482</td>
<td>15,586</td>
<td>15,283</td>
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<td>4</td>
<td>4</td>
<td>5</td>
<td>22,265</td>
<td>17,812</td>
<td>17,711</td>
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<tr>
<td>FBP</td>
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<td>7</td>
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<td>6,680</td>
<td>8,350</td>
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<tr>
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<td>7</td>
<td>11,133</td>
<td>8,906</td>
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<tr>
<td>SCL</td>
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<td>6</td>
<td>8,350</td>
<td>6,680</td>
<td>16,699</td>
</tr>
<tr>
<td></td>
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<td>5</td>
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<td>13,359</td>
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<tr>
<td></td>
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<td>4</td>
<td>5</td>
<td>19,482</td>
<td>15,586</td>
<td>34,114</td>
</tr>
</tbody>
</table>

Equations and a large number of variables) allowing for detailed simulation, leading to extensive data sets as presented in this paper.

A computer model was designed and implemented to enable the detailed analysis of performance of the binary distillation column for separation of benzene and toluene. The values of $R_{\min}$, $R/R_{\min}$ and number of stages strongly depend on $x_F$ and feed thermal conditions, with $R/R_{\min}$ increasing with $x_F$ for all feed thermal conditions. The number of stages decreases with $x_F$ for all feed thermal conditions, being highest for vaporized feed compared to other feed thermal conditions. The number of stages decreases with $x_F$ from 14.5 to 8.8 for VF being highest and sensitive to $x_F$ for this feed thermal condition compared to SCF and FBP.

The condenser duty increased with $x_F$ for total and partial condenser (independent of feed thermal condition). The increase in reboiler duty with $x_F$, however, depends strongly on feed thermal conditions. It was further observed that for SCF, the specific power consumption for distillate ($D/Q_R$, kmol distillate per kWh consumed in the reboiler) increased with $x_F$ while for VF and FBP, the ratio shows very slight change with $x_F$. On the other hand, the specific power consumption for bottoms ($B/Q_R$, kmol bottoms per kWh consumed in the reboiler) decreases with increasing $x_F$ for all feed thermal conditions. The cooling water flow rate and steam mass flow rate into condenser and reboiler, respectively, increased with increasing $x_F$.

The boil-up ratio increased with the feed composition, $x_F$, being highest for SCF than FBP and VF, attributable to the fact that when SCL is fed to the column, there is higher demand of vapor generation in the reboiler in order to balance the internal flows. This indicates also that
the reboiler duty is highest for SCL feed.

The locus of the $q$-lines and stripping section operating lines which fall along the rectifying section have been developed and presented graphically and in tabular form for different feed thermal conditions (VF, FBP and SCL) at increasing $x_r$ for the first time in this paper. This was accomplished also for the point $(x_b, x_d)$ where $q$-lines meet regardless of $x_r$ for vaporized feed.

Presentation of results has been carefully tailored, using specially designed graphical presentations and tabular formats to improve the readability of the paper. The study results and its methodology forms an important tool or training package for operators and other chemical and process engineering professionals, and imparts new knowledge in the understanding of the distillation process.

CONFLICT OF INTERESTS

The author has not declared any conflict of interests.

REFERENCES


