

INTEGRATED COMPUTATIONAL MODELING OF FEED COMPOSITION AND THERMAL VARIABLES IN DISTILLATION PLANTS

Elias David Mnyandu

Department of Chemical and Mining Engineering, University of Dar es Salaam, Tanzania

Abstract

Binary distillation, a fundamental process in chemical engineering, involves the separation of a liquid or vapor mixture containing two substances into its component fractions of desired purity through the application and removal of heat. While the concept of distillation has ancient roots, its refinement into a systematic method for separation emerged in the 16th century when it was recognized that the process could be enhanced through multiple stages of vapor-liquid contacting. This advancement paved the way for the widespread adoption of multiple-stage distillation as the predominant industrial technique for liquid mixture separation in the 20th century. In this paper, we delve into the historical evolution of distillation, highlighting its transition from batch distillation, primarily used for producing alcoholic beverages, to the more efficient and versatile multiple-stage distillation method. By exploring the contributions of pioneers in distillation theory and practice, such as Lone and Rather (2015), we aim to elucidate the principles underlying binary distillation and its significance in modern chemical engineering processes. Through a comprehensive review of the literature and theoretical frameworks, we discuss the key factors influencing the efficiency and effectiveness of binary distillation, including stage design, heat exchange mechanisms, and thermodynamic considerations. Furthermore, we examine contemporary advancements in distillation technology, such as the integration of computational tools and optimization algorithms, which have revolutionized process design and operation. By synthesizing historical perspectives with current research trends, this paper provides insights into the evolution, principles, and applications of binary distillation, laying the groundwork for further advancements in separation science and engineering.

Keywords: Distillation, Binary distillation, Separation processes, Multiple-stage distillation, Chemical engineering

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, 2005). Due to its use for a long time, and also due to being well studied and intensively published in literature, it is regarded as technically the most mature separation process.

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 (Bhusnure 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 (C₂'s to C₅'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 shortcut or approximate methods (Diwekar and Madhavan, 1991; Sundaram and Evans, 1993; Barolo and Guarise, 1996; Salomone et al., 1997; Narvaes-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 condensed material and the vapor flow upward is decreased. 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; Narvaes-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_B ; 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.

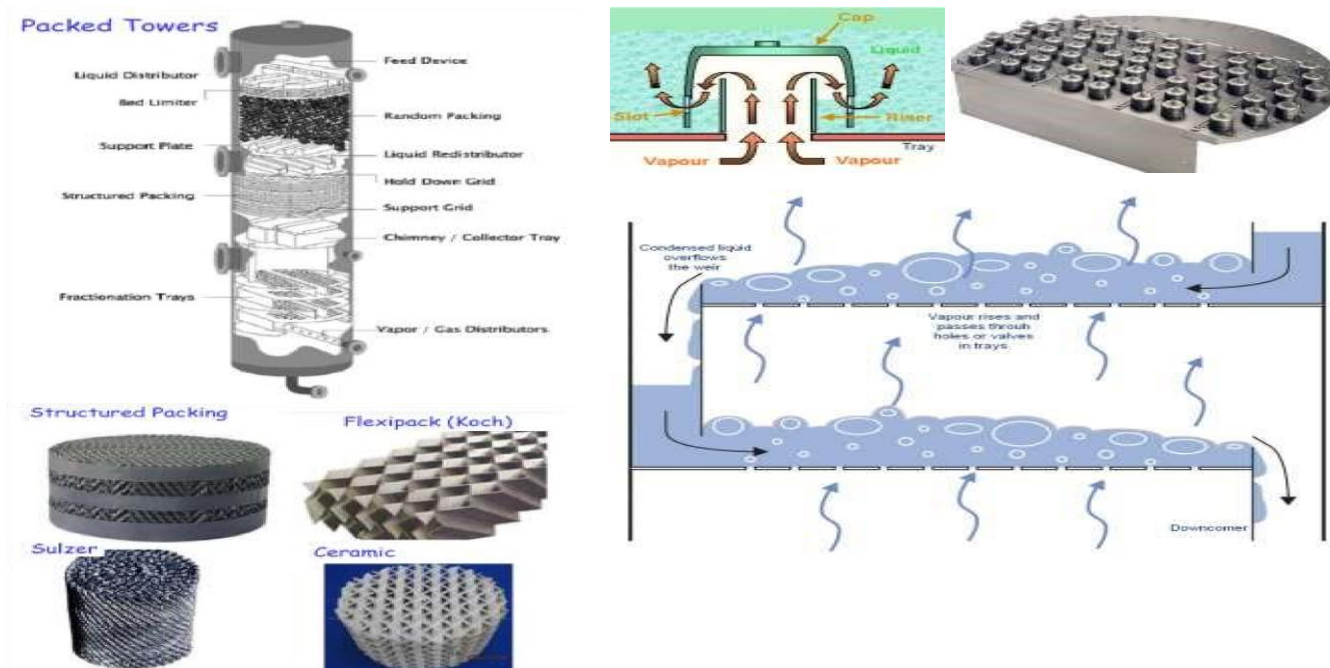
Techniques for increasing the energy efficiency of a distillation column exist (Li et al., 2008; Patil and Patil, 2016) including vapor recompression (Pribic et al., 2006), internal heat integration in distillation column (Nakaiwa et al., 2000; Jansens et al., 2001), changing feed thermal conditions and feeding mechanisms (Soave and Feliu, 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_1 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.

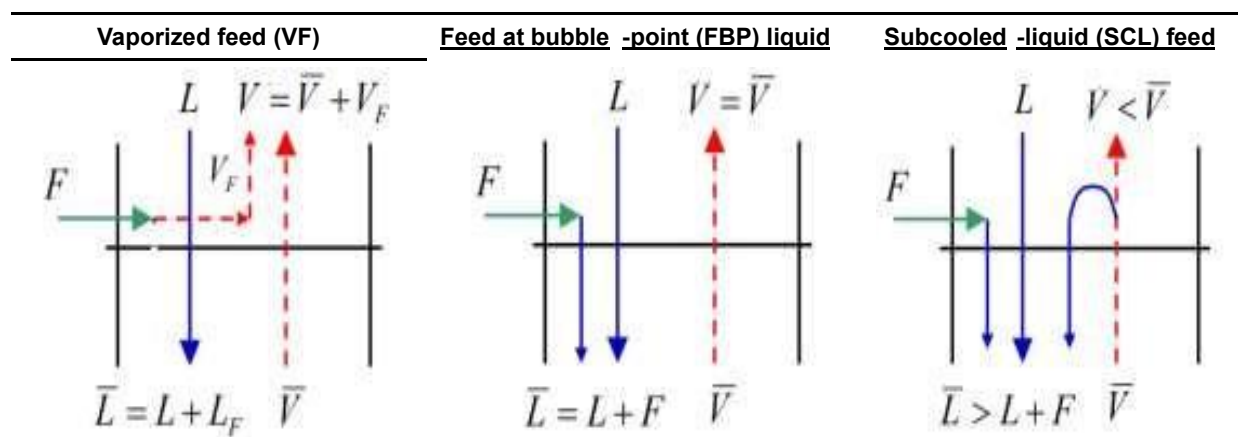
Most reboilers are partial reboilers, that is, they only vaporize part of the liquid in the column base allowing the vapors to flow upwards while the remaining liquid forms the bottoms stream. Partial reboilers also provide an ideal separation stage. Reboilers take several forms: they may be thermosiphon 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 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).



Packed tower design features Trayed tower design features and trayed distillation columns designs.
Figure 1. Comparison between packed



able 1. Feed-plate consideration for different thermal conditions of the feed.

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_D , and the bottoms containing more of the HLC 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_{cw} and m_s are cooling water and steam flow rates are denoted as m_{cw} and m_s , 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 modeling work.

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:

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} \quad (1)$$

The material and energy balance equations were developed as:

Overall mole balance:

$$F = D + B \quad (2)$$

Light key mole balance:

$$F.x_F = D.x_D + B.x_B \quad (3)$$

or, based on the distillate flow rate and composition,

$$D.x_D = F.x_F - B.x_B \quad (4)$$

Combining Equations 2 and 3 gives:

$$D = F \left(\frac{x_F - x_B}{x_D - x_B} \right) \quad (5)$$

where $x_B < x_F < x_D$.

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

$$F + L = V_I + B \quad (6)$$

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

$$F.x_F + L.x_D = V_I.x_D + B.x_B \quad (7)$$

The mole balance around the condenser gives:

Table 2. Model set-up and fixed variables for studying the effects of feed composition on the distillation column performance.

Parameter	Formula or symbol	Range or fixed values
Feed composition range	x_F	0.2 - 0.45 mol/mol
Distillate composition	x_D	0.95 mol/mol
Bottoms composition	x_B	0.05 mol/mol
Feed flow rate	F	1000 kmol/h

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:

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

	$\frac{R}{R+1}$	4.0
	$\frac{x_D}{R+1}$	0.8
Y intercept for ROL, y_i	$\frac{x_D}{R+1}$	0.19
Minimum of number of stages	N_{min}	6

The McCabe-Thiele method for analysis of distillation process uses graphical method with the following important lines: VLE curve,

Reflux ratio

Slope of the ROL

$$y = \left(\frac{L}{V}\right)x - \left(\frac{B}{V}\right)x_B \quad (17)$$

while an LKC balance gives:

$$F.x_F + L.x = V.y + B.x_B \quad (10)$$

Equation 10 leads to ROL equation as per Equation 11:

$$y = \left(\frac{L}{V}\right)x + \left(\frac{F.x_F - B.x_B}{V}\right)x_D \quad (11)$$

Combining Equations 12 and 5 simplifies to:

$$y = \left(\frac{L}{V}\right)x + \left(\frac{D}{V}\right)x_D \quad (12)$$

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

$$N_{th} = N_{mc} + 1 \quad (19)$$

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:

$$F + L = V + B \quad (9)$$

$$y \left(\frac{V_B + 1}{V_B} \right) x + \left(\frac{1}{V_B} \right) x_B \left(\frac{y_n - y_{n+1}}{y_n^* - y_{n+1}} \right) = \left(\frac{x_n - y^* x_{n-1}}{x_n^* - y^* x_{n-1}} \right) \quad (18)$$

$$E_m = (20)$$

where L and V are the liquid and vapor total molar flow rates, which

$\left(\frac{R}{R+1} \right) x + \left(\frac{1}{R+1} \right) x_D$ $V_L = L + D$ (8) 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,

$$y = \quad (13)$$

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:

$$R_{min} = \left(\frac{x_D}{y_i} - 1 \right) \quad (14)$$

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

$$L = V + B \quad (15)$$

while an LKC balance gives in this section gives:

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, $(H_v - H_L)$. The feed quality can be varied from superheated vapor condition (that is, $q < 0$) to SCL condition (that is, $q > 1$). Defining V' = 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:

$$Lx = Vy + Bx_B \quad (16)$$

Combining Equations 15 and 16 gives the SOL equation as per

Equation 17: (21)

For a given feed thermal condition, x_F and q are fixed; therefore, the q -line is a straight line with slope $-q/(1-q)$ 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:

$$q = 1 + \frac{C_{pl}(T_{bm} - T_F)}{\Delta H_{vap}} \quad (22)$$

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

$$q = \frac{(F - V_F)}{F} \quad (23)$$

where $D/F = V_F/F$ 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:

$$F.h_f + QR = D.h_D + B.h_B + QC + Q_{loss} \quad (24)$$

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

$$Q_c = D(R+1) \Delta H^{vap} \quad (25)$$

where ΔH^{vap} 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:

$$Q_c = D \Delta H^{vap} \quad (26)$$

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

$$Q = m_{cw} C_{pw} (T_{out} - T_{in}) \quad (27)$$

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

$$m_{cw} = \frac{Q_c}{C_{pw} (T_{out} - T_{in})} \quad (28)$$

where Q_c = condenser duty/rate of heat transfer, T_{out} , T_{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 1 and 2, respectively, as per Equation 29:

$$\dot{m}_{water} = \frac{V[\lambda_1 x_D + \lambda_2 (1 - x_D)]}{C_{PH2O} (T_{out} - T_{in})} \quad (29)$$

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

$Q_R = BV_B \Delta H^{vap}$ (30) When the feed is at the bubble point and a total condenser is used, using the relationship that $V_B = (L + D - V_F)/B$, that is, $BV_B = L + D = D(R+1)$, 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:

$$Q_R = Q_C \left(1 - \frac{V_F}{D(R+1)}\right) \quad (31)$$

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:

$$Q_R = m_s \lambda_s \quad (32)$$

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:

$$m_s = \frac{m_s Q_R}{\Delta H_s^{vap}} \quad (33)$$

where Q_R is the reboiler duty or rate of heat transfer, m_s = molecular weight of steam and ΔH_s^{vap} = molar enthalpy of vaporization of the steam, as per Equation 34:

$$\dot{m}_{steam} = \frac{V^f [\lambda_1 x_D + \lambda_2 (1-x_D)]}{\lambda_{water}} \quad (34)$$

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:

$$\text{Specific energy for distillate} = \frac{D}{Q_R} \left(\frac{\text{kmol}}{\text{kWh}} \right) \quad (35)$$

$$\text{Specific energy for bottoms} = \frac{B}{Q_R} \left(\frac{\text{kmol}}{\text{kWh}} \right) \quad (36)$$

$$\text{Specific steam consumption} = \frac{B}{m_s} \left(\frac{\text{kmol}}{\text{kg}} \right) \quad (37)$$

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 was 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.

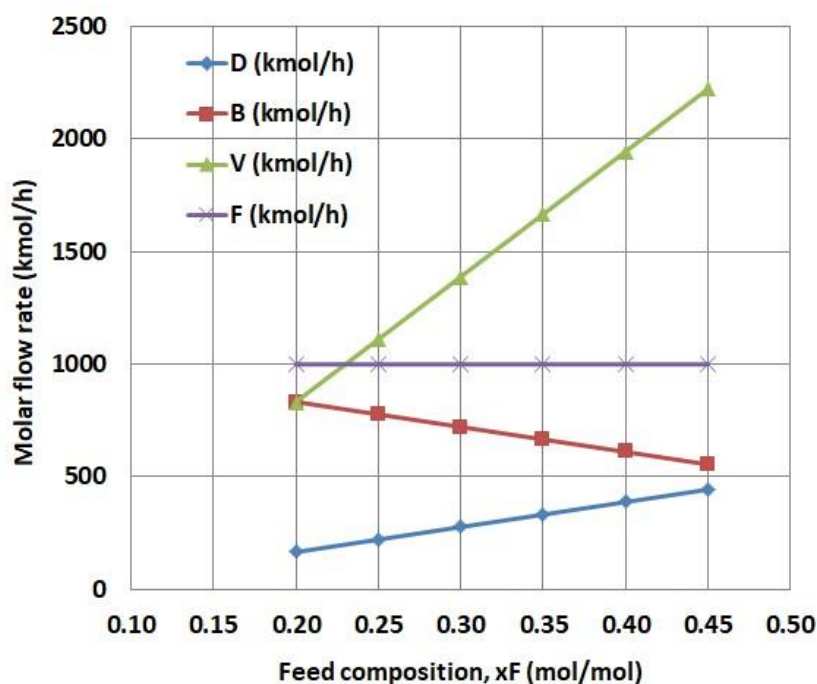


Figure 3. Variation of molar flow rates of distillate, bottoms and total vapors with feed composition at a fixed feed flow rate, based on mass balances.

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_B , and the characteristics of the equilibrium curve, that is, . 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_{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_{min} , x_F , x_B , x_D and q must be known. While the slope of the q -line depends on feed thermal conditions, the R_{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_{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_{min} values equal to 2.39, 1.97 and 1.32, respectively. Thus, at a fixed feed composition of $x_F = 0.3$, R_{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.

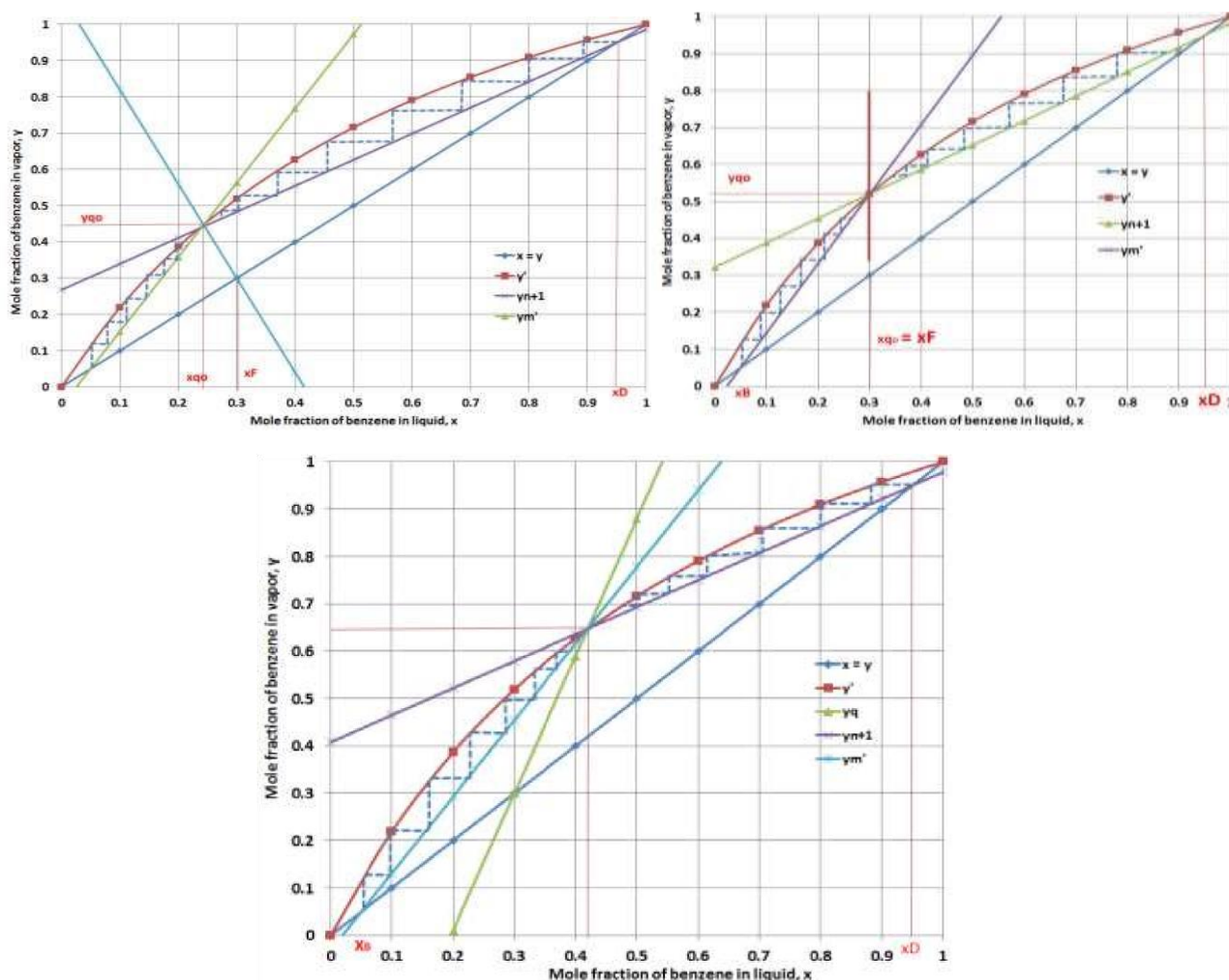


Figure 4. Number of stages and loci of PoI between SOL,ROL and q -line for three different feed thermal conditions used for determination of minimum reflux ratio.

Effect of feed composition on minimum reflux ratio, R_{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_{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_{min} . For a fixed reflux ratio, R/R_{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_{min} showing that R_{min} decreases as x_F increases towards x_D . This was observed for all feed thermal conditions. Moreover, higher values of R/R_{min} were observed for SCF followed by FBP, while VF shows lowest values of R/R_{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_{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 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_{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 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 (Kulkarni, 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.

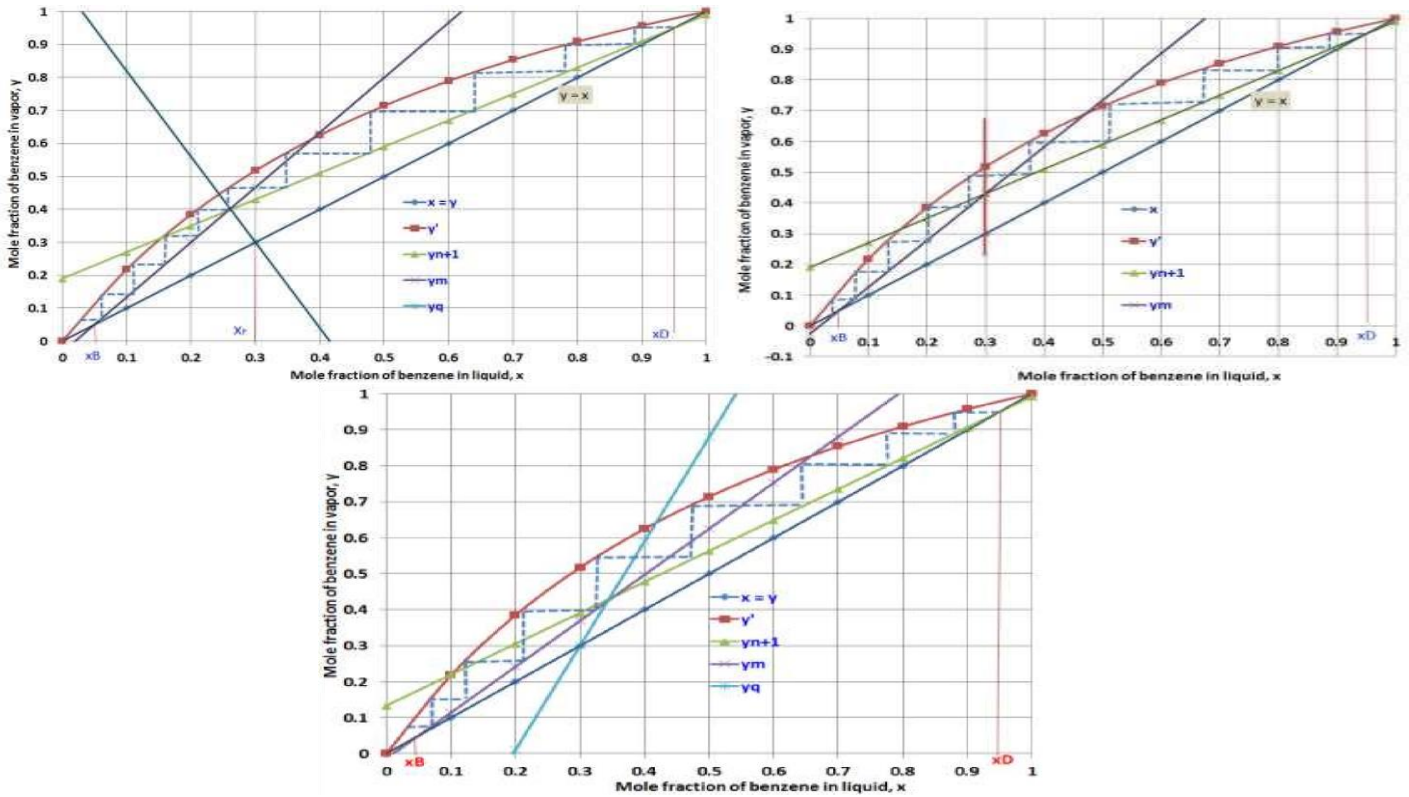


Figure 5. Variation of minimum number of stages, minimum reflux ratio and equilibrium number of stages with feed thermal conditions (VF, FBP, and SF) at a fixed feed composition $x_F = 0.3$.

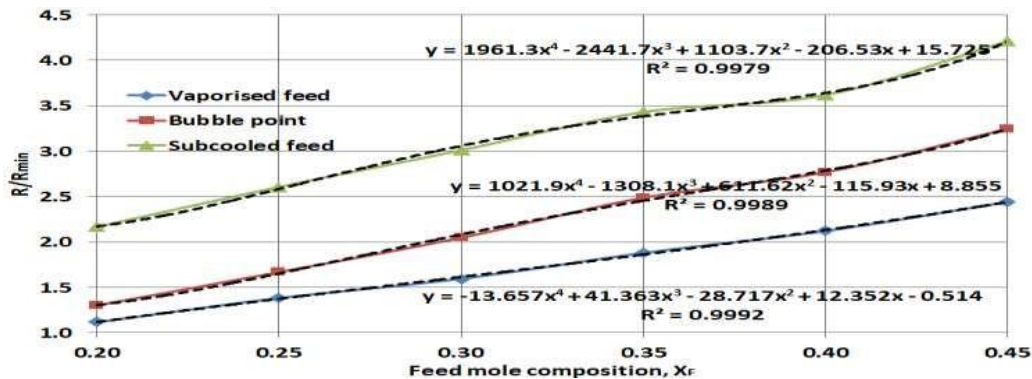


Figure 6. Effect of varying feed composition on minimum of reflux ratio for different feed thermal conditions ($R = 4.0$).

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 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:

$$m_{cw} = \begin{cases} 2379x_F - 119.85 \\ 0.0431 Q_{tc} \\ 0.0538 Q_{pc} \end{cases} \quad (38)$$

$$Q_{pc} = \frac{0.0431}{0.0538} Q_{tc} = 0.8 Q_{tc} \quad (39)$$

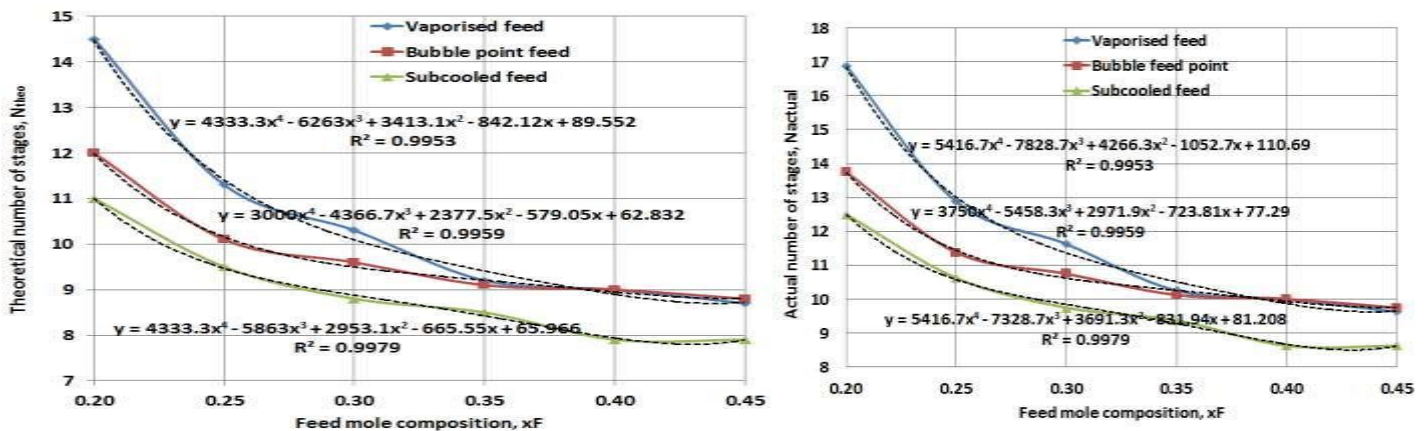


Figure 7. Effect of varying feed composition on the theoretical and actual number of stages

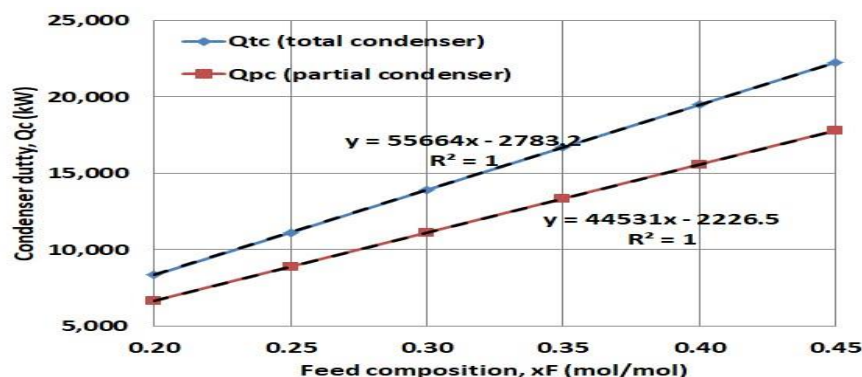


Figure 8. Effect of varying feed composition on the total and partial condenser duties.

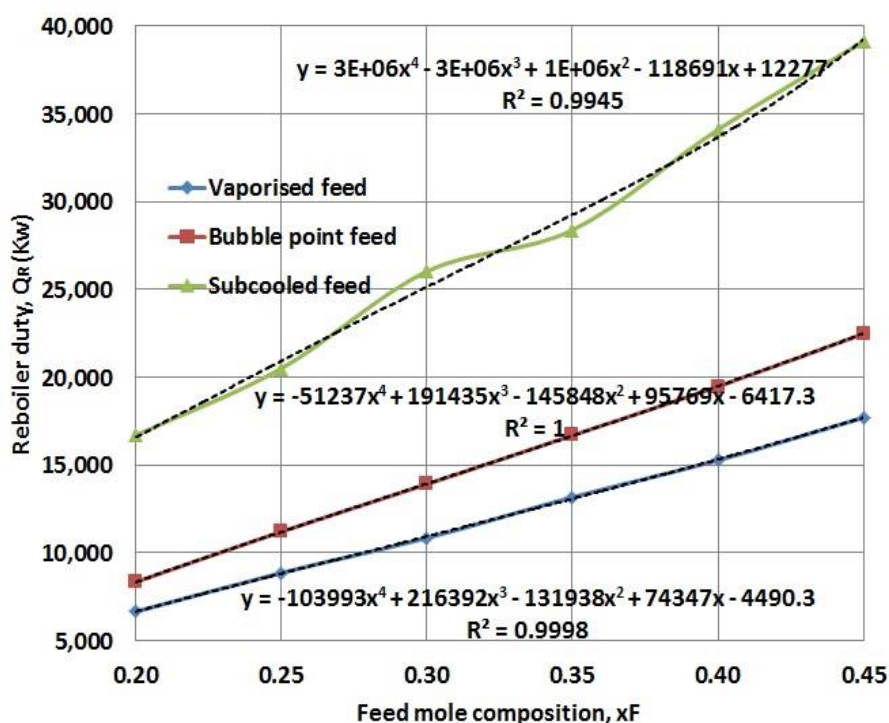


Figure 9. Effect of increasing x_F on reboiler duty for different feed thermal conditions.

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_R , 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_R . 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_R , 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_R , 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_R . 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.

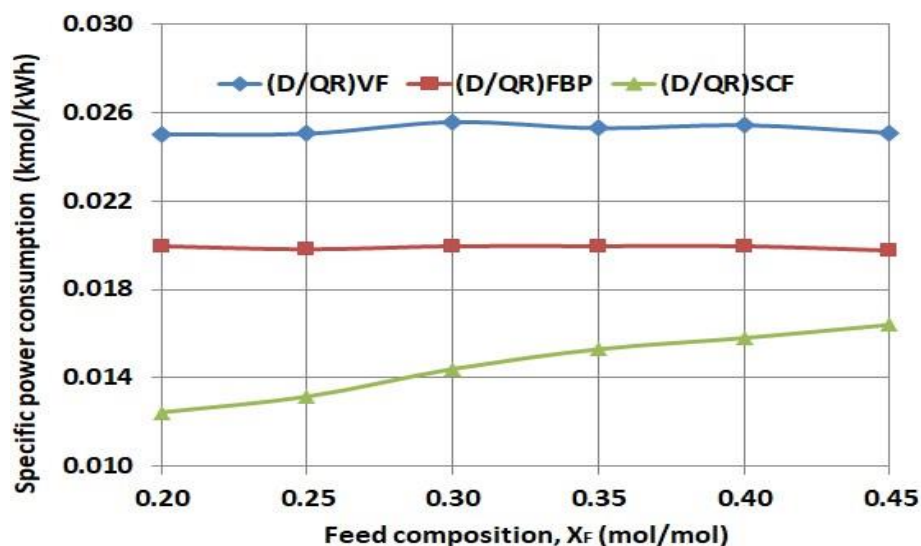


Figure 10. Specific energy consumption in the reboiler in relation to the distillate produced

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.

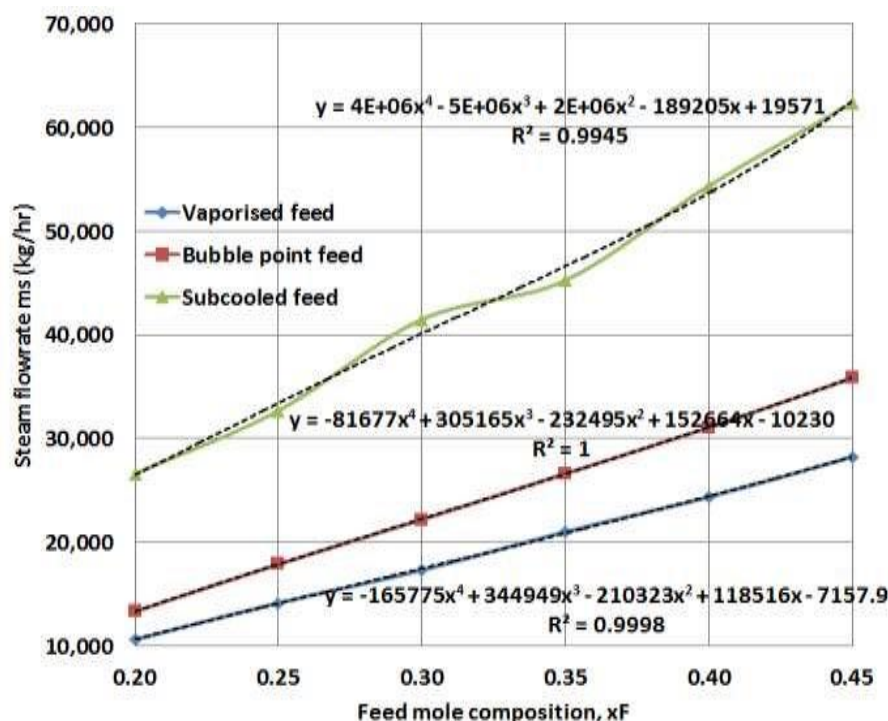


Figure 11. Effect of varying feed composition on the steam flow rate into the reboiler.

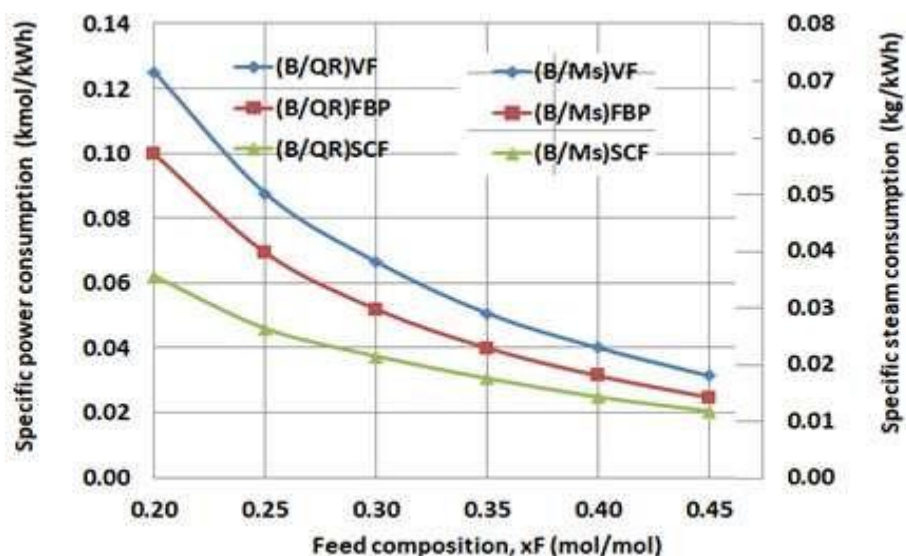


Figure 12. Variation of bottoms flow rate per kWh reboiler duty and per kg steam with x_F

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 the 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 the reboiler to maintain a constant molal 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, R/R_{min} , QR, ms 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 R/R_{min} , QR, ms 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.

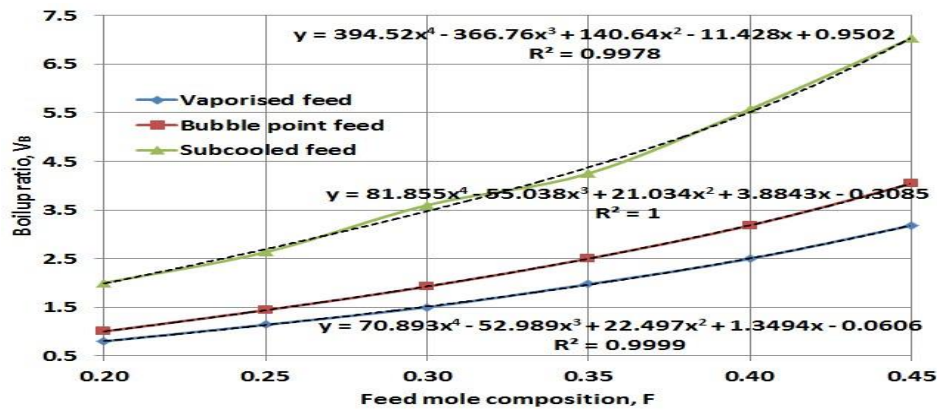


Figure 13. Effect of varying feed composition on the boil-up ratio.

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, $(V_B + 1)/V_B$ and x_B/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 $(V_B + 1)/V_B$ and x_B/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, $(V_B + 1)/V_B$ and x_B/V_B decreases with x_F .

Effect of varying x_F and feed thermal conditions on the q -line equation

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.

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

Parameter	SCF	VF	FBP	Increasing x_F
R/R_{min}	Highest	Lowest	-	Increases
N_{th}	Lowest	Highest	-	Decreases
N_{th}/N_{min}	Lowest	Highest	-	Decreases
N_{actual}	Lowest	Highest	-	Decreases
Q_R	Highest	Lowest	-	Increases
m_s	Highest	Lowest	-	Increases
V_B	Highest	Lowest	-	Increases

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

x_F	V_B			$(V_B + 1)/V_B$			x_B / V_B		
	VF	FBP	SCL	VF	FBP	SCL	VF	FBP	SCL
0.20	0.80	1.00	2.00	2.254	2.00	1.500	0.063	0.050	0.025
0.25	1.14	1.44	2.63	1.879	1.695	1.380	0.044	0.035	0.019
0.30	1.50	1.92	3.6	1.667	1.52	1.278	0.033	0.026	0.014
0.35	1.97	2.50	4.25	1.507	1.40	1.235	0.025	0.020	0.012
0.40	2.50	3.18	5.57	1.401	1.314	1.179	0.02	0.016	0.009
0.45	3.18	4.04	7.03	1.314	1.248	1.142	0.016	0.012	0.007

Effect of increasing feed composition on q-lines and SOL for vaporized 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_B) on the $y = x$ line while the q -lines meet at a point (x_B, x_D) . The two points adds 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 pas through (x_B, x_B) , 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 SCL, 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 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_B) 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.

Table 5. Variations in the q -line equation parameters due to varying feed composition and conditions.

x_F	q			$q/(q-1)$			$x_F/(q-1)$		
	VF	FBP	SCL	FBP			VF	FBP	SCL
0.45	0.833	1	1.53				-1.200	∞	0.38
	0.778	1	1.53				-1.125	∞	0.475
	0.722	1	1.53				-1.080	∞	0.57
	0.667	1	1.53				-1.050	∞	0.665
	0.611	1	1.53				-1.029	∞	0.759
	0.556	1	1.53	-1.25	∞	2.9	-1.013	∞	0.854

				VF	SCL	
0.2				-5.00	∞	2.9
0.25	-3.50	∞	2.9	0.30	-2.60	∞
2.9	0.35	-2.00	∞	2.9		
0.40				-1.57	∞	2.9

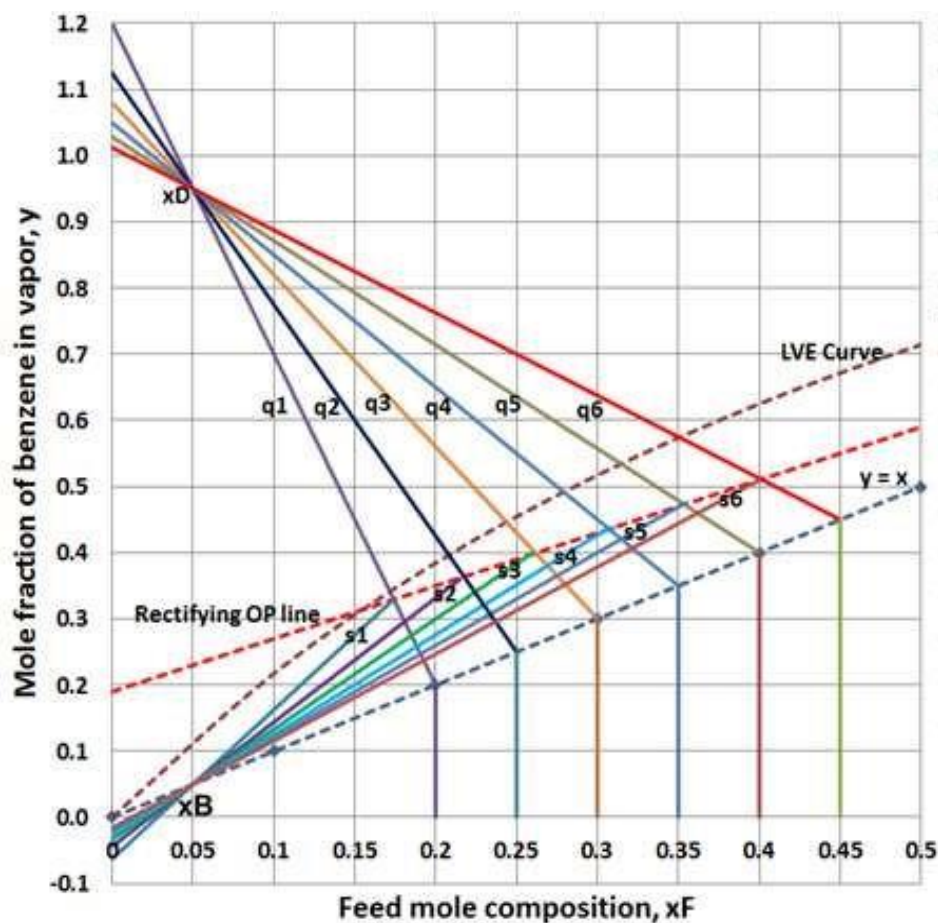


Figure 14. Loci of q -lines and SOL for increasing composition of vaporized feed.

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

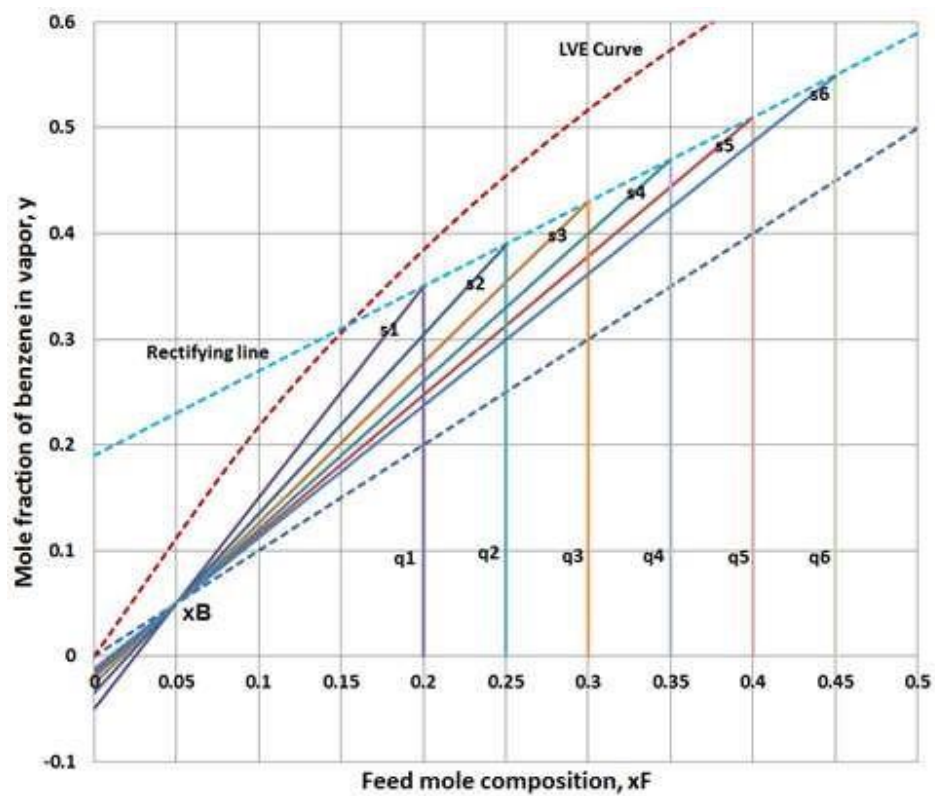


Figure 15. Loci of SOL and q lines for increasing composition of feed at its boiling point.

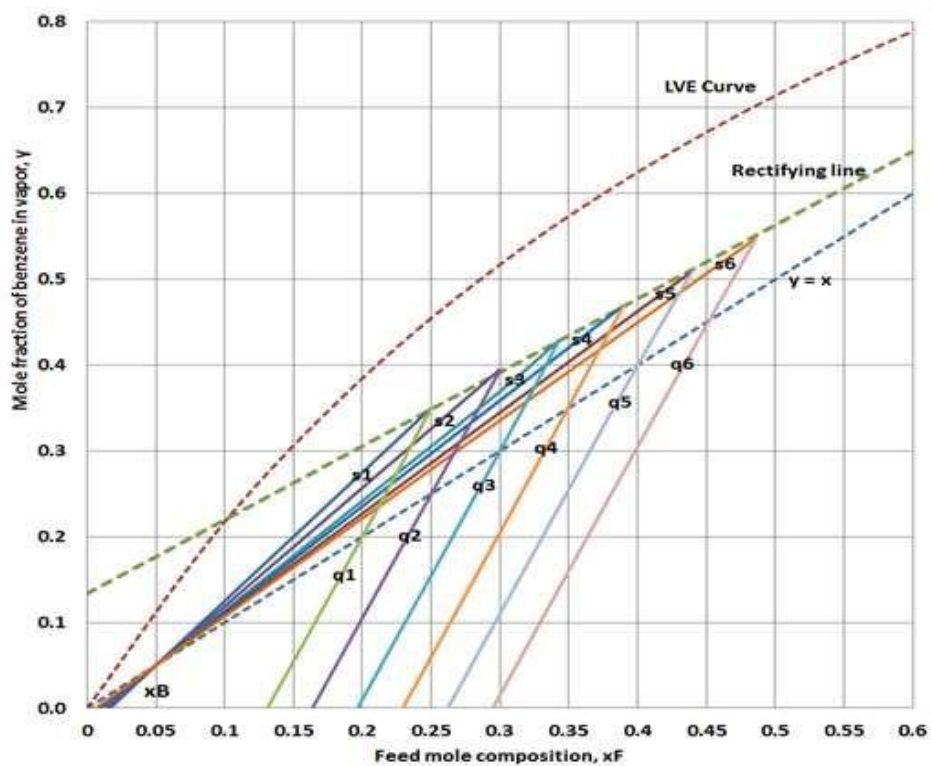


Figure 16. Loci of SOL and q lines for increasing composition for sub cooled liquid feed.

Table 6. Loci of Point of Intersection between SOL, ROL and q -line.

x_F	VF	FBP	SCL
0.20	0.33	0.35	0.34
0.25	0.36	0.38	0.39
0.30	0.40	0.44	0.43
0.35	0.44	0.47	0.46
0.40	0.48	0.52	0.52
0.45	0.51	0.55	0.55

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

Key parameters for distillation process		Increasing x_F	Affected by feed thermal conditions
Mass balances	D	Increases	Independent
	B	Decreases	Independent
	V	Increases	Independent
Minimum reflux, R_{min}		Decreases	Dependent
Theoretical number of stages, N_{theo}		Decreases	Dependent
Actual number of stages, N_{actual}		Decreases	Dependent
N_{theo}/N_{min}		Decreases	Dependent
Condenser duty	Partial condenser, Q_{pc}	Increases	Independent
	Total condenser, Q_{tc}	Increases	Independent
Reboiler duty, Q_R		Increases	Dependent

Steam requirements in the reboiler, m_s	Increases	Dependent
For light key, A		
Absorption factor, A_i <i>benzene</i>	Decreases	Dependent
For heavy key, $A_{toluene}$	Independent	Independent
Boil-up ratio, V_B	Increases	Dependent
q -lines	Moves to the right	Independent
Stripping operating line, SOL	Moves to the right	Independent
Rectifying operating lone, ROL	Moves to the right	Independent
PoI between SOL, ROP and q -line	Moves to the right	Dependent

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 s 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 PoI 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 PoI. Any combination of x_F and these values gives the coordinates of the PoI in the form of (x, y) . For example, at $x_F = 0.4$ kmol/kmol, the corresponding PoI 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

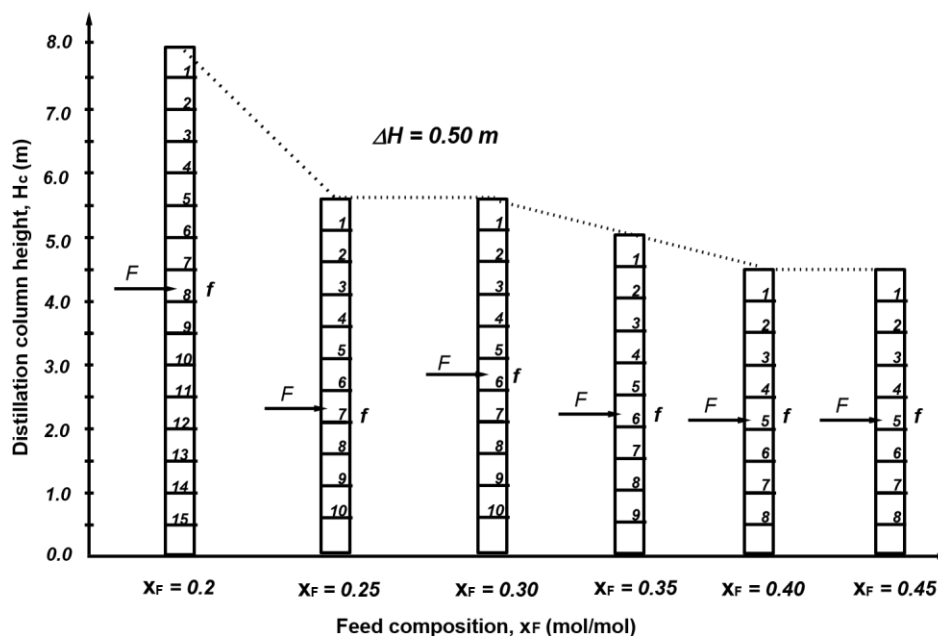


Figure 17. Graphical presentation of variation of the distillation column height, number of stages and feed plate location with feed composition or vaporized feed (VF).

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_R and Q_C 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_B, 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.

		Number of stages				f	Condenser and reboiler duty (kW)				Cooling water
and steam flow rates											
Feed condition (m ³ /h)Partial ms	xF	N_{str}	N_{rect}	N_{feed}						m_{cw}	
					Total	Q_C Partial	Partial Q_R	Total			
					kg/h) condenser	condenser	reboiler	condenser	(		
					condenser						
VF	0.20	6	8	9	8,350	6,680	6,658	360	288	10,613	
	0.25	4	6	7	11,133	8,906	8,868	479	384	14,136	
	0.30	5	5	6	13,916	11,133	10,854	599	479	17,303	
		0.40	4	4	5	19,482	15,586	15,283	839	671	
		0.45	4	4	5	22,265	17,812	17,711	959	767	
		0.20	5	6	7	8,350	6,680	8,350	360	288	
		0.25	4	6	7	11,133	8,906	11,213	479	384	
		0.30	4	5	6	13,916	11,133	13,916	599	479	
	FBP	0.35	5	4	5	16,699	13,359	16,699	719	575	
		0.40	4	4	5	19,482	15,586	19,482	839	671	
		0.45	4	4	5	22,265	17,812	22,490	959	767	
		0.20	4	5	6	8,350	6,680	16,699	360	288	
		0.25	3	5	6	11,133	8,906	20,508	479	384	
	SCL	0.30	4	4	5	13,916	11,133	26,033	599	479	
		0.35	4	4	5	16,699	13,359	28,388	719	575	

	0.40	3	4	5	19,482	15,586	34,114	839	671
0.35	4	5	6	16,699	13,359	13,171	719	575	20,996

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_F 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_F 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

- Asiedu NY, Hildebrandt D, Glasser D (2014). Batch distillation targets for minimum energy consumption. *Industrial and Engineering Chemistry Research* 53(7):2751-2757.
- Barolo M, Guarise GB (1996). Batch distillation of multicomponent systems with constant relative volatilities. *Chemical Engineering Research and Design* 74(8):863-871.
- Bernot C, Doherty MF, Malone MF (1993). Design and operating targets for non-ideal multicomponent batch distillation. *Industrial and Engineering Chemistry Research* 32(2):293-301.
- Bhusnure O, Mali S (2015). Recent Trends In Ion- Exchange ChromatoGraphy. *The International Journal of Drug Policy* 403-416.
- Diwekar UM, Madhavan KP (1991). Multicomponent batch distillation column design. *Industrial and Engineering Chemistry Research* 30(4):713-721.

- Gustinelli G, Eliasson L, Svelander C, Andlid T, Lundin L, Ahrné L, Alminger M (2018). Supercritical Fluid Extraction of Berry Seeds: Chemical Composition and Antioxidant Activity. *Journal of Food Quality* 2018, <https://doi.org/10.1155/2018/6046074>
- Jana AK, Khan NM, Maiti D (2013). Improving energy efficiency and cost-effectiveness of batch distillation for separating wide boiling constituents. II: Internal versus external heat integration. *Chemical Engineering and Processing: Process Intensification* 72:122-129.
- Jansens PJ, Fahkri F, Graauw J, Olujic Z (2001). Energy saving potential of a heat integrated distillation column. *Proceedings of the Topical Distillation Symposium, AIChE 2001 Spring Meeting, Houston* pp. 19-25.
- Jawad SK, Husien NSM (2018). Solvent Extraction Method for Separation and Determination of Zn (II) by Using of Imidazole Derivative. *International Journal of Engineering and Technology* 7(4.36):553-556. 10.14419/ijet.v7i4.36.24136.
- Khan MN, Babu GUB, Jane A (2012). Improving Energy Efficiency and Cost – Effectiveness of Batch Distillation for Separating Wide Boiling Constituents. 1.Vapor Recompression Column. *Industrial and Engineering Chemistry Research* 51(47):15413-15422.
- Kulkarni SJ (2017). Various aspects of distillation with emphasis on modeling, optimization and simulations - a review. *International Journal of Scientific Research in Chemistry (IJSRCH)* 2(1):1-4.
- Li QS, Song CY, Wu HL, Liu H, Qian YQ (2008). Performance and applications of flow-guided sieve trays for distillation of highly viscous mixtures. *Korean Journal of Chemical Engineering* 25(6):1509-1513.
- Lone SR, Rather MA (2015). Modeling and Simulation of a Distillation Column using ASPEN PLUS for separating methanol/water mixture. *International Journal of Scientific and Engineering Research* 6(3):619-627
- Luyben WL (2005). Effect of feed composition on the selection of control structures for high-purity binary distillation. *Industrial and Engineering Chemistry Research* 44:7800-7813.
- Manzo F Tzouanas V, Barbieri E (2012). Modeling, simulation, and control of heat integrated distillation columns: a case study. *American Society for Engineering Education (ASEE)* 1:1-6.
- Nakaiwa M, Huang K, Naito K, Endo A, Owa M, Akiya T, Nakane T, Takamatsu T (2000). A new configuration of ideal heat integrated distillation columns. *Computers and Chemical Engineering* 24:239245.
- Narvaes-Garcia A, Loria JCZ, Marin AR, Quiroz AVC (2014). Simple multicomponent batch distillation procedure with a variable reflux policy. *Brazilian Journal of Chemical Engineering* 31(2):531-542.

- Olujic Z, Fakhri F, de Rijke A, de Graauw J, Jansens PJ (2003). Internal heat integration—the key to an energy conserving distillation column. *Journal of Chemical Technology and Biotechnology* 78:241-248.
- Patil NP, Patil VS (2016). Operational and economic assessment of distillation column from the performance of tray, *International Conference on Global Trends in Engineering, Technology and Management (ICGTETM-2016)* 500-505.
- Popoola LT, Adeniran JA, Akinola SO (2012). Investigations into optimization models of crude oil distillation column in the context of feed stock and market value. *Advances in Chemical Engineering and Science* 2(4):474-480.
- Pribic P, Roza M, Zuber L (2006). How to improve the energy savings in distillation and hybrid distillation-pervaporation systems. *Separation Science and Technology* 41(11):2581-2602.
- Roffel B, Betlem BHL, de Blouw RM (2003). A comparison of the performance of profile position and composition estimators for quality control in binary distillation. *Computers and Chemical Engineering* 27:199-210.
- Salomone HE, Chiotti OJ, Iribarren OA (1997). Short-cut design procedure for batch distillations. *Industrial and Engineering Chemistry Research* 36:130-136.
- Sharmila M, Mangaiyarkarasi MV (2014). Modeling and Control of Binary Distillation Column. *International Journal Of Advanced Research In Electrical, Electronics and Instrumentation Engineering* 3(4):105-111.
- Soave G, Feliu JA (2002). Saving energy in distillation towers by feed splitting. *Applied Thermal Engineering* 22(8):889-896.
- Soave GS, Gamba S, Pellegrini LA, Bonomi S (2006). Feed-splitting technique in cryogenic distillation. *Industrial and Engineering Chemistry Research* 45:5761-5865.
- Sundaram S, Evans LB (1993). Shortcut procedure for simulating batch distillation operations. *Industrial and Engineering Chemistry Research* 32:511-518.
- Thurton R, Bailie RC, Whiting WB, Shaeiwitz JA (2003). *Analysis, Synthesis, and Design of Chemical Processes*. Prentice Hall.
- Wankat PC (2007). Balancing diameters of distillation column with vapor feeds. *Industrial and Engineering Chemistry Research* 46:8813-8826.
- Wankat PC (2014). Improved rectifying columns. *Industrial and Engineering Chemistry Research* 53(22):9158-9168. Wankat PC (2015). Economic Analysis for Improved Rectifying Columns. *Separation Science and Technology* 50(16):2525-2531.

Zhu G, Henson MA, Megan L (2001) Low-order dynamic modeling of Cryogenic distillation columns based on nonlinear wave phenomenon, Separation and Purification Technology 24(3):467-487.