

The effect of reflux ratio and feed thermal conditions on ethanol-water distillation process performance

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Abstract

Demand for ethanol has increased globally due to the need for energy and consumer chemicals, necessitating use of distillation to concentrate dilute sources. This paper presents the effect of reflux ratio, number of stages, feed thermal conditions (FTCs), feed composition (X_F), and feed plate location on the performance of a normal distillation column separating ethanol-water mixtures ranging between 0.1 and 0.6 mol/mol. The model was created using Aspen Plus® Software. The FTCs studied include: feed at room temperature (FRT), partially vaporized feed (PVF), feed at its boiling point (FBP), superheated vapor (SHV) and feed at dew-point (FDP). The performance factors studied were: distillate composition (X_D), reboiler and condenser duties. The axial profiles of temperature and ethanol concentration in the liquid across the column revealed stronger dependence on X_F in the stripping section and on feed plate location. Increasing reflux ratio increased distillate composition, reboiler and condenser duties. Increasing feed composition increased distillate composition and lowered reboiler and condenser duties depending on the FTCs. Locating the feed plate further down the column increased the distillate composition. The Q_R was highest for FRT while Q_C values were highest for FTC and SHV. The FBP led to minimum energy demands for both Q_R and Q_C . To minimize energy, switch all FTCs to FBP was recommended, with highest savings observed for switching from FRT to FBP.

Keywords: Ethanol-water mixtures, Feed composition, Feed thermal conditions, Reflux ratio, Condenser and reboiler duties.

DOI: <http://dx.doi.org/10.4314/ijest.v16i4.6>

Cite this article as:

Manyele S.V. 2024. The effect of reflux ratio and feed thermal conditions on ethanol-water distillation process performance. *International Journal of Engineering, Science and Technology*, Vol. 16, No. 4, pp. 66-90. doi: 10.4314/ijest.v16i4.6

Received: February 14, 2024; Accepted: June 15, 2024; Final acceptance in revised form: December 2, 2024

1. Introduction

1.1. Global necessity of ethanol

Although it is a simple alcohol, ethanol (with chemical formula C_2H_5OH) has become a globally significant substance due to its multiple applications, spanning across energy production, industrial use and medical purposes. This necessity is driving large scale production processes (including distillation) to meet a global demand. Ethanol has renewable energy and environmental benefits as a biofuel (US-DOE, 2020). When used in gasoline as ethanol-blended fuels, it helps to reduce carbon monoxide and nitrogen oxides due to presence of 35% oxygen. The adoption of ethanol as a fuel is part of global efforts to transition towards more sustainable energy sources and mitigate climate change. The production of ethanol has significant economic implications (RFA, 2020). The ethanol industry supports agriculture by providing a stable market for crops like corn, cassava and sugarcane, as the primary raw materials for ethanol production and job creation (RFA, 2020).

Ethanol has wide industrial and consumer applications. It is a key solvent in the manufacture of personal care products, pharmaceuticals and cosmetic and also an excellent solvent for resins, oils and other organic compounds (Klein and Klein, 2011). In the medical field, ethanol is widely used as an antiseptic and disinfectant. Its ability to denature proteins makes it effective in killing bacteria, viruses and fungi, thus used in sanitizers and cleaning solutions (WHO, 2020). The production of ethanol on a large scale is primarily through fermentation (Naik *et al.*, 2020) and distillation. Distillation purifies the ethanol from fermentation broth, usually in low concentration, making it suitable for various applications (Mosier *et al.*, 2005). The distillation process can accept very dilute solutions and effectively raise the purity (Manyele, 2021), and when conducted repeatedly, higher concentration closer to azeotropic can be attained.

1.2. Purification of ethanol-water mixtures by distillation

Distillation remains the sole viable process for production of concentrated ethanol solution from dilute solutions due to its unmatched efficiency in achieving high purity levels (Kiss and Ignat, 2012). Despite the effectiveness, the energy required to heat the mixture and subsequent cooling processes are substantial, necessitating research for optimization (Kiss and Ignat, 2012). For ethanol to be used in various applications, it must meet specific purity standards. In the fuel industry for instance, ethanol needs to be anhydrous (less than 1% water content) to blend effectively with gasoline. Similarly, in pharmaceuticals and cosmetics, high-purity ethanol is essential to ensure product safety and efficiency. Distillation is the only process that can consistently achieve these high-purity levels, necessitating its use despite its energy intensity (Olbrich *et al.*, 2012; Sholl and Lively, 2016). Distillation is well-suited for large scale and continuous production, which is vital for meeting the global ethanol demand. Modern distillation systems, including multi-stage distillation and continuous distillation column, allow for the efficient handling of large volumes of dilute ethanol solutions. Research in this area focuses on improving the design and operation of these systems to enhance throughput and reduce operational costs (Huang *et al.*, 2008; Sholl and Lively, 2016; Taylor *et al.*, 2018).

Distillation is a unit operation that involves mass and heat transfer to achieve separation of two or more components of a liquid mixture. The separation is based on differences in boiling temperatures between the components. Two product streams are generated, that is, the liquid bottoms product and the distillate that may be a liquid or a vapor or both. Energy transfer is used as the driving force to achieve separation, by effecting vaporization of a liquid mixture. The aim is to separate the components of a liquid into individual components, in this case, ethanol and water, so that a concentrated ethanol solution can be obtained for further uses (Mosier *et al.*, 2005; Klein and Klein, 2011; WHO, 2020). The distillation of ethanol-water mixture aims at achieving a higher concentration of ethanol in the distillate, for which several operating variables including reflux ratio must be maintained (Chen and Lin, 2001; Arrieta *et al.*, 2017; Manyele, 2021). The process is carried out in a normal distillation column, which is widely used in the industry. Although new separation techniques are being developed, such as extractive or azeotropic distillation, membrane techniques, solvent extraction, etc., distillation remains the most important separation method in the petrochemical, food, beverage and pharmaceutical industries today.

Separation of liquid mixtures by using distillation method requires formation of a second phase, that is the vapor phase. Both liquid and vapor phases are then intensively contacted across each stage within a column. Because of having different volatilities, the ethanol and water will partition differently between the two phases (Redlich and Kwong, 1949; Soave, 1972; Peng and Robinson, 1976). This leads to different concentrations in the liquid and vapor phases that are being contacted, denoted as x and y , representing mol ethanol/mol mixture in liquid and vapor phases, respectively (Luyben, 2006). The two phases behave differently under gravity, such that vapor flows upwards and liquid flows downwards inside the column. The countercurrent flow between liquid and vapor enhances mixing (Khoury, 2004).

After entering the column via a feed plate, the liquid mixture flows into a reboiler. Heat is used in the reboiler to partially vaporize the mixture. The reason for partial vaporization is to allow for separation of ethanol and water between liquid and vapor phases. The vapor is returned to the bottom of the column, coming in contact with the down-flowing liquid as it rises towards the top, and exiting towards the condenser. The basic method of operation is to take the vapors to a condenser across stages of down-flowing refluxed liquid. The vapor that leaves the reboiler is supposed to be in equilibrium with the liquid. The concentration of ethanol which is the more volatile component (MVC) in the vapor increases as the vapor rises to the top (Wankat, 2014). Because of the axial temperature gradient, the compositions of liquid and vapor are not constant and changes along the column (Luyben, 2006; Battisti *et al.*, 2019). This is expressed using axial profiles of ethanol concentration in the liquid. At the top of the column, part of the distillate is returned to the column (the reflux). This study investigates the effect of the reflux ratio on the distillation plant performance (that is, distillate composition, condenser and reboiler duties, and number of stages required to achieve a given separation).

The amount of liquid to be refluxed down the column is part of the condensed distillate, forming two streams denoted as L (reflux) and D (distillate or product to be withdrawn). The quantity of reflux is always expressed by the ratio to the distillate ($R = L/D$). This variable affects the column performance strongly, necessitating detailed studies. The quantity of the reflux, and hence the reflux ratio has a strong effect not only on the performance, but also on the design and control of the distillation plant (Skogestad, 2000). This study, however, has a stronger contribution to knowledge as it focusses on ethanol-water mixtures, which have a tendency to form azeotropic mixture complicating the normal distillation process when the distillate composition approaches azeotrope. Due to complexity in setting up distillation process, modeling and simulation is necessary to determine the optimal conditions and performance analysis.

1.3. Challenges facing ethanol-water distillation

Ethanol water distillation faces significant challenges related to energy consumption (Huang *et al.*, 2008; Kiss and Ignat, 2012; Olbrich *et al.*, 2012), azeotrope formation (Kiss and Ignat, 2012), environmental impacts (Sholl and Lively, 2016), equipment corrosion (Taylor *et al.*, 2018), the need for equipment or process integration (Kiss and Ignat, 2012) and process complexity due to a large number of variables. Azeotrope formation significantly complicates the ethanol-water distillation due to the unique behavior of the azeotrope (formed at 0.895 mol ethanol/mol), which boils at 78.1%. Conventional distillation applied in this study cannot produce pure ethanol since when this point is approached, a large number of trays is required, posing a significant challenge. To achieve high-purity ethanol, more complex, energy intensive and costly separation methods are required.

Addressing these issues via ongoing research and technological innovations is crucial for improving the efficiency, sustainability and economic viability of ethanol production (Sholl and Lively, 2016). Advancements in heat integration, alternative separation technologies and materials science are the key to overcoming these challenges. The complexity of the distillation column increases by large number variables such as reflux ratio, number of stages, feed thermal conditions (FTCs), feed composition, feed plate location, required distillate composition, condenser and reboiler duties (Manyele, 2021), necessitating use of simulation packages to support experimental work (Taylor *et al.*, 2003; Taqvi *et al.*, 2016; Kulkarni, 2017).

1.4. Importance of reflux ratio on distillation process performance

The reflux ratio is a pivotal operating variable in the distillation of ethanol-water mixtures due to its significant impact on the efficiency, purity and economic viability of the separation process. Despite the presence of other operational variables, the reflux ratio stands out because of its direct influence on the key performance metrics such as product purity, energy consumption and operational costs (Chen and Lin, 2001; Patil and Patil, 2016; Arrieta *et al.*, 2017). The reflux ratio, defined as the ratio of the liquid returned to the column to the liquid collected as distillate, directly affects the purity of the distilled ethanol. A higher reflux ratio generally results in better separation efficiency, enabling the production of higher purity ethanol. This is crucial for applications that demand high-purity ethanol, such as pharmaceutical and fuel industries. Optimizing the reflux ratio is essential for achieving the desired product specifications without excessive energy use (Skogestad, 2000). The reflux ratio significantly influences the energy required for the separation (Kiss *et al.*, 2012). Higher reflux ratios can enhance separation efficiency but at the cost of increased energy consumption due to the higher volume of liquid being vaporized and condensed. Conversely, lower reflux ratios reduce energy usage but may compromise product purity. The purity of the product depends on number of trays and reflux ratio. Since for an operating column the number of trays is fixed, the suitable operating variable that can be maneuvered for successful separation is the reflux ratio (Chen and Lin, 2001), which balances energy efficiency with separation performance. The economic implications of the reflux ratio are profound. Thus, the cost of operating a distillation column includes energy costs, which are directly impacted by the reflux ratio (Taylor *et al.*, 2018). Additionally, the reflux ratio affects the capital costs associated with the size of the distillation column and auxiliary equipment which must be addressed during design. An optimized reflux ratio can lead to significant cost savings by reducing both operational and capital expenditures. The reflux ratio is also a critical variable for the dynamic behavior and control of the distillation column. It influences the column's response to changes in feed composition, flow rates and other disturbances (Skogestad, 2000). Effective control strategies often rely on adjusting the reflux ratio to maintain stable operation and ensure consistent product quality. Given its critical role, the reflux ratio has been a focal point of the research aimed at optimizing distillation processes, which have explored various aspects, including the development of advanced control algorithms, integration with heat recovery systems and the use of hybrid separation technologies (Huang *et al.*, 2008).

1.5. The need for modeling the ethanol-water distillation

Modeling of distillation columns helps in predicting various parameters for a given separation, which is, however, complex due to a large number of variables in a real plant. Setting up a model with all its complexity is a challenging area necessitating use of commercial software like Aspen Plus (Taylor *et al.*, 2003; Taqvi *et al.*, 2016; Manyele, 2021). Modeling and simulation of a distillation process is important in the context of improving efficiency, process scale-up, and control. Where validated models exist, modeling is applied to save experimental costs for pilot plants and reagents. The role of modeling and simulation prior to design, installation and operation of distillation columns cannot be overemphasized. This is due to complex dynamics in the way the distillation process performance is affected by a large number of variables. As a result, to fully understand some of its dynamics, modeling and simulation is essential (Sharmilla and Mangaiyarkarasi, 2014; Kulkarni, 2017; Manyele, 2021). Modeling gives chemical and process engineers a deep insight of the factors affecting the design features of the unit operations whether existing or new. An initial design of a distillation tower involves specifying the separation (that is X_D and X_B) from the given feed of known composition and feed thermal conditions (FTCs). This is followed by setting the pressure and other operating condition (Khan and Kumar, 2021).

1.6. Research gap to be filled by the study

The objectives of this study were: to establish the maximum X_D that can be reached using a normal distillation column and hence prepare ethanol-water solutions of higher concentration (from dilute solutions) as feeds to the azeotropic distillation plant. The study involved maximizing X_D mainly by manipulating the reflux ratio and other operating conditions such as: feed molar concentration of ethanol and FTCs. In addition, theoretical number of stages (denoted as N) were also determined. The study aimed at assessing the effects of reflux ratio and number of stages on the distillation column operational performance (X_D , Q_C and Q_R), given X_F , X_B , N

and FTCs. The study was conducted by creating a computer simulation model using Aspen Plus software to enable informed design of the azeotropic process, which utilizes two normal distillation columns. Similarly, Taqvi *et al.* (2016) used this software to study optimization and dynamics of the distillation column. The design features of the distillation process such as reboiler and condenser types were suggested and assessed to establish cooling water and steam mass flow rates (denoted as, m_{cw} and m_s), respectively.

The novelty of this study is based on the need to fill research gaps identified in the former research reports in the literature. A number of research papers were visited as summarized in Table 1. While this study assessed the performance of the distillation column across a wide range of feed composition (from 0.1 to 0.6 mol/mol) former studies used fixed values or narrow ranges of feed composition (X_F) (Li *et al.*, 2019; Wang *et al.*, 2019; Inoue and Kaminaka, 2020; Zhang *et al.*, 2021). The values of X_F reported in the former studies were 0.05 mol/mol (Micale *et al.*, 2004), 0.1 mol/mol (Taylor and Krishna, 2000; Aguilar *et al.*, 2002; Smith, 2005; Kiss, 2013; Górak and Olujić, 2014; Turton *et al.*, 2018), 0.15 mol/mol (Doherty and Malone, 2001; Van Gerven and Stankiewicz, 2009). Table 1 shows more values of X_F fixed in the former studies including 0.2, 0.3 and 0.5 mol/mol.

Literature shows also limited range of reflux ratios used, that is, 1 to 10 as listed in Table 1, compared to the range used in this study, that is 1 to 16. Furthermore, in the former studies a single feed thermal condition was used in each study, as shown in Table 1, while five FTCs were studied in this work. Finally, it is intended to fill the gap by studying distillation processes with high duties, Q_R and Q_c , observed for ethanol-water mixtures which ranged from 0.33 to 19.0 MW and 3.0 to 22.5 MW, respectively, compared to literature values which ranged only from 0.2 to 4.0 MW for Q_R and 0.1 to 3.5 MW for Q_c .

Table 1. Operating variables used by different researchers during ethanol-water distillation studies.

Study	Aim	Variables Studied	Problems Addressed	Number of Stages	Range of Reflux Ratio	Feed Compositions	Feed Thermal Conditions	Reboiler Duty (MW)	Condenser Duty (MW)
Aguilar <i>et al.</i> (2002)	Analyze distillation column dynamics	Reflux ratio, dynamic simulation, control response	Dynamic simulation and control response	20-30	1-6	0.1	Saturated vapor	0.5-3.0	0.4-2.5
Chen and Yu (2008)	Optimize column performance	Reflux ratio, column height, distillate rate	Column efficiency and separation performance	30-40	1-7	0.3	Subcooled liquid	1.0-3.5	0.7-2.8
Doherty and Malone (2001)	Study conceptual design of distillation systems	Reflux ratio, design methodologies, process optimization	Conceptual design and optimization	15-35	2-6	0.15	Saturated liquid	0.8-2.5	0.5-1.8
Dutta <i>et al.</i> (2020)	Apply AI in process modeling	Reflux ratio, AI algorithms, process control	Nonlinear behavior and prediction accuracy	20-30	2-6	0.2	Saturated vapor	0.8-4.0	0.4-3.0
Górák and Olujić (2014)	Assess distillation equipment and processes	Reflux ratio, process efficiency, equipment design	Process efficiency and equipment design	20-30	2-7	0.1	Superheated vapor	0.5-3.0	0.4-2.0
Kiss (2013)	Investigate advanced distillation technologies	Reflux ratio, feed composition, energy efficiency	Energy efficiency and cost optimization	10-50	1-10	0.1	Saturated liquid	0.5-3.0	0.3-2.0
Luyben (2006)	Study distillation design and control (Aspen Simulation)	Reflux ratio, column pressure, temperature	Dynamic control during transient states	20-40	2-8	0.2	Subcooled liquid	1.0-5.0	0.5-3.5
Micale <i>et al.</i> (2004)	Model complex distillation processes	Reflux ratio, feed impurities, column efficiency	Non-ideal behavior in mixtures	15-35	1-6	0.05	Superheated vapor	0.2-4.0	0.1-3.0
Olujić <i>et al.</i> (2003)	Evaluate process integration	Reflux ratio, column internals, efficiency	Process intensification and efficiency	10-20	3-8	0.2	Superheated vapor	0.5-2.0	0.3-1.5
Seader and Henley (2011)	Analyze separation process principles	Reflux ratio, feed quality, column configuration	Separation efficiency	20-40	2-8	0.2	Subcooled liquid	0.8-4.0	0.5-3.5
Smith (2005)	Design and integrate chemical processes	Reflux ratio, heat integration, feed temperature	Energy integration and sustainability	10-30	3-9	0.1	Saturated liquid	0.5-2.5	0.3-1.8
Taylor and Krishna (2000)	Explore multicomponent distillation	Reflux ratio, multicomponent systems, efficiency	Multicomponent system behavior	25-35	2-8	0.1	Saturated liquid	0.5-3.5	0.3-2.5
Turton <i>et al.</i> (2018)	Provide comprehensive chemical process design	Reflux ratio, equipment sizing, economic analysis	Equipment design and economic analysis	15-45	2-8	0.1	Subcooled liquid	0.8-3.5	0.5-2.5
Van Gerven and Stankiewicz (2009)	Examine fundamentals of process intensification	Reflux ratio, process intensification parameters	Environmental impact and economic performance	25-50	1.5-10	0.15	Subcooled liquid	0.5-3.5	0.3-2.5
Wankat (2012)	Educate on chemical process equipment design	Reflux ratio, column design, operational strategies	Educational approach to column design	10-50	1-10	0.2	Saturated liquid	0.5-3.0 MW	0.3-2.5 MW

2. Literature Review

2.1. Effect of varying reflux ratio on distillation process performance

There is, however, a difference between heat addition and removal rates (Zhu *et al.*, 2001). A temperature gradient along the column is needed because a uniform temperature throughout the column will lead to vapor and liquid composition (at same temperature) to be at equilibrium everywhere in the column, reducing separation efficiency. Thus, refluxing part of the distillate is important (Zhu *et al.*, 2001). Inside the tower, the down flowing reflux liquid provides cooling and condensation of the up-flowing vapors thereby increasing the efficiency of the distillation tower (Adeleke *et al.*, 2013). The efficiency increases because the LKC escapes the liquid into vapor while the HKC remains more in the liquid flowing downwards.

For a given separation, increasing the reflux ratio will increase the gradient of the rectifying operating line and move its intercept with the y -axis downwards, moving it away from the equilibrium line closer to being parallel with the $y = x$ line. Therefore, increasing reflux ratio decreases the number of stages required to achieve the separation. On the other hand, as reflux is decreased, the operating line for the rectification section moves towards the equilibrium line. The 'pinch' between operating and equilibrium lines becomes more pronounced and more and more trays are required (Patil and Patil, 2016). Moreover, Dasan *et al.* (2014) investigated this phenomenon by presenting parametric variation of number of stages (actual and theoretical) under different feed conditions.

Therefore, there is an inverse relationship between the reflux ratio and the number of theoretical stages required to achieve a given separation. For a new design, the reflux ratio and number of theoretical stages can both be varied to achieve an optimum balance via modeling. For an existing column, the number of trays used is fixed, so that a higher distillate concentration can only be obtained by increasing the reflux ratio (Chen and Lin, 2001). Alternatively, for a fixed number of stages in a real column, adjusting the reflux ratio will control the purity of the distillate, such that the higher the reflux ratio the purer the distillate (Chen and Lin, 2001; Seader and Ernest, 2006; Eldirderi, 2015). The desired separation can be achieved with relatively low energy requirements by using a large number of trays and lower reflux ratio, thus incurring larger capital costs (Chen and Lin, 2001). Thus, to avoid extra equipment costs, modeling techniques are used to assist in setting up operation condition that aids separation at low cost, in this case, by establishing the reflux ratio.

In particular, the optimization of reflux ratio is attractive for distillation columns that operate with high reflux ratio, high differential product values between overhead and bottom, high utility costs, low relative volatility, and also feed with the LKC far below 50%. Luyben (2005) and Manyele (2021) studied the effect of feed composition on the distillation column design and performance. On the other hand, by increasing the reflux ratio, the overhead composition specification can be met using a fewer number of trays but with higher energy costs (Chen and Lin, 2001; Patil and Patil, 2016). This study, therefore, focuses on the effect of reflux ratio on energy consumption (reboiler and condenser duties).

There are a large number of variables involved when operating a distillation tower that are difficult to analyze experimentally. It is thus necessary to complement the experimental practices with the help of a computer-based modeling that help to analyze the effect of many variables on the final product, for instance, reflux ratio, FTC, feed mole fraction and distillate composition (Arrieta *et al.*, 2017; Manyele, 2021). The reflux ratio is indeed a sensitive operating variable and affects a daily profit achievable. The reflux ratio is also closely related to the relative volatility and separation factor (Chen and Lin, 2001). Researchers have determined the optimum value of the reflux ratio by evaluating the annualized capital costs (column, condenser and reboiler) and operating costs (steam and cooling water) (Chen and Lin, 2001). This study focused on parametric studies without emphasis on optimization function, using ethanol-water mixtures, as a case study. The more reflux provided for a given number of theoretical plates, the better is the column's separation of lower boiling material (ethanol) from the higher boiling material (water). The relationship between distillate molar fraction (X_D) and the reflux ratio (R), for different tray numbers (N) shows the importance to work with a high number of plates or to work with higher reflux ratio to obtain the needed distillate molar fraction (Arrieta *et al.*, 2017). Physically, increasing R means more and more liquid that is rich in the MVC is being recycled back into the column. In this case, a better separation is attained and fewer trays are needed to achieve the same degree of separation (Khoury, 2005). However, operating too close to the minimum reflux ratio can make the process highly sensitive to operational fluctuations or errors in the design calculations, e.g., estimated tray efficiencies or predicted phase equilibrium behavior. If heating and cooling are inexpensive, e.g., where recovered heat is used in the reboiler, higher reflux ratios may be suitable.

Although a higher reflux ratio is desired to produce a higher concentration of the LKC in the distillate, it must be considered that a higher reboiler duty, and in turn a higher operating cost, is required to accomplish this (Jansens *et al.*, 2001; Khan *et al.*, 2012; Eldirderi, 2014). In order to obtain these operating lines, the reflux ratio must be known (Eldirderi, 2014). Other studies related R with X_D to assess the concentration of LKC in the distillate. As the reflux ratio was increased from 2.36 to 7.3, the concentration of ethanol in the distillate increased by 15% to 20% (Eldirderi, 2014).

2.2. The effect of feed characteristics on distillation column performance

The feed to a distillation column can be liquid or vapor, or both, depending on the temperature, pressure, and composition of the feed. To quantify the thermal condition of the feed, the parameter q is defined as the fraction of the feed that is liquid. The magnitude of q is related to the FTCs of the feed. Adjusting operating conditions, such as reflux ratio, FTCs, feed concentration, etc., is also an effective way to increase the capacity of distillation columns (Wang *et al.*, 2012). Table 2 summarizes the characteristics of the feed thermal conditions studied. Increasing feed q -value the required reflux ratio is reduced as the feed is made colder (that is, as q increases) but energy input to the reboiler increases.

Table 2. Characteristics of the feed thermal conditions used in this study.

Feed thermal condition		q-value range	Enthalpy range	Phases present	Source
Feed at room temperature	FRT	$Q > 1$	$H_F < h_L$	Sub-cooled liquid (SCL)	Chen and Yu (2008), Luyben (2006), Seader and Henley (2011), Turton <i>et al.</i> (2018), Van Gerven and Stankiewicz (2009).
Partially vaporized feed	PVF	$0 < q < 1$	$h_L < H_F < H_V$	Vapor liquid mixture	-
Feed at its boiling point	FBP	$q = 1$	$H_F = H_V$	Saturated liquid at bubble point	Doherty and Malone (2001), Harvianto <i>et al.</i> (2018), Hernandez <i>et al.</i> (2011), Kiss (2013), Smith (2005), Taylor and Krishna (2000), Wankat (2012).
Superheated vapor	SHV	$q < 0$	$H_F > H_V$	Vapor	Górak and Olujić (2014), Micale <i>et al.</i> (2004), Olujić <i>et al.</i> (2003).
Feed at dew-point	FDP	$q = 0?$		Saturated vapor at dew point	Aguilar <i>et al.</i> (2002), Dutta <i>et al.</i> (2020).

In this paper, a more intensive analysis is presented, whereby, five FTCs were studied, that is, FBP, FRT, PVF, FDP and SHV, compared to Manyele (2021), who studied only three FTCs including FBP, VF and SCL. Depending on the feed composition and FTCs, there is a variation in the amounts of both LKC and HKC in the vapor and liquid flows inside the column. While distillate and bottoms composition (X_D and X_B) can be selected independently, the reflux ratio, R , and vapor flow rate in the column, V , are related to the FTCs. The condition of the feed stream F determines the relation between the flow rates in the stripping and rectifying sections. Manyele (2021) reported a study on the effect of FTCs and composition ($X_F = 0.1$ to 0.45 mol/mol) for benzene-toluene mixtures, while this study extends the analysis from 0.1 to 0.6 mol ethanol/mol. The state of the feed mixture which depends on temperature and feed composition affects the operating lines and hence the number of stages required for separation. It also affects the location of feed tray. In this study, three different feed locations were implemented to assess the effect of feed locations on distillate composition (X_D), condenser duty (Q_c) and reboiler duty (Q_R). While varying the FTCs affects the heat duty requirements, feed location and number of stages, this study incorporates the effects of these conditions at various reflux ratio settings. Dasan *et al.* (2014) reported a similar analysis, but for limited operating conditions (only 10 stages, small throughput, low reflux ratio value from 0.2 to 0.4). To overcome the problems associated with the FTCs, some columns are designed to have multiple feed points when the feed is expected to contain varying amounts of components (Tham, 2006). Also, columns are designed to receive feeds of different conditions based on temperature in relation to boiling and dew point temperatures, expressed using a parameter denoted as q .

2.3. Energy management during continuous distillation

Energy management during distillation of ethanol water mixtures is critical (Huang *et al.*, 2008; Kiss and Ignat, 2012; Olbrich *et al.*, 2012). Also, Zhu *et al.* (2001) carried out rigorous mass and energy balances for modelling of the reboiler and condenser systems. Because of high heat duties in these two units, other researchers suggest use of heat integrated columns within the plant (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).

The advantages of distillation over other separation processes are: a) high purity products (Kiss and Ignat, 2012); b) economies of scale; c) well-established technology and competitive supply of equipment (Luyben *et al.*, 2006); d) use of low temperature, low-cost energy; e) well suited for energy integration into the surrounding processes (Olbrich *et al.*, 2012). Integration involves utilization of heat from the condenser and supply of reboiler heat from other parts of the plant (Pulido *et al.*, 2011a, 2011b; Olujić *et al.*, 2003). Moreover, the bottoms leaving the column at high temperature can be used to heat other process streams, such as the incoming feed. It is generally-accepted that if it is possible to achieve a separation by distillation, then distillation will be the most economical method to use. For that reason, distillation processes are largely used in petroleum refining and alcohol industries. Distillation columns consume a huge amount of energy in terms of reboiler heating (steam mass flow rate) and condenser duty (cooling water mass flow rate). Therefore, the concept of heat-integrated distillation column (HIDiC) is normally incorporated in the distillation process studies using simulation techniques in order to overcome operational drawbacks (Nakaiwa *et al.*, 2000; 2003; Olujić *et al.*, 2003; Pulido *et al.*, 2011a, b; Manzo *et al.*, 2012).

Thus, the top cold reflux is supplied to bring down the temperature at the column top, leading to column temperature profile (Zhu *et al.*, 2001; Huang *et al.*, 2008; Kiss and Ignat, 2012; Olbrich *et al.*, 2012). Therefore, to maintain temperature profile in the column,

heat is taken away by cold top reflux as well as by the cooling water in the condenser and also heat is provided by feed preheaters and bottom reboilers (Luyben *et al.*, 2006; Battisti *et al.*, 2019). Reflux is required in a distillation column to maintain the quality of distillate product by controlling the temperature at the top of the column (Kiss and Ignat, 2012). This allows for a feed of given composition to be separated into a desired top and bottom product meeting a specific requirement.

The reflux ratio is a key variable in the performance of a distillation column. This is the ratio of the liquid flow in the rectifying section to the distillate flow rate. The gradient of the rectifying section operating line is a function of the reflux ratio, that is, $R/(R+1)$ (Chen and Lin, 2001; Seader and Ernest, 2006; Eldirderi, 2015). Reflux ratio will control the product purity and determine the energy input required in the reboiler and energy withdrawal from the condenser and can affect the separation efficiency (Dasan *et al.* (2014). Reflux do not only maintain the temperature and pressure profile in the column, but also provides high mass transfer through diffusion of MVC in the reflux liquid to vapor and condensing LVC in the vapor into the liquid due to concentration gradient (Zhu *et al.*, 2001). Reflux produces vapors rich in MVC due to mass transfer and also due to lowering of temperature which allows more of the MVC to enter vapor phase and condenses the LVC. The refluxed liquid controls the speed of boil and boilup ratio, as it drains into the reboiler. Thus, the reflux ratio can affect the purity of the product and can be improved by slowing the boil up rate. The composition profile along the column is also determined by the reflux rate and the distillate withdrawal rate (Luyben 2006; Ballisti *et al.*, 2019). Hence, the sharpness of the separation is determined by the reflux ratio. Since, the reflux rate is limited by hydraulics considerations, higher reflux ratios would require lowering the distillate withdrawal rate, thus lengthening the distillation cycle (Khoury, 2005). Most columns are, however, designed to operate between 1.0 to 1.5 times the minimum reflux ratio because this is approximately the region of minimum operating costs (more reflux means higher reboiler and condenser duty) (Seader and Ernest, 2006; Kaama *et al.*, 2008).

2.4. Energy efficiency analysis based on selection of the FTCs

A total condenser is used to produce liquid reflux and distillate product. The selection between total and partial condenser is a crucial decision, as the nature of the products generated differs significantly (Luyben, 2006). Several studies on condenser performance in distillation and other applications exist in literature, which can provide design and operational details to accommodate ethanol-water distillation requirements (Anozie and Odejobi, 2011; Zhao *et al.*, 2013; Kara, 2014; Attia, 2015; Naik and Muthukumar, 2017). Energy is required to pump the cooling water at a higher rate to condense the vapors containing higher concentrated of ethanol. The heat rejection rate from the vapors, denoted as Q_c , is expressed in MW. Cooling the vapors from a distillation column in a condenser is a critical step for improved process performance and energy efficiency. Research has been conducted intensively to establish optimum cooling water flow rate (Anozie and Odejobi, 2011), influence of cooling water inlet temperature on thermal efficiency (Attia, 2015), modeling of shell-and-tube condensers (Kara, 2015; Zhao *et al.*, 2013) and testing the empirical correlation models (Naik and Muthukumar, 2017).

The reboiler, on the other hand, is a “partial reboiler” (vapor is boiled off a liquid pool). This is necessary to allow for the withdrawal of the liquid bottoms from the reboiler. The composition of this liquid pool is the same as the bottom product composition, based on the principle of completely stirred tank reactor (CSTR) (Taylor and Krishna, 2000; Doherty and Malone, 2001; Seader and Henley, 2011). The mostly used reboiler types for distillation are kettle reboilers due to several advantages, including easy of separation of the vapors and high heat transfer rate. Studies to improve heat transfer coefficient in the kettle reboilers has been conducted by investigating the effect of steam temperature (Kumar *et al.*, 2013; Chan *et al.*, 2016; Shao *et al.*, 2018; Ghanbarpour *et al.*, 2021). Application of organic solvents (Zhang *et al.*, 2008) and heat transfer oils (Gupta, 2019) have been tested for heat transfer rate improvements.

Distillation column can be fed with different feed thermal conditions, that is, FBP, FDP, FRT, SHV feed or PVF, all of which have an impact on the energy requirements for reboiler and condenser. Another feed condition is the concentration of the LKC in the feed which determines the location of the q-point and number of stages for rectifying and stripping sections (Wankat, 2014; 2015). The diameter of the column must be designed in such a way that it balances the vapor flow rate (Wankat, 2007). The feed composition on the other hand, not only affects the selection of control structures for distillation process, but also the final distillate composition, condenser and reboiler duties (Manyele, 2021).

3. Methodology

3.1. Process description

The layout of a distillation column is shown in Figure 1 (modified from Manyele, 2021). The process flow diagram includes the energy input from FRT in order to attain FBP, SHV or PVF and heat removal to attain FDP. After preparing the selected feed conditions, the feed enters the column with properties described by flow rate (F), composition (X_F), molar enthalpy (H_F), and feed temperature (T_F). A section of the feed plate is also shown on the right-hand side, to indicate the details of liquid and vapor flow at the feed plate (Manyele, 2021). 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 or MVC, X_D , and the bottoms containing more of the HKC is removed from the bottom at a molar flow rate B , and composition of the LKC or MVC, X_B . Heat for evaporation of the liquid is supplied to the reboiler (in this case, steam) and heat is again removed (through cooling water) at the top in the condenser. The nomenclature used in this paper is 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, m_{cw} and m_s are cooling water and steam flow respectively, in kg/h. Figure 1 shows also the energy input to the feed stream to attain feed thermal conditions (FTCs) used in this study. In order to maintain constant separation in the distillation column, it should be well instrumented and controlled. The treatment of instrumentation and control techniques are, however, not covered in this paper.

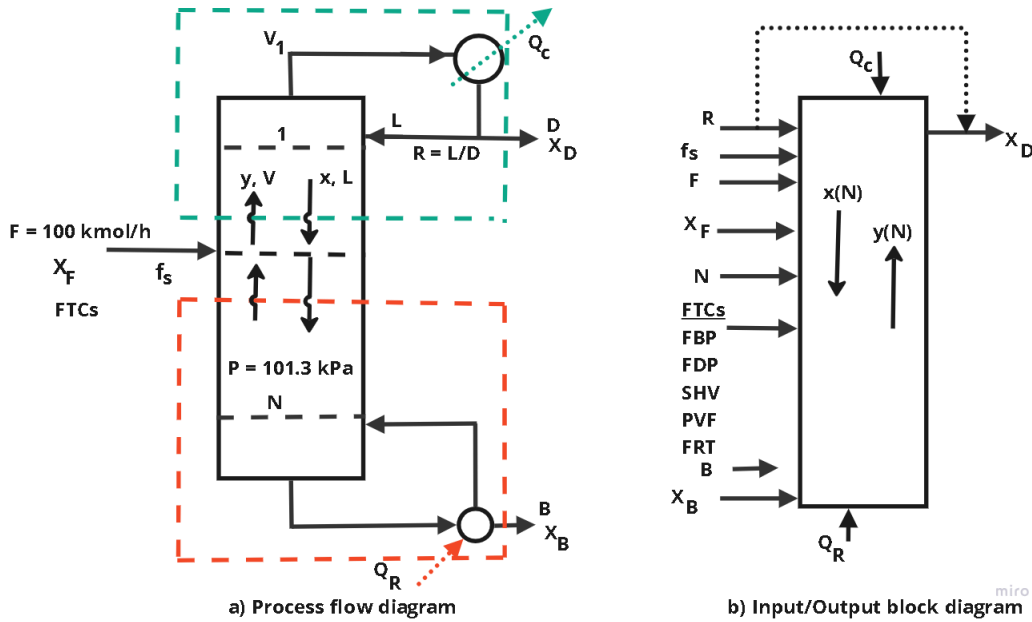


Figure 1. Process flow diagram for the distillation process used in this modeling work

A feed mixture of two components (in this case ethanol and water), was separated into two streams, that is, overhead distillate with composition X_D , and bottoms at a concentration 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 or liquid distillate at a bubble-point temperature (total condenser). Heat is transferred into the process in the “reboiler” (typically a shell-and-tube heat exchanger) to vaporize some of the liquid from the base of the column. The heat-transfer rate is Q_R energy units/time (that is, MW). The vapor coming from the top of the column is liquefied in another shell-and-tube heat exchanger called a condenser. Heat is transferred out of the condenser at a rate Q_C , measured in MW.

Liquid from the condenser drops into the reflux drum. Distillate product is removed from this drum. In addition, the reflux is fed back to the top tray of the column. This liquid reflux and the vapor boilup in the base of the column are necessary to achieve the separation or “fractionation” of chemical components, in this case ethanol and water. The energy required to make the separation is approximately the heat added to the reboiler.

At the bottom of the column, a partial re-boiler is used to produce vapor boil up with boil-up ratio $V_B = V/B$ where V is the vapor flow rate from the reboiler to the column bottom and B is the liquid bottoms product withdrawn from the reboiler. This liquid exits at the reboiler temperature, heat content of which is worth recovering by preheating the feed. The partial reboilers function as additional theoretically stage since the vaporization follows the equilibrium relationship between, expressed by the relationship between the concentration of ethanol in vapor and liquid (y and x relationship).

The phase condition (thermal condition) of the feed is determined at the feed tray pressure by an adiabatic flash calculation across the feed valve. The feed contains a MVC and LKC and, and enters the column at a feed stage. At the feed-stage pressure, five feed thermal conditions studied were: feed at room temperature (FRT), also called sub-cooled liquid depending on temperature, partially vaporized feed (PVF), feed at its boiling point (FBP), feed as superheated vapor (SHV) and feed at dew-point (FDP).

3.2. Distillation process mathematical model formulation

In order to obtain the operating lines, the reflux ratio, or amount of top product returned to the column, must be known. Manyele (2021) presented the mathematical relationships for modeling a binary distillation system, covering equilibrium and mass balance relationships, feed thermal conditions identifier (the q -values), condenser and reboiler duties based on energy balances and steam and cooling water mass flow rates for benzene-toluene mixture. The overall molar composition of the feed with respect to the light component (ethanol), denoted by X_F , was varied between 0.1 and 0.6 mol/mol, in order to establish how close the distillate can approach the azeotropic molar concentration of ethanol, for the product to be used as the feed to the azeotropic distillation plant.

3.3. Effect of FTCs and the q -line equation

The condition of the feed stream(FTC),and the feed flow rate, F , determines the relation between the flow rates in the stripping and enriching sections. Let q be the ratio of the moles of saturated liquid in the feed to the total amount of the feed, then

$$F = qF + (1 - q)F \quad (1)$$

The molar liquid overflow in the bottom section, \bar{L} , is given by:

$$\bar{L} = L + qF \quad (2)$$

where L is the constant molar flow rate of the liquid across the column. Equation (2) leads to:

$$\bar{L} - L = qF \quad (3)$$

The left-hand side of Equation (3) shows the additional liquid downflow due to feed conditions. The vapor flow rate above the feed plate, on the other hand, is given by:

$$V = \bar{V} + (1 - q)F \quad (4)$$

which leads to:

$$\bar{V} - V = (q - 1)F \quad (5)$$

Where V is the average vapor molar flow rate across the column and \bar{V} is the total vapor flow due to additional vapor in the entering feed and the steady state flow rate. Similarly, the LHS of Equation (5) shows the additional vapor flow rate due to FTC.

The magnitude of q is related to the thermal condition of the feed, as stated earlier. The relationships between flows above and below the feed plate can be used to study the effect of FTCs. Making enthalpy and material balance around the feed plate leads to Equation (6):

$$H_F F + H_V \bar{V} + H_L L = H_L \bar{L} + H_V V \quad (6)$$

where:

H_V = specific enthalpy of the feed at the dew point (saturated vapor)

H_F = specific enthalpy of the feed at its entrance conditions

h_L = specific enthalpy of feed at the bubble point (saturated liquid).

Taking the total mole balance around the feed plate gives Equation (7):

$$F + \bar{V} + L = \bar{L} + V \quad (7)$$

Assuming $H_V = H_V$ and $h_L = h_L$, then Equation (6) becomes:

$$H_F F + H_V (\bar{V} - V) = H_L (\bar{L} - L) \quad (8)$$

Substituting $\bar{V} - V = (q - 1)F$ and $\bar{L} - L = qF$ in Equation (8), gives:

$$H_F F + H_V (q - 1)F = h_L qF \quad (9)$$

Solving for q , gives:

$$q = \frac{H_V - H_F}{H_F - H_L} \quad (10)$$

where:

$H_V - H_F$ = heat needed to vaporize 1 mole of feed at its entrance conditions

$H_V - h_L$ = molar latent heat of vaporization of feed.

The feed-line or q-line equation, which is the focus of the intersection of the enriching/rectification and stripping operating-line equations, can be defined based on the solute mola balance around the top section excluding the feed plate, which leads to Equation (11):

$$y_{n+1}V = X_oL + X_D D \quad (11)$$

where y_{n+1} is the composition of the vapor entering an n^{th} plate and X_o is the composition of the liquid entering the feed plate, and X_D is the distillate composition. Also, taking a solute balance around the bottom section (also excluding the feed plate) yields Equation (12):

$$y_{m+1}\bar{V} = x_m\bar{L} - X_B B \quad (12)$$

where y_{m+1} is the composition of the vapor entering the feed plate and x_m is the composition of the liquid leaving the feed plate, and X_B is the bottoms composition. At the intersection of the two operating lines, where the feed plate is located, $y = y_{n+1} = y_{m+1}$ and $x = x_n = x_m$, and therefore:

$$yV = xL + X_D D \quad (13)$$

and

$$y\bar{V} = x\bar{L} - X_B B \quad (14)$$

Subtracting Equation (13) from (14) leads to Equation (15):

$$y(\bar{V} - V) = x(\bar{L} - L) - (X_B B + X_D D) \quad (15)$$

After substituting $\bar{V} - V = (q - 1)F$, $\bar{L} - L = qF$, and $(X_B B + X_D D) = X_F F$ into Equation (14) and rearranging leads to Equation (16):

$$y = \frac{q}{q-1} x \frac{X_F}{q-1} \quad (16)$$

Equation (16) is referred to as the q -line or feed plate equation, which varies according to FTCs.

3.4. Modeling of the effect of reflux ratio on distillate composition

Starting with Equation (13), the relationship between molar composition of ethanol in the gas and liquid phases across the column can be established by substituting $R = L/D$, which simplifies to:

$$y = \left(\frac{1}{R+1} \right) x + \frac{X_D}{(q+1)} \quad (17)$$

Equation (17) is commonly referred to as operating line equation. The focus of this study is to establish how the distillate composition X_D is affected by the reflux ratio, R , both in Equation (17), which can be transformed into:

$$X_D = y(R+1) - x \quad (18)$$

Since, however, both y and x are functions of the stage number or axial level across the column, represented by stage number N , Equation (18) can be changed to:

$$X_D = y(N)(R+1) - x(N) \quad (19)$$

It is evident that all input variables shown in the block diagram, Figure 1, affect the X_D via changes in the $y(N)$ and $x(N)$ across the column, until the very top value of $y(N = 1)$ is established (noting that plates are numbered from the top), leading to the composition of the condensed vapors, that is $y_1 = y_N = X_D$ for a total condenser. During simulation, therefore, the computer software (i.e., Aspen Plus) simulates the resulting flow dynamics and phase compositions in the distillation column to finally establish the distillate composition. In practice, Aspen Plus uses rigorous thermodynamic models and iterative calculations to estimate distillate composition when all other variables are fixed. The operating conditions used to set up the simulation model are summarized in Table 3.

Table 3. Operating conditions for the distillation column

Parameter	Value or range
Feed flow rate, kmol/h	1,000
Lighter component	Ethanol, C ₂ H ₅ OH
Heavier component	Water, H ₂ O
System pressure, kPa	101.325
Mole fraction of the lighter component in the bottoms	variable
Mole fraction of the lighter component in the distillate product	variable
Mole fraction of the lighter component in the feed, X_F , mol/mol	0.1 – 0.6
Condenser cooling water temperature (in), T_{in} , °C	28
Condenser cooling water temperature (out), T_{out} , °C	75
Number of stages, N	8 - 20
Reflux ratio	1 - 16
Distillate composition X_D (mol/mol)	0.72 - 0.88
Condenser duty (MW)	3 – 22.5
Reboiler duty (MW)	0.33 - 19.0

Table 4 summarizes the models used by Aspen Plus in establishing the distillate composition, given all input variables. Some variables are actually established internally using mass and energy balances and used to estimate X_D , such as Q_C and Q_R .

Table 4. Models used by Aspen Plus for estimation of distillate composition

Model	Description
Thermodynamic models	Aspen Plus utilizes various thermodynamic models (e.g., NRTL, UNIQUAC, etc.) to predict the equilibrium behavior of the mixture. These models incorporate activity coefficient and vapor-liquid equilibrium (VLE) data to simulate the behavior of the components in the distillation column.
Mass and energy balances	Aspen Plus solves mass and energy balance equations for each stage of the distillation column. These equations consider factors such as vapor and liquid flow rates, heat exchange, phase equilibrium and tray efficiencies.
Tray-to-tray calculations	Aspen performs tray-to-tray calculations to predict the composition profiles ($x(N)$ and $y(N)$) across the stages of the distillation column. These profiles are influenced by factors such as reflux ratio, feed composition, tray efficiencies and operating conditions.
Convergency iterations	Aspen iteratively adjusts the tray compositions until convergency criteria are met. This iterative process ensures consistency between the predicted compositions and the specified operating conditions.
Distillate composition estimation	Once the tray compositions have been converged, Aspen Plus calculates the overall distillate composition based on the predicted composition profiles and the operating conditions of the distillation column. The distillate composition is typically estimated as a weighted average of the compositions from the top stages of the column.
Error analysis	Aspen Plus performs error analysis to assess the accuracy of the calculated distillate composition compared to specified criteria or experimental data. Adjustments are then made to the model parameters or operating conditions to improve the accuracy of the predictions.

4. Results and Discussion

4.1. The effect of number of stages on distillate composition

Increasing the number of stages leads to higher distillate composition, that is, increase in X_D for all set values of reflux ratio and feed composition. The key problem being addressed here is how close can X_{AZ} be approached by (as a final distillate composition) increasing the number of stages at constant feed composition and reflux ratio. The effect of increasing N on X_D was stronger for $N \leq 15$, where X_D increased faster with N .

The maximum X_D reached was 0.86 mol/mol at $N = 20$ and $X_F = 0.6$ mol/mol, which is, practically expensive to reach given the height of the column required. Even at $N = 20$, at the highest reflux ratio, $R = 7$, X_D did not closely approach the azeotropic ethanol concentration. With $N = 10$ stages, the X_D reached around 82% ethanol. The effect of X_F was more pronounced for lower number of stages. At lower feed concentration, the effect of reflux ratio was minimal, as shown in Figure 2. Thus, for FRT, and 10 stages in the column, any feed concentration in the studied range will lead to $X_D \geq 0.82$ mol/mol.

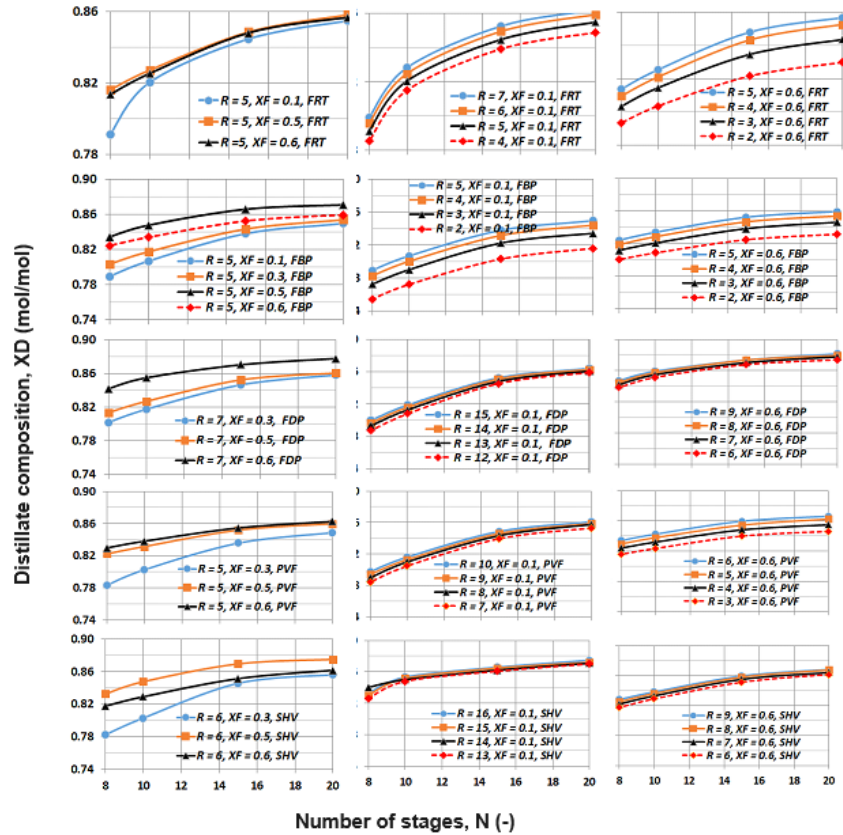


Figure 2. Effect of increasing on Variation of distillate composition with number of stages at constant reflux ratio and feed composition for different FTCs.

Figure 2 shows the variation of distillate molar composition, X_D , with the number of stages at constant reflux ratio and feed concentration, for FBP. Compared to FRT, the FBP takes place at lower reflux ratio (2 to 5). In only one set of operating parameters ($R = 5, X_F = 0.6$) the X_D exceeded 0.86 mol/mol only when $N > 14$ stages. Despite the energy input to raise the temperature of the feed to the boiling point, X_D was still lower than the values attained using FRT. The effect of reflux ratio for lower and higher X_F was similar for both higher and lower X_F (that is 0.1 and 0.6 mol/mol), as shown in Figure 2. Increasing X_F only increased X_D slightly at lower number of stages, $N = 8$, from 0.78 at $X_F = 0.1$ mol/mol to 0.82 mol/mol at $X_F = 0.6$ mol/mol.

Figure 2 shows the effect of increasing the number of stages on X_D at constant reflux ratio and feed composition for feed at dew point (FDP). In this case, separation was achieved at higher reflux ratio compared to FBP and FRT. At lower $X_F = 0.1$ mol/mol, higher reflux ratios ($R = 12$ to 15) were required to achieve the required separation. Higher distillate quality was obtained for lower reflux ratio ($R = 6$ to 9) ranging from $X_D = 0.83$ to 0.88 mol/mol. For a column with lower number of stages (8 to 10), the feed with ethanol concentration of 0.6 mol/mol leads to $X_D = 0.84$ to 0.86 mol/mol), which falls in the higher range compared to FBP and FRT, although high reflux ratio is required ($R = 6$ to 9), which may hinder distillate withdrawal rate.

Figure 2 shows also the effect of increasing the number of stages on X_D at constant reflux ratio and feed composition for SHV feed. At lower feed concentration ($X_F = 0.1$ mol/mol), separation was achieved at higher reflux ratios $R = 12$ to 16, variation of which, however, did not influence X_D . The effect of X_F was observed at $R = 6$, which is lower for SHV, while $X_F = 0.6$).

4.2 Effect of feed composition on distillate composition

In an effort to increase the X_D towards X_{AZ} at constant N and for different FTCs, the feed composition was increased from 0.1 to 0.6 mol/mol at constant number of stages, as shown in Figure 3. Increasing the concentration of ethanol in the feed improves the distillate composition or purity for a given number of stages. Highest values of X_D were observed at $X_F = 0.5$ and 0.6 mol/mol. The distillate molar concentration also increased with number of stages, being highest at $N = 20$. The effect of X_F was stronger at lower number of stages at which, X_D increases faster (for $N = 8$ and 10) than for larger number of staged (for $N = 15$ and 20). In Figure 3, there was no data for FDP and SHV because $R = 5$ do not converge, the minimum reflux ratio for these two conditions being $R = 6$.

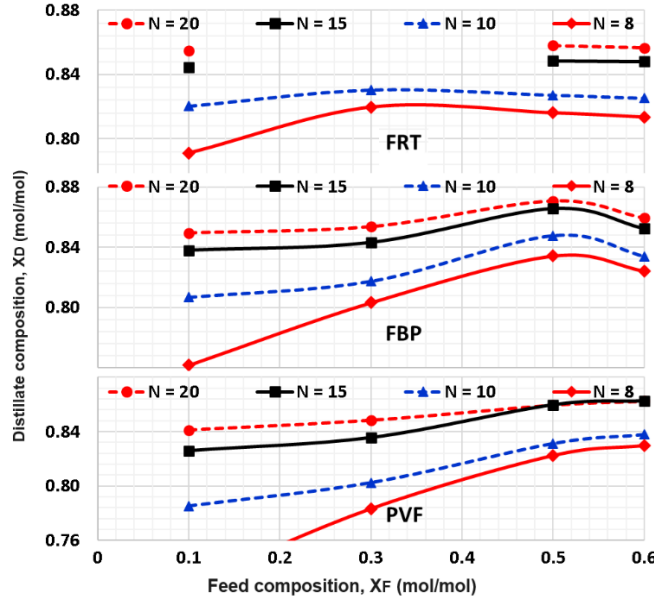


Figure 3. Variation of distillate composition with feed composition at fixed number of stages ($N = 8 - 20$) and constant reflux ratio ($R = 5$) for selected FTCs (FRT, FBP and PVF).

The profiles of X_D were different for each feed thermal condition. Due to lack of convergence of the simulation setup, no data was obtained at $X_F = 0.1$ for PVF, although the profiles were still clear. For the feed at its boiling point, the X_D values were not the highest at highest $X_F = 0.6$ mol/mol as expected, and instead the highest values were those at $X_F = 0.5$ mol/mol. The smaller difference in X_D between $N = 15$ and 20 to that observed for $N = 8$ and 10 , indicates that higher equipment costs at larger number of stages is not justifiable and can be avoided by utilizing a column with lower number of stages.

Figure 4 shows the effect of increasing the feed composition from 0.1 to 0.6 mol/mol on distillate molar composition at constant reflux ratio for different feed thermal conditions and $N = 10$ stages. The highest X_D values were observed at $X_F = 0.5$ mol/mol for FBP, FRT and SHV and at $X_F = 0.6$ mol/mol for FDP and PVF thermal conditions of the feed. The operating range for reflux ratio was different depending on the feed thermal conditions, being lower for FRT, FBP and PVF and higher for FDP and SHV (that is, $R = 2$ to 6 and $R = 5$ to 9 , respectively). Based on the need for convergence of the simulation, data for X_D was obtained from 0.1 to 0.6 mol/mol for FRT and FBP and from 0.3 to 0.6 only for FDP, SHV and PVF. In general, the results show that changing feed thermal conditions leads to complex dynamics in the distillation column affecting the separation performance and changes in the necessary operating conditions such as reflux ratio.

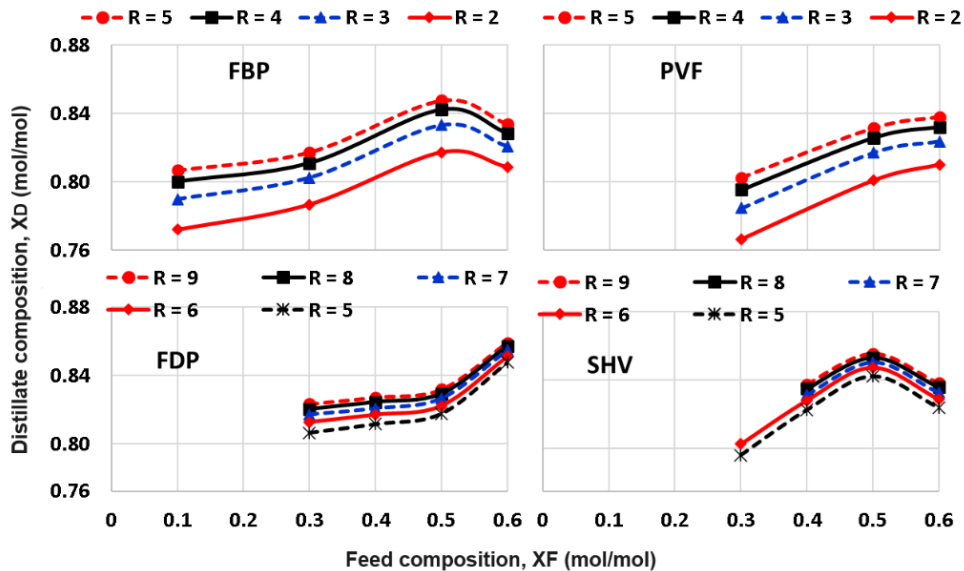


Figure 4. Variation of distillate composition with feed composition at constant reflux ratio for different feed thermal conditions (for $N = 10$ stages).

4.3 Effect of reflux ratio on distillate molar composition

Figure 5 shows the variation of distillate composition with reflux ratio for FRT and FBP of different compositions. The distillate composition increases with reflux ratio for all set values of X_F and number of stages. At constant $N = 20$, the effect of X_F on X_D was small, but the range of R leading to the observed X_D values shifted from left to right. The range of reflux ratio required to attain the required separation depends strongly on X_F than on number of stages as observed for FRT and FBP, in Figure 5. For $X_F = 0.1$ mol/mol, regardless of number of stages, the operating range of R was 3 to 7. For larger number of stages, say $N = 20$, increasing feed concentration shifts the range of reflux ratio towards the right. Higher feed concentration, on the other hand requires wider but lower range of reflux ratio, from $R = 1$ to 5, leading to higher X_D .

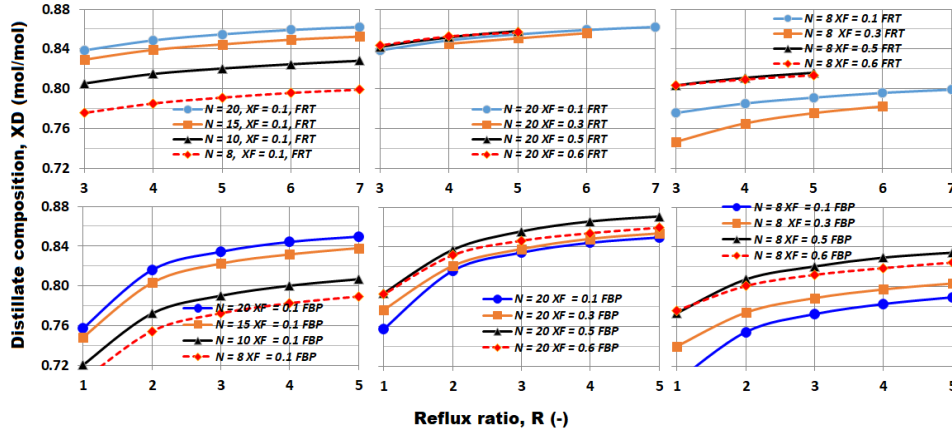


Figure 5. Variation of distillate molar composition with reflux ratio at constant values of number of stages and feed composition for FRT and FBP.

Figure 6 shows the effect of increasing reflux ratio on distillate molar composition, X_D , at constant values of number of stages and feed composition for feed at boiling point (FBP). The results show that increasing R increases X_D for any number of stages and feed concentration. Different from other feed thermal conditions, the range of R which led to achieving the required separation for FBP was 1 to 5 only. The effect of N was stronger at lower $X_F = 0.1$ mol/mol, when N was varied from 8 to 20. For larger number of stages, the effect of X_F on X_D was small, even when X_F was varied from 0.1 to 0.6 mol/mol.

The profiles of X_D as the reflux ratio were increased from 1 to 5 were similar in shape for all operating conditions studied using FBP. Results show that further increase in R would not have caused an increase in X_D for this feed thermal condition. Higher distillate purities were observed at higher reflux ratio, $R = 5$, for the range of X_F studied using FBP. Therefore, for FBP, $R = 5$, $N = 8$ to 10 are sufficient to concentrate the feeds of different strengths (0.1 to 0.6 mol/mol) to $X_D = 0.86$ mol/mol.

The results for X_D were located into two different ranges of R , that is higher range ($R = 11$ to 15 for $X_F = 0.1$ mol/mol) and lower range ($R = 5$ to 9 for $X_F = 0.3, 0.5$ and 0.6 mol/mol) for all number of stages. Moreover, at the lowest feed concentration, $X_F = 0.1$ mol/mol, the effect of the number of stages on X_D was stronger, changing from $X_D \approx 0.78$ to 0.80 to $X_D \approx 0.85$ to 0.87 mol/mol, observed at highest reflux ratios ($R = 11$ to 15). Figure 6 shows the effect of increasing reflux ratio on distillate molar composition, X_D , at constant number of stages and feed composition for FDP, SHV and PVF. For SHV, three distinct ranges of reflux ratio were observed, that is 3 to 6 (for $X_F = 0.3$ mol/mol), 5 to 9 (for $X_F = 0.5$ and 0.6 mol/mol) and 12 to 16 for $X_F = 0.1$ mol/mol. The values of X_D lower than 0.8 were observed for $X_F = 0.3$ mol/mol for $R = 3$ to 5 and $N = 8$ to 10. At $X_F = 0.1$ mol/mol, with number of stages increasing for 8 to 10, X_D values ranged from 0.82 to 0.88 when R was ranged between 12 and 16. The range of R between 4 and 9, was found to suit the separation of feed solution at $X_F = 0.5$ and 0.6 mol/mol for any given number of stages with higher distillate composition.

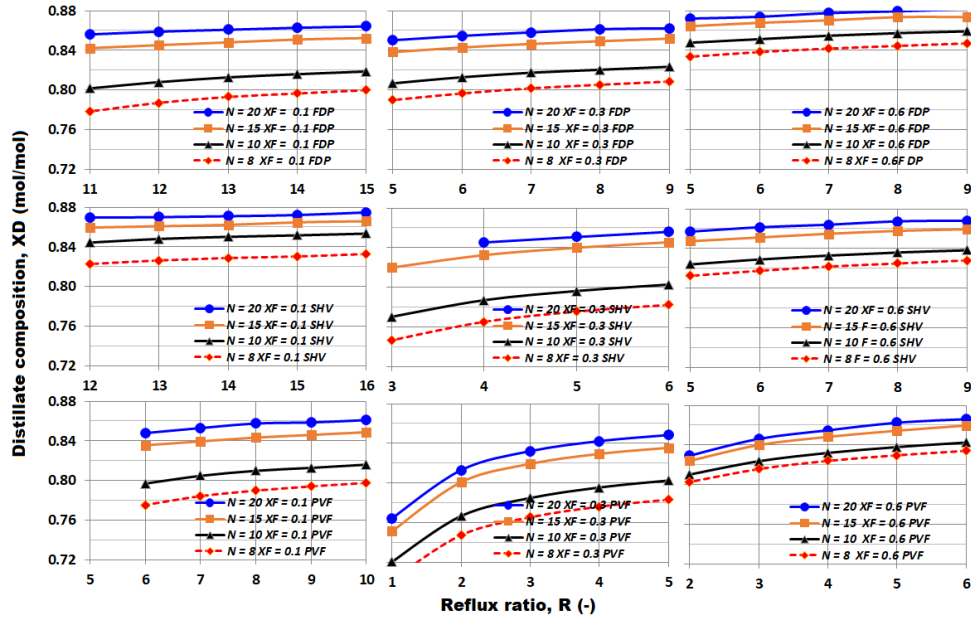


Figure 6. Variation of distillate composition with reflux ratio at constant number of stages ($N = 8 - 10$) and feed composition for FDP, SHV and PVF.

In Figure 6, the effect of increasing reflux ratio on distillate molar composition, X_D , at constant values of reflux ratio and feed composition for partially vaporized feed (PVF) is also presented. As stated for other feed thermal conditions, X_D increases with reflux ratio for all feed concentration and number of stages. The suitable reflux ratio range was from 1 to 10. Similarly, for PVF, there were three distinct ranges of reflux ratio required to achieve the desired separation. Different from SHV, the demarcation between R ranges for $X_F = 0.1$ and for 0.5 or 0.6 mol/mol was at $R = 6$, that is $2 \leq R \leq 6$ for $X_F = 0.5$ and 0.6 mol/mol and $6 \leq R \leq 10$ for $X_F = 0.1$ mol/mol. The lowest values of X_D were observed for $X_F = 0.3$ for R between 1 and 2, regardless of the number of stages. Higher X_D values were also observed at $X_F = 0.1$ when the highest reflux ratio was applied, that is, $6 \leq R \leq 10$. However, highest X_D values were observed for R ranging between 4 and 5 for $X_F = 0.6$ mol/mol. Increasing product purities (raising X_D , and/or decreasing X_B) the number of trays required in the column is increased. Conversely, highest X_D values were recorded when the number of stages was highest, that is, $N = 20$, as shown in Figure 6.

Figure 7 shows the effect of changing feed plate location on the distillate composition at different feed concentrations and FTCs for $R = 5$ and $N = 10$ stages. Feeding the solution in the lower section of the column, that is, towards the bottom increases the distillate composition for all FTCs and feed compositions. Highest values of X_D were observed when the feed was introduced in the 7th stage. The increase in X_D due to increasing f_s , was highest for $X_F = 0.1$ mol/mol compared to $X_F = 0.3$ and 0.5 mol/mol. Moreover, the variation of X_D due to changes in X_F was smallest at $f_s = 7$ than at $f_s = 4$, where X_D varied widely. With dilute feed solution, $X_F = 0.1$ mol/mol, higher distillate compositions were observed for FRT and FBP and lowest for PVF, FDP and SHV. This indicates that for higher X_D , FRT should be used (without thermal processing of the feed) with feed plate located closer to the bottom. Feeding FRT in the lower stages ($f_s = 7$) allows the vapors to be further rectified by condensing the LVC in the vapor stream back to liquid leaving the MVC at higher concentration in the vapors. Using $f_s = 7$ extends the rectifying section further downwards, leading to purer distillate stream.

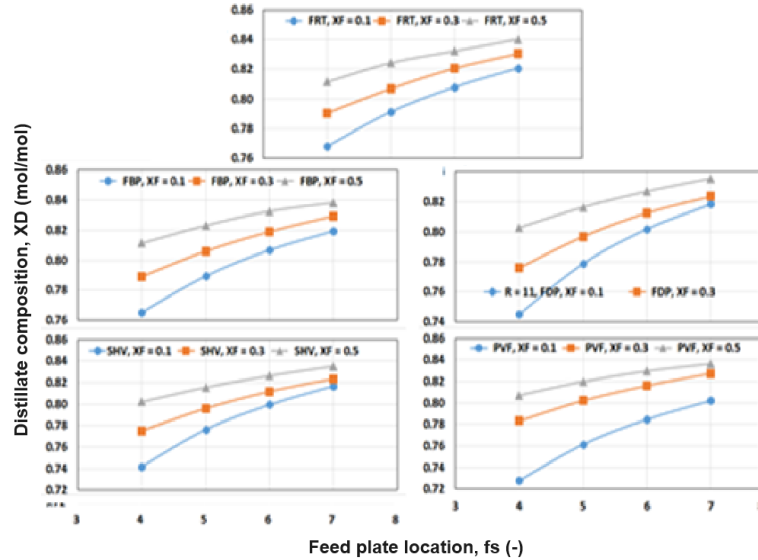


Figure 7. Effect of feed plate location on the distillate composition at different feed composition and FTCs for $R = 5$ and $N = 10$ stages

4.4. The effect of reflux ratio and feed composition on reboiler duty

In general, the reboiler duty increases with reflux ratio for all X_F and all feed compositions and thermal conditions, as shown in Figure 8. Lower energy requirements were observed for SHV and FDP followed by FBP and PVF. The highest energy consumption in the reboiler was for FRT. For FRT, on the other hand, lower $X_F = 0.1$ mol/mol required higher range of reflux ratio to attain separation from 3 to 7, while $X_F = 0.3$ to 0.6 the range was from 1 to 5 only. Separation at lower X_F took place at lower reboiler duties than at higher X_F . The effect of X_F was observed to shift the range of R from low (between 1 and 6, for PVF, FBP and FRT) at high X_F to higher reflux ratio range of 12 to 16 and 11 to 11 at lower $X_F = 0.1$ mol/mol (for PVF and FDP), respectively. Separation took place at lower reflux ratio for FRT and FBP, that is, between $R = 1$ and 7 only. Thus, distillation of feed solutions at $X_F = 0.1$ require high values of R although the reboiler duty was lower, but leads to low X_D .

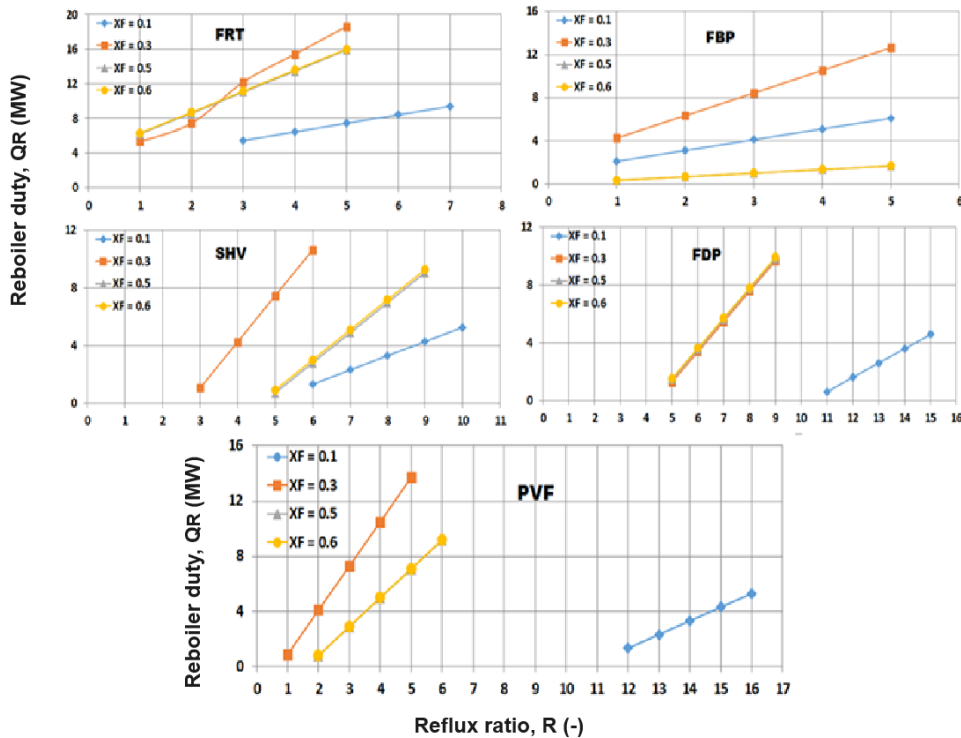


Figure 8. Variation of the mean reboiler duty (averaged across $N = 8-15$ stages) with reflux ratio for constant values of feed composition and for different FTCs.

Figure 9 presents the effect of reflux ratio on distillate composition at different fixed feed composition and for three different FTCs. Results show that distillate composition increases with reflux ratio for all distillation column operating conditions, that is, higher distillate composition results from applying higher reflux ratio. The highest distillate composition above 0.84 mol/mol was observed at $X_F = 0.5$ mol/mol for feed at boiling point. The effect of feed composition was not appreciable for FRT, where all curves were closer together. Higher distillate composition was possible at lower reflux ratio, $R = 1$, only for FRT, even for dilute feed solution. A feed composition, $X_F = 0.3$ mol/mol led to lower distillate composition for PVF, even at higher reflux ratios. The feed thermal conditions and feed composition show strong effect on X_D which need to be selected properly during operation of the distillation column.

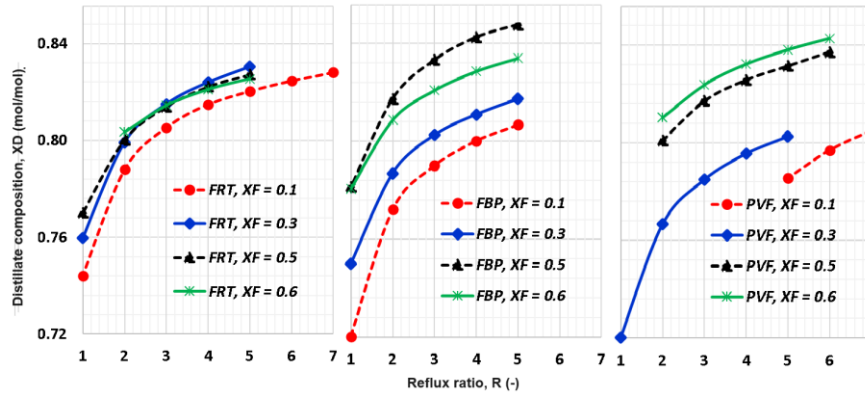


Figure 9. Effect of reflux ratio on the distillate composition at different feed concentration and FTCs (FRT, FBP and PVF) for a distillation column with $N = 10$ stages.

4.5. Effect of increasing reflux ratio on reboiler duty

Figure 10 shows the effect on increasing reflux ratio on reboiler duty at fixed values feed composition and different FTCs (that is, FRT, FBP and PVF). The reboiler duty increased linearly with reflux ratio for all operating conditions, with slope depending on feed composition. Increasing reflux ratio has a strong effect on Q_R for at $X_F = 0.3$ mol/mol feed composition (steeper increase) compared to concentrated feed solutions at $X_F = 0.5$ and 0.6 mol/mol. The highest demand for energy is the reboiler was observed at $X_F = 0.3$ mol/mol for all FTCs and the lowest energy demand at $X_F = 0.1$ mol/mol, as per Figure 10. The low energy demand in the reboiler at $X_F = 0.1$ mol/mol can be attributed to changes in specific heat capacity (increases with increasing X_F), decrease in boiling point with increasing X_F , and a slight decrease in latent heat of vaporization with increasing X_F . Therefore, the fixed FTC, such as FRT, with high C_p at higher X_F , required to heat the mixture from room temperature to boiling point, the reboiler duty will be highest, as shown also in Figure 10. Comparing the FTCs, shows that FRT will require high condenser duty due to high specific heat capacity required for sensible heat to raise the temperature to boiling point, while FBP and PVF do not have the sensible heat requirement, and hence lower condenser duty for the latter compared to FRT.

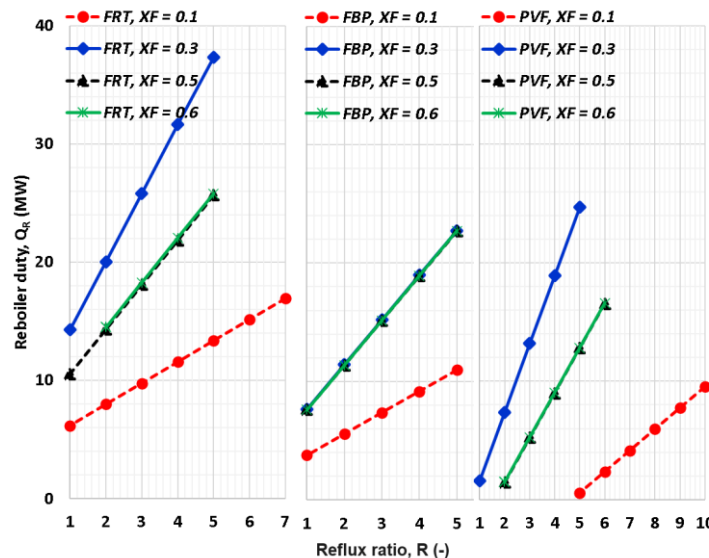


Figure 10: Effect of increasing reflux ratio on the reboiler duty at fixed values of feed composition and FTCs.

Figure 11 shows the maximum and minimum values of condenser duty at different feed thermal conditions and feed composition. The lowest reboiler duties were observed for FBP, especially at $X_F = 0.5$ and 0.6 mol/mol. This can be attributed to the feed being ready to separate into vapor and liquid as it enters the column at FBP. Also, there is less sensible heat required to reach the boiling point when such a feed enters the reboiler, leading to lower heat requirement in the reboiler. For $X_F = 0.3$ mol/mol, highest maximum condenser duty is required attributable to appreciable changes in specific heat, latent heat and boiling points of the feed solution. The FRT shows largest minimum and maximum condenser duties for all feed compositions, also attributable to the sensible heat required to raise the temperature of the feed from room temperature to the boiling point.

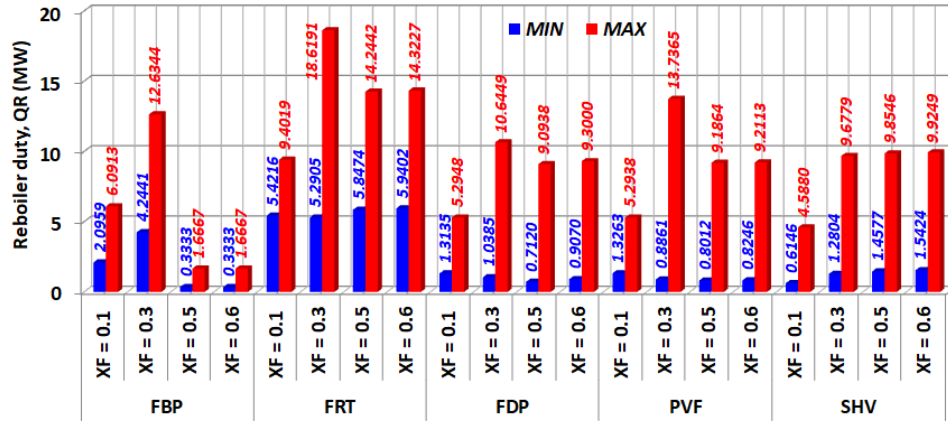


Figure 11: Maximum and minimum average energy demand in the reboiler (across $N = 8$ to 20 stages) for different feed thermal conditions and ethanol concentration.

Figure 12 summarizes the variation of reboiler duty with X_F for fixed reflux ratios and for different feed thermal conditions. For all feed thermal conditions, the maximum reboiler duties were observed at $X_F = 0.3$ mol/mol. For all feed thermal conditions, FBP, SHV, FBP, the minimum reboiler duties were observed at higher ethanol concentration, that is, $X_F = 0.5$ and 0.6 mol/mol, similar to the results presented in Figures 10 and 11. For FRT and FDP, the minimum Q_R values were however observed at $X_F = 0.1$ mol/mol.

For FBP and PVF, similar profiles were obtained for all values of R . On the other hand, for FDP and FRT, the profiles were different depending on the fixed values of reflux ratio. Moreover, the FDP was separated at higher reflux ratios of $R = 6$ to 10 , compared to 1 to 5 for FRT, FBP and PVF. Lowest Q_R values were observed for FDP, separation of which was achieved at higher reflux ratios compared to other feed thermal conditions. In all cases presented in Figure 12, highest Q_R were required to achieve separation at highest reflux ratios of 10 and 5 , respectively. To minimize steam consumption in the reboiler, while maximizing distillate composition, higher feed compositions, $X_F = 0.5$ and 0.6 should be used.

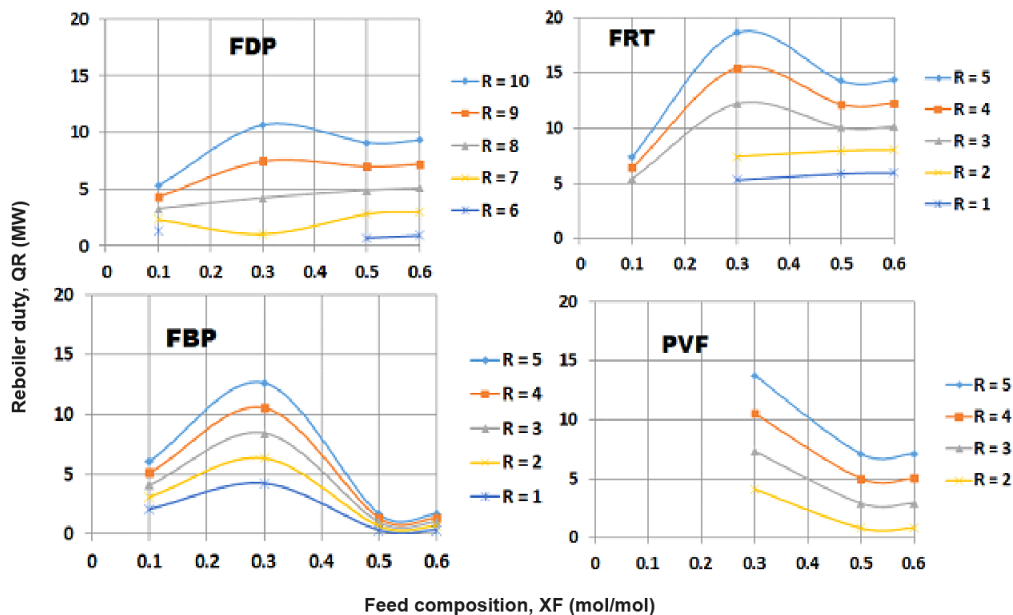


Figure 12. Variation of reboiler duty with feed composition at fixed values of reflux ratio for different FTCs.

4.6 Variation of condenser duty with reflux ratio and feed composition

When the condenser duties were compared at increasing number of stages from 8 to 20, there was no appreciable difference. This can be attributed to the fact that the condenser receives the vapors and condenses them regardless of number of stages in the column. The only major factors were feed composition and reflux ratio, which determines the temperature, composition and flow rate of the vapors from Stage 1. Thus, the average values of Q_c across the number of stages were determined as shown in Figure 13. The condenser duty increased linearly with reflux ratio for all feed thermal conditions.

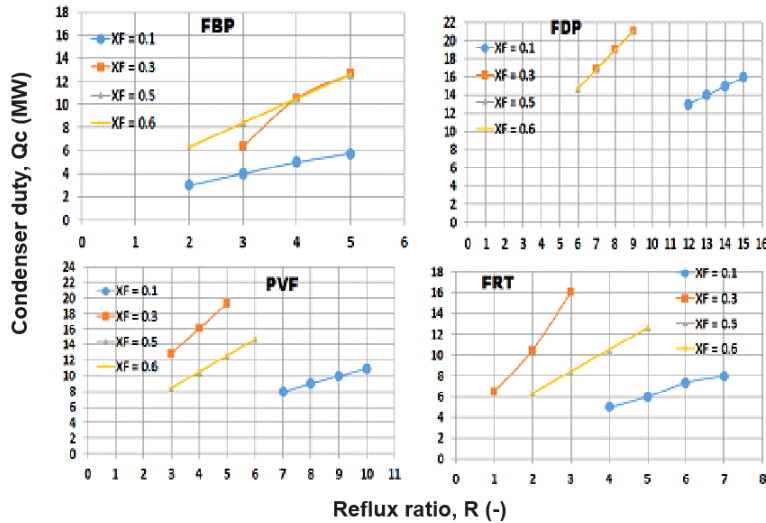


Figure 13. Variation of the condenser duty (across $N = 8$ to 20) with reflux ratio at constant feed compositions for different feed thermal conditions

For SHV, PVF and FDP, at lower $X_F = 0.1$ mol/mol, the average condenser duty was lowest and required separation was achieved at higher reflux ratio range that is 13 to 16, 7 to 10 and 12 to 15, respectively. Highest condenser duties were observed for SHV, PVF and FDP compared to FRT and FBP. Increasing X_F decreased the range of reflux ratio required to achieve separation. For instance, when SHV feed was introduced into the column, the range of reflux ratio required shifted from 13 to 16 to 9 and 4 to 6 for $X_F = 0.1, 0.5$ and 0.3 , respectively. The highest condenser duties were observed for $X_F = 0.3$ mol/mol for all feed thermal conditions.

Figure 14 compares the maximum and minimum average condenser duties (averaged for $N = 8$ to 20) for five different feed thermal conditions and compositions. Lowest, condenser duties were observed for feed at boiling point (FBP), especially at $X_F = 0.1$ mol/mol, while the highest duties were observed for FDP and SHV feed thermal conditions. The condenser duties for FRT and PVF were observed to lie within the two extremes. With respect to feed composition, the highest condenser duties were observed for $X_F = 0.3$ mol/mol for all feed thermal conditions, as reported also in Figures 8 and 12. Compared to Figure 8, condenser duties are higher than reboiler duties for all feed thermal conditions and feed compositions. This is again attributable to the mode of operation of the reboiler, which is operated in partial vaporization mode, while at the top, a total condenser was used. With SHV and FDP, the condenser duties in the range of 20-22 MW, significantly higher cooling water flow rates will be required to produce the distillate. Such feed thermal conditions should be avoided to save energy consumption in the condenser. Moreover, these feed thermal conditions require higher energy input (sensible and latent heats depending on the FTC prior to feeding), as summarized in Figure 1.

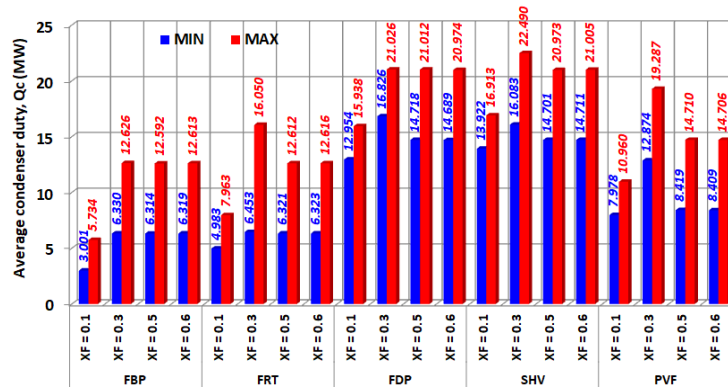


Figure 14. Maximum and minimum average energy demand in the condenser (across $N = 8$ to 20) for different feed thermal conditions.

4.7 Energy efficiency analysis for reboiler based on feed thermal conditions

The energy management in the chemical and process industry involves assessing for the means to achieve minimum energy consumption for profit maximization. In the distillation process, this necessitates critical analysis of the reboiler and condenser duties so as to select the feed conditions, reflux ratio, etc. Energy efficiency assessment leads to operational and economic insights and savings (Popoola *et al.*, 2012; Patil and Patil, 2016). Comparing results presented in Figure 11 for reboiler duties and Figure 14 for condenser duties, the feed thermal condition leading to lower reboiler and condenser duties was the FBP. Thus, it was important to determine the energy saving realized by shifting the respective feed thermal conditions to FBP. The analysis of the energy saving using single reference (FBP in this case) is based on the fact that both reboiler and condenser serve the same feed.

When the savings in energy were arranged for Q_R and Q_C by switching the respective feed thermal conditions to the FBP in both cases, similar results were obtained, as summarized in Figure 15. Thus, the total saving is the sum of the saving realized in the reboiler and condenser, which implies twice the values presented in Figure 15. In the plot, negative values indicate that there is no energy saving, and instead extra energy is required for the given feed composition.

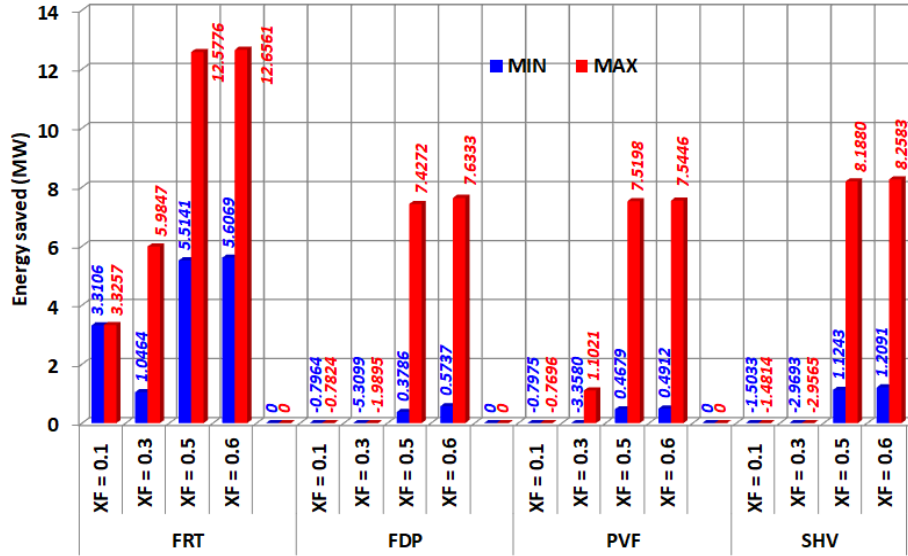


Figure 15. Energy saving in the reboiler or condenser by switching respective feed thermal conditions to FBP.

The highest energy saving can be achieved by switching FRT to FBP for the whole range of feed compositions, followed by SHV. Since the maximum for both reboiler and condenser duties occur at higher reflux ratio, the results shows that maximum saving is duties also occur at higher reflux ratios. Conversely, where higher energy consumption occurs, focused saving efforts will lead to high savings as well. Switching from any feed thermal condition to FBP is more economical especially where higher reflux ratios are required to achieve the required separation. Also, higher energy savings is realized at higher feed concentration when any feed thermal condition is switched to FBP mode. Figure 16 shows also that there are cases whereby, switching to FBP adds more cost, where negative savings are realized. Such cases should be identified and avoided. For example, switching to FBP from FDP, PVF and SHV at $X_F = 0.3$ mol/mol, should be avoided as negative savings are indicated. Based on Figure 15, the feed molar ethanol concentration at $X_F = 0.5$ and 0.6 mol/mol are recommended, since largest energy savings can be realized when shifting to FBP from any FTC. For chemical and process industries, energy efficiency and product yield are generally the key to profitability and emissions abatement. For example, ExxonMobil achieved a 35% reduction in the energy intensity of its global refining and chemical operations from 1974 to 1999 and has identified a further 10–15% cost-effective energy-savings opportunity in all plants around the world (NAS, 2010).

Benchmarking data indicate that most petroleum refineries can economically improve energy efficiency by 10–20% (NAS, 2010), and analysis of individual refining processes indicate energy savings ranging from 23–54% (EIA, 2006). Common technologies include high-temperature reactors, distillation columns for liquid-mixture separation, gas-separation technologies, corrosion-resistant metal- and ceramic-lined reactors, sophisticated process-control hardware and software, pumps of all types and sizes, steam generation, and many others. In the EIA (2006) petroleum bandwidth study, the largest potential bandwidth savings are found in crude distillation, with savings of up to 54% of current average energy for atmospheric distillation (39% for vacuum distillation). Alkylation follows closely, with a potential bandwidth savings of 38%, and the remaining processes also exhibit significant potential for improving energy efficiencies. According to experts working in the field of petroleum refining and energy management, identifying plant-wide energy savings of approximately 30% would be typical. However, these savings estimates are calculated on a relative basis. The absolute energy consumption of petroleum refineries in the United States must be adjusted to account for increasingly heavy crude slates over the coming years. When one adjusts for the use of heavier crude slates, the energy consumption of a refinery increases per equivalent amount of refined product.

5. Conclusions

For ethanol-water mixtures, increasing the number of stages slightly increases the distillate composition, below X_{AZ} , the closest being 0.86 mol/mol for most FTCs and 0.88 mol/mol for FDP at $N = 20$ stages. On the other hand, increasing the feed ethanol concentration increases the distillate composition, up to 0.86 mol/mol when X_F was increased from 0.1 to 0.6 mol/mol, irrespective of the FTCs and reflux ratio. Increasing reflux ratio increases the distillate composition up to 0.86 mol/mol. Depending on FTC and X_F , acceptable ranges of reflux ratio was established for which the model converged. Due to the nature of vapor-liquid equilibrium (VLE) relationship, the distillate composition could not closely approach the azeotropic concentration, X_{AZ} . Locating the feed plate closer to the column bottom increases the distillate composition for all FTC and feed composition (for fixed reflux ratio and number of stages). An increase in X_D when f_s values were changed from 4 to 7 in a 10-stage column increased X_D from up to 0.84 from 0.72 mol/mol. The reboiler duty increases linearly with reflux ratio for all FTCs and number of stages. Increasing N from 8 to 20 does not affect the reboiler duty. Thus, averaging the reboiler duty for $N = 8$ to 20 simplifies the analysis of data with reduced number of variables.

The highest reboiler duties were observed for FRT, at $X_F = 0.3$ mol/mol, and lowest for FBP (especially for $X_F = 0.5$ and 0.6 mol/mol), which forms the optimal feed condition. For all FTCs, dilute feed conditions ($X_F = 0.1$ mol/mol), leads to a wide variation of temperature across the distillation column and also to a higher reboiler temperature (that is higher reboiler duty). Highly uniform axial temperature profiles were observed at higher feed concentration ($X_F = 0.5$ and 0.6 mol/mol). Across the distillation column, ethanol concentration increases upwards, being highest at the condenser, i.e., X_F . The concentration of ethanol in the liquid approaches X_F in the rectifying section (forming a single profile) for all X_F , while in the stripping section, each X_F assumes distinct profiles, increasing with X_F and decreasing with axial elevation towards the lowest in the reboiler. The condenser duty increases linearly with reflux ratio for all values of X_F and FTCs. However, the loci of the curves along the horizontal axis or reflux ratio strongly depend on X_F and FTC. The lowest condenser duties for different feed conditions were observed for FBP while highest duties were observed for FDP and SHV. Thus, the choice of FTC should involve considerations of reboiler and condenser duties, based on which, FBP was identified to be the suitable FTC. Highest energy saving was realized when switching from FRT to FBP, especially at higher $X_F = 0.5$ and 0.6 mol/mol.

Acknowledgement

The financial support from the University of Dar es Salaam Research Grant is highly acknowledged. Special thanks to Mr. Emmanuel Stephen Monge for his assistance in setting up the Aspen Plus® Model.

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