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Simulation of a Plate Distillation Column for Separation of Ethanol-water Mixture Based on Feed Composition Using DWSIM

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Abstract: The study explores the effect of mole fraction of ethanol in feed on the performance and energy efficiency of a distillation column used for ethanol-water separation by simulation using DWSIM. Key parameters, including the molar flow rates of distillate and bottom products, condenser and reboiler duties, minimum reflux ratio, and tray requirements, were analysed by maintaining the following parameters constant: 100 kmol/h of feed, Non-Randon Two-Liquid (NRTL) thermodynamic model, mole fraction of ethanol in distillate is 0.9 and in bottom is 0.05, reflux ratio of 2.5, partial condenser and pressure and vapour fraction flash specification. As the feed ethanol mole fraction increases from 0.4 to 0.6, the distillate flow rate rises, while the bottom flow rate decreases, demonstrating enhanced ethanol recovery. However, energy requirements exhibit a non-linear trend, peaking near a mole fraction of 0.5 due to azeotropic tendency. The minimum reflux ratio progressively increases with ethanol content in feed, highlighting the energy trade-off necessary for achieving desired separation. Additionally, the number of minimum trays, feed tray position, and actual number of trays all increase with feed ethanol concentration, reflecting the rising separation difficulty. These findings provide valuable insights into optimizing column design and operation for maximum efficiency and product quality while minimizing energy consumption.

Keywords: *Distillation, Ethanol-water, Simulation, Molar flowrates of products, Energy duties, Number of trays.*

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Introduction

Distillation is a widely used separation process in the chemical industry, designed to separate components of a liquid mixture based on differences in their boiling points (Meng et al., 2023). The process involves vaporizing the liquid mixture, followed by condensation to achieve the desired separation (Santoro et al., 2022). Distillation plays a critical role in purifying chemicals, producing fuels, and separating alcohols, such as ethanol from water (Tian et al., 2024). Key parameters, such as the reflux ratio, feed composition, and tray design, significantly impact its efficiency. Despite its effectiveness, distillation is energy-intensive, which has led to research focused on optimizing energy use and minimizing its environmental impact. Its versatility makes it an indispensable tool in both industrial applications and research (Velasco et al., 2021).

Ethanol-water mixture is a widely studied binary system, crucial in industries such as biofuel production, pharmaceuticals, and beverages. Due to hydrogen bonding, ethanol (C_2H_5OH) and water (H_2O) form a complex mixture with non-ideal behaviour (Mekala et al., 2022). One of the most notable characteristics of this mixture is the presence of an azeotrope at approximately 95.6% ethanol by volume, where the mixture boils at a constant composition. This azeotropic point complicates separation via simple distillation. Therefore, advanced techniques, such as azeotropic distillation or the use of molecular sieves, are required for complete separation (Carravetta et al., 2022; Su et al., 2020; Cheng et al., 2023). A thorough understanding of thermodynamic properties of this mixture is essential for optimizing distillation and separation processes (Valverde et al., 2022).

Simulation using Graphical User Interface (GUI) tools allows for the modelling and analysis of complex systems without the need for extensive programming knowledge. These tools provide visual interfaces with intuitive drag-and-drop components, pre-built templates, and interactive environments, making it easier to configure system parameters, flow diagrams, and process models (Buditjahjanto, 2022). In chemical engineering, GUI-based simulation tools, such as DWSIM, Aspen Plus, and others, help design and optimize processes like distillation, heat exchangers, and reactors. These platforms simplify simulation workflows, making them accessible to users without advanced programming expertise, while offering powerful capabilities for sensitivity analysis, parameter optimization, and scenario testing (Ramirez et al., 2020; Subramanian and Neelameggham, 2023). The visual nature of GUI tools enhances understanding of system behaviour and decision-making, improving both the speed and accuracy of simulation (Mutlu and Zeng, 2020).

Studies by Seader et al. (2016) highlight that a higher reflux ratio generally improves separation efficiency but at the cost of increased energy consumption. In addition, feed composition and the number of trays significantly affect both separation efficiency and operational costs (Smith, 2005). However, traditional distillation remains an energy-intensive process with a considerable environmental impact, driving ongoing research to

enhance energy efficiency and reduce its carbon footprint (Yadav et al., 2021). Rodríguez-Bencomo (2016) discusses several strategies for breaking azeotropes, such as azeotropic distillation, which involves adding a third component to alter the relative volatilities of the mixture's components. Another approach is the use of molecular sieves, which selectively adsorb water, allowing ethanol to be produced with purity exceeding the azeotrope point (Karimi et al., 2021). However, both methods typically require substantial energy input and may involve complex equipment, increasing operational costs and environmental impact.

ecent advances have focused on energy-efficient distillation techniques, such as pressure-swing distillation (Zhang et al., 2024) and membrane-based separation (Santoro et al., 2022). While these methods show promise in improving separation efficiency and reducing energy consumption, they are still in the experimental or early commercial stages. The use of simulation tools, such as Aspen Plus, DWSIM, and CHEMCAD, allows for the modeling of complex distillation processes, helping to predict performance, identify optimal operating conditions, and reduce the need for costly pilot-scale experiments. These tools incorporate thermodynamic models, such as NRTL (Non-Random Two-Liquid), which accurately predict the phase behavior of non-ideal mixtures like ethanol-water. However, while these tools have facilitated significant advancements in distillation optimization, they still struggle to fully capture the non-linear behavior of azeotropic mixtures under varying operational conditions (Jasinski et al., 2019; Lynd et al., 2022).

Wang et al. (2024) and Liu et al. (2023) investigated the use of heat integration techniques to recover energy from reboilers and condensers, thereby improving overall energy efficiency. Pinheiro et al. (2024) proposed the implementation of variable reflux ratios and advanced control strategies to reduce energy consumption in real-time operations. However, these techniques are often difficult to implement in practice due to their complexity and the need for precise control systems.

The present study offers a novel approach by comprehensively simulating performance and energy efficiency of a distillation column. It focuses on analysing how the ethanol mole fraction in the feed influences performance across a wide range of operating conditions. Using DWSIM and a rigorous thermodynamic model (NRTL), the research provides a deeper understanding of the non-linear energy behaviour associated with azeotropic mixtures. The primary aim of this study is to analyse the relationship between the ethanol mole fraction in the feed and key distillation column parameters, including the distillate and bottom product flow rates, condenser and reboiler duties, minimum reflux ratio, and the number of trays required by simulation in DWSIM at the process conditions of 100 kmol/h of feed, Non-Randon Two-Liquid (NRTL) thermodynamic model, mole fraction of ethanol in distillate is 0.9 and in bottom is 0.05, reflux ratio of 2.5, partial condenser and pressure and vapour fraction flash specification.

Simulation Procedure

DWSIM is an open-source process simulation software designed for modelling and optimizing chemical processes. It supports both steady-state and dynamic simulations, enabling users to model unit operations like distillation columns, reactors, heat exchangers, and pumps. This versatility makes it an essential tool for process engineers, researchers, and educators (Adha and Rahmadi, 2024). A standout feature of DWSIM is its extensive selection of thermodynamic models, such as Peng-Robinson, Soave-Redlich-Kwong, and NRTL, allowing users to accurately represent the behaviour of fluids and mixtures under varying conditions (Chantasiriwan, 2023). The software also includes tools for dynamic simulation, which models system behaviour over time, crucial for studying processes during startup, shutdown, and disturbances. Its intuitive graphical user interface (GUI) enables users to easily create process flowsheets by dragging and dropping unit operations and connecting them with streams. This helps visualize and analyse material and energy balances, thermodynamic properties, and overall system performance (Tangsriwong et al., 2020; Sreemahadevan et al., 2024).

To begin the simulation of a distillation column in DWSIM, first, open the software and create a new simulation file. The user interface allows to select ethanol and water from a variety of compounds and thermodynamic models, depending on the nature of the mixture working with. For ethanol-water mixture, the NRTL (Non-Random Two-Liquid) model is commonly chosen, as it accurately represents non-ideal mixtures. Next, specify the operating conditions, including the temperature, pressure, and flow rates for the feed streams entering the column. The molar flowrate of feed at 100 kmol/h and required feed composition with default values of temperature and pressure have been set. It is important to ensure that the feed stream conditions are realistic, as these will directly influence the performance of the distillation column. At this stage, select the distillation column unit operation from the unit operation library in DWSIM, which can be dragged and dropped onto the simulation flowsheet.

After placing the distillation column in the simulation, the next step is to configure its specifications. In DWSIM, the distillation column can be modelled with a range of options, including the selection of light and heavy key components and their composition in distillate and bottom products as 0.9 and 0.05, respectively (Figure 1). For reflux, define a fixed reflux ratio of 2.5 for the desired purity of the top product. Partial condenser was chosen for the present study.

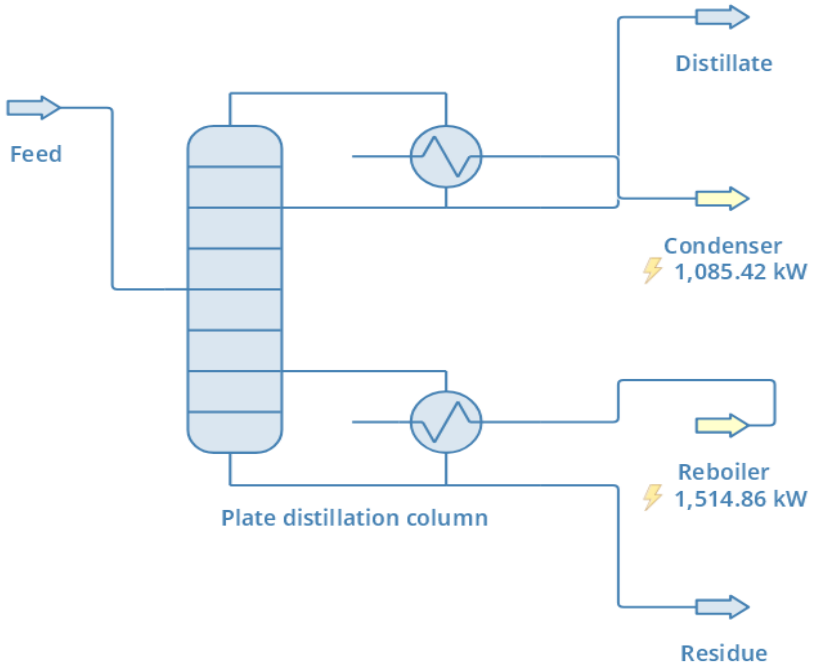

Figure 1. Simulation of a plate distillation column for separation of ethanol-water mixture in DWSIM

Once the column configuration is complete, it is time to run the simulation. DWSIM will use the thermodynamic model and feed conditions to calculate the operation and separation performance of column. The simulation proceeds by solving mass and energy balances across each stage of the distillation column, iterating until convergence is achieved. The convergence process checks if the mass flow rates, compositions, and energy balances match the input and output conditions across the column, ensuring that the system is operating as expected.

After the simulation has converged, DWSIM provides various results that allow you to assess the performance of the distillation column. These include the composition of the top and bottom products, minimum reflux ratio, and the number of trays, as well as energy consumption in the reboiler and condenser. The software generates detailed output tables, which can be used to evaluate the separation efficiency and energy usage. Once the simulation is complete and satisfactory, DWSIM allows to generate reports summarizing all key results, including column configurations, feed and product compositions, energy consumption, and overall system performance. These reports can be exported in various formats (such as Excel, PDF, or CSV), making it easier to document and communicate the simulation results for further analysis or presentation.

Results and Discussion

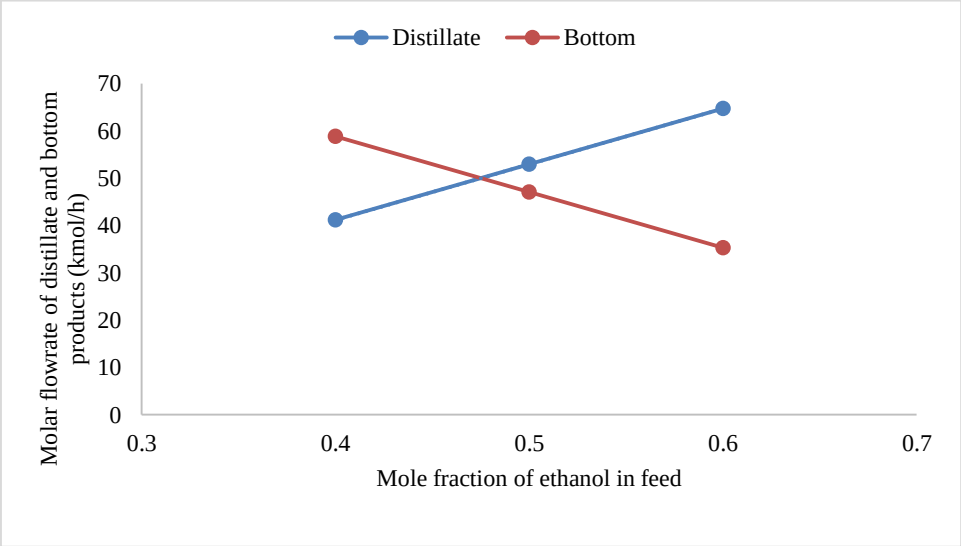

Figure 2. Effect of mole fraction of ethanol in feed on molar fluorite of distillate and bottom products

Figure 2 illustrates the simulation results of a distillation column separating an ethanol-water mixture, focusing on the relationship between the mole fraction of ethanol in the feed and the molar flow rates of distillate and bottom products. The mechanism behind the increase in the molar flow rate of the

distillate and the decrease in the molar flow rate of the bottoms with an increase in the mole fraction of the ethanol in the feed is explained by the principles of distillation and component separation. In a distillation column, components are separated based on their volatilities, the ethanol being the more volatile component, which tends to preferentially vaporize and rise to the top of the column, while the water remains more concentrated in the liquid phase at the bottom (Ngoma and Antonio André, 2023).

When the mole fraction of the ethanol in the feed increases, the overall volatility of the feed mixture also increases. This results in a greater tendency for the light key to vaporize and be carried into the distillate phase. Since the distillation column operates by separating the more volatile components (the light key) from the less volatile ones (the heavy key), a higher mole fraction of the light key in the feed means more of it will be drawn into the distillate.

As a consequence, the molar flow rate of the distillate increases because the column is more efficient at separating the light key component from the feed, and a larger proportion of the feed is now being converted into distillate. On the other hand, as the mole fraction of the light key increases in the feed, the relative amount of the heavy key (the less volatile component) in the feed decreases. Since the distillation process tends to concentrate the heavy key in the bottoms product, a reduction in the heavy key content in the feed means that less of the heavy key will be separated and collected in the bottoms.

As a result, the molar flow rate of the bottoms decreases because less of the less volatile component remains in the liquid phase at the bottom of the column. Thus, the increase in the mole fraction of the light key in the feed shifts the distribution of components in the distillation process, leading to an increase in the molar flow rate of the distillate (which contains more of the light key) and a decrease in the molar flow rate of the bottoms (which contains more of the heavy key). This dynamic is a direct consequence of the separation behaviour driven by differences in volatility between the components.

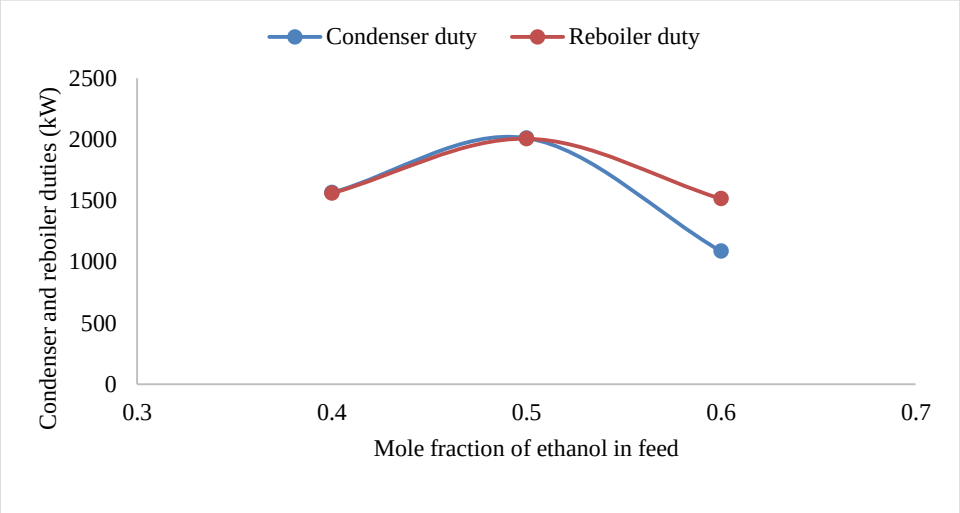

Figure 3. Effect of mole fraction of ethanol in feed on condenser and reboiler duties

Figure 3 represents the condenser and reboiler duties (in kW) as a function of the mole fraction of ethanol in the feed for a distillation column separating an ethanol-water mixture. The mechanism behind the increase and subsequent decrease in condenser and reboiler duties with an increase in the mole fraction of the light key (LK) component in the feed could be understood in terms of the energy balance and the changes in the separation behaviour within the distillation column. In a distillation column, the condenser and reboiler play crucial roles in maintaining the thermal equilibrium required for the separation of components. The condenser is responsible for cooling and condensing the vapor at the top of the column, while the reboiler provides heat to vaporize the liquid at the bottom of the column. When the mole fraction of the light key (LK) component in the feed increases, the overall volatility of the mixture in the column increases. This means that the light key is more easily vaporized and moves toward the top of the column, requiring more cooling and condensation at the top (condenser duty). At the same time, more of the light key is carried over to the distillate, which results in a greater separation of the light key from the heavy key (Sivalingam, 2023).

The reboiler, which is responsible for providing heat to the bottom of the column, also experiences an increase in duty. As the light key concentration in the feed increases, the overall composition of the column becomes more volatile, which means more vapour must be generated at the bottom to maintain the necessary separation between the light key and heavy key components. The increased flow of vapor from the reboiler ensures that the column operates with sufficient vapor flow to maintain the desired separation and to facilitate the transfer of heat needed to vaporize the mixture. Thus, when the mole fraction of the light key in the feed increases, the duties of both the condenser and the reboiler initially rise to handle the increased need for vaporization and condensation of the more volatile light key component. However, as the mole fraction of the light key continues to increase further, a point is eventually reached where the system becomes more efficient in separating the light key from the heavy key. At this stage, the amount of light key in the feed is sufficiently high that the distillation column can reach an optimal separation without requiring as much additional heat input from the reboiler or cooling from the condenser.

In this case, the condenser duty may begin to decrease. Since the light key is more volatile, the distillation column becomes more efficient at separating the components, and less energy is needed to condense the vapor at the top of the column.

Similarly, the reboiler duty begins to decrease because less heat is needed to vaporize the liquid at the bottom. The increased concentration of the light key in the feed means that a larger proportion of the vapor at the top of the column consists of the light key, and less energy is required to maintain the necessary vaporization and condensation rates. This decreasing duty phenomenon is related to the reduced need for thermal energy as the system becomes more efficient in handling a higher concentration of the light key. Once the feed contains a sufficiently high proportion of the light key, the system reaches a point where the thermal energy input and removal are optimized, and both the condenser and reboiler duties start to drop.

The increase in the mole fraction of the light key in the feed initially leads to higher condenser and reboiler duties because more vaporization and condensation are needed to separate the more volatile light key from the heavy key. However, as the mole fraction of the light key continues to rise, the system becomes more efficient at separating the components, and the required thermal duties decrease. The condenser and reboiler duties initially increase due to the need for more energy to handle the greater volatility of the feed but eventually decrease as the separation becomes more efficient with increasing light key concentration in the feed.

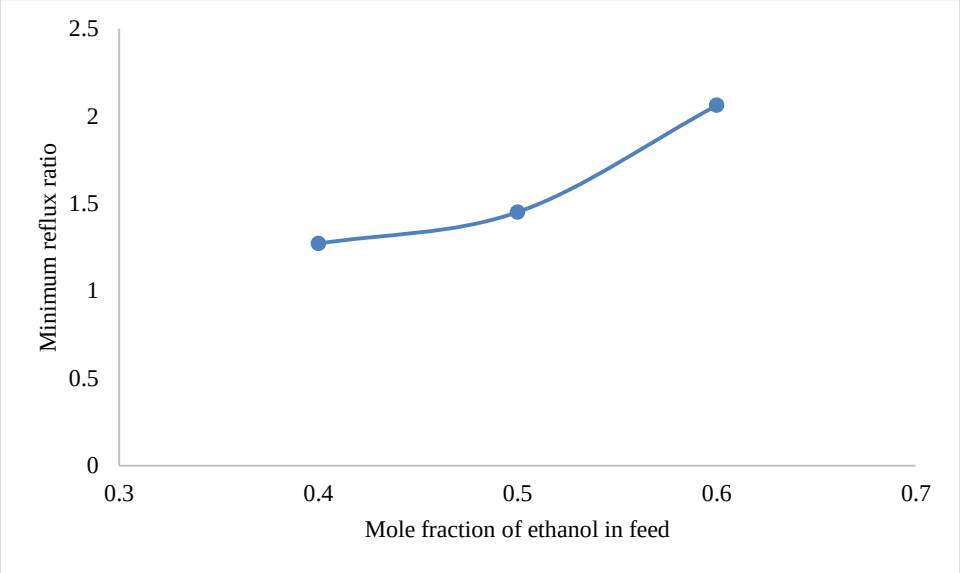

Figure 4. Effect of mole fraction of ethanol in feed on minimum reflux ratio

Figure 4 depicts the variation of the minimum reflux ratio as a function of the mole fraction of ethanol in the feed for a distillation column. The mechanism behind the increase in the minimum reflux ratio with an increase in the mole fraction of the light key (LK) component in the feed could be understood in terms of the principles of distillation and the column's operating conditions, specifically the relationship between feed composition, separation efficiency, and energy requirements (Koteswari and Kumar, 2021).

In distillation, the reflux ratio is the ratio of the liquid returned to the column (reflux) to the liquid taken as distillate. The minimum reflux ratio is the lowest reflux ratio at which the desired separation can be achieved. If the reflux ratio is below this minimum value, it is impossible to achieve the required separation, and the column will not work as intended. The minimum reflux ratio depends on the relative volatility of the components in the feed and the degree of separation needed. The relative volatility is a measure of how much more volatile one component is compared to another. A higher relative volatility means a more efficient separation, and a lower reflux ratio can achieve the same degree of separation. Conversely, a lower relative volatility requires a higher reflux ratio for the same separation.

- Increased Volatility of the Feed: As the mole fraction of the light key (LK) component in the feed increases, the overall volatility of the mixture also increases. The light key is more volatile and more easily vaporized than the heavy key, so with more light key in the feed, the mixture becomes more volatile overall. This leads to a higher difference in volatility between the light key and the heavy key, which should, in principle, reduce the minimum reflux ratio required to achieve the same separation.
- Increased Separation Efficiency: When the mole fraction of the light key increases, the distillation process becomes more efficient in separating the components. More of the light key is carried into the distillate, and less of the heavy key remains in the liquid phase. In theory, this would suggest that less reflux is needed to achieve the same separation. However, this is not always the case.
- Effect of Higher Feed Concentration of Light Key: As the mole fraction of the light key increases in the feed, the composition of the feed becomes closer to that of the distillate. In other words, the light key is already more concentrated in the feed, and the heavy key is less concentrated. To achieve the required separation, the distillation column needs to further concentrate the light key in the distillate and remove the heavy key in the bottoms. As the light key becomes more abundant in the feed, the difference in composition between the top (distillate) and bottom (bottoms) of the column becomes smaller. This means that achieving a high degree of separation between the light and heavy keys requires a larger number of theoretical stages and more reflux to "fine-tune" the separation.

- Thermodynamic Considerations: As the light key increases in the feed, the operating line (the relationship between the liquid and vapor compositions at different stages) becomes steeper because the light key is more easily vaporized. To achieve the desired separation with the increased light key concentration in the feed, the column needs to operate with a higher reflux ratio to ensure the light key is sufficiently concentrated in the distillate and the heavy key is sufficiently concentrated in the bottoms. This increase in the reflux ratio is required to maintain the separation efficiency as the feed composition shifts.

The key factor is that as the mole fraction of the light key in the feed increases, the relative volatility between the components decreases. This means that, although the light key is more volatile, the difference in volatility between the light key and the heavy key becomes smaller, making it harder to separate them efficiently. To compensate for this reduced volatility difference, the column needs to operate at a higher reflux ratio to achieve the same level of separation.

The increase in the reflux ratio ensures that the column can produce a distillate with a high concentration of the light key and a bottoms product with a high concentration of the heavy key, even as the difference in volatility between the two components becomes smaller. In other words, the system requires more reflux (and thus more energy) to overcome the reduced volatility difference and achieve the same separation as the feed composition shifts toward higher light key concentration.

As the mole fraction of the light key component in the feed increases, the volatility difference between the light key and heavy key components decreases, which reduces the separation efficiency. To compensate for this reduced separation efficiency, the minimum reflux ratio required to achieve the same separation increases. Essentially, a higher reflux ratio is needed to provide the additional number of stages or equivalent separation work needed to achieve the desired product purity and maintain the column's performance.

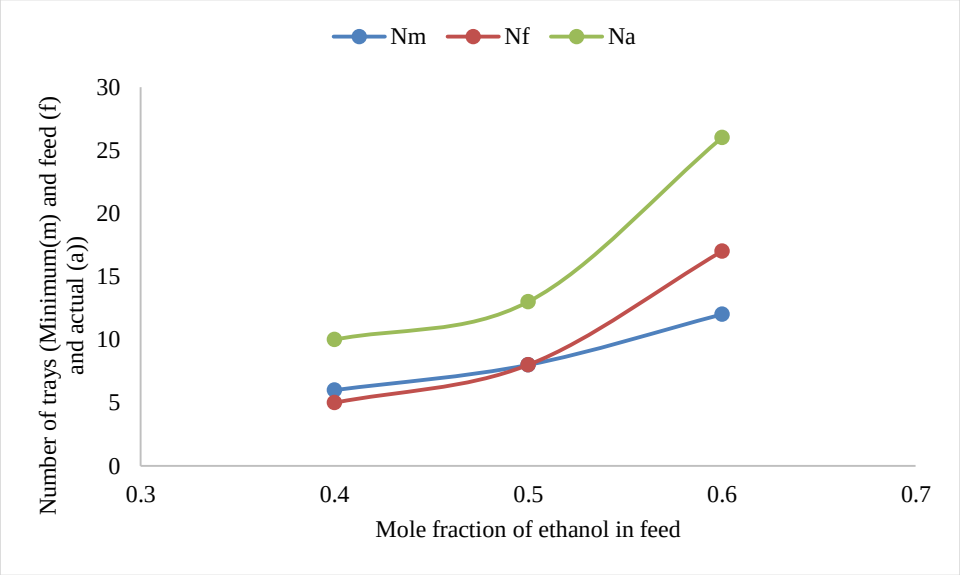

Figure 5. Effect of mole fraction of ethanol in feed on minimum trays, feed tray location, and actual number of trays

Figure 5 indicates the relationship between the ethanol mole fraction in the feed and the distillation column parameters: minimum trays, feed tray location, and the actual number of trays. The mechanism behind the increase in the minimum number of trays, the feed tray location, and the actual number of trays with an increase in the mole fraction of the light key (LK) component in the feed is rooted in the changing separation dynamics and the efficiency of the distillation process as the feed composition shifts. To understand these changes, considering the principles of distillation, including relative volatility, the vapor-liquid equilibrium, and the behaviour of the light key and heavy key components within the column (Gupta and Yadav, 2021).

As the mole fraction of the light key in the feed increases, the relative volatility between the light key and the heavy key generally decreases. Relative volatility is a measure of how easily the two components can be separated based on their differences in volatility. When the light key increases in the feed, it causes the column to become less effective at separating the two components because the volatility difference between the light key and heavy key narrows. To achieve the same degree of separation between the components, more theoretical trays (or stages) are required. The minimum number of trays is determined by the difficulty of achieving the desired separation, which is influenced by the relative volatility of the components. With a reduced volatility difference, the distillation process needs more stages to achieve the same separation efficiency. Therefore, as the mole fraction of the light key increases, the minimum number of trays required for the column to meet product specifications increases.

The location of the feed tray in the distillation column is critical for optimal separation. The feed tray is typically placed at the point where the composition of the feed best matches the composition of the column’s internal vapor-liquid equilibrium. The goal is to maximize the separation of the light key in the distillate and the heavy key in the bottoms. As the mole fraction of the light key increases, the composition of the column shifts towards a higher concentration of the light key at the top and the heavy key at the bottom. The optimal feed tray location is usually at a point where the vapor and liquid compositions are similar to the feed

composition, as this minimizes the energy required for separation. With an increasing mole fraction of the light key, the composition of the feed becomes closer to the distillate composition, meaning the feed tray should be located higher in the column. This ensures that the heavier components (which are less volatile) are better separated from the more volatile light key component. If the feed tray is placed too low, too much heavy key might be carried over to the distillate.

As the mole fraction of the light key increases, the actual number of trays in the column often needs to be increased to accommodate the changes in the separation dynamics. The increase in the minimum number of trays (due to reduced relative volatility) and the shift in feed tray location typically require an increase in the actual number of trays in the column. The increase in trays is needed to improve the separation process. With a higher light key concentration in the feed, the column needs to operate with more stages to achieve a sufficient concentration of the light key in the distillate and the heavy key in the bottoms. The column's ability to achieve these separations effectively depends on the available stages for vapor-liquid contact, and with more trays, the system can achieve the necessary separation more efficiently. Furthermore, as the feed contains more of the light key, the column needs more contact between vapor and liquid to refine the separation. The additional trays allow for more equilibrium stages, improving the separation of the light and heavy components.

As the mole fraction of the light key component in the feed increases, several adjustments occur in the distillation column design and operation:

- The minimum number of trays increases because the reduced relative volatility between the light key and heavy key makes it more difficult to achieve the desired separation, requiring more theoretical stages to accomplish the same separation.
- The feed tray location moves higher in the column, reflecting the shift in the composition of the feed closer to the distillate, which ensures that the separation of the light key and heavy key is more efficient.
- The actual number of trays increases to accommodate the additional stages needed for separation and to enhance the separation efficiency, as the column must work harder to achieve the required product purity.

In essence, with an increase in the mole fraction of the light key, the column becomes more difficult to operate efficiently, requiring more trays and an adjusted feed tray location to ensure that the separation is still achieved effectively.

Conclusion

The study reveals the intricate relationship between mole fraction of ethanol in feed and the operational efficiency of a distillation column for ethanol-water separation. As the ethanol mole fraction increases, the distillate flow rate rises, while the bottom flow rate decreases, demonstrating effective ethanol recovery. The condenser and reboiler duties exhibit a peak at a mole fraction of 0.5, attributed to the challenging azeotropic characteristics of the ethanol-water system. Beyond this point, energy demands decline as separation becomes easier for ethanol-rich feeds. The minimum reflux ratio and tray requirements (minimum, feed, and actual) increase steadily with ethanol content, reflecting the need for more intense separation efforts. These results underscore the importance of optimizing distillation column design and operation based on feed composition. Proper adjustments to tray numbers, feed tray position, and reflux ratio significantly enhance energy efficiency and product purity. The study emphasizes the need for energy-conscious design strategies, particularly when processing intermediate feed compositions, to strike a balance between separation performance and operational cost. These insights serve as a foundation for future research on sustainable and efficient distillation column design.

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