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Simulation of the separation process of Toluene/n-Heptane mixture using the organic solvent N-methyl-2-pyrrolidone by Aspen Hysys software

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الملخص

يُعدّ النفط الخام ومشتقاته من أهم مصادر الطاقة ودعم للاقتصاد المحلي. ولذلك، يُركّز الاهتمام على تطوير صناعة البترول، بما في ذلك فصل خليط الهيبتان العادي والتولوين، الشائع في عمليات الفصل والتكرير في مصافي البترول، وخاصةً في فصل المذيبات العضوية. ونظرًا لأهمية هاتين المادتين في الصناعة الكيميائية، يُعدّ فصلهما أمرًا بالغ الأهمية. في هذا البحث، استُخدم برنامج **Aspen Hysys** لمحاكاة فصل هاتين المادتين من خلال تصميم برجي تقطير باستخدام مذيب عضوي مناسب، وهو **N**–ميثيل–2–بيروليدون **(NMP)**، بواقع 14 و10 مراحل فصل على التوالي. وقد كان هذا ضروريًا نظرًا لصعوبة الفصل ووجود حالة متجانسة في خليط التولوين/الهيبتان العادي. في هذه العملية، يتم ضخ ما يقرب من 962 كجم/ساعة من الخليط، بتركيز 50% لكل مادة، إلى برج التقطير ومعالجته بمذيب بمعدل تدفق دوري يبلغ حوالي 2947 كجم/ساعة، مما ينتج عنه ما يقرب من 460 كجم/ساعة من التولوين بتركيز 99.9%.

الكلمات المفتاحية : أسبن هايسيس، مذيب عضوي، تقطير متساوي الخواص، تقنية فصل

Abstract

Crude oil and its derivatives are among the most important sources of energy and support for the local economy. For these reasons, attention is focused on developing the petroleum industry, including the separation of the normal heptane and toluene mixture, which is commonly found in separation and refining processes in petroleum refineries, especially in organic solvent separation. Given the importance of these two substances in the chemical industry, their separation is crucial. In this research, the Aspen Hysys software was applied to simulate the separation of these two substances by designing two distillation towers using a suitable organic solvent, N-Methyl-2-

Pyrrolidone (NMP), with 14 and 10 separation stages, respectively. This was necessary due to the difficulty of separation and the presence of an isotropic state in the Toluene/n-Heptane mixture. In this process, approximately 962 kg/h of the mixture, at a concentration of 50% for each substance, is flowed into the distillation tower and treated with a solvent at a cyclic flow rate of approximately 2947 kg/h, resulting in approximately 460 kg/h of toluene at a concentration of 99.9%.

Keywords : Aspen Hysys, Organic Solvent, Isotropic Distillation, Separation Technique

Introduction

Distillation is a basic separation technique that is used in the chemical industry for the separation of two or more components in an effective manner. Among industrial facilities, the distillation columns represent the highest energy users to more than 50% of the total energy usage, whose accurate operation and design are therefore vital to guarantee economic energy-related aspects of the process [8]. While simple distillation is sufficient for most mixtures, isotropic mixtures, with the same liquid-vapor phase composition, cannot be broken down by this method. Conventional distillation would yield a high purity and high product recovery, but if separation was needed, advanced techniques such as extractive, variable pressure distillation, isotropic distillation, and liquid-liquid extraction would be used [4][8]. Among the methods, e.g., the variable pressure distillation method, the extractive distillation method is an economic and energy-saving process. But it needs the careful determination of the suitable solvent, which profoundly influences the separation efficiency and the purity of the end-product [2][5][6]. The solvent/feed ratio and the reflux ratio should be sufficiently high for the best solvent and feed combination in the design of extraction distillation columns. Higher purity of the target component and consequently lower content of the impurities in the distillate and the overall energy consumption decrease with increasing these ratios in most cases. Studies also indicated that an increased flow rate of solvent lowers the reboil heat in the extraction distillation column and elevates the heat of reboiling in the solvent recovery column. A suitable solvent flow rate is to be selected so that the total energy consumption of the process is minimized [6][7]. The separation of aromatics (benzene, toluene, and xylene, BTX) from naphtha is significant in the petrochemical industry due to the value of the aromatics, and the need to satisfy environmental regulations limiting aromatic contents in fuels

[1][3].Using simulation software tools such as Aspen Plus or Aspen Hysys, some work related to the design and simulation of the extraction distillation process, considering the influence of different types of solvents and the heat integration for the process improvement in terms of efficiency, cost, and energy consumption [1][2][3][8]. Recent studies have also shown the ability of ionic liquids to act as green solvents with high efficiency in breaking isotropic behavior and minimizing the loss of solvent and energy when compared to traditional solvents [1]. So, extraction distillation is a high-tech and powerful technique for the separation of isotropic mixtures and holds great promise for further improvement in economic and environmental performance.

The inspiration of these research enthusiasts, Numerous commonalities between extractive distillation and its optimization were seen in the literature review and are outlined as:

• The Extractive Distillation process is more economical in terms of capital investment and energy requirement [9]. On the other hand, the pressure swing distillation does not suffer from the potential problem of product contamination by an extractive solvent which must be added to binary systems.

• The Solvent/Feed (solvent to feed ratio) and reflux ratio optimization are the two most crucial design specifications or parameters of the distillation columns that necessarily need to be optimized in extractive distillation [10].

• The selection of solvent is the most important in extractive distillation process design.

• The optimization of extractive distillation frequently demands the consideration of the influence of number of theoretical stages on the purities of components from homogeneous isotropic mixtures, as also to examine the cost to be incurred for obtaining a component purity within specification limit.

• It could be generally seen that the higher the flow rates of solvent, the higher would be the purity of desired component in distillate or equivalently speaking; lower would be impurities of rest of components in distillate at column T-100 during extractive distillation.

• Reboiler heat duty in extractive distillation column decreases with the entrainer flow rate, while reboiler in solvent recovery column is noticed to increase as more solvent is fed. Therefore, a solvent flow rate should be selected in such way that the total heat reboiler duty or energy of separation process is minimized [11-12].

Simulation Process for N-Heptane and Toluene System

Toluene present in crude oil is dominantly obtained as an intermediate product during the gasoline production through a catalytic reformer/ethylene cracker or during the coke production from coal [13]. It is one of the leading chemicals that is used in various chemical industries. n-Heptane a larger extent through dehydration of 2-heptanols into Heptene, which is further converted into n-Heptane through hydrogenation or produced alternatively during hydrogenation of Heptene into n-Heptane. n-Heptane is in continuous demand by various chemical industries. n-Heptane forms a homogenous isotropic mixture with Toluene; further separation of the former and the latter through the normal distillation technique cannot be effectively worked out. In our research study, we had concentrated on the ED technique for the effective separation of n-Heptane and toluene using N-Methyl-2-Pyrrolidone (NMP). The properties of Toluene and n-Heptane are also shown in Table1:

Table 1. Properties of n-Heptane and Toluene compounds [14-15]

Properties	**Toluene**	**n-Heptane**
Molecular Weight	92.14 gm/mole	100.2 gm/mole
Density	0.867 gm/cm^3 at 20˚C	0.68 gm/cm^3 at 20˚C
Boiling Point	110.6˚C	98.4˚C
Melting Point	-94.9˚C	-90.6˚C
Solubility in water	0.52 g/L at 25˚C	3.4 mg/L at 25˚C

In the simulation of the n-heptane-toluene extractive distillation system, we focused on two distillation columns. The primary column, referred to as the Extractive Distillation Column (T-100), plays a crucial role in breaking down the isotropic components of the feed. The second column, designated as the Entrainer Recovery Column (T-101), is responsible for recovering the solvent

used in the process. In the context of T-100, the isotropic feed (detailed in Table 2) was uniform across all solvents, ensuring a consistent basis for comparing the effectiveness of different solvents informed by our optimization results.

Table 2. Isotropic feed stream parameters for Column (T-100)

Vapor Phase Fraction	Temperature (°C)	Pressure (kpa)	Molar Flow Rate (kgmole/h)	Mole Fraction	
				Toluene	n-Heptane
0	43.33	12	10	0.5	0.5

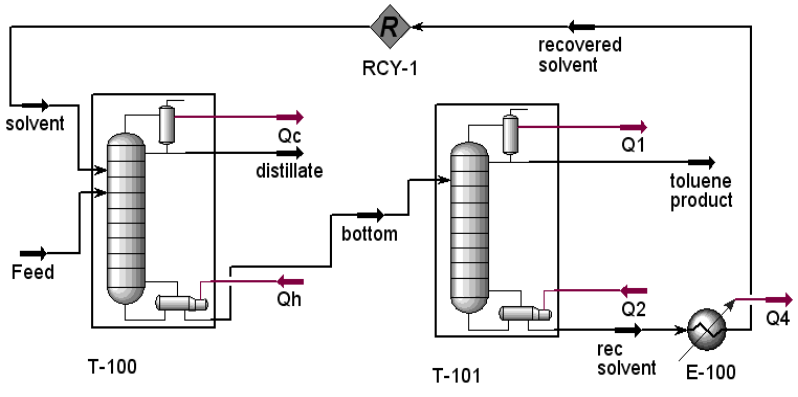

Figure 1. Aspen Hysys Schematic Process Flow Diagram for the n-Heptane/Toluene system using N-Methyl-2-Pyrrolidone (NMP) as a solvent [16]

Addition of isotropic components, solvent, followed by input of the thermodynamic model (UNIQUAC), and Peng-Robinson equation of state (PR) which makes equation widely applied in engineering. The expression is as follows in equations 1 to 4 [17]:

$$P = \frac{RT}{(V-b)} - \frac{\theta_{PR}}{V^2+2bV-b^2} \quad (1)$$

$$\theta_{PR} = a''[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{0.5})]^2 \quad (2)$$

$$a'' = \frac{0.45724R^2T_c^2}{P_c} \quad (3)$$

$$b = \frac{0.07780RT_c}{P_c} \quad (4)$$

Defining solvent and isotropic feed streams, followed by the addition of Extractive Column (T-100), and defining the necessary column parameters. Run the simulation till the column T-100 converges with the required distillate purity (n-Heptane) of a minimum 99%. Adding the Entrainer Recovery Column (T-101) and adding the bottom product of the T-100 as feed to T-101. Run the simulation till T-101 converges with the required distillate purity (Toluene) of a minimum 99%.

Comparison of the use of solvent (NMP) with some other solvents

The efficiency of aromatic recovery processes is highly dependent on the thermodynamic and physical properties of the solvent. Sulfolane exhibits the highest industrial selectivity for Toluene over paraffins, ensuring superior product purity at the column bottom [18]; however, its high viscosity (10.3 cP) can lead to a 15% increase in pressure drop, impacting hydraulic stability [19]. In contrast, N-Methyl-2-pyrrolidone (NMP) offers a balanced operational profile with low viscosity and high chemical stability, making it ideal for maintaining linear pressure profiles in recovery columns [20], [21]. While Dimethyl Sulfoxide (DMSO) provides acceptable hydraulic performance, its inherent thermal sensitivity above 150°C poses significant risks to simulation accuracy and process reliability [22]. Therefore, the selection between these solvents necessitates a trade-off between the high-purity yield of Sulfolane and the energy-efficient, stable operation provided by NMP [18], [21].

Table 3. shows the differences between some solvents

Feature	N-Methyl-2-pyrrolidone (NMP)	Sulfolane	Dimethyl Sulfoxide (DMSO)
Selectivity	High selectivity for aromatics (Toluene) over paraffins (Heptane).	Highest industrial selectivity; often yields higher Toluene purity at the bottom [24].	Moderate to high; slightly lower than NMP in this specific system.

Boiling Point	202(̊C) ensures stable separation in the recovery column.	287(̊C) extremely high, prevents solvent loss but increases reboiler energy duty.	189(̊C) relatively close to Toluene, which may complicate downstream recovery.
Hydraulic Impact	Low viscosity 1.89cP ensures a linear pressure profile.	Higher viscosity 10.3cP may increase pressure drop by 15\% [25].	Acceptable viscosity; provides a pressure profile similar to (NMP).
Chemical Stability	Very stable and non-corrosive under standard conditions.	May require additives to prevent acidic decomposition at high temperatures.	**Thermally sensitive;** may decompose above 150(C), affecting simulation accuracy [26].

Results and Discussion

The mole fraction distribution of liquid in the distillation column trays for the separation of n-heptane and toluene using the non-volatile solvent NMP is shown in figure 2. n-Heptane is the most volatile component and is found to have a mole fraction close to one in the upper trays. The mole fraction drops rapidly around tray 6 and more gradually in the lower trays. This shows that n-heptane is concentrated in the distillate. On the upper stages, the concentration of toluene diminishes, and then, it starts rising to the peak concentration in stages 13-14 (the middle part). The concentration of NMP, the least volatile compound, is non-existent in the rectifying section and sharply rises below stage 6 in the bottom stage. This strong change of slope at stage 6 is the position of the solvent feed, and also explains the great influence of this solvent feed on the column performance. In general the profiles show good clear separation as n-heptane on top, NMP on subtracting stage and toluene is the intermediates stage and the main body of the distillation column. The simulated tray composition profiles agree with experimental literatures for n-heptane/toluene/NMP system, NMP is an efficient selective solvent separation of aromatics and aliphatics is strengthened [23]. The mole fraction distribution shows that the solvent (NMP) is fed at Tray 5, which changes the relative volatility of the mixture and leads

to the sudden drop of the n-Heptane concentration. In terms of solvent efficiency for this extractive system, NMP has a superior compromise of separation selectivity and hydraulic stability [24]. NMP has higher efficiency in reducing the energy consumption of the reboiler than that of Sulfolane attributed to the lower boiling point and viscosity, which is also in consistent with the linear pressure profile in the primary results [25]. Yet, contemporary experimental patterns hint that substitutes such as DMSO could be a greener received profile if reboiler temperatures are rigorously monitored to avoid thermal degradation leading to erratic component mole fractions [26].

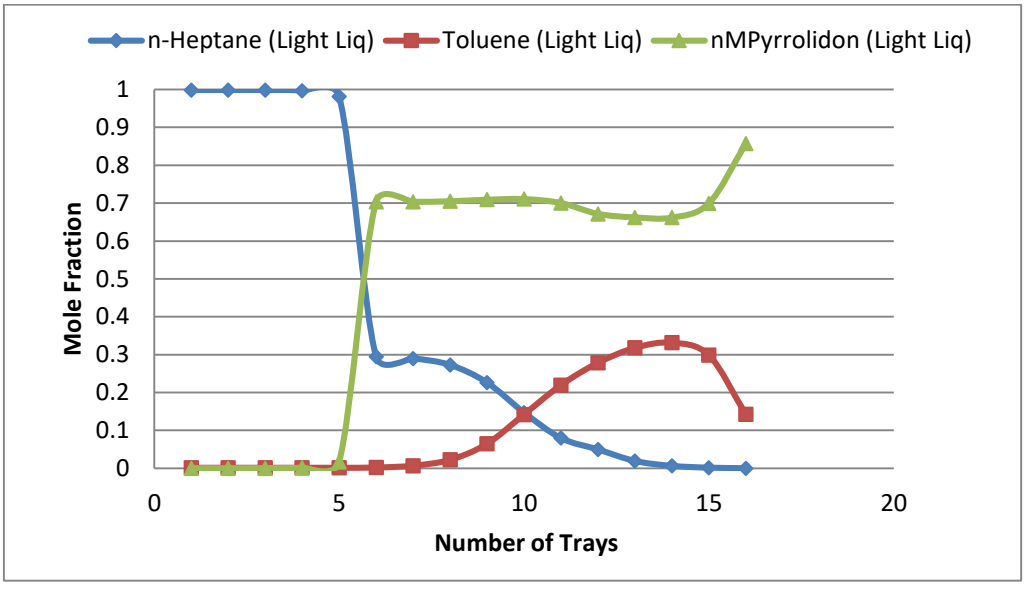

Figure 2. Change in the mole fraction of Toluene, n-Heptane, and NMP versus the Number of Trays in the first column T-100

The distributions of molar flow rates of both vapor and liquid within the stages of the distillation column are shown in Figure 3 for various feed and solvent inputs to the column, which also illustrates the effect of feed and solvent addition on the internal column hydrodynamics. The vapor flow rate rises rapidly along the upper stages to about 24 kmol/h, and it drops gradually along the lower stages to about 10–12 kmol/h at the bottom of the column. This depression may be due to the condensation effect and vapor–liquid mass transfer in the column. On the other hand, the liquid flow is almost constant in

the high section (18~19 kmol/h) and sharply increases at about stage 6 up to 43~46 kmol/h. Such an abrupt increase marks the location of feed (solvent) injection, a fact which causes the internal liquid traffic to be considerably greater there. In this zone, the liquid flow remains very high, and it decreases slightly near the bottom, near the reboiler. In summary, the rate of flow results illustrate that two very different types of regions exist above and below the feed stage, giving rise to a feed stage recompiling process with significant changes in vapor-liquid traffic that led to potential variations in mass transfer behavior and separation of. The simulated tray composition profiles are consistent with literature experimental data for the n-heptane/toluene/NMP system, where NMP acts as an effective selective solvent and increases the separation between aromatics and aliphatic [23],[27].

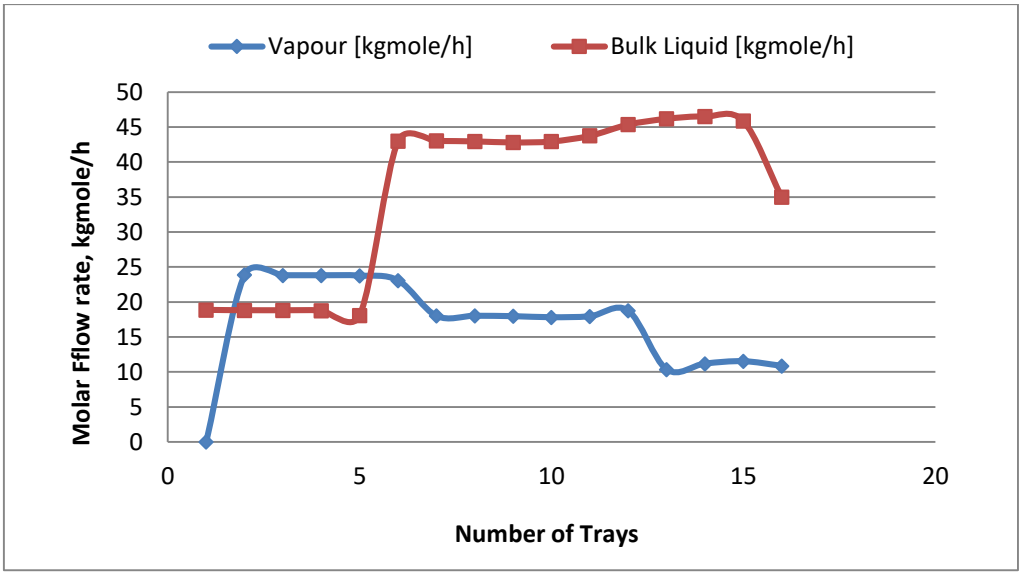

Figure 3. Change in the molar flow rate of vapor and liquid versus the Number of Trays in the first column T-100

Pressure (in kPa) is shown as a function of experimental phases (or time/phase) in Figure 4. We note that the pressure begins at about 12 kPa and then increases in an almost linear manner to about 15–15.2 kPa in the next phases. This escalating trend means that the system is moving towards a linear increase of pressure, with no dramatic jumps, or in other words, a kind of relative stability of the developing stable operating conditions. The steady rise

in pressure may also be due to the temperature rise or vapor accumulation in the system, which is usual in heat and mass transfer operations like distillation or in separation operations like crystallization. In short, the behavior of the curve indicates a gradual increase in pressure in the process, where the pressure variation is tempered and considered gradual. The simulation results generated via Aspen HYSYS demonstrate a progressive pressure increase from 12 kPa at the column top to 15 kPa at the sump, indicating a total pressure drop of 3 kPa across the 16 stages. This linear profile exhibits a high degree of concordance with established experimental benchmarks for tray hydraulics, where the pressure gradient is fundamentally governed by vapor-liquid resistance and static head [28].

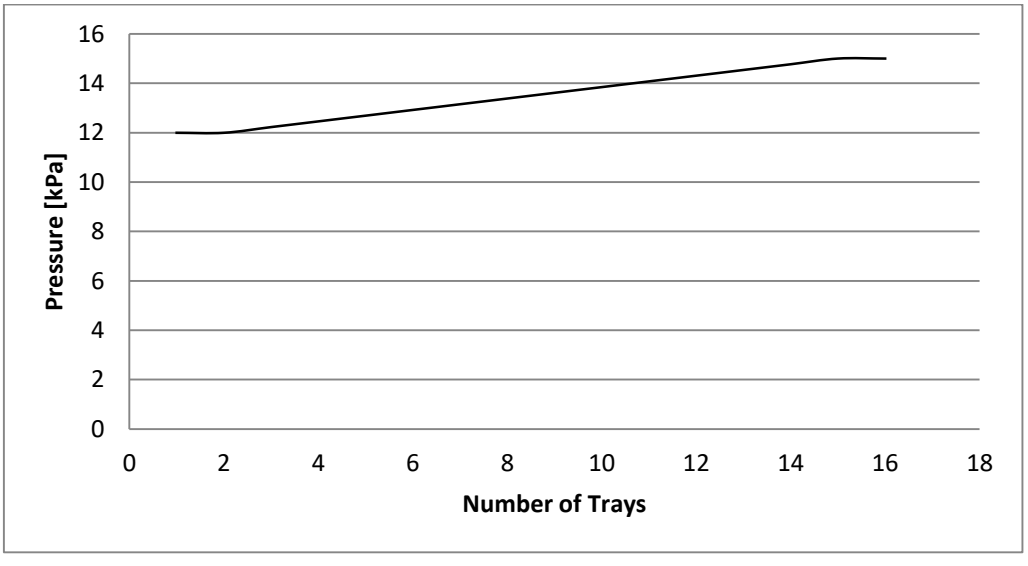

Figure 4. Change in the Pressure in the column versus the Number of Trays in the first column T-100

The temperature profile along the stages of the distillation column is shown in the Figure 5. The result is that the temperature steadily rises during the distillation. 1–5) Temperature is almost constant at about 40 °C (the most volatile components of the mixture are evaporated). This fairly constant temperature indicates that compounds with low boiling points were dominant in the vapor phase. From stage 6 to 14, the temperature rises gradually from about 45 °Cup to almost 80 °C as the distillation is also carried out. This slow increase is indicative of a gradual removal of the more volatile constituents and

introduction of compounds with higher boiling points to the evaporation. Increasing temperature corresponds to changes in vapor–liquid equilibrium as vapor composition becomes dominated by heavier components. In the end of distillation (15–16), the increasing temperature reached 100 °C. This represents a big increase and implies that most of the lighter fractions have by then been removed, and that only fractions with somewhat higher boiling points remain in the material. This kind of behavior is typical in fractional distillation, where components are separated based on the difference in their volatilities, and the temperature curve gives an important clue to the composition variation that is happening inside the column. In general, the temperature trend validates the incremental separation of the components of the mixture as the boiling point difference increases, which is an essential concept of distillation and the general principle of the process itself. The temperature profile rises monotonically from almost 40 °C at the top to 110 °C at the bottom, which corresponds to a temperature increase of around 70 °C over 18 trays. Such a behavior is in line with experimental observations found in the literature, where the higher temperature at the lower stages was ascribed to the enrichment of heavier components with higher boiling points [29]. Experimentally verified like trends of increasing temperature profiles on sieve tray columns, good agreement between plant and HYSYS simulations [30]. This temperature profile indicates that the simulated column is performing as expected for a multi-component separation with moderate relative volatility.

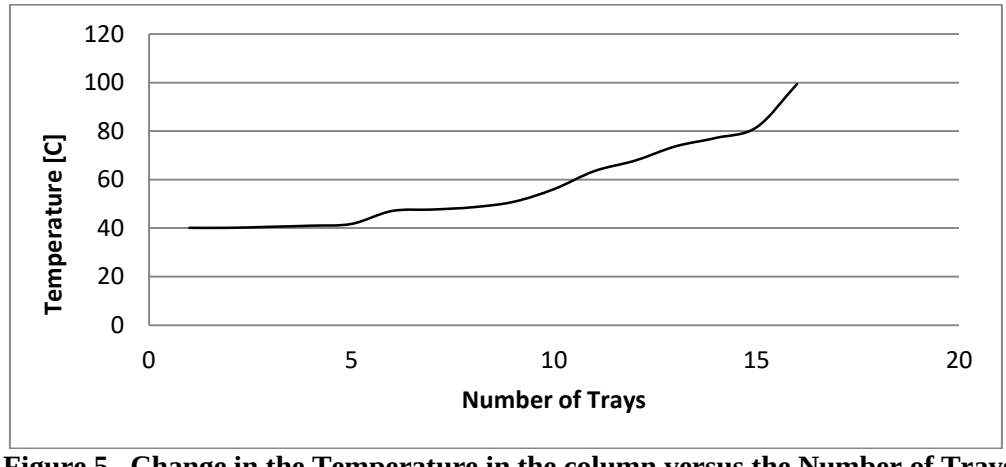

Figure 5. Change in the Temperature in the column versus the Number of Trays in the first column T-100

Figure 6 illustrates the light liquid mole fraction change in various stages of the isotropic separation column. Toluene is the major component of the initial stages, and the mole fraction is extremely close to unity, indicating that toluene is abundant in the upper portion of the column. On the other hand, the aromatic concentration (toluene) decreases dramatically along the column top. The solvent (n-methyl pyrrolidone, NMP) concentration gradually increases to become a major component in the bottom stages. This behavior indicates that the solvent (toluene) is extremely selectively to extract toluene from the column, thus transferring to a phase with a greater amount of solvent and hydrocarbon compounds. However, the n-heptane concentration in the liquid phase in the column is negligible because n-heptane has a strong tendency to stay in the light phase and is removed as the overhead product. These results suggest that the isotropic separation may be applied to separate, for instance, components that significantly differ in their solubility in the solvent. The separation simulation for the n-heptane/toluene/NMP system shows that the results are in good agreement with experimentally established vapor-liquid equilibrium for the n-heptane–toluene mixture and experimentally based extractive distillation using NMP as a selective solvent. This good agreement is also an indication of the accuracy of the simulation and confirms the effectiveness of NMP in extracting toluene from the hydrocarbon [31],[32],[33].

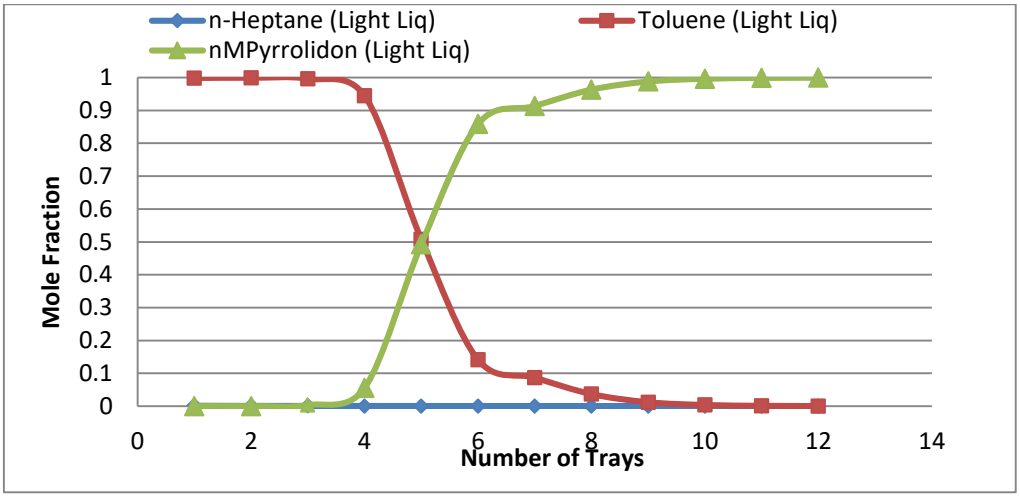

Figure 6. Change in the mole fraction of Toluene, n-Heptane, and NMP versus the Number of Trays in the second column T-101

Conclusion

The simulation carried out with Aspen Hysys Software shows that extractive distillation is an excellent technique for the separation of a toluene / normal heptane mixture that is an azeotrope-like mixture and has quasi-isotropic behavior and therefore is difficult to separate by ordinary distillation. The relative volatility of the components was greatly increased with the N-methyl-2-pyrrolidone as a selective solvent, and they could be separated easily. The developed process includes two distillation columns, one with fourteen theoretical stages and the other with ten. The result showed that a mixture of 50% toluene and 50% normal heptane as a feed was processed at about 962 kg/h with a circulating solvent flow of about 2947 kg/h by the toluene recovery under given conditions. The achievable purity and recovery of the solvent are also simulated, and the feasibility of obtaining high-purity toluene (≈99.9%) at a recovery rate of 460 kg/h is demonstrated. These findings suggest that the NMP-based extractive distillation would have a superior separation capability with a lower solvent-to-feed ratio and better separation performance, and these are also comparable to the best available results for the separation of aromatic compared to aliphatic hydrocarbons using petroleum solvent for refining and extracting processes.

Recommendations:

1. Some further optimization of operating conditions (solvent/feedstock ratio, reflux ratio, number of theoretical stages) is still possible to decrease energy consumption and increase the efficiency of the overall process.
2. In the coming, an economic analysis of the extractive distillation process should be considered to evaluate the investment and operating costs for its application on an industrial scale.
3. Investigation of other selective solvents with lower energy demands or with higher selectivity may lead to better separation performance.
4. Dynamic simulation and process control study in Aspen Hysys is suggested to verify dynamic stable operation over feedstock and operating condition changes.
5. Laboratory or pilot-scale experiments are recommended to validate the simulation findings and to investigate the real process performance.

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