

Research Article

Muntadher Sallah Hussain*, Mohammad N. Fares and Mohammad A. Taher

Optimization and design of a new column sequencing for crude oil distillation at Basrah refinery

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Abstract: The utilization of distillation stands as a predominant separation method within the chemical and petroleum industries, prominently influencing operational costs and environmental impact due to energy consumption. Enhancing energy efficiency holds paramount significance in elevating the sustainability and overall efficacy of distillation operations. Within this study, we introduce an innovative approach termed “marginal vapor flow (MVF)” to optimize the distillation column sequence for crude oil processing, focusing on the third distillation unit at the Basra Refinery. This research evaluates diverse column designs through streamlined simulations using Aspen HYSYS V11 software. The study determines total energy consumption as a benchmark, comparing it against the optimal sequence recommended by the MVF methodology. A novel application of the downward reduction equation to crude oil guides the selection of light and heavy components. Key findings from this comprehensive analysis showcase the potency of combining MVF with Aspen HYSYS for optimizing crude oil distillation column sequences. Aspen HYSYS, a widely recognized process simulation tool, accurately represents distillation processes. Simultaneously, MVF facilitates the determination of optimal column sequences based on marginal vapor flow rates. Notably, the results reveal that within the studied sequences, sequence 9 exhibits the lowest total MVF of (1393.4 kmol/h), signifying its optimality, while sequence 2 displays the highest total MVF of (4827.3 kmol/h), representing the least favorable scenario. Simulation of the optimal sequence derived through the MVF approach exhibits a remarkable 35% reduction in

energy consumption compared to real-life operations. Conversely, simulating the least favorable sequence demonstrates a substantial 32% increase in energy consumption compared to actual operations. This study underscores the pivotal role of MVF methodology in optimizing distillation sequences for enhanced energy efficiency, providing actionable insights for refining operations to significantly reduce energy consumption and operational costs while advancing sustainability goals.

Keywords: marginal, hysys, optimal, distillation, sequence

1 Introduction

The foundation of chemical engineering lies in process design, a crucial element enabling efficient separation and manufacturing of pure products based on specific criteria [1,2]. The significance and economic benefits of process design have grown with the scale of chemical manufacturing, particularly in response to escalating environmental concerns [3,4]. Process design, rooted in knowledge derived from existing processes and modified through case-based reasoning, has evolved alongside technological advancements, especially with the advent of computers facilitating process modeling [5,6]. The introduction of computers has not only enabled process modeling but has given rise to process systems engineering, optimizing design and enhancing chemical processes. As these tools became more accessible, sophisticated mathematical models emerged, enhancing process modeling accuracy and fostering improved adaptability for exploring design alternatives [7,8]. Recognizing the immense value of proper process design is paramount, as it not only leads to significant cost savings but also contributes to energy conservation [4]. The foundation of chemical engineering is process design, which enables the efficient and effective separation and production of pure products according to specific requirements. The importance of process design and its economic advantages have gained recognition as the production of chemicals increases,

* **Corresponding author: Muntadher Sallah Hussain**, College of Engineering, Basra University, Basra, Iraq, e-mail: pgs.muntadher.sallah@uobasrah.edu.iq

Mohammad N. Fares: College of Engineering, Basra University, Basra, Iraq, e-mail: mahmod.faris@uobasrah.edu.iq

Mohammad A. Taher: College of Oil and Gas Engineering, Basra University for Oil and Gas, Basra, Iraq, e-mail: moh.may@buog.edu.iq

simultaneously with escalating environmental concerns and energy consumption. The chemical and petroleum industries use distillation more frequently than any other separation method. Distillation, being the most widespread separation system, is also the most energy-consuming with 40–60% of the energy used in chemical and refining industries, accounting for about 3% of global energy consumption [9–11]. Energy expenditure is a critical factor that affects the operational cost of distillation operations and the environmental impact. Implementing energy-saving methods is therefore an important aspect of increasing the overall efficiency and sustainability of distillation operations. Reducing energy costs in distillation operations is critical to improving efficiency and sustainability. Ways to reduce energy use include thermal integration (reuse of waste heat); use of high-efficiency distillation column trays; optimization of process parameters such as feed flow rate and reflux ratio; and implementation of advanced control systems. One important method to consider is sequential or multi-stage distillation. This method uses multiple distillation columns in a sequence or stage to separate mixtures into their different components. Each distillation column focuses on the separation of a specific fraction or component, thus increasing efficiency and reducing energy use. Multicomponent distillation sequencing, a challenging combinatorial problem, has been extensively studied [12–15]. As the number of components in the feed stream increases, the number of viable solutions grows [1,13,16], with fixed and operating costs varying significantly even among sequences yielding the same products [17–19].

The distillation column sequence, a vital process in chemical engineering, involves interconnected columns operating at different pressures and temperatures to optimize separation [20,21]. It offers enhanced efficiency and improved product purity compared to single distillation columns [20]. The specific arrangement of columns depends on the characteristics of the mixture and desired separation objectives [21].

To reduce energy consumption during distillation, some researchers have used step distillation, which involves two sets of columns. The first set of columns is arranged in a direct sequence, while the second set is in an indirect sequence. Studies conducted by Steven *et al.* (2009), Anita *et al.* (2014), and Shankar *et al.* (2018) showed that this technique is cost-effective and low-energy efficient [22–24]. In addition to what has been mentioned, several researchers have studied reducing energy consumption in distillation systems by finding an appropriate distillation sequence that guarantees energy saving. Gadalla *et al.* introduced a retrofitting design for simple and complex columns and crude oil distillation columns [25]. Gadalla introduced a new method to determine critical components based on

distillates' specifications of crude oil columns. Chen (2008) introduced a new configuration of crude oil distillation and compared it with different configurations [26]. The results showed the advantages of new designs in terms of energy efficiency. The heat integration of three different arrangements of sequential distillation columns for the separation of benzene, toluene, xylene, and C9+ was studied by Masoumi and Kadkhodaie in 2012. These arrangements include different combinations of indirect sequence and forward and backward heat integration [27]. Rahimi *et al.* (2015) found the best sequence of distillation columns using the driving force method, which consists of four hierarchical steps: Step 1: Analysis of the current sequence energy; Step 2: Determine the optimal sequence; Step 3: Optimum sequence energy analysis; and Step 4: Energy comparison. The authors found that this method reduced energy consumption by about 39.6% [28]. In 2021, Louhi *et al.* conducted a study to improve the composition of the distillation column. They applied it to gas-to-liquid distillation by separation matrix, achieving the lowest operating costs, capital costs, and energy losses [29]. Ibrahim *et al.* (2018) also used alternative column models and support vector machines to choose an optimal crude oil distillation tower design, reducing energy expenditure [30].

Previous research has highlighted the importance of sequential distillation systems as cost-effective alternatives to conventional distillation. As mentioned above, various techniques have been used to determine optimal configurations, such as driving force, marginal vapor flow, mathematical modeling, and simulation software. These techniques have been applied extensively to binary and multi-component systems of pure components. However, crude oil distillation systems have not been well covered, and the marginal vapor flow rate has not been fully exploited for selecting a proper distillation configuration.

In our study, the MVF method was employed to select an appropriate distillation column sequence based on the relative volatility of the constituents, avoiding the need for complete column designs or cost calculations. As part of our work plan, we focused on improving energy consumption in the third crude oil distillation unit at the Basrah refinery.

2 Methodology and procedure

2.1 Materials

2.1.1 Basra crude oil

The crude oil properties were provided by the third crude oil refining unit, which is a unit of the Basrah Refinery in

Iraq. However, the crude oil used in this unit is considered a light oil. These characteristics were measured and calculated by the manufacturer of this unit (Technoexport company). Table 1 shows the characteristics of Basra crude oil.

2.1.2 Crude oil distillation unit products

The Basra refinery's third crude oil distillation unit produces five products within the specifications set by the company that designed this unit. These products are listed in Table 2.

2.1.3 Equipment selection of the methodology

In this section, details of some of the equipment inside the third crude oil distillation unit of interest to us in research

Table 1: The characteristics of crude oil

| Feed – crude oil | kg/h | 397,000 |
|----------------------------|----------------------|-------------|
| Basrah | | |
| API Gravity at 15.6°C | | 33.6 |
| Spec. Gravity at 15.6°C | | 0.855 |
| Kinematic viscosity | | |
| at 20°C | cSt | 9.66 |
| at 37.8°C | cSt | 6.13 |
| Sulfur content | wt% | 2.11 |
| H2S | wt% | 0.0012 |
| Pour point | °C | <-20 |
| R. V. P. | kg/cm ² a | 0.34 |
| Water & sediment | vol% | 0.051 wt% |
| Salt content | ppm | 80 mg/lmax. |
| Light ends | | |
| C2 | wt% | 0.01 |
| C3 | wt% | 0.27 |
| i-C4 | wt% | 0.181 |
| n-C4 | wt% | 0.92 |
| i-C5 | wt% | 0.72 |
| n-C5 | wt% | 1.24 |
| Distillation T.B.P. | | |
| At 50°C | wt% | 3.8 |
| At 60°C | wt% | 4.1 |
| At 70°C | wt% | 5.8 |
| At 80°C | wt% | 6.4 |
| At 100°C | wt% | 9.2 |
| At 120°C | wt% | 11.6 |
| At 150°C | wt% | 17.1 |
| At 180°C | wt% | 22.24 |
| At 200°C | wt% | 25.04 |
| At 250°C | wt% | 33.85 |
| At 300°C | wt% | 42.33 |
| At 350°C | wt% | 50.57 |
| At 400°C | wt% | 58.14 |

and experimental work are described including the selection of parameters for all components of the equipment as well as the operational conditions under which the equipment operates. All parameters and operating conditions were provided from the third crude oil distillation unit at the Basrah Refinery, in addition to the assistance of the designer company (Technoexport company). The specification of the equipment is shown in Table 3.

2.1.4 Simulation procedures for a third crude oil distillation unit

This section will discuss simulation procedures for the third crude oil distillation unit in Basrah Refinery. The objective of the experimental simulation is to carry out the experimental work to validate the theoretical model of the unit.

The procedures are as follows:

1. Open the Aspen Hysys simulation software.
2. Through the (Oil Manager) command, add the characteristics of the crude oil in Table 1, and this is the simulated feed to the unit.
3. Insert the heat exchanger equipment through the list (Model Palette), and add the specifications in Table 3.
4. Insert the Fired heater equipment through the list (Model Palette), and add the specifications in Table 3.
5. Insert Distillation column equipment through the list (Model Palette), and add the specifications in Table 3.
6. After completing the simulation of the feeding and equipment used, press the Run command to run the simulation process for the entire unit.

2.2 Number of distillation sequences

One important method for conserving energy during the distillation procedure is distillation sequence synthesis. When looking for the best distillation sequence in process synthesis, an estimation of the total number of potential sequences is crucial information. According to the simple column hypothesis, which states that one feed is divided into two streams in each column without component mixing between the two output streams or sharp split, the distillation sequence has been thoroughly investigated [31]. The basic column distillation sequence number's general term formula has been attained [8]. The work presents splits for five-component separations by a sequential enumeration technique [32]. There are multiple solutions for a single case because it was conducted for a particular

Table 2: The characteristics of Crude oil distillation unit products

| Product | Boiling temperature (°C) | Spec. gravity at 15°C | Flash point (°C) | Sulfur content (wt%) |
|---------------|--------------------------|-----------------------|------------------|----------------------|
| Naphtha + LPG | 35–175 | 0.710–0.725 | — | 0.007–0.015 |
| Kerosene | 170–230 | 0.785–0.800 | 40 min. | — |
| LGO | 230–300 | 0.825–0.840 | 70 min. | — |
| HGO | 300–340 | 0.870–0.885 | 90 min. | — |
| RCR | 340+ | 0.950–0.965 | 120 min. | — |

industrial application. The discussion based on the premise of a sharp split, however, has theoretical relevance to separation issues in general.

According to Seider, the recursive formula and general term formula for the number of distillation sequences using only basic columns are as follows [21]:

$$R_s = \sum_{j=1}^{s-1} R_j R_{s-j}, \quad (1)$$

$$R_s = \frac{[2(S-1)]!}{S!(S-1)!}, \quad (2)$$

where R_s is the number of different sequences of the ordinary distillation column, S is the number of products, and j is the number of final products that must be developed from the distillate of the first column.

2.3 Marginal vapor flow method

Modi and Westerberg recommended this strategy (1992). This method can be used without requiring complete

column designs or cost calculations and is superior to previous methods for determining the optimal distillation column sequence. The minimal sum of column MVs is used to define the sequence. Vapor rate, which is a key determinant of column diameter, reboiler, and condenser areas (and, consequently, column and heat exchanger construction costs), as well as reboiler and condenser tasks, makes for a good prediction of cost (thus, heat exchanger annual operating costs).

To accommodate the total vapor flow, we need to solve each of the Underwood equations for each column of the distillation sequence for all the sequences.

$$V_{\min, \text{top}} = Ds(R_{\min} + 1) = \sum_{i=1}^{Nc} \frac{\gamma_{i,j} Ds X_{i, Ds}}{\gamma_{i,j} - \phi}, \quad (3)$$

$$V_{\min, \text{bottom}} = R_{\min} Bo = - \sum_{i=1}^{Nc} \frac{\gamma_{i,j} Bo X_{i, Bo}}{\gamma_{i,j} - \phi}, \quad (4)$$

where $V_{\min, \text{top}}$, $V_{\min, \text{bottom}}$ is vapor molar flow rate, kmol/h, R_{\min} is the minimum reflux ratio, Ds , Bo is the molar flow rate at distillate and bottom, kmol/h, $\gamma_{i,j}$ is the relative

Table 3: Specifications of distillation unit equipment

| The specification | Heat exchange | Fired Heater | Distillation Column |
|--|---------------|--------------|---------------------|
| Temperature Inlet (°C) | 40 | 266 | 349 |
| Temperature outlet (°C) | 266 | 349 | — |
| Pressure inlet (kg/cm ² g) | 23.3 | 14.9 | 1.6 |
| Pressure outlet (kg/cm ² g) | 14.9 | 1.6 | — |
| Mass flow (kg/h) | 397,000 | 397,000 | 397,000 |
| Air temperature (°C) | — | 40 | — |
| Air pressure (kg/cm ² g) | — | 1.05 | — |
| Fuel temperature (°C) | — | 40 | — |
| Fuel pressure (kg/cm ² g) | — | 5 | — |
| Condenser pressure (kg/cm ² g) | — | — | 1.2 |
| Condenser pressure drop (kg/cm ² g) | — | — | 0.2 |
| Number of trays | — | — | 46 |
| S.S Kerosene (kg/h) | — | — | 18,700 |
| S.S LGO (kg/h) | — | — | 30,900 |
| S.S HGO (kg/h) | — | — | 7,200 |
| PA1 (kg/h) | — | — | 300,480 |
| PA2 (kg/h) | — | — | 300,000 |

volatility of the light key component to the heavy key component, ϕ is the root of Underwood's equation. These two equations would suggest that $V_{\min, \text{top}}$ is increased by an amount $\sum_{\text{non Key } i}^{Nc} \frac{y_{i,j} Ds X_{i,Ds}}{y_{i,j} - \phi}$ for the presence of components in distillate lighter than the light key (LK). $V_{\min, \text{bottom}}$ is increased by an amount $-\sum_{\text{non Key } i}^{Nc} \frac{y_{i,j} Bo X_{i,Bo}}{y_{i,j} - \phi}$ for the presence of components in the bottoms heavier than heavy key (HK).

Assumptions:

The nonkey components are lighter than LK or heavier than HK. They will be essentially recovered in the respective products so that we can substitute the product flows with the feed flows. Also, we assume the interval halving: the root ϕ is located in the middle of the LK and HK relative volatilities.

$$v = \left| \frac{y_{i,j} Fi}{y_{i,j} - \left(\frac{y_{LK,j} + y_{HK,j}}{2} \right)} \right|. \quad (5)$$

The marginal vapor flow in a column with LK and HK as light and heavy key components is the added vapor flow required in the column because of the presence of the nonkey components.

$$MFV_{LK/HK} = \sum_{\text{non key } j} v_{LK/HK} = \sum_{\text{non key } j} \left| \frac{y_{i,j} Fi}{y_{i,j} - \left(\frac{y_{LK,j} + y_{HK,j}}{2} \right)} \right|. \quad (6)$$

Due to the commonality of all sequences' binary splits, this amount can be compared across all. The existence of other species differentiates the sequences.

3 Results and discussions

3.1 Simulation of a crude oil distillation unit

In the first step, crude oil was simulated using simple, concise, and reliable software (Aspen Hysys V11; Figure 1) [33]. The crude oil distillation unit was simulated in the second step, producing five products with different boiling points. The energy used in the main distillation column is analyzed and taken as a reference (Table 4).

After completing the simulation process for the third crude oil distillation unit in the Aspen Hysys program and making sure that the process works correctly, the amount of energy consumed is now calculated. The simulation results showed that the total energy consumed to produce 885.5 kmol/h of naphtha, 235.4 kmol/h of kerosene, 300.7 kmol/h of LGO, 35.67 kmol/h of HGO, and 395.1 kmol/h of RCR is about 1.37×10^8 kJ/h. This energy will be taken as a reference to find the best distillation column sequence.

3.2 Potential distillation column sequences

The marginal vapor flow method will be applied to the distillation column in the crude oil distillation unit of the Basra refinery (Table 5).

In the first step, the number of possible sequences for the distillation column is found using equation (2), and when applied to the products of the distillation column in the Basra Refinery, the number of possible sequences is obtained as shown in Table 6 (Figure 2).

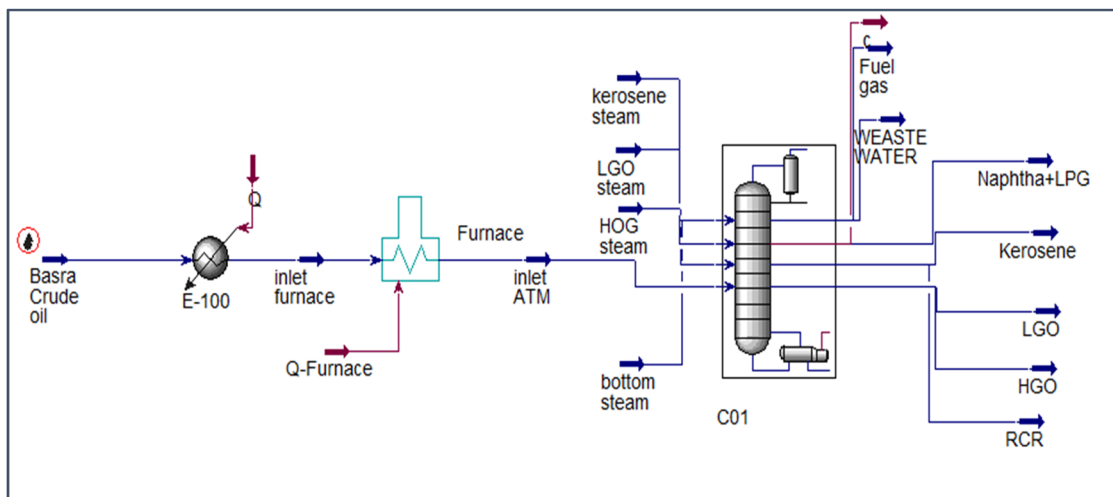


Figure 1: The basic flowsheet of crude oil distillation in Hysys.

Table 4: Compare product specifications

| Product name | Crude distillation unit | | Simulated results | |
|---------------|--------------------------|--------------------|--------------------------|--------------------|
| | Boiling temperature (°C) | Flow rate (kmol/h) | Boiling temperature (°C) | Flow rate (kmol/h) |
| Naphtha + LPG | 35–175 | 898.4 | 68.49 | 885.5 |
| Kerosene | 170–230 | 246.7 | 211.7 | 235.4 |
| LGO | 230–300 | 308.27 | 274.4 | 300.7 |
| HGO | 300–340 | 40.8 | 316 | 35.67 |
| RCR | 340+ | 383.2 | 343.9 | 395.1 |

Table 5: Distillation column products in Basra refinery

| Distillation tower products | Abbreviated | Molar flow rate (kmol/h) |
|-----------------------------|-------------|--------------------------|
| Naphtha + LPG | A | 897.5 |
| Kerosene | B | 247.4 |
| LGO | C | 307.7 |
| HGO | D | 39.67 |
| RCR | E | 385.1 |

Table 6: Possible separation sequences

| Number of Distillates, S | Number of separators in each sequence | Number of sequences, R_s |
|----------------------------|---------------------------------------|----------------------------|
| 5 | 4 | 14 |

3.3 Volatility of crude oil distillation column products

In the second step, process simulation software (Aspen Hysys V11) was used for the determination of k values. It is worth noting that each of the five products consists of a set of pseudo components. The mole fraction distribution of pseudo components for each product is presented in Figure 3. The pseudo component with the highest mole fraction was used to determine the volatility of the product [34].

3.4 Optimization steps distillation column sequencing

Equation (5) is used to calculate the vapor flow as shown in Table 7.

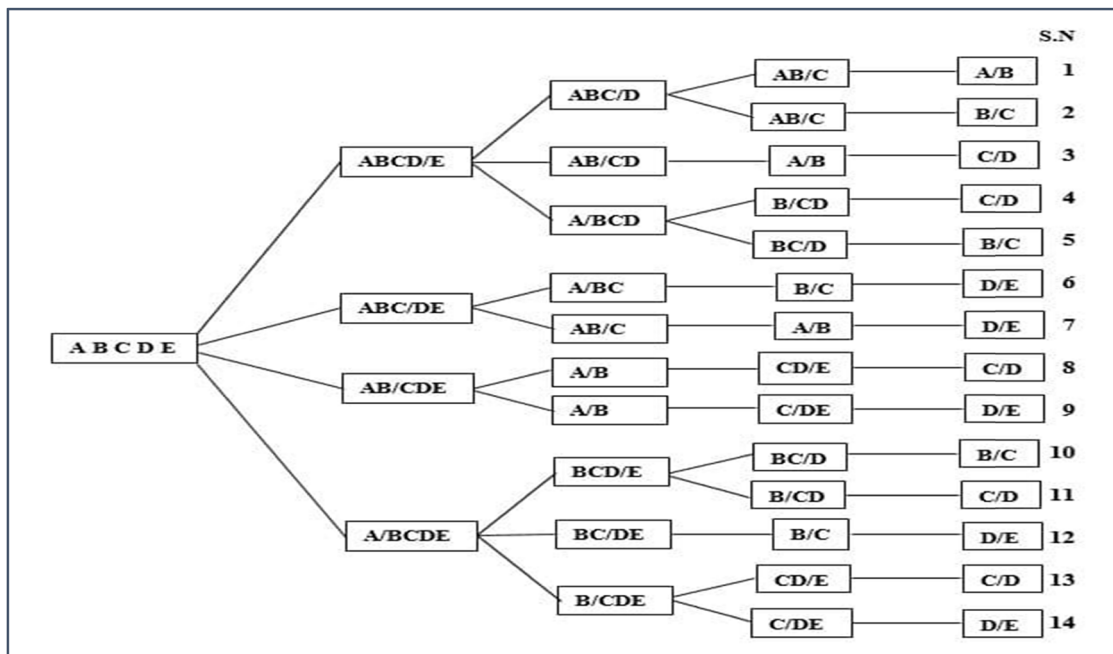


Figure 2: Potential distillation column sequences.

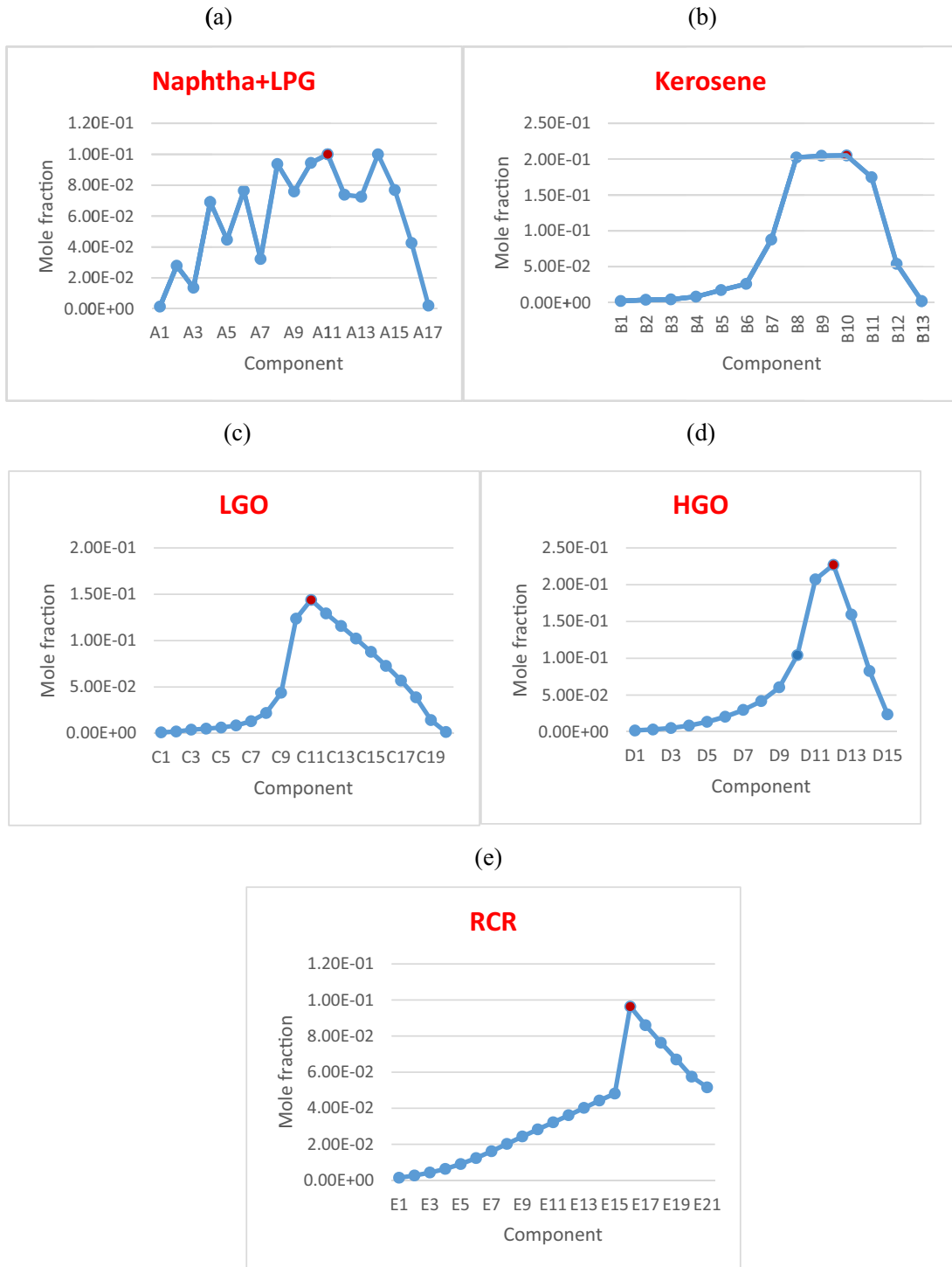


Figure 3: (a-e) Components of the product.

Starting from the above table, we can evaluate each sequence’s total marginal vapor flow (Figure 4; Table 8).

The results identified sequence 9 as optimal due to its lower total marginal vapor flow of 1,393 kmol/h. A simulation was conducted using the program Aspen HYSYS V11 to

determine the optimal sequence based on the minimum total marginal vapor flow. To validate the claim of the marginal vapor flow method, the simulation was also conducted for the best and worst possible sequences within this method. The simulated results proved the validity of

Table 7: Calculation of the vapor flow for each product

| Key Split (LK/HK) | $1/2(Y_{LK} + Y_{HK})$ | V_A (kgmol/h) | V_B (kgmol/h) | V_C (kgmol/h) | V_D (kgmol/h) | V_E (kgmol/h) |
|-------------------|------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| A/B | 2.47 | — | — | 2003.28 | 1.56 | 8.62 |
| B/C | 1.42 | 1134.71 | — | — | 7.83 | 62.94 |
| C/D | 5.35 | 970.34 | 339.47 | — | — | 187.89 |
| D/E | 1.98 | 903.41 | 254.08 | 356.71 | — | — |

the marginal vapor flow method in determining the optimal sequence where the required heating duty was 35% less in the minimum vapor flow sequence compared to the conventional distillation system (Figures 5 and 6; Tables 9 and 10).

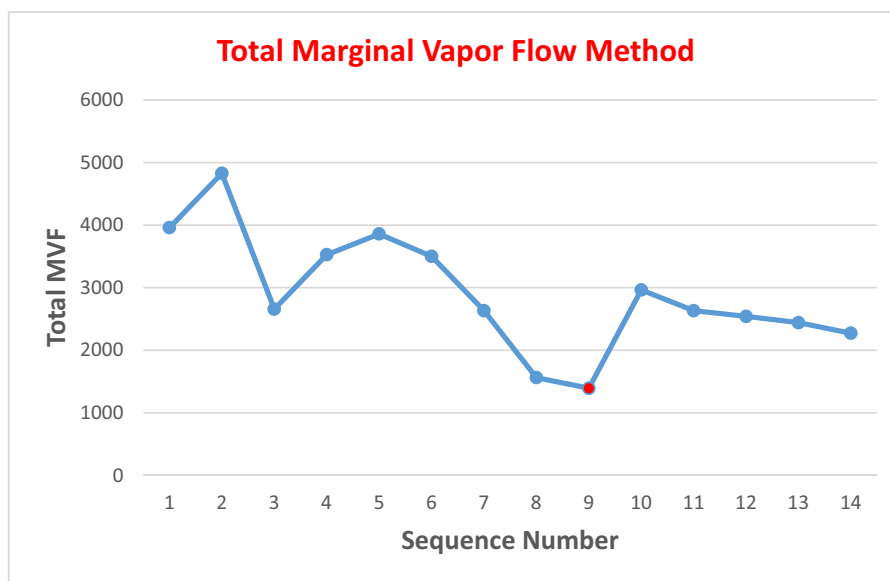
4 Conclusions

This study delved into the utilization of the Marginal Vapor Flow Method (MVF) alongside Aspen HYSYS simulation software to ascertain the most efficient column sequence for crude oil distillation. Through a comprehensive analysis of diverse parameters and performance indicators, pivotal insights were gleaned. The amalgamation of MVF with Aspen HYSYS showcased a robust and effective strategy for optimizing column sequences in crude oil distillation. Aspen HYSYS, renowned as a widely employed process simulation tool, provided an authentic portrayal of the distillation process. Concurrently, MVF enabled the identification of the optimal column sequence predicated on marginal vapor flow rates. The findings underscored the substantial

Table 8: Calculation of the marginal vapor flow of each sequence

| Sequence | MVF_{C1} (kgmol/h) | MVF_{C2} (kgmol/h) | MVF_{C3} (kgmol/h) | Total MVF (kgmol/h) |
|----------|----------------------|----------------------|----------------------|---------------------|
| 1 | 1514.20 | 1309.81 | 1134.71 | 3958.72 |
| 2 | 1514.20 | 1309.81 | 2003.28 | 4827.28 |
| 3 | 1514.20 | 1142.54 | 0.00 | 2656.74 |
| 4 | 1514.20 | 2004.83 | 7.83 | 3526.87 |
| 5 | 1514.20 | 2004.83 | 339.47 | 3858.50 |
| 6 | 1497.70 | 2003.28 | 0.00 | 3500.97 |
| 7 | 1497.70 | 1134.71 | 0.00 | 2632.41 |
| 8 | 1205.49 | 0.00 | 356.71 | 1562.19 |
| 9 | 1205.49 | 0.00 | 187.89 | 1393.38 |
| 10 | 2013.46 | 610.79 | 339.47 | 2963.71 |
| 11 | 2013.46 | 610.79 | 7.83 | 2632.08 |
| 12 | 2013.46 | 527.36 | 0.00 | 2540.81 |
| 13 | 2013.46 | 70.78 | 356.71 | 2440.94 |
| 14 | 2013.46 | 70.78 | 187.89 | 2272.12 |

impact of the optimal column sequence on energy consumption, separation efficiency, and product quality during crude oil distillation. The integrated approach not only facilitated the identification of the most efficient arrangement but also

**Figure 4:** Best and worst sequence for total marginal vapor flow method.

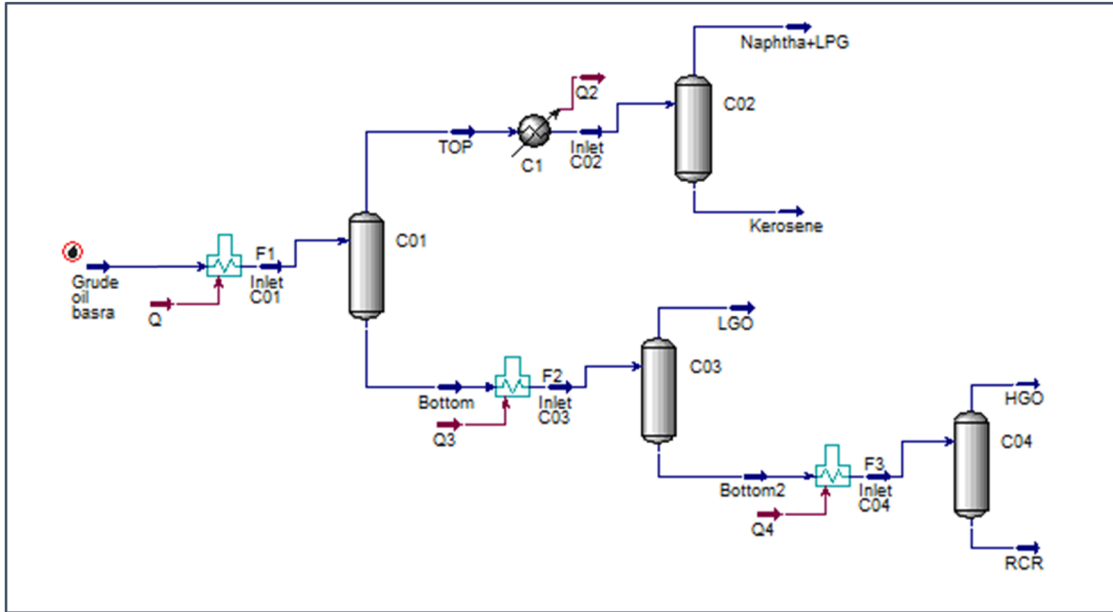


Figure 5: Best sequence (sequence 9).

resulted in heightened energy efficiency and increased product yields. Aspen HYSYS' capacity to consider diverse process parameters such as temperature, pressure, and feed compositions significantly bolstered the accuracy and dependability of the optimization process. The dynamic nature of Aspen HYSYS also allowed for scenario simulations, enabling an evaluation of their implications on the optimal column sequence. The outcomes of this research bear practical implications for the petroleum refining industry. The implementation of MVF alongside Aspen HYSYS empowers refineries to optimize their crude oil distillation processes, leading to heightened operational efficiency, reduced energy consumption,

Table 9: Compare total duty between conventional distillation and distillation sequence (9)

| | |
|--|--------------------|
| Total duty for distillation sequence (9), MW | 8.81×10^4 |
| Total duty for conventional distillation, MW | 13.7×10^4 |

Table 10: Compare total duty between conventional distillation and distillation sequence (2)

| | |
|--|---------------------|
| Total duty for distillation sequence (2), MW | 20.16×10^4 |
| Total duty for conventional distillation, MW | 13.7×10^4 |

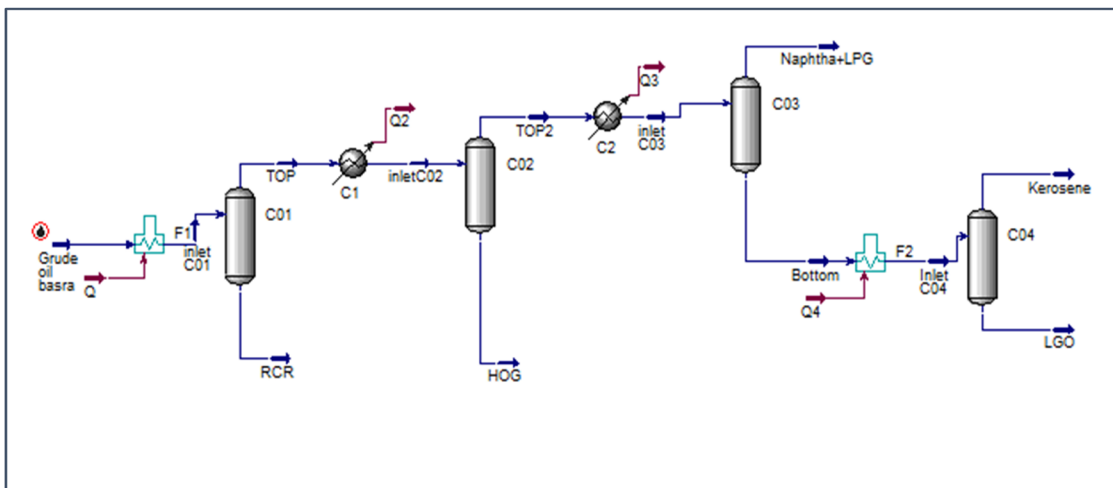


Figure 6: Worst sequence (sequence 2).

and augmented product yields. These enhancements bring about substantial economic and environmental benefits for the industry. Moreover, the study revealed that Sequence 9 demonstrated the minimum total MVF (1393.4 kmol/h), signifying its status as the optimal sequence, while Sequence 2 exhibited the maximum total MVF (4827.3 kmol/h), marking it as the least optimal sequence. Simulating the optimal sequence illustrated a remarkable 35% reduction in energy consumption compared to reality. Conversely, simulating the worst sequence resulted in a substantial 32% increase in energy consumption compared to reality. In conclusion, this research not only underscores the crucial impact of column sequence on crude oil distillation efficiency but also highlights the potential for significant energy savings and operational enhancements through the application of the MVF method in conjunction with Aspen HYSYS. Future studies could further explore additional variables and scenarios to refine and expand upon these findings, paving the way for continued advancements in refining processes and sustainability within the industry.

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Data availability statement: Most data sets generated and analyzed in this study are comprised in this submitted manuscript. The other data sets are available on reasonable request from the corresponding author with the attached information.

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