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Enhancement of Ternary LNG Mixture Separation Process by Using Dividing Wall Column

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ABSTRACT

The dividing wall column (DWC) represents a form of process intensification that offers the potential to lower energy usage and initial investment costs in distillation practices. This research undertakes a systematic optimization and economic comparison between DWC and a traditional distillation column process for the separation of a three-component mixture of N-Pentane, N-Hexane, and N-Heptane. The analysis delves into the exergy flows and economic aspects of these two processes in detail. In this study the sequential quadratic programming (SQP) optimization method was used to minimize the total reboiler and condenser duties and the Peng Robinson model is applied to predict the vapor-liquid equilibrium (VLE) of the systems under study. In this study, DWC is evaluated against a conventional two-column distillation setup in terms of total annual cost (TAC) and energy consumption under the same feed ratio conditions. The results show that implementing DWC leads to a 37% decrease in TAC and a 38% reduction in energy requirements. This research proposes the use of dividing wall columns as an alternative to traditional distillation columns, providing a new method for separating hydrocarbons that emphasizes economic efficiency and encourages the adoption of innovative practices for energy conservation and environmental protection.

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1. Introduction

The increase in energy costs and economic difficulties has highlighted the necessity for natural gas and liquid recovery facilities to improve their sophistication and efficiency. Essentially, the latest NGL plants are structured to lower both fixed and operational expenses without compromising on their production levels. Two crucial factors that can significantly impact process performance are process configuration and plant operation (Mehrpooya, Vatani et al. 2010). Distillation is widely recognized as one of the most frequently utilized processes in chemical industries and petrochemical (Shahruddin, Uzuman et al. 2025).

Distillation is recognized as one of the most energy-demanding separation methods, responsible for consuming more than 40% of the energy consumed in the petrochemical and chemical industry. Additionally, it constitutes roughly 95% of the total energy used for separation in both the refining and chemical processing sectors. Despite its significant energy requirements, distillation continues to be a fundamental separation technique because of its straightforwardness and efficiency. As of now, there are approximately 40,000 operational distillation columns utilized in more than 200 distinct processes (Biasi, Zemp et al. 2024). In today's energy-conscious society, conventional distillation processes are both cost and energy intensive. It is crucial to enhance the sustainability and economic viability of distillation systems. Heat-integrated distillation columns, such as the dividing-wall column (DWC), have been proposed and investigated for NGL recovery processes. Dividing-wall column, as a practical intensification technology, demonstrates significant advantages in this regard. Because of its compact equipment design and minimized remixing effects, a DWC necessitates lower capital and operating costs for the separation of multicomponent mixtures compared to traditional distillation setups (Li, Guan et al. 2024). The Dividing Wall Column was first designed by R.O. Wright in 1949 as an improved column setup. It includes a vertical partition wall that divides the column into a main section and a pre-fractionation section. This wall helps reduce the remixing of intermediate components, leading to higher energy efficiency compared to traditional distillation sequences. The inaugural industrial deployment of a DWC occurred at BASF in 1985. Since then, only over 200 DWCs have been erected globally. One obstacle hindering widespread DWC adoption is the challenging task of tightly managing the vapor split ratio, which typically operates within a narrow range (Song, Cui et al. 2024). With reference to Fig 1. the distinction between the Dividing Wall Column (DWC) and the Simple Distillation Column (SDC) is clearly visible. The DWC features a vertical dividing wall that separates it into two sections: the prefractionator on the left side and the main column on the remaining side. The ternary feed is initially introduced into the prefractionator, where it is separated into two primary binary mixtures. These mixtures then flow into the main column, bypassing the dividing wall, for further refinement and separation into three pure products. (Yuan, Zhang et al. 2024). the three-component feed (A, B, C) enters from the pre-fractionator side. In this section, the heaviest and lightest are separated. The lightest composition (A) and part of the composition with the middle boiling point (B) travel to the top of the wall and the lightest component (A) leave the top of the tower as a distillate. The heaviest composition (C) along with a part of (B) deflected towards the bottom of the wall and the heaviest composition exits from the bottom of the tower. The middle boiling point (B), which moves up and down the wall along with the light and heavy currents, is separated on the back side of the wall and exits from the middle of the tower by a tensile flow (Ränger, Halvorsen et al. 2025). Therefore, the DWC is two different distillation columns in one unit separated by a wall. Since two separation steps are being merged into one unit, it can be referred to as process integration. So, compared with conventional distillation columns, DWCs reduce plant space, equipment investment, and energy consumption (Kolbe and Wenzel 2004, Liu, Zhao et al. 2022). This innovative column design effectively addresses the issue of re-mixing the intermediate component, setting it apart from conventional direct or indirect SDC sequences.

When evaluating design options for multi-component separation, the primary measure is often used total annual cost (TAC). Processes with lower TAC are generally more energy-efficient, as energy usage is a key factor influencing costs. However, a more comprehensive insight can be gained by examining metrics directly linked to energy analysis and TAC. Researchers have employed energy analysis and TAC to assess the effectiveness of various distillation alternatives a wide range of systems including hydrocarbons, alcohols, aldehydes, ketones, amines. Yanyang et al.(Wu, Zhang et al. 2020) optimized TAC and total energy loss simultaneously for separation of the three diols. In this study, DWC was evaluated against both a side rectifier configuration and a conventional distillation column in terms of energy consumption and total annual costs, while using an equal number of stages. The findings revealed a 47.60% reduction in energy requirements and a 35.40% decrease in TAC when using DWC compared to the traditional distillation column. Furthermore, compared to the side rectifier configuration, DWC exhibited a 48.00% reduction in energy consumption and a 34.11% decrease in total annual costs. Li et al. (Li, Zhang et al. 2020)optimized DWC to separate ternary mixtures of alcohol systems. In this work, used response surface methodology (RSM) to obtain optimal operation parameters and compared with to the conventional process. Result showed that DWC can decrease energy consumption and total annual cost by 25.43%, 33.39%, and 28.73% respectively and increase thermodynamic efficiency. In an tray to reduce the costs related with DWC, Wu et al. (Wu, Zhang et al. 2020) precented Sequential quadratic programming (SQP) to optimize the separation of the ternary components. As a result, illustrated that DWC can reduce total annual costs (TACs) and energy requirements significantly compared with traditional two-column distillation process. In another work, to separate azeotrope three components, Wang et al. (Wang, Song et al. 2023) proposed the use DWC. They obtained an energy saving of 37% and TAC 43.5% compared conventional azeotrope distillation. The advantages of this new technology are reducing energy consumption, reducing investment costs, high thermodynamic efficiency, and reducing the required space. Natalie et al. (Czarnecki, Giannetti et al. 2024) conducted research on how the positioning of walls affects the economics and energy consumption in a simulated chemical system. Their goal was to create an azeotropic composition of water and isopropanol. Different wall placement sequences such as direct conventional, indirect conventional, middle wall divided wall column (DWC), top wall DWC, and bottom wall DWC were analyzed through Aspen Plus simulations. The results showed that the middle wall DWC option required a fixed capital investment of at least 8% less, while achieving energy savings of 14% compared to conventional sequences. In order to improve the intensification process, Andrade et al.(Andrade, Andrade et al. 2024) compared two improved setups for the downstream separation phase of the Methanol-to-Olefins (MTO) process to enhance the intensification process. They found that the configuration with two DWCs was more efficient, saving 15.56% energy in the reboiler, cutting total annual costs by 7.68%, and lowering daily CO_2 emissions by 11.33 tons, representing a 14.19% reduction compared to the traditional method.

To design DWC, in 1992 Triantafyllou and Smith presented the first methods to design DWCS (FUGK) (Di Pretoro, Ciranna et al. 2021). The minimum vapor flow rate (V_min) was presented by Halvorsen (Halvorsen and Skogestad 2011). In another research, Lavasani et al. (Lavasani, Rahimi et al. 2018) used response surface methodology (RSM) to design and optimize the parameters of the DWC. In a similar work (2020), Chunli et al. studied (RSM) method to obtain optimal parameters (Li, Zhang et al. 2020). Finally, Ceron et al. (Buitimea-Cerón, Hahn et al. 2021) evaluated three methodologies to design and optimize DWCs. They showed that the Sotudeh and Shahraki (S&S) method was the most efficient technique.

In distillation sequences, intricate columns that are thermally connected and operate based on the concept of process enhancements are employed to reduce the remixing of non-essential elements. As a result, this leads to a more energy-efficient separation process and the potential for reducing operational and investment costs. Among these complex columns, dividing-wall columns (DWC) are commonly considered as a favored option in distillation sequence design scenarios (Li, Finn et al. 2023). By eschewing remixing, DWCs typically achieve a 20-40% reduction in energy consumption compared to the most efficient conventional two-column sequence. Each single DWC shell substitutes for two traditional columns, along with their related ancillary equipment (such as one condenser, one reboilers, and fewer pumps and vessels), resulting in potential capital cost savings of up to 30%. This decreased energy usage not only results in a diminished carbon footprint and lower greenhouse gas emissions but also aligns with the principles of green engineering.

The main importance of this study lies in introducing novel methods for separating a ternary mixture of N-Pentane, N-Hexane, and N-Heptane. New methods against traditional techniques, considering criteria such as energy consumption, initial investments, and greenhouse gas emissions were evaluated. The most effective operational conditions were determined by simulation. The final separation technique is developed by analyzing economic, environmental, overall energy consumption, and thermodynamic efficiency indicators.

1.1. Example of Application

The distillation process plays a key role in chemical, petrochemical, and refinery industries, despite high energy consumption. DWCs can be the best alternative to traditional distillation columns (Battisti, Machado et al. 2020). In 1985, BASF installed the first industrial DWC. In 2010 Asprion et al. (Asprion and Kaibel 2010) reported more than 60 DWCs were put in by BASF. In 2010 Yildirim et al reported. In 2010 Yildirim et al reported there are 125 DWCs in the world which 116 are to separate ternary components. The author expected this number to increase to 350 in 2015 (Yildirim, Kiss et al. 2011). Later, Li et al. (Li, Li et al. 2019) expressed there were more than 300 DWCs. It was promised that DWC could be a popular distillation device in 2070 (Schultz, Stewart et al. 2002, Wu, Zhang et al. 2020). Most of the DWCs are of the packing type and some of them are of the tray type. Reported that the diameter of these columns is 0.6 to 4 meters and the largest middle wall tower with a height of 107 meters and a diameter of 5 meters is active in Africa. DWCs can be used in the azeotropic process, extractive process, and reactive distillation process which will be investigated in the following sections (Yildirim, Kiss et al. 2011). However, one of the strategies to intensify the process is to set up and use the DWC towers, but their application is minuscule on the industrial and pilot scale (Shi, Zhao et al. 2020).

In this study, two setups, including a traditional distillation column and a DWC process, were utilized to separate N-Pentane, N-Hexane, and N-Heptane. The Aspentech Aspen Plus was used to acquire the operation conditions and accurate design variables. The effective sensitivity analysis device sensitivity analysis was adopted to minimize the total condenser and reboiler duties needed in the simulations. Several optimization variables were adopted: split vapor ratio and liquid ratio, reflux ratio, divided wall location, feed stage, side stream location and total number of stages. DWC and conventional distillation column were compared to indicate the advantage of DWC process for separation of hydrocarbon mixtures in terms of (total annual cost) TAC, exergy loss (El) and CO_2 emissions.

2. Simulation and Performance Evaluation Methods

2.1. Simulation Condition and Methods

In this work, the simulation software Aspen Plus was applied to execute a steady-state simulation and optimization of the separation of N-Pentane (A), N-Hexane (B), and N-Heptane (C) systems in a DWC and conventional distillation column. In addition, the feed fresh mol ratio of A, B and C was 0.3,0.3 and 0.4 and feed ratio was 3600 Kmol/h. The boiling point of A, B and C was 35.9 °C, 68.3 °C and 98 °C. degrees centigrade at one atmospheric pressure (Figure 1). All the product purities are set as 99.5 mol% in two processes. In this simulation, the two columns are assumed to be at atmospheric pressure for easy operation. Process simulations were carried in Aspen Plus V8.0. The Peng Robinson model is applied to predict the vapor-liquid equilibrium (VLE) of the systems under study, with the binary interaction parameters carefully selected from Aspen Plus default databank.

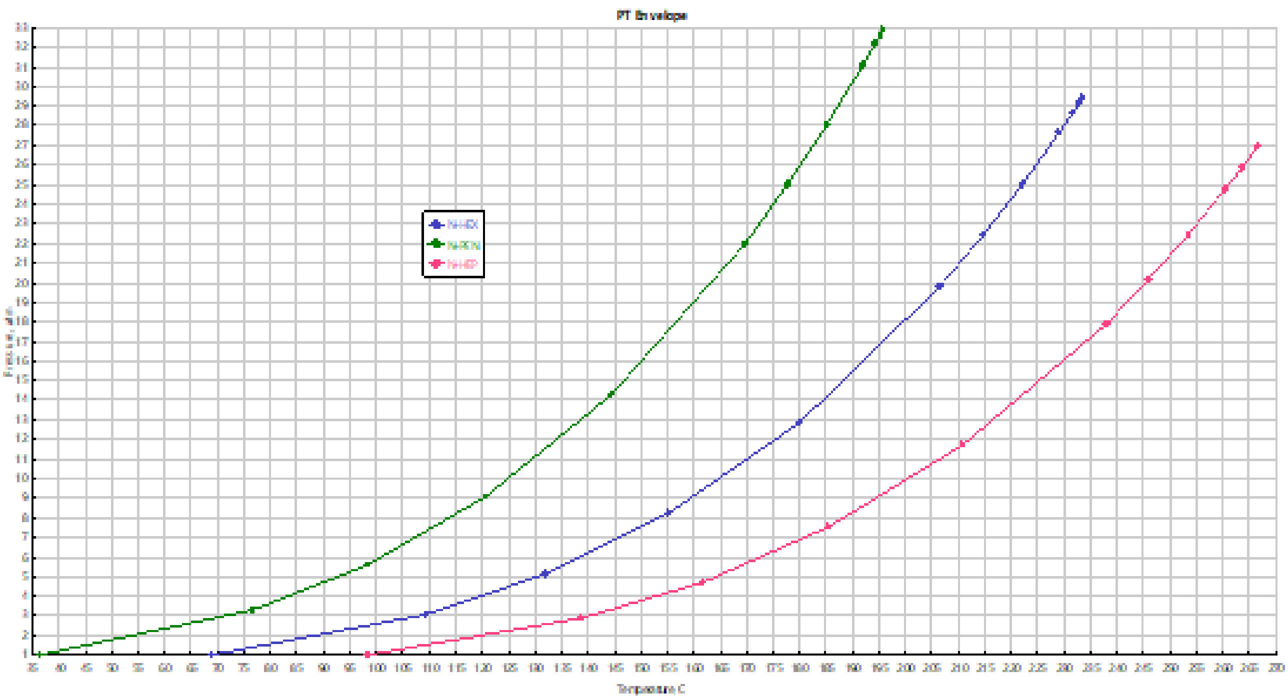

Figure 1. Boiling Point of Ternary Mixture

2.2. Framework of Energy Consumption, Economics and Environmental Impact

2.2.1. Total Energy Consumption

The estimated total energy consumption (TEC) indicates the external energy usage for the reboiler and condenser.

2.2.2. Total Annual Cost

The overall yearly expense is utilized to assess the economic estimation. TAC consists of energy expenses and yearly capital investments, as demonstrated below.

$$TAC = \frac{capital\ cost}{payback\ period} + energy\ cost$$

The study's initial investment includes expenses for columns and heat exchangers, such as reboilers and condensers. The analysis assumes a payback period of three years and an annual operating time of 8000 hours. The comprehensive design and assessment procedure for Total Annual Cost (TAC) is summarized in (Table 1-2) of the Supplementary material.

2.2.3. Environmental Impact

In distillation systems, the main contributors to CO_2 emissions are furnaces, boilers, and electricity use. There are also indirect emissions associated with the process, such as those from refrigerant use, which are affected by the power needed to cool and circulate these fluids, as well as emissions from manufacturing equipment like the steel used in distillation columns. Additional emissions arise from transportation during construction and operation, along with those related to water consumption (Andrade, Andrade et al. 2024). This study evaluates the energy consumption of the reboiler and condenser in both tower types and, based on these values, identifies the tower with the lowest pollution.

2.3. Conventional Distillation Process

In this research, the feasibility of a distillation system was assessed using the Residue Curve Map (RCM). (Figure 2) displays the RCM for the hydrocarbon blend, demonstrating that traditional distillation could successfully achieve the separation process due to the absence of azeotropic and distillation boundaries. (Figure 3) presents a flow diagram showing the feasibility of a conventional distillation column for separating the ternary mixture of n-pentane, n-hexane, and n-heptane. In the CDC process, the first component or lightest component is separated from the top of the first column, and the other two compounds that came out from the bottom of the first tower enter the second column as feed. After establishing steady-state simulation, the liquid composition, temperature profiles and optimal design parameters were obtained. The results were shown in (Table 1).

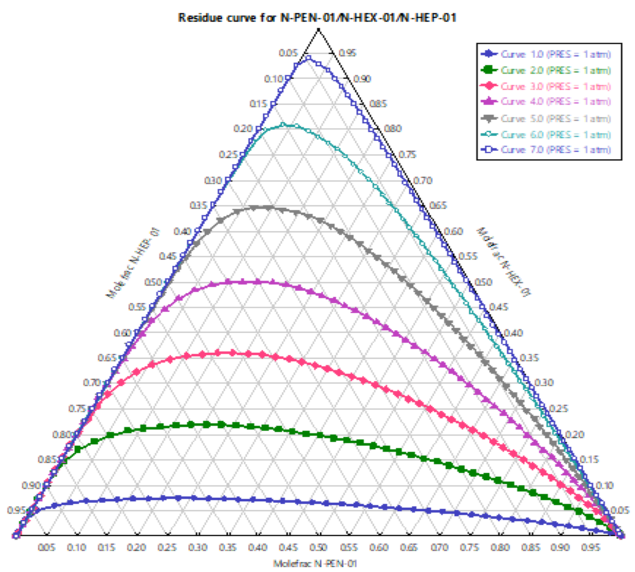

Figure 2. RCM of Ternary Mixture

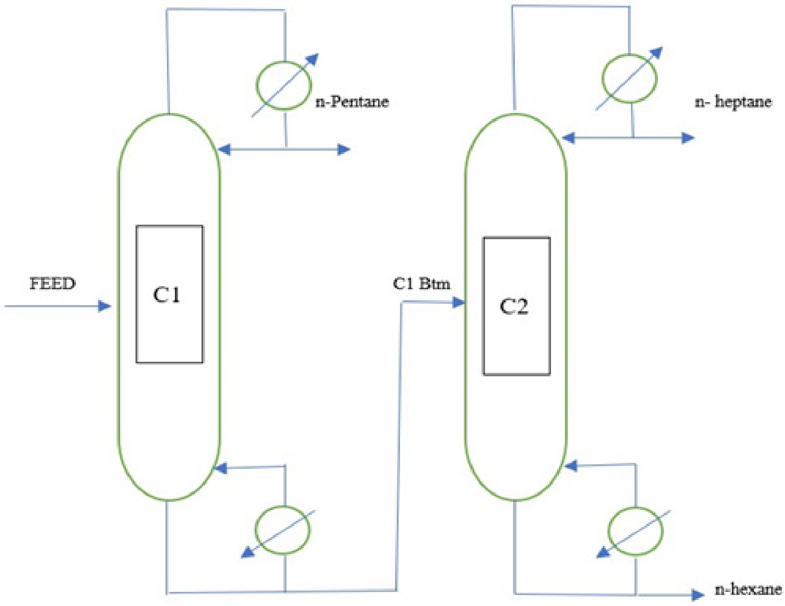

Figure 3: Flow Diagram of the Direct Sequence

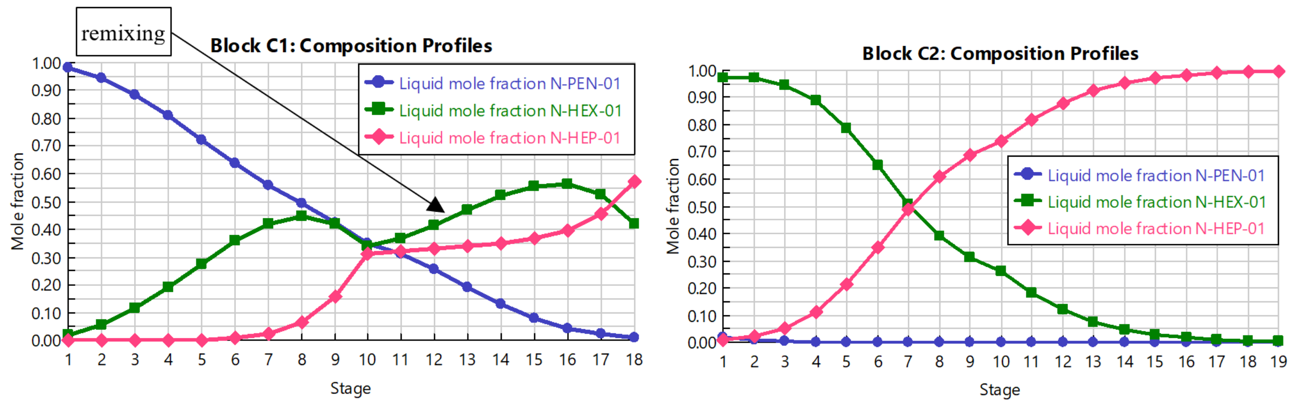

Figure 4: Composition Profiles in C1 and C2 Units of the Conventional Distillation Column

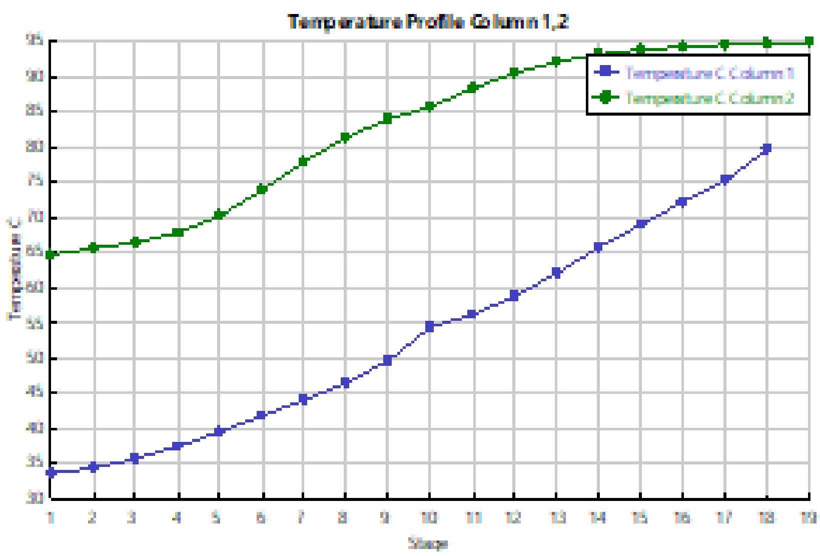

Figure 5: Temperature Profiles in C1 and C2 Units of the Conventional Distillation Column

Table 1: Optimal Design Parameters of the Direct Sequence of Two Columns

Design parameters	Value	Unit
Flow rate of feed stream	3600	Kmol/h
Feed compositions		
n-Pentane. n-Hexane and n-Heptane	0.3:0.3:0.4	_
Vapor Fraction	0	_
Pressure of feed stream	1	atm
Operating pressure(C1)	1	atm
Operating pressure(C2)	1	atm
Column diameter(C1)	6.7	m
Column diameter(C2)	5.6	m
Total number of stages(C1)	18	_
Total number of stages(C2)	19	_
Feed stage(C1)	10	_
Feed stage(C2)	10	_
Reflux ratio(C1)	1.32	_
Reflux ratio(C2)	3.2	_
Distillate to feed ratio(C1)	1080	Kmol/h
Distillate to feed ratio(C2)	1083.86	Kmol/h
n-Pentane product purity	98.0	%wt
n-Hexane product purity	96.6	%wt
n- Heptane product purity	99.2	%wt
Reboiler duty(C1)	25.870284	MW
Reboiler duty(C2)	37.741526	MW
Condenser duty(C1)	18.245788	MW
Condenser duty(C2)	37.115258	MW
Capital cost	8019529	USD
TAC	12101668	$/y

2.4.DWC Process

In order to address the drawbacks associated with using CDC to separate the ternary mixture of n-Pentane, n-Hexane, and n-Heptane - which include high energy consumption, TAC, exergy loss (El), and CO_2 emissions - this study introduced the divided wall column as a solution. DWC can product high purity in the one column with the one reboiler and one condenser. (Figure 5) illustrated the DWC structure. N-Pentane was separated as distillate, n-Heptane bottom product and n-Hexane as side stream. The presence of walls in these types of columns has increased the freedom of the system and also complicated the design of these types of towers compared to conventional towers. Research on the design and physical implementation of DWC has received attention in recent years. One of the ways to reduce the investment cost for setting up thermally coupled column is to use a DWC tower instead of the Petlyuk column. If the heat transfer through the wall is not taken into account, this particular tower is essentially the same as the Petlyuk tower from a thermodynamic perspective. (Cui, Zhang et al. 2020). DWC efficiency is significantly affected by degrees of freedom. Important design parameters (degrees of freedom) include the reflux ratio, the quantity of stages in every section, the feed stage, the side draw position, the amount of heat supplied to the reboiler, the rate at which side products flow, and vapor and liquid split ratios. These parameters are the basic requirement of an accurate simulation (Buitimea-Cerón, Hahn et al. 2021). The existence of 12 degrees of freedom in the configuration of fully thermally coupled distillations and DWCs has caused complexity in the design of these types of towers (Kiss and Rewagad 2011). Selecting the column configuration, thermodynamic model and operating pressure is the first step in designing a DWC column. The second step is to choose detailed models or shortcut models to optimize the equipment sizing and system control. A suitable initial guess of the design parameters and some guidelines are necessary for the convergence of the simulation (Dejanović, Matijašević et al. 2011, Di Pretoro, Ciranna et al. 2021). Triantafyllou and Smith disseminated the first DWC design based on a minimum reflux ratio, minimum number of equilibrium stages, feed stage, and number of stages (FUGK) (Tavan, Shahhosseini et al. 2014, Di Pretoro, Ciranna et al. 2021). Long N et al (Long, Lee et al. 2010) investigated the purification process of acetic acid and focus on the design of DWC. They proposed the interior recycle flow around the wall as the main optimization variable. Later, Seihoub F Z et al. (Seihoub, Benyounes et al. 2017) In their work to improve the shortcut design approach, while using Underwood's and Gilliland's equations, presented an accurate model for the design of each section of the DWC.

2.4.1. Optimal Steady-State Processes

In this study, the optimal design of the DWC was achieved using the Sequential Quadratic Programming (SQP) method integrated with Aspen Plus's sensitivity analysis tool. SQP is a well-established, robust approach for addressing nonlinearly constrained optimization problems (Wu, Zhang et al. 2020). These SQP techniques have been extensively applied throughout chemical engineering, demonstrating clear benefits. This study focuses on optimizing the process to minimize the total reboiler duty, as defined below:

$$Min(Q) = f(N_T, N_F, N_{SS}, N_{DWS}, N_{DWC}, V, RR, r_V, r_L)$$

$$Subject\ to\ \overrightarrow{y_m} \geq \overrightarrow{x_m}$$

The optimization variables consisted of the total stage count (N_T), feed stage (N_F), side-draw location (N_{SS}), dividing wall dimensions (N_{DWS})

and position (N_{DWC}), boilup rate (V), reflux ratio (RR), and the vapor and liquid splits (r_V,r_L). The vectors y_m and x_m represent the actual and target purities for the mproducts, respectively (Wu, Zhang et al. 2020). Temperature and liquid composition profiles for the DWC unit are illustrated in (Figure 7), while the optimal design values are summarized in (Table 2).

In the simulation, the DWC process was optimized. The total number of stages including reboiler and condenser is 46. The feed is fed at Stage 12 in the prefractionator column. Apparently the most important issue in the Petlyuk column in simulation is the definition of stages where the two liquids and two vapors leave and enter the main column prefractionator column. Two streams leave, including one vapor at the bottom and one liquid at the top of the prefractionator. The vapor streams at 1 stage leave prefraction section and inter at 10 stages in the main column. The liquid streams at 24 stages leave bottom of the prefractionator and go 34 stages in the main column. On the other hand, two streams of liquid and vapour from trays 9 and 34, respectively, leave the main tower and enter trays 1 and 24 of the prefraction column. The purities of n-pentane, n-hexane, and n-heptane products meet the required criteria, with purity levels of 99.8%, 99.9%, and 99.6% respectively.

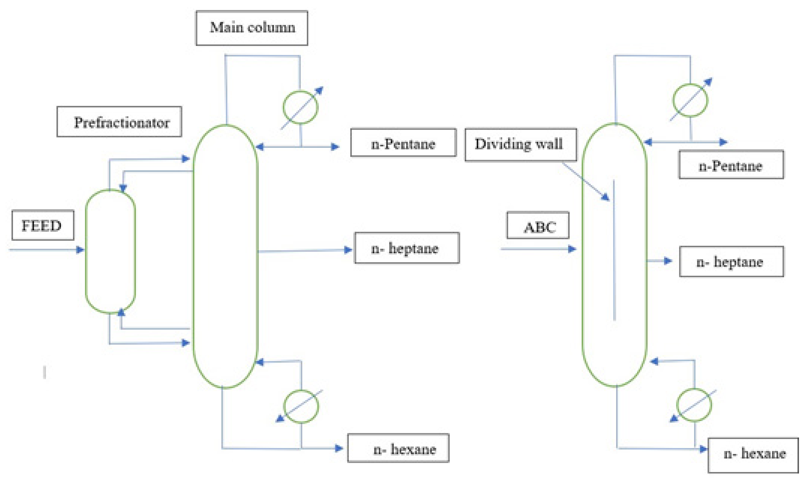

Figure 6: Petlyuk Configuration and DWC Configuration

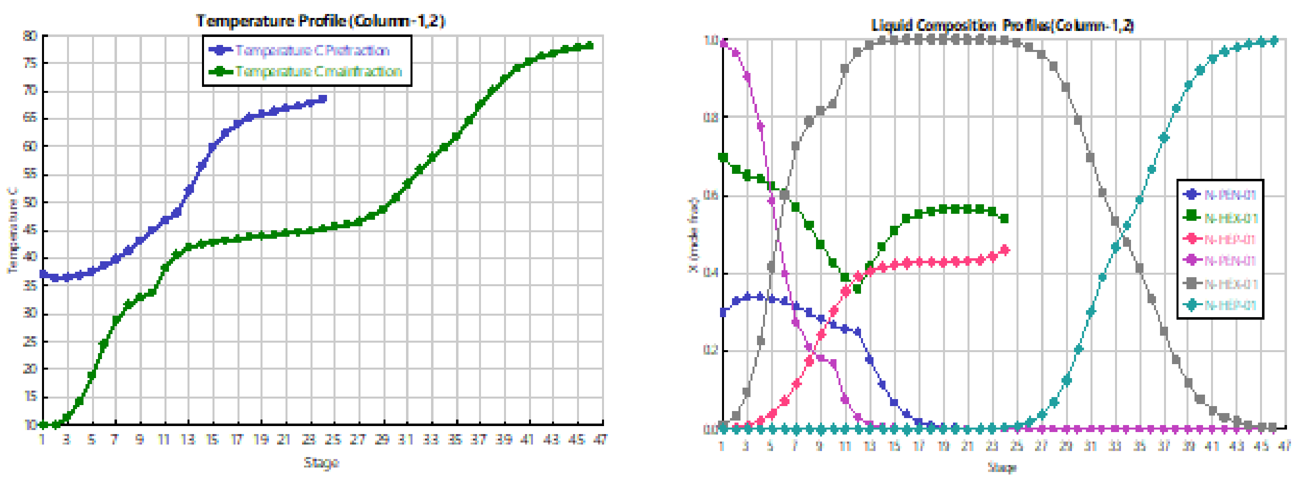

Figure 7: Temperature and Composition Profiles in the Dividing Wall Column

Table 2: Optimal Design Parameters of Dividing Wall Column

Design parameters	Value	Unit
Flow rate of feed stream	3600	Kmol/h
Feed compositions		
n-Pentane. n-Hexane and n-Heptane	0.3: 0.3 :0.4	_
Vapor Fraction	0	_
Pressure of feed stream	1	atm
Operating pressure	0.9	atm
Column diameter	8.83	m
Number of stages pre-fractionator side	24	_
Total number of stages DWC	70	_
Feed stage pre- fractionator side	12	_
Side stream withdrawal stage	20	_
Distillate rate	0.289948288	Kmol/sec
Reflux ratio	8.59	mol/mol
n-Pentane product purity	99.8	%wt
n-Hexane product purity	99.9	%wt
n- Heptane product purity	99.6	%wt
Reboiler duty	39.126925	MW
Condenser duty	36.201479	MW
Capital cost	4591648	USD
TAC	7329911	$/y

3. Results and Discussion

3.1. Simulation Results

3.1.1. Composition Profiles and Temperature Profiles

In distillation, the difference in boiling point and relative volatility causes the concentration of components in the trays to be different. Investigating the concentration of the ingredients on the trays can be helpful because it can be found in the maximum concentration of one the creator of a side stream removed that creator from the corresponding tray. In the conventional distillation column, N-pentane is released from the top of the first tower. Therefore, it is expected that its concentration is higher at the top of the column. The concentration of the middle component reaches the maximum in the first column under the feed tray and then decreases at the bottom of the column. Such an effect is known as remixing and causes more energy consumption (Figure 4-5). To re-purify the binary mixture N-Hexane, and N-Heptane in the second column through conventional distillation, the process will necessitate additional energy. This remixing can be viewed as a thermodynamic inefficiency in energy utilization. Finally, two other components leave the bottom of the first tower and enter the second tower as feed. (Figure 6) shows the concentration distribution of three key components in the pre-separator tower of the Petlyuk column. The light key component moves to the upper trays of the prefraction tower and its concentration decreases in the lower feed trays and its concentration becomes zero at the bottom of the column. The intermediate component is distributed almost continuously throughout the prefraction tower. In this tower, the phenomenon of remixing has wholly disappeared. The range of changes in the concentration of the intermediate material in the prefraction tower is minimal, and the intermediate material is appropriately distributed, distributed correctly in the prefraction column. In the main column of the dividing wall column, N-Pentane naturally moves to the top of the tower because it is lighter. Its amount reaches the desired level in the trays at the top of the tower, and it is removed in the upstream product, and as we move to the bottom of the tower, the concentration of this component decreases to zero arrives. Hexane is taken from the middle trays of the tower, so naturally, the concentration of this component reaches its maximum in the middle trays and tends to zero in the upper and lower trays of the tower. N-Heptane as a heavy substance in the tower moves to the lower trays until it reaches the desired concentration in the lowest tray. Its amount in the upper trays of the tower decreases until it reaches zero. In the DWC, the recycling streams can effectively minimize remixing and reduce the energy needed for ternary separations.

The temperature distribution in both the main and prefraction columns, as illustrated in (Figure 7), suggests that the temperature difference from the top to the bottom of the prefraction column falls within the range of the temperature difference in the main column, a logical finding. The temperature profile in a Dividing Wall Column (DWC) is a key defining characteristic due to its reflection of complex internal heat and mass transfer processes across both the pre-fractionator and the main column side. Given the integration of two columns within a single shell in a DWC, the temperature profile is not represented by a simple linear or sigmoidal curve; instead, it is a coupled distribution where the temperatures in the prefractionator section need to closely align with their counterparts in the main column sections to minimize entropy production and maximize energy efficiency. In the context of this ternary separation simulation involving N-pentane as the light element, N-hexane as the intermediate element, and N-heptane as the heavy element, it is noteworthy that the temperature profile typically exhibits three distinct segments.

The top section of the distillation column, known as the Rectifying Zone, follows a typical temperature profile where it begins at the boiling point of the lightest component (N-Pentane) and gradually increases towards the feed stage. In the Dividing Wall Zone, the profile takes on a unique characteristic. Within the Prefractionator Side, the temperature profile is influenced by the feed composition with a steeper gradient observed when the feed is rich in the intermediate component (N-Hexane). On the Main Column (Side Stream) Side, the temperature profile must align with the side-draw product, ideally reaching the boiling point of the pure intermediate component (N-Hexane) at the side-draw tray. Finally, in the Bottom Section or Stripping Zone, the temperature steadily rises until it reaches the boiling point of the heaviest component (N-Heptane) at the reboiler.

3.2. Process Comparison

The total annual cost, thermodynamic efficiency and energy consumption were used to analyze predomination of DWC instead of conventional column based on performance quantification method. (Table 3) illustrates the economic comparison results of traditional columns of distillation and DWC processes.

3.2.1. Comparisons of Economic and Energy Cost

The Total Annual Cost (TAC), calculated using Eq. (1), serves as a benchmark for assessing the economic viability of each of the two configurations.

$$TAC = Energy\ cost + Capital\ cost \div 3 \quad (1)$$

The analysis incorporates operating costs (OPEX) derived from utility expenses (as previously calculated) and an assumed operational lifespan of 8000 hours per year. Capital expenditures (CAPEX) for the distillation columns are established using design parameters.

The detailed calculations are presented in (Tables 1-2), while the evaluation criteria are visually compared in (Table 3). (Table 1-2) demonstrate that the purity levels of N-Pentane, N-Hexane, and N-Heptane were all consistently high at 99.0% in both setups. Looking at (Table 3), the total condenser duty and reboiler duty for the traditional distillation column and DWC were 55.37MW, 63.61MW, and 36.2MW, 39MW, respectively. The total annual cost (TAC) for the direct distillation sequence and DWC were $12,101,668/year and $7,329,911/year, respectively. These findings indicate that the energy consumption in the conventional distillation column setup was significantly greater than that in the DWC configuration, making the latter a more suitable option for separating the ternary system. The findings indicate that in dividing wall columns, there is a decrease in investment costs attributed to fewer column vessels, reboilers, and condensers. Moreover, energy consumption is significantly lowered as a result of reduced back-mixing within this tower configuration, leading to decreased energy expenses and carbon dioxide emissions.

The energy conservation level serves as an additional measure for assessing DWC compared to conventional two-column distillation. We utilize the following formula to determine the decrease in energy usage as a percentage (Li, Zhang et al. 2020):

$$Energy\ saving\ rate\ (\%) = \frac{Q_{reb,CD} - Q_{reb,DWC}}{Q_{reb,CD}} \times 100 = 38\%$$

Limited research has been conducted on ternary LNG mixture separation using direct thermal coupling. Mostofian et al. (Mostofian, Noori Keshtkar et al. 2023) recently investigated the energy consumption and exergy loss during the separation process of n-pentane, n-hexane, and n-heptane. Their findings indicated a 69% reduction in energy consumption and a 55% decrease in exergy loss with the use of direct thermal coupling.

Table 3. Comparison of the Two Configurations in Condenser and Reboiler Duties

Flow Regime	Conventional distillation column		DWC
Condenser duty (MW)	C1=18.255788	C2=37.115258	36.201479
Reboiler duty (MW)	C1=25.870284	C2= 37.741526	39.126925
TAC($/y)	**12101668**		**7329911**

4. Conclusion

Distillation is a physical separation process based on the difference in the boiling points of compounds. Studies have shown that almost 5% of the world's energy is spent on distillation towers. The increase in energy costs, the production of greenhouse gases, the reduction of natural resources, and the pressure on the natural gas industry have led researchers to look for a suitable solution. One of the practical solutions is process intensification. Thermally coupled distillation columns (Petlyuk) have been introduced as advanced distillation technology and the best alternative for process intensification.

In this research, a conventional distillation column and a DWC process were utilized to separate and purify a mixture of N-Pentane, N-Hexane, and N-Heptane hydrocarbons. The study used three distillation columns based on the FUGK model to determine initial design parameters for the DWC. Subsequently, the Sequential Quadratic Programming optimization method and Aspen Plus efficient sensitivity analysis tool were employed to minimize the total reboiler and condenser duties. The findings demonstrated that adopting the DWC configuration led to significant improvements in side product purity, energy efficiency, total annual cost (TAC) reduction, and a decrease in CO_2 emissions by 37% and 38% respectively compared to traditional distillation columns. The advantages of this new technology are reducing energy consumption, reducing investment costs, high thermodynamic efficiency, and reducing the required space. The superior performance and compact design of the proposed process set it apart from other methods.

Appendix A. Column Cost Correlations

Total annual cost (TAC) was calculated as follows:

(A)Capital cost

Luyben method was applied (Luyben, 2006). The cost of a distillation column was mainly made up of the investment of the column vessel and heat exchangers. The cost of trays was usually small compared to the cost of the vessel and heat exchangers and was neglected.

$$L = 1.2\times 0.61\times (N-2) \quad (A.1)$$

$$Shell = 17640 \times D^{1.066}\times L^{0.802} \quad (A.2)$$

$$Ar=qr\times 1.055\times 2.54\times exp(6)\div 3600\div 0.7457\div dtr\div ur \quad (A.3)$$

$$Ac=qc\times 1.055\times 2.54\times exp(6)\div 3600\div 0.7457\div dtr \div ur \quad (A.4)$$

$$Hx=7296 \times (Ar^{0.65}+ Ac^{0.65}) \quad (A.5)$$

$$Capital\ cost = shell + Hx \quad (A.6)$$

where L, D were the length and diameter of the column, respectively, both with unit of meters. Shell with unit of $ was the cost of the column vessel. Ar and Ac were the heat transfer areas of the reboiler and the condenser, respectively and their unit was m^2. qr and qc were the heat duty of the reboiler and the condenser, respectively, both with unit of MW. dtr and dtc were the differential temperature in the reboiler and the condenser, respectively, both with unit of K. ur and uc were heat transfer coefficients of the reboiler and the condenser, respectively, and their unit was Kw/K. m^2. Hx was the capital cost of heat exchangers with a unit of $.

(B)Energy cost

$$Energy\ cost = qr\times 4.7\times 3600\times 24\times 365\div 1000 \quad (B.1)$$

(C)Total annual cost (TAC)

$$TAC = Energy\ cost + Capital\ cost \div 3 \quad (C.1)$$

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بهبود جداسازی یک مخلوط سه جزئی هیدروکربنی با استفاده از برج تقطیر دیوار میانی

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چکیـــــده

برج تقطیر دیوار میانی (DWC) به‌عنوان یکی از راهکارهای پیشرفته در تشدید فرآیند، پتانسیل بالایی برای کاهش مصرف انرژی و هزینه‌های سرمایه‌گذاری اولیه در سیستم‌های تقطیر دارد. این مطالعه با هدف بهینه‌سازی سیستماتیک و مقایسه اقتصادی، عملکرد برج تقطیر دیوار میانی را در مقایسه با فرآیند تقطیر متداول برای جداسازی مخلوط سه‌جزئی نرمال‌پنتان، هگزان و هپتان ارزیابی می‌کند. در این راستا، تحلیل جریان‌های اگزرژی و ابعاد اقتصادی هر دو فرآیند به‌تفصیل بررسی شده است. به‌منظور کمینه‌سازی مجموع بارهای حرارتی ریبویلر و کندانسور، از روش بهینه‌سازی «برنامه‌ریزی درجه دوم متوالی» (SQP) استفاده و برای پیش‌بینی تعادل بخار-مایع (VLE) سیستم، مدل ترمودینامیکی پنگ-رابینسون به کار گرفته شد. درنهایت، با در نظر گرفتن شرایط یکسان خوراک، عملکرد برج تقطیر دیوار میانی در مقایسه با سیستم تقطیر دو ستونی مرسوم، از نظر کل هزینه سالانه و مصرف انرژی سنجیده شد. نتایج نشان می‌دهد که به‌کارگیری برج تقطیر دیوار میانی منجر به ۷۳ درصد کاهش در کل هزینه سالانه و ۸۳ درصد کاهش در مصرف انرژی می‌شود. در مجموع، این پژوهش ضمن تأکید بر بهره‌وری اقتصادی و راهکارهای نوآورانه در بهینه‌سازی مصرف انرژی و حفاظت از محیط‌زیست، استفاده از ستون‌های دیواره جداکننده را به‌عنوان جایگزینی کارآمد و عملیاتی برای برج‌های تقطیر متوالی پیشنهاد می‌کند.

واژگان کلیدی: برج دیوار میانی، بهینه‌سازی، جداسازی مخلوط سه جزئی، کل هزینه سالانه، بازدهی انرژی، تشدید فرآیند، اسپن پلاس