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Simulation and Economic Analysis for Separating Propylene and Propane Based on Distillation Column

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Abstract: The distillation column represents an important unit in industrial processes to separate the mixture into multi products. This work shows simulation and economic analysis to separate propylene from propane to meet the required purity, besides to determine the cost of the process. The simulation process of distillation column is carried out via mass and energy balances for separating the propylene from propane using Aspen HYSYS®. The economic analysis conducted to define the total module cost for predicting the cost estimation of the process according to the Chemical Engineering Plant Cost Index (CEPCI) in 2022. The simulation results showed that the required purity in propylene was 99.2 mole percent (mol%), which was accomplished by having a distillation column comprising 148 trays and 74 as feed trays at 17°C and 2.3 MPa and the column operating at a pressure of 1.4 MPa with column height around 67m. Energy consumption of the condenser and re-boiler were 17.46 GJ/hr and 17.69 GJ/hr, respectively. The total module cost of a new construction process was USD$ 10,043,039.

Keywords: Simulation; Economic Analysis; Propylene/Propane; Distillation Column

1. Introduction

Propylene represents one of the most important raw materials in modern industry and as a basic component in the petrochemical industry. Pure propylene is obtained by separating the mixture of propylene and propane formed in a propane rectification column [1, 2]. Propylene is commonly used in the manufacture of many commercial products such as fibers, elastomers, resins and other chemicals. Propane/propylene separation is one of the most expensive and energy consuming processes in the petrochemical industry. Propylene and propane have very similar properties [3]. Propylene is homogenously polymerized in two mixed flow reactors using a highly active catalyst [4]. Separation is essential in chemical plants, dividing substances for processes like raw material prep, gas removal, and product purification. Common methods include distillation, stripping, and extraction, all based on equilibrium between two phases. Distillation columns, with multiple equilibrium trays, are widely used for both simple and complex mixtures [5]. Cost estimation is vital for design engineers, aiding in project evaluation and design selection. In chemical plants, it involves assessing investment and production costs. Capital costs cover design, construction, equipment, and infrastructure, emphasizing the importance of total equipment costs for effective planning [6]. Cost estimation methods vary with the design stage, including capacity-based, parametric, and detailed models. Feasibility studies guide cost estimation, aiding management decisions and budget planning. A common approach involves using equipment cost factors, making method selection crucial [7].

For previous in the literature review about the separation of propylene and propane by distillation column. Liao et al. investigated a novel method for separating propylene and propane by extractive distillation using aqueous acetonitrile. They chose an acceptable vapor-liquid equilibrium model and used PRO/II software to simulate the process. The new method, extractive distillation, uses fewer trays, uses less energy, and has a smaller column diameter. They discovered that the new method significantly enhances the industrial separation of propylene and propane [8]. Using Aspen Plus simulation, Mauhar et al. examined optimizing the propylene-propane distillation process based on actual operating data collected from the factory .They discovered that by combining pressure and reflux rate, they could achieve the desired product purity while improving column characteristics and minimizing energy usage [4]. Response surface methodology was used by Rostamiyan et al. to model and optimize a Propene/Propane distillation column. The number of theoretical stages, the reflux ratio, the condenser pressure, and the recovery of propylene in the top product are the four input variables they suggested for the distillation column. Propylene purities (as high as 99%) have been achieved at high reflux ratio and low pressures while the propylene recovery in the top product was very high. The results were the best conditions for operating the column with 60 theoretical stages as the best number of stages of the column, condenser pressure being 100psia, and propylene purities (as high as 99%) [9].

In order to produce polymer grade, Jiménez et al. (2016) investigated the model and simulation of a distillation column for a propylene/propane mixture. They focused on the behavior of the fractionation column with his temperature and mixture composition profiles. They found that the distillation method proposed has advantages because of its high efficiency, which enables obtaining for maximum performance and directly impacts operating costs, enabling their reduction. On the other hand, they discovered that this type of column was simple to use, given that all that was required was to maintain the operating conditions, which were simple to follow [10]. Kazemi et al. studied the distillation without hot utilities for the mixture separation of propylene and propane in order to conserve energy and costs. This study used vapor recompression (VRC), a method that has attracted a lot of interest recently for improving the energy efficiency of distillation systems. They contrasted their proposed arrangements for distillation without hot utilities to earlier ones, such the traditional distillation column. The discovered distillation can outperform traditional distillation without the use of hot utilities design [11]. Alcheikhhamdon et al. studied propylene propane separation using a zeolitic imidazolate framework (ZIF-8) membrane as a technocommercial model. They looked into and evaluated the performance of single-stage and two-stage membrane processes in comparison to distillation. Propylene of the chemical grade (93 weight percent) could be produced using the single-stage technique, but not the polymer grade (99.5 weight percent). Instead, the two-stage method produced both propylene grades with encouraging recovery and cost rates [3].

Yamaki et al. [12] studied design and evaluation of propylene–propane mixtures separation process to minimize energy consumption. They used two-stage membrane- processes to evaluate the separation processes, which included two indicators CO_2 emissions and total annual costs. These outcomes were benchmarked against distillation techniques, and the benefits of the membrane-separation approach were superior. Using a specially designed ionic liquid solvent, Lei et al. investigated the environmentally hazardous and high energy-consuming separation of propylene and propane. They conducted an economic analysis of the traditional propane/propylene separation process using simulation and optimization techniques based on mixed-integer nonlinear programming (MINLP).When compared to the usual technique, this one saves 68.9% more energy and saves 74.7% more money [13]. Kazemi et al. investigated close-boiling distillation systems, specifically focusing on the separation of propylene/propane and isobutane/n-butane. Their study found that bottom flashing systems outperformed vapor recompression methods in terms of economic efficiency, particularly for isobutane/n-butane separation. By employing a new heat recuperated bottom flashing arrangement, they achieved a 19.0% reduction in total annual expenditures. Additionally, the bottom flashing systems' annualized costs were 10.9%, 4.2%, and 7.3% lower than those of comparable vapor recompression procedures, demonstrating the cost-effectiveness of this approach [14]. Zhang et al. demonstrated that the Permylene™ membrane in a PDS unit achieves over 98.5% propylene purity and operates efficiently for 1200 hours. Their case study showed that the PDS process consumes just 8% of the energy required by conventional distillation, making it a highly energy-efficient alternative for propylene separation [15].

This work focused on the simulation and economic analysis for separating propylene from propane besides to estimate the cost of the process. Simulation process of distillation column carried out via mass and energy balances using Aspen HYSYS®. The economic analysis implemented by the module costing technique for predicting the cost estimation of the process.

2. Separation Process Description

The input stream mixture of gases (i.e. comes from catalytic cracking unit in refinery plant) was fed into distillation column at 2.3 MPa and 17 °C and it is100 % liquid [4]. The distillation column has 148 trays and feed tray is 74 [16]. The light key component in mixture feed is propylene where obtained from top of column and heavy key component is propane where obtained from bottom of column. The condenser and re-boiler operating at 1.4 MPa [4]. Propylene, propane, methane, ethylene, C-4 fraction, hexane, water, hydrogen, nitrogen, and a few more ingredients from a petrochemical factory make up raw material. Pure propylene must be separated from propane and the other impurities in the distillation column due to a high feed stream. The mixture, which may have had a tiny quantity of water, moves from the drying portion to the distillation column, where it is separated to produce high-purity propylene. The distillation column used to separate propane and propylene is shown in Figure 1.

3. Methodology

Simulation process of distillation column carried out via mass and energy balances for separating the propylene from propane using Aspen HYSYS®. The economic analysis conducted to define the total module cost for predicting the cost estimation of the process according to the Chemical Engineering Plant Cost Index (CEPCI) in 2022.

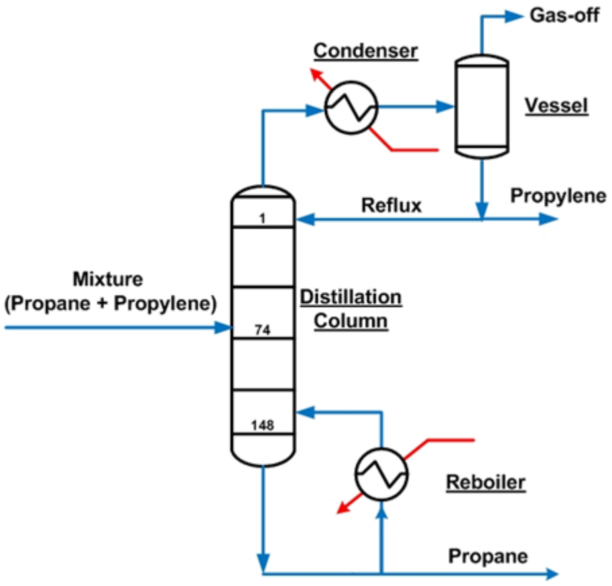


Figure 1. Distillation column for separating propylene and propane

3.1 Process simulation analysis

Process simulation analysis of the distillation column for separating propane and propylene applied Aspen HYSYS®. Mixture components were identified as first step for simulation. To suit defined components and to predict thermodynamic properties of propane/propylene mixture, Peng Robinson equation of state (EOS) from thermodynamic property package was used. For a fluid mixture of the process, the Peng-Robinson equation is given as [17]:

$$P = \frac{R\,T}{V-b} - \frac{a}{V(V+b)+b(V-b)} \tag{1}$$

Where:

$$a = \frac{0.45724\,\alpha(T)R^2T_c^2}{P_c} \tag{2}$$

$$b = \frac{0.07780RT_c}{P_c} \tag{3}$$

$$\alpha(T) = [1 + k(1-\sqrt{T_r})]^2 \tag{4}$$

$$k = 0.37464 + 1.5422\omega - 0.26992\omega^2 \tag{5}$$

Where P: pressure (Pa), T: Temperature (K), n: number of moles (mole), V: molar volume (m^3/mole), R: gas constant (J/mol·K), a and b are the coefficients of Peng-Robinson associated to the mixture, ω: acentric, T_c: critical temperature (K), P_c: critical pressure (Pa) and T_r: reduced temperature.

For material balance of the distillation column, the streams data for simulating the process is specified. The distillation column for separating of the mixture is described in Figure 2 on Aspen HYSYS. There is one input stream as feed stream (mixture) and are three-output stream, namely top product, gas flow rate and bottom product. The flow rate, composition, temperature, and pressure of this stream must be specified.

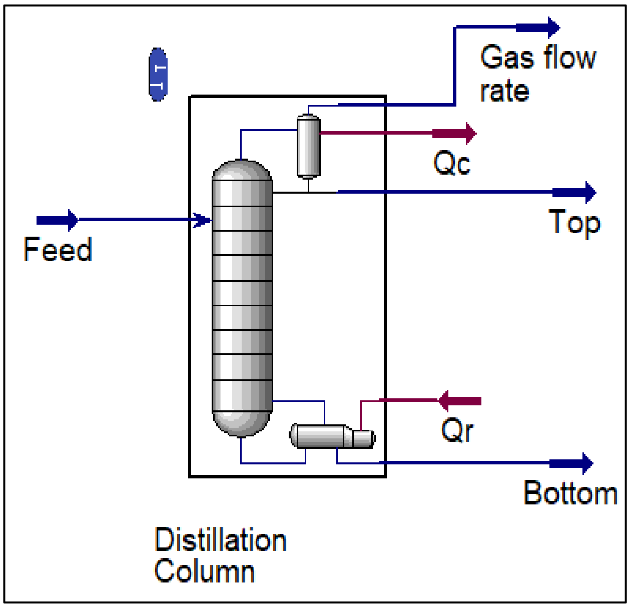


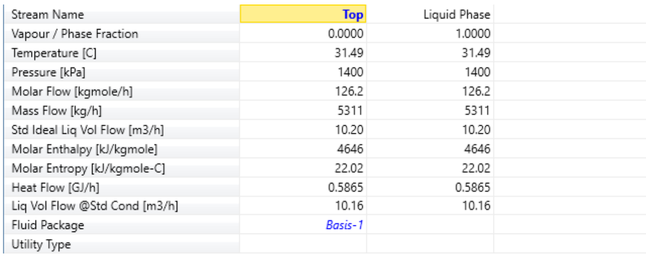
Figure 2. Diagram of distillation column on Aspen HYSYS

Moreover, additional input streams such as steam for heating and cooling water for condenser. The parameters for the opening column distillation are identified. Figures 3,4,5,6 and 7 show the stream data.

Stream Name	Feed	Liquid Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	17.00	17.00
Pressure [kPa]	2300	2300
Molar Flow [kgmole/h]	130.4	130.4
Mass Flow [kg/h]	5496	5496
Std Ideal Liq Vol Flow [m3/h]	10.56	10.56
Molar Enthalpy [kJ/kgmole]	-217.9	-217.9
Molar Entropy [kJ/kgmole-C]	18.80	18.80
Heat Flow [GJ/h]	-2.841e-002	-2.841e-002
Liq Vol Flow @Std Cond [m3/h]	10.52	10.52
Fluid Package	Basis-1	
Utility Type		

Figure 3. Feed stream of distillation column on Aspen HYSYS

For energy balance of the distillation column, the streams data for simulating the condenser and re-boiler are specified. Condenser was used to condense the vapor comes from top of tower at 33.03 °C to 31.49 °C using refrigerated water at 5°C and it is riser to 10 °C. The heat transfer coefficients are U = 850 W/(m^2℃) for condenser and U = 1140 W/(m^2℃) for re-boiler. Re-boiler used to boil the liquid comes from bottom of tower at 41.48 °C to 45.8 °C using low pressure steam at 5.2 bar gage and 160 °C [6].



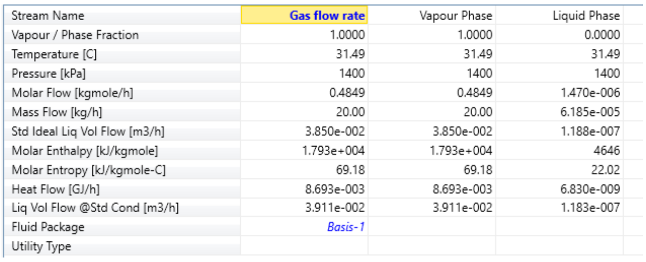
Stream Name	Top	Liquid Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	31.49	31.49
Pressure [kPa]	1400	1400
Molar Flow [kgmole/h]	126.2	126.2
Mass Flow [kg/h]	5311	5311
Std Ideal Liq Vol Flow [m3/h]	10.20	10.20
Molar Enthalpy [kJ/kgmole]	4646	4646
Molar Entropy [kJ/kgmole-C]	22.02	22.02
Heat Flow [GJ/h]	0.5865	0.5865
Liq Vol Flow @Std Cond [m3/h]	10.16	10.16
Fluid Package	Basis-1	
Utility Type		

Figure 4. Top stream of distillation column on Aspen HYSYS

3.2 Cost Estimation of Process

For estimating cost of the process, the module costing method is carried out by Turton et al. [6]. The main relation in this method is as shown in equation 6. For other items the related relations are given in table 1.

$$C_{TM} = 1.18 \sum_{i=1}^{n} C_{BM,i} \qquad (6)$$



Stream Name	Gas flow rate	Vapour Phase	Liquid Phase
Vapour / Phase Fraction	1.0000	1.0000	0.0000
Temperature [C]	31.49	31.49	31.49
Pressure [kPa]	1400	1400	1400
Molar Flow [kgmole/h]	0.4849	0.4849	1.470e-006
Mass Flow [kg/h]	20.00	20.00	6.185e-005
Std Ideal Liq Vol Flow [m3/h]	3.850e-002	3.850e-002	1.188e-007
Molar Enthalpy [kJ/kgmole]	1.793e+004	1.793e+004	4646
Molar Entropy [kJ/kgmole-C]	69.18	69.18	22.02
Heat Flow [GJ/h]	8.693e-003	8.693e-003	6.830e-009
Liq Vol Flow @Std Cond [m3/h]	3.911e-002	3.911e-002	1.183e-007
Fluid Package	Basis-1		
Utility Type			

Figure 5. Gas flow rate stream of distillation column on Aspen HYSYS

Where C_{TM} represents total module cost ($), n represents number items equipment and $C_{BM,i}$ represents bare module cost ($). The bare module cost can be reported as:

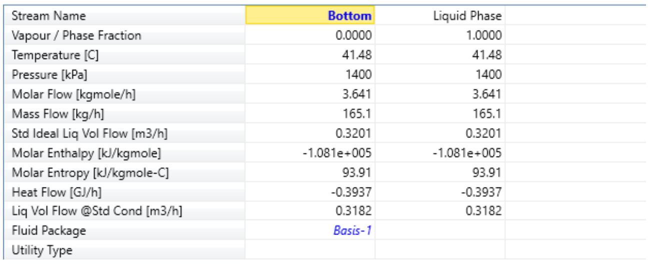
$$C_{BM} = C_P^O F_{BM} \qquad (7)$$

Where C_P^O refers to the base costs of equipment and F_{BM} is the bare module cost factor. It accounts for operating pressures and specific materials of construction of equipment. The base costs of equipment and the bare module cost factor are given by equation (8) and (9), respectively.

$$\log C_P^O = K_1 + K_2 \log(A) + K_3 (\log(A))^2 \qquad (8)$$

$$F_{BM} = (B_1 + B_2 F_P F_M) \qquad (9)$$

Where A is the capacity or size parameter for the equipment. The constants values for K_1, K_2, K_3, B_1 and B_2 are given in Table 1. F_p and F_M refer pressure factor and material of construction of equipment, which are calculated in the Table 1.



Stream Name	Bottom	Liquid Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	41.48	41.48
Pressure [kPa]	1400	1400
Molar Flow [kgmole/h]	3.641	3.641
Mass Flow [kg/h]	165.1	165.1
Std Ideal Liq Vol Flow [m3/h]	0.3201	0.3201
Molar Enthalpy [kJ/kgmole]	-1.081e+005	-1.081e+005
Molar Entropy [kJ/kgmole-C]	93.91	93.91
Heat Flow [GJ/h]	-0.3937	-0.3937
Liq Vol Flow @Std Cond [m3/h]	0.3182	0.3182
Fluid Package	Basis-1	
Utility Type		

Figure 6. Bottom stream of distillation column on Aspen HYSYS

For trays, the bare module cost is given by equation:

$$C_{BM,trays} = C_P^O N F_{BM} F_q \qquad (10)$$

Where N represents number of trays in the column and F_q is constant factor depending on number of trays. The components of the process are tower and trays, condenser, re-boiler and reflux drum. Chemical Engineering Plant Cost Index (CEPCI), which is widely used to evaluate equipment and plant costs for the chemical and process industries was 824.5 in 2022 Aug Prlm [18]. For updating cost data using cost indices (CEPCI), the equation (11) can convert from base year (i.e., 2001) into the current year (i.e., 2022). The most straightforward manner to update historical data is by means of composite cost indices, using the equation and that is acceptable:

$$\frac{C_j}{C_i} = \left(\frac{I_j}{I_i}\right) \qquad (11)$$

Where C_j refers to the cost in current year, C_i refers to the cost in base year, I_j refers to the cost indices in current year and I_i refers to the cost indices in base year.

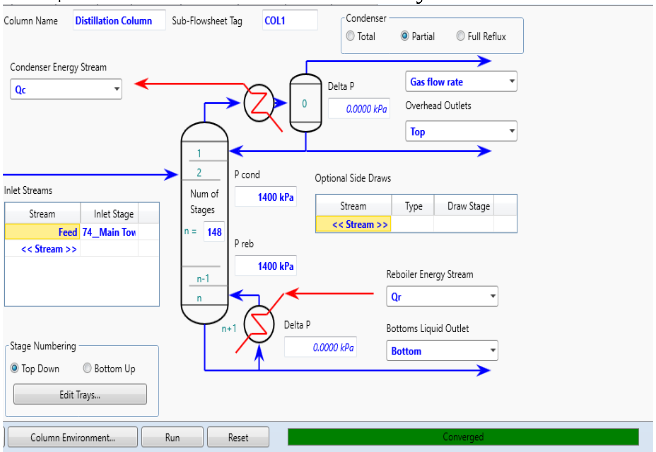


Figure 7. Parameters distillation column on Aspen HYSYS

Table 1. Values of constants related relations and some is calculated*

Equipment Constants	Tower	Tray	Condenser	Re-boiler	Reflux drum
K_1	3.4974	2.9949	4.8306	4.8306	3.5565
K_2	0.4485	0.4465	-0.8509	-0.8509	0.3776
K_3	0.1074	0.3961	0.3187	0.3187	0.0905
B_1	2.25	-	1.63	1.63	1.49
B_2	1.82	-	1.66	1.66	1.52
C_1	-	-	0.03881	0.03881	-
C_2	-	-	-0.11272	-0.11272	-
C_3	-	-	0.08183	0.08183	-
* F_p	3.27	-	1.034	1.034	3.01
* F_M	3.2	-	2.8	2.8	3.2
F_q	-	1	-	-	-
N	-	148	-	-	-
* F_{BM_trays}	-	1.8	-	-	-

4. Results and Discussion

For the purpose of process evaluation to separate propylene from mixture, a summary of results for simulating of distillation column was developed as given in Table 2. It can be seen that the propylene purity reached 99.2 mol%. As a result, it was found that it is possible to energy requirements for duties of condenser and re-boiler 17.46 GJ/hr and 17.69 GJ/hr, respectively.

Table 2. Summary of material and energy balance for purity

	Input		Output					
	Feed		Top		Bottom		Gas flow rate	
Composition	Kg/hr	Mol%	Kg/hr	Mol%	Kg/hr	Mol%	Kg/hr	Mol%
Propane	178.73	3.11	39.5095	0.71	139.0849	86.62	0.1356	0.63
Propene	5304.48	96.69	5269.4678	99.2	15.3209	10	19.6913	96.49
Ethane	0.16	0.000	0.1586	0.000	0	0.000	0.0014	0.01
Butane	2.2	0.03	0	0.000	2.2	1.04	0	0.000
Heptane	8.54	0.07	0	0.000	8.54	2.34	0	0.000
Hydrogen	0.13	0.05	0.1132	0.04	0	0.000	0.0168	1.72
Nitrogen	1.76	0.05	1.6048	0.05	0	0.000	0.1552	1.14
Total	5496		5496					
Duty of condenser	17.46 GJ/hr							
Duty of re-boiler	17.69 GJ/hr							

From Table 2, it can be seen that material balance of the distillation column for the input and the output was equalled around 5496 kg/h. Furthermore, it could be noted that the purchase costs and the bare module cost for the components of the process as tower and trays, condenser, re-boiler and reflux drum is estimated in Table 3. Also, the total module cost of the process reached about USD$ 10,043,039.

4.1 Comparison results of this work with previous study.

The comparison results of this work with previous studies related to simulation of the process for separating propylene and propane is shown in Table 4. It is clearly observed that both processes used feed about 5496 kg/hr, but in this work studied one distillation with 148 trays is better by compared with the another author [4].

Table 3. Summary of equipment cost in 2022

Equipment	Size	C_p^o (USD$)	C_{BM} (USD$)
Tower and trays	234.2 m3 / 3.5 m2	144544 / 2290.9	7,404,441
Condenser	256.4 m^2	42657.9	551,170
Re-boiler	41.2 m^2	7585.8	98,014
Reflux drum	16.3 m^3	14125.4	457,425
Total			8,511,050
Total module cost (CTM)	USD$ 10,043,039		

Table 4. Comparison results between this work and previous study of the process

Separation process	**Feed input (kg/h)**	**Number of columns**	**Working pressure (MPa)**	**Number of stages**	**Energy consumption (GJ/h)**	**Column height (m)**	**Total module cost ($)**	**References**
Distillation column	5496	Two	1.4	241	14.31	-	-	[4]
Distillation column	5496	one	1.4	148	17.69	67	10,043,039	This work

Table 5. Comparison of simulated material stream composition with data of previous study

Components	**Input**		**Output**					
	Feed		**Top column**		**Bottom column**		**Gas flow rate**	
	Data (kg/hr)	*Simulated (kg/hr)*	*Data (kg/hr)*	*Simulated (kg/hr)*	*Data (kg/hr)*	*Simulated (kg/hr)*	*Data(kg/hr)*	*Simulated (kg/hr)*
Propane	178.73	178.73	37.57	39.51	141.10	139.08	0.06	0.13
Propene	5304.48	5304.48	5262.43	5269.46	28.16	15.32	13.89	19.69
Ethane	0.16	0.16	0	0.16	0	0	0.16	0.0014
Butane	2.2	2.2	0	0	2.2	2.2	0	0
Heptane	8.54	8.54	0	0	8.54	8.54	0	0
Hydrogen	0.13	0.13	0	0.11	0	0	0.13	0.017
Nitrogen	1.76	1.76	0	1.6	0	0	1.76	0.16
	5496	5496	5300	5310.85	180	165.14	16	20
Total		5496		5496				

In addition, this work linked the total module cost with simulation to identify the height of column for estimating the process cost, while another author did not mention it. For Table 5, it can be seen that the comparison of simulated material stream composition with data of previous study by Mauhar et al. was valid and acceptable.

5. Conclusion

Propylene represents a valuable and used as fuel gas and produce polypropylene. Due to the increasing purity of propylene, it is necessary to switch to separation alternatives. Distillation column was chosen in this project as the most suitable. Using a 148 number of trays and 74 as feed tray for the process, a 5269.4678 kg/hr product is produced on distillate, of which 99.2 mole percent (mol%) is purity. Energy consumed of condenser and re-boiler are 17.46 GJ/hr and 17.69 GJ/hr, respectively to obtained 99.2 mole percent (mol%) of propylene. For cost estimation, the construction of a new process or alterations to exiting process is USD$ 10,043,039.

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Conflicts of Interest

"The authors declare that they have no conflicts of interest to report regarding the present study."

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محاكاة وتحليل اقتصادي لفصل البروبيلين والبروبان على أساس عمود التقطير

الملخص: يمثل عمود التقطير وحدة مهمة في العمليات الصناعية لفصل الخليط إلى منتجات متعددة. يوضح هذا العمل المحاكاة والتحليل الاقتصادي لفصل البروبيلين عن البروبان لتلبية النقاوة المطلوبة، بالإضافة إلى تحديد تكلفة العملية. تتم عملية محاكاة عمود التقطير من خلال موازنات الكتلة والطاقة لفصل البروبيلين عن البروبان باستخدام.®Aspen HYSYS تم إجراء التحليل الاقتصادي لتحديد إجمالي تكلفة الوحدة للتنبؤ بتقدير تكلفة العملية وفقاً لمؤشر تكلفة مصنع الهندسة الكيميائية (CEPCI) في عام 2022. أظهرت نتائج المحاكاة أن النقاوة المطلوبة في البروبيلين كان 99.2 مول في المائة(mol%) ، والذي تم تحقيقه من خلال وجود عمود تقطير يتألف من 148 صينية و 74 صينية تغذية عند 17 درجة مئوية و 2.3 ميجا باسكال والعمود يعمل عند ضغط 1.4 ميجا باسكال وارتفاع العمود حوالي 67 متراً. بلغ استهلاك الطاقة للمكثف والغلاية 17.46 جيجاجول/ساعة و17.69 جيجاجول/ساعة على التوالي. وبلغت التكلفة الإجمالية للوحدة لعملية البناء الجديدة 10,043,039 دولارًا أمريكيًا.