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Research Article

Total Net Energy Assessment for Rule-of-Thumb Applications in Multicomponent Distillation Separation Strategy

I. Istadi*[1], Teguh Riyanto[2]

[1]Department of Chemical Engineering, Faculty of Engineering, Universitas Diponegoro, Semarang, Indonesia.
[2]Industrial Chemical Engineering Technology, Vocational College, Universitas Diponegoro, Semarang, Central Java, 50275, Indonesia.

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Abstract

Energy saving in separation systems, particularly in distillation systems, is a research field that has attracted considerable innovative approaches. A distillation system is an essential separation process, yet it is inefficient in using thermal energy, and may operate with adverse environmental impact as it discharges a large amount of thermal energy into the environment. In this work, several Sequences Designs of Distillation Column Network are proposed to be compared with respect to Total Net Energy of each sequence design. Applying the Rule of Thumb of Distillation Strategy for separating multicomponent mixtures is important by performing the easiest separation first (largest relative volatility), that is, the one least demanding of trays and reflux, and leaving the most difficult to the last. From all sequence designs results, Sequence-A shows the lowest Total Net Energy (9,750,720.88 kJ/h), because the Sequence-A follows the strategy/procedure for separation of multicomponent using distillation column network. Decreasing the relative volatility affects on increasing number of tray and recycle ratio required for distillation process and decreasing the Net Energy.

Keywords: Distillation; Multicomponent; Separation; Rule of Thumb; Total Net Energy

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1. Introduction

Distillation is the predominant technology employed for various separations in the chemicals and petrochemicals industries — such as crude petroleum, hydrocarbons, air, natural gas liquids, alcohols, etc. To identify which are energy-efficient for a given separation, each distillation configuration must be optimized and compared. While several process simulators have in-built optimizers for evaluating a distillation configuration, the solution process often gets trapped in local optima, and a sensitivity analysis of the operating conditions can take days if not weeks [1]. Coupled with the vastness of the search space, this makes the process simulator approach impractical for the identification of energy-efficient distillation configurations.

There are a few existing works in the literature for identifying configurations for multicomponents distillation separations. Aggarwal and Floudas [2] proposed an multicomponents distillation formulation considering a superstructure of possible splits and connections between streams, splits, and products. However, it was demonstrated with at most three splits for four products, while configurations with up to ten splits are known to be energy-efficient for four-product separations [3,4]. Ryu and Maravelias [5] presented a formulation for basic distillation configurations coupled with reactors and demonstrated it on examples containing up to nine-component feed streams with three splits and four product streams. However, their formulation implicitly evaluates all possible pairs of key

* Corresponding Author.
Email: istadi@che.undip.ac.id (I. Istadi)

components in each split, which can limit computational tractability for separations with higher number of product streams. While the formulation of Ryu and Maravelias [6] also considers thermal coupling, only bypasses from submixture streams are allowed as multicomponent products, which restricts the space of feasible process products. Floudas and Anastasiadis [7] use ten splits in their multiproduct distillation superstructure, but each split is restricted to be a sharp split. For reference, sloppy split configurations are well-known to be capable of achieving lower energy consumption than sharp split configurations [3]. Cheng and Liu [8] proposed heuristics for selecting multiproduct distillation configurations. We remark that bypassing a portion of each stream in the configuration and blending products streams are some of the features commonly used in the process flowsheets of the aforementioned works.

Thus, many efforts have been made to develop systematic and effective frameworks to synthesize optimal distillation networks [9,10]. In early works, distillation network synthesis has been addressed by heuristic rules obtained from numerical studies [11,12]; a thermodynamic approach to synthesizing distillation trains, focusing on minimizing energy consumption and maximizing separation efficiency (thermodynamic insights) [13]; later, heuristic rules are combined with evolutionary algorithms, where several initial flow sheets are generated and changed based on heuristic rules until there is no improvement [14,15].

Energy saving in separation systems, particularly in distillation systems, is a research field that has attracted considerable innovative approaches. A distillation system is an essential separation process yet it is inefficient in using thermal energy, and may operate with adverse environmental impact as it discharges a large amount of thermal energy into the environment. Innovative research incorporating the principles of thermodynamics for energy efficient distillation systems is in an advanced stage through pinch analysis, exergy analysis, and equipartition principle. In this work, several Sequences Designs of Distillation Column Network are proposed to be compared with respect to Total Net Energy of each sequence design. The sequence design following Rule of Thumb of separation process should show the minimum Total Net Energy.

2. Methods

2.1 Rules of Thumb or Heuristic Rules of Distillation Strategy

Distillation usually is the most economical method of separating multicomponent liquids, superior to extraction, adsorption, crystallization, or others. For ideal mixtures, relative volatility or separation factor is the ratio of vapor pressures (P_i^{sat}) of each component ($\alpha_{12}=P_2^{sat}/P_1^{sat}$), used for choosing criteria for separation method.

Sequencing of columns for separating multicomponent mixtures by distillation are: (a) performing the easiest separation first (largest α_{12}), that is, the one least demanding of trays and reflux, and leaving the most difficult to the last; (b) when neither relative volatility nor feed concentration vary widely (larger α_{12}), removing the components one by one as overhead products; (c) when the adjacent ordered components in the feed vary widely in relative volatility, sequencing the splits in the order of decreasing volatility (start from larger α_{12}); (d) when the concentrations in the feed vary widely but the relative volatilities do not, removing the components in the order of decreasing concentration in the feed (start from larger concentration).

2.2 Distillation Simulation Strategy

Aspen HYSYS V11 was used to simulate and modify the distillation column strategy. We used Shortcut Column Method to predict Minimum Number of Trays (Fenske minimum number of trays, Equation (1)), while Actual Number of Trays was calculated using the Gilliland method (Equation (2)). Estimation of the theoretical optimal feed stage by the Fenske equation (Equation (3) or Kirkbridi equation (Equation (4)).

$$N_{min} = \frac{\ln\left(\left[\frac{x_{LKD}}{x_{HKD}}\right]\left[\frac{x_{HKB}}{x_{LKB}}\right]\right)}{\ln \alpha_{LKHK}} \quad (1)$$

$$\frac{100(N-N_{min})}{N+1} = f\left(\frac{100(R-R_{min})}{R+1}\right) \quad (2)$$

$$\frac{N_n}{N_m} \cong \frac{N_{n,min}}{N_{m,min}} \quad (3)$$

$$\log\frac{N_n}{N_m} = 0.206 \log\left[\frac{n_B}{n_D}\left(\frac{x_{HK}}{x_{LK}}\right)_F\left(\frac{x_{LKB}}{x_{HKD}}\right)^2\right] \quad (4)$$

The detail distillation simulation was conducted using Rigorous Distillation Column in Aspen HYSYS by entering Actual Number of Trays, Optimal Feed Stage, and Reflux Ratio predicted/provided by the Shortcut Column Method. The Rigorous Distillation Column model involve complex unit performance predictions, including equilibrium- or rate-based mass and/or heat transfer. A major barrier in the optimization of these systems is that the models are typically implemented in black boxes in which only function evaluations can be performed. The bulk of interest in rigorous models has been related to the synthesis of distillation sequences.

All material-equilibrium-summation-heat (MESH) equations involved in the calculation of rigorous distillation stage-by-stage is explained as follow (Figure 1):

$$M_{i,j} = n_{Lj-1}x_{i,j-1} + n_{Vj+1}y_{i,j+1} + n_{Fj}x_{Fi,j} - (n_{Lj} + n_{SLj})x_{i,j} - (n_{Vj} + n_{SVj})y_{i,j} = 0 \quad (5)$$

or

$$M_{i,j} = n_{Li,j-1} + n_{Vi,j+1} + n_{Fi,j} - n_{Li,j} - n_{SVi,j} - n_{SLi,j} + n_{SVij} = 0 \quad (6)$$

$$E_{i,j} = y_{i,j} - K_{i,j}x_{i,j} = 0 \quad (7)$$

Efficiency of stage j (η_j):

$$\eta_j = \frac{y_{i,j} - y_{i,j+1}}{K_{i,j}x_{i,j} - y_{i,j+1}} \quad (8)$$

The selected thermodynamic model are:

$$S_{x,j} = \sum_{i=1}^{k} x_{i,j} - 1 = 0 \quad (9)$$

$$S_{y,j} = \sum_{i=1}^{k} y_{i,j} - 1 = 0 \quad (10)$$

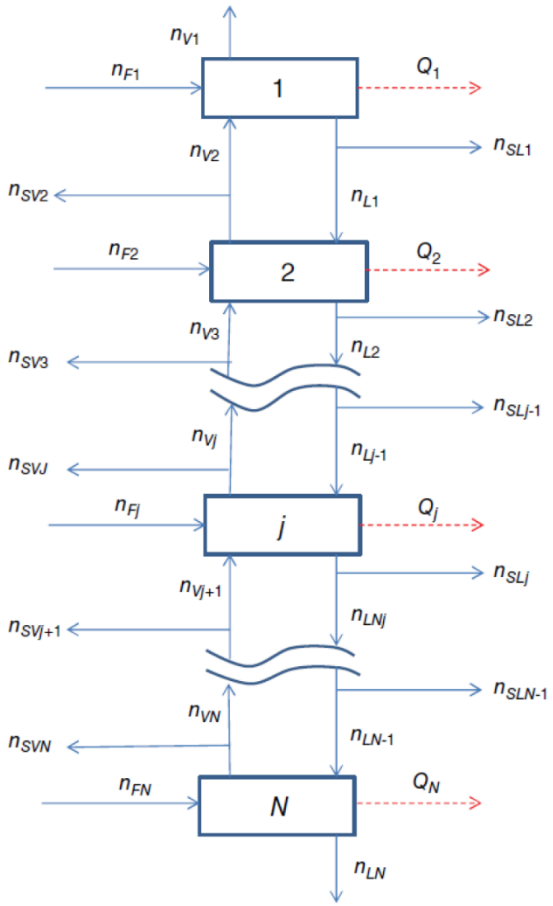

Figure 1. General scheme of multistage and multicomponent (rigorous) distillation.

The enthalpy equation is:

$$H_j = n_{Lj-1}h_{Lj-1} + n_{Vj+1}h_{Vj+1} + n_{Fj}h_{F,j} - (n_{Lj} + n_{SLj})h_{Lj} - (n_{Vj} + n_{SVj})h_{Vj} - Q_j = 0 \quad (11)$$

In these equations, n represents mole flow, x mole fraction in the liquid phase, y mole fraction in the vapor phase, K equilibrium constant, h molar enthalpy, and Q heat flow. Subscript i represents component, j stage, L liquid, V vapor, SV side vapor, SL side liquid, F feed, and N last stage, respectively.

The specified criteria for distillation simulation were: (a) Reflux Ratio (based on calculated minimum reflux), and (b) Distillation Column Component Recovery (0.999 per a separated component). Feed operating conditions are temperature of 60 °C (333 K), total pressure of 2000 kPa, and total molar flowrate of 977.7 kgmol/h, while feed composition is tabulated in Table 1 as a case study. We are targeted to separate of each component with 99.9% component recovery. Thus, Condenser and Reboiler Duties (kJ/h) were calculated by HYSYS.

2.3 Comparison of Various Sequence Design of Distillation Network

We compare five sequence design of distillation network with respect to a criterium namely Total Net Energy. Net Energy is defined as net energy between energy required in reboiler (Qreb) and energy released in condensor (Qcond) with unit of kJ/h of each distillation column. The Total Net Energy (kJ/h) is calculated as summation of Net Energy of all distillation columns in the network. Therefore, we compared the Total Net Energy of each sequence design if distillation column network. Figures 2-6 depicted five sequence design of distillation column network. The Total Net Energy (kJ/h) of all Sequence Designs (Sequence-A, Sequence-B, Sequence-D, and Sequence-E) were compared. The best Sequence Design was indicated by the lowest Total Net Energy.

Table 1. Feed composition as a case study.

Component	Formula	Molar Flow Rate (kgmol/h)
Nitrogen	N_2	10.5
Propane	C_3H_8	105.4
Isobutane	C_4H_{10}	136.1
n-butane	C_4H_{10}	226.8
i-pentane	C_5H_{12}	181.4
n-pentane	C_5H_{12}	317.5
	Total	977.7

3. Results and Discussion

3.1 Strategy for Separation of Multicomponent using Distillation Column Network

According to the Rule of Thumb of Distillation Strategy, we propose following procedures: (1) Estimating Saturated Vapor Pressure per component (P_i^{sat}) using Antoine Equation as function of temperatur ($P_i^{sat} = f(T)$); (2) Ordering the component from higher to lower value of Saturated Vapor Pressure (P_i^{sat}); (3) Calculating K-value (y_i/x_i), by estimating $K_i=P_i^{sat}/P$; (4) Calculating relative volatility, ($\alpha_{i,i+1}$), where $\alpha_{i,i+1} = K_i / K_i+1$; (5) Separating by distillation column network starting from the highest value of $\alpha_{i,i+1}$; thus (6) Calculating Net Energy (kJ/h) of each distillation column as energy efficiency consideration. The distillation column indicates lower energy efficiency when the Net Energy is minimum. The calculation of relative volatility ($\alpha_{i,i+1}$) according to Saturated Vapor Pressure (P_i^{sat}) and K-value is tabulated in Table 2.

From all Sequence Designs (Sequence-A, Sequence-B, Sequence-D, and Sequence-E), we compared by calculating Total Net Energy (kJ/h) of all distillation column in the separation network. The best Sequence Design was indicated by the lowest Total Net Energy. Figures 7-11 depicted simulation of all Sequence Designs (Sequence-A, Sequence-B, Sequence-D, and Sequence-E) using rigorous distillation simulation in Aspen HYSYS.

3.2 Total Net Energy Calculation and Comparison from All Sequence Designs

The distillation column indicates lower energy efficiency when the Net Energy is minimum. The Net Energy of each distillation column of each sequence design are presented in Tables 3-7. Total Net Energy (kJ/h) of all distillation column in the separation network is compared among all Sequence Designs (Sequence-A, Sequence-B, Sequence-D, and Sequence-E) as presented in Table 8 and Figure

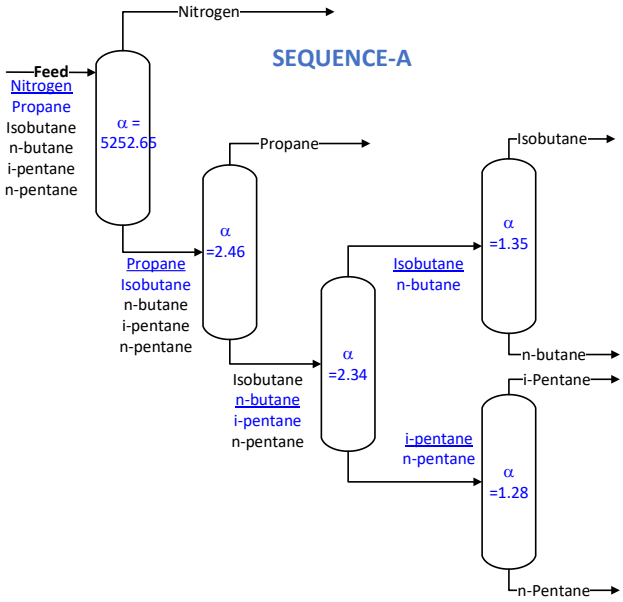

Figure 2. Sequence-A design of distillation column network.

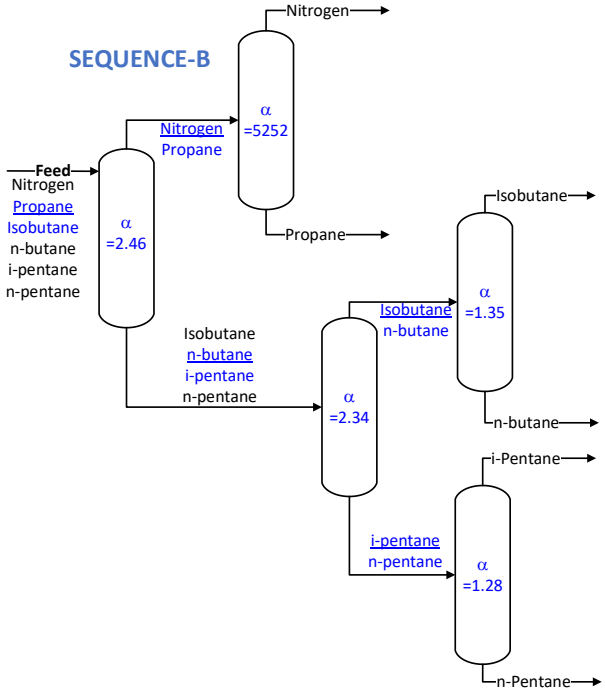

Figure 3. Sequence-B design of distillation column network.

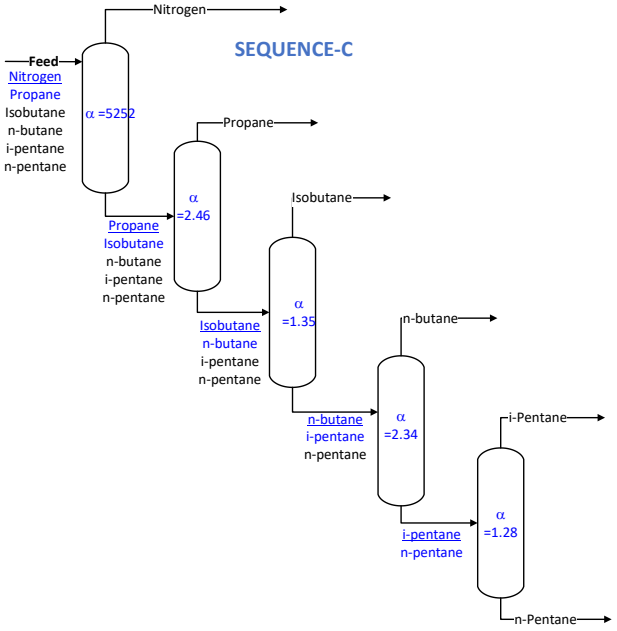

Figure 4. Sequence-C design of distillation column network.

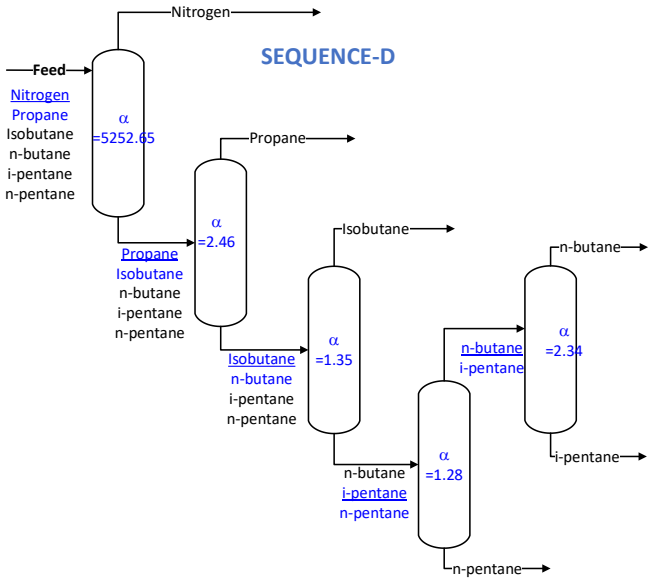

Figure 5. Sequence-D design of distillation column network.

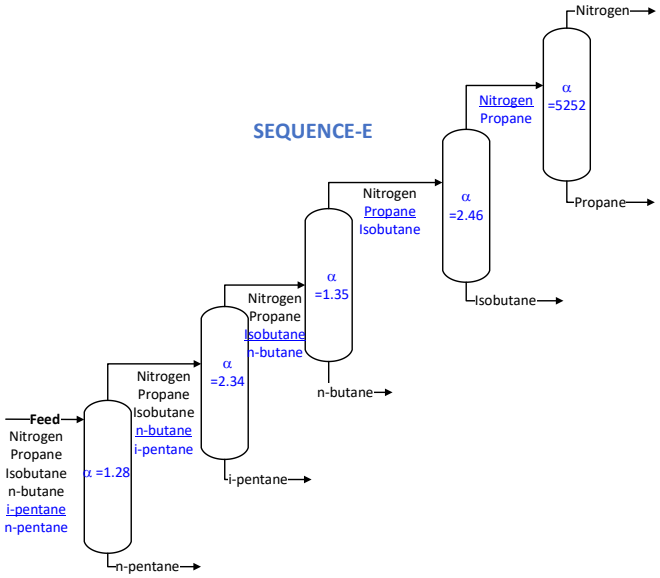

Figure 6. Sequence-E design of distillation column network.

Table 2. The calculation of relative volatility ($\alpha_{i,i+1}$) according to Saturated Vapor Pressure (P_i^{sat}) and K-value.

Component	Formula	Normal Boiling Point (°C)	Coefficient of Antoine Vapor Pressure						Vapor Pressure (P_i^{sat}) (kPa)	$K_i=P_i^{sat}/P$	$\alpha_{i,i+1} = K_i/K_{i+1}$
			a	b	c	d	e	f			
Nitrogen	N_2	-195.8	35.4113	-966.243	0	-4.31849	7.93E-05	2	11104585.61	5552.29	**5252**
Propane	C_3H_8	-42.1	52.3785	-3490.55	0	-6.10875	1.12E-05	2	2114.09	1.0570	**2.46**
Isobutane	C_4H_{10}	-11.73	58.7845	-4136.68	0	-7.01666	1.04E-05	2	860.72	0.4304	**1.35**
n-butane	C_4H_{10}	-0.502	66.945	-4604.09	0	-8.25491	1.16E-05	2	636.68	0.3183	**2.34**
i-pentane	C_5H_{12}	27.88	66.7563	-5059.18	0	-8.08935	9.25E-06	2	271.95	0.1360	**1.28**
n-pentane	C_5H_{12}	36.06	63.3315	-5117.78	0	-7.48305	7.77E-06	2	213.01	0.1065	

Table 3. The calculation of Net Energy of each distillation column of Sequence-A.

Distillation Column	Energy Required by Reboiler (Qreb, kJ/h)	Energy released by Condensor (Qcond, kJ/h)	Net Energy of Distillation Column (kJ/h)	Number of Trays	Reflux Ratio
Alfar-5252	15,262,297.78	-6,795,536.91	8,466,760.87	6	0.29
Alfar-2.46	20,302,401.77	-19,377,161.52	925,240.24	45	7.5
Alfar-2.34	23,323,000.88	-23,096,373.20	226,627.68	61	4.67
Alfar-1.35	26,948,661.72	-26,775,380.86	173,280.86	378	20.16
Alfar-1.28	77,260,872.21	-77,302,060.99	-41,188.78	497	42.17
		Total Net Energy of Sequence-A =	9,750,720.88		

Table 4. The calculation of Net Energy of each distillation column of Sequence-B.

Distillation Column	Energy Required by Reboiler (Qreb, kJ/h)	Energy released by Condensor (Qcond, kJ/h)	Net Energy of Distillation Column (kJ/h)	Number of Trays	Reflux Ratio
Alfar-2.46	32,331,017.57	-22,530,833.94	9,800,183.63	20	1.16
Alfar-5252	3,204,694.40	-410,276.14	2,794,418.26	25	8
Alfar-2.34	15,130,149.10	-15,094,384.32	35,764.77	61	4.67
Alfar-1.35	5,730,862.83	-5,656,165.42	74,697.41	236	19.5
Alfar-1.28	53,906,203.24	-53,858,000.21	48,203.04	459	42.71
		Total Net Energy of Sequence-B =	12,753,267.11		

Table 5. The calculation of Net Energy of each distillation column of Sequence-C.

Distillation Column	Energy Required by Reboiler (Qreb, kJ/h)	Energy released by Condensor (Qcond, kJ/h)	Net Energy of Distillation Column (kJ/h)	Number of Trays	Reflux Ratio
Alfar-5252	15,262,297.78	-6,795,536.91	8,466,760.87	6	0.29
Alfar-2.46	17,453,167.97	-16,700,373.67	752,794.30	64	8.88
Alfar-1.35	36,129,667.84	-35,831,138.94	298,528.91	212	28.59
Alfar-2.34	23,472,899.75	-23,173,911.98	298,987.78	71	7.08
Alfar-1.28	82,127,155.26	-82,156,426.15	-29,270.89	497	42.65
		Total Net Energy of Sequence-C =	9,787,800.97		

Table 6. The calculation of Net Energy of each distillation column of Sequence-D.

Distillation Column	Energy Required by Reboiler (Qreb, kJ/h)	Energy released by Condensor (Qcond, kJ/h)	Net Energy of Distillation Column (kJ/h)	Number of Trays	Reflux Ratio
Alfar-5252	15,262,297.78	-6,795,536.91	8,466,760.87	6	0.29
Alfar-2.46	17,453,167.97	-16,700,373.67	752,794.30	64	8.88
Alfar-1.35	36,129,667.84	-35,831,138.94	298,528.91	212	26.59
Alfar-1.28	59,705,763.90	-59,529,073.25	176,690.66	375	16.68
Alfar-2.34	9,500,929.39	-9,307,601.77	193,327.62	91	4.48
		Total Net Energy of Sequence-D =	9,888,102.35		

Table 7. The calculation of Net Energy of each distillation column of Sequence-E.

Distillation Column	Energy Required by Reboiler (Qreb, kJ/h)	Energy released by Condensor (Qcond, kJ/h)	Net Energy of Distillation Column (kJ/h)	Number of Trays	Reflux Ratio
Alfar-1.28	126,558,927.93	-117,294,664.33	9,264,263.60	233	7.25
Alfar-2.34	23,028,260.27	-22,229,377.36	798,882.91	50	1.78
Alfar-1.35	30,431,389.00	-30,597,449.27	-166,060.27	80	4.58
Alfar-2.46	3,745,062.11	-557,583.04	3,187,479.07	15	0.8
Alfar-5252	250,999.87	-97,872.62	153,127.25	10	2
	Total Net Energy of Sequence-E =		13,237,692.57		

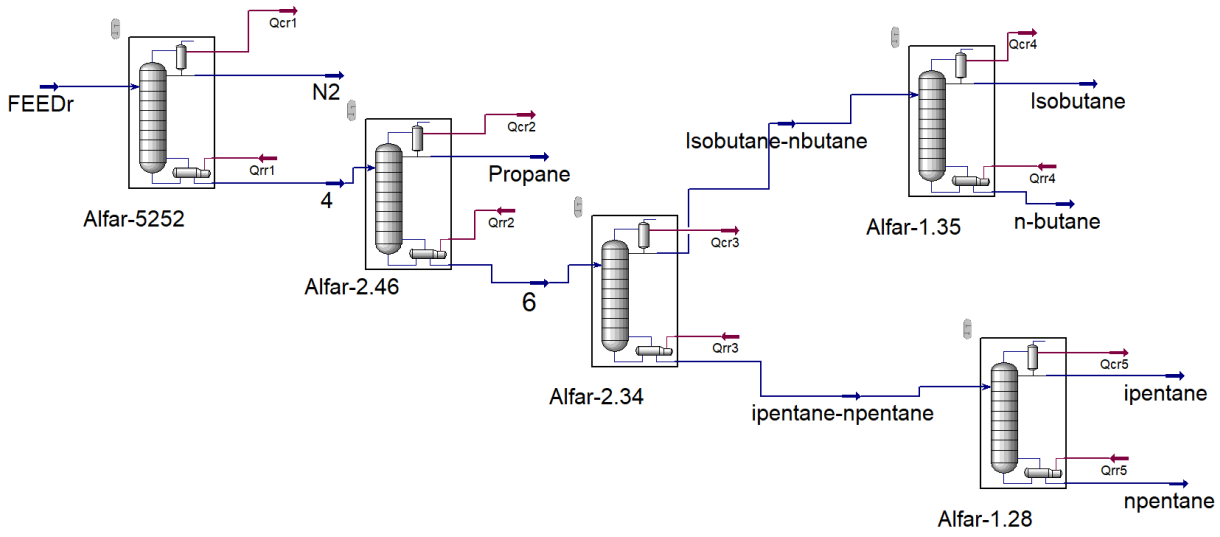

Figure 7. Simulation of rigorous distillation column network for Sequence-A design

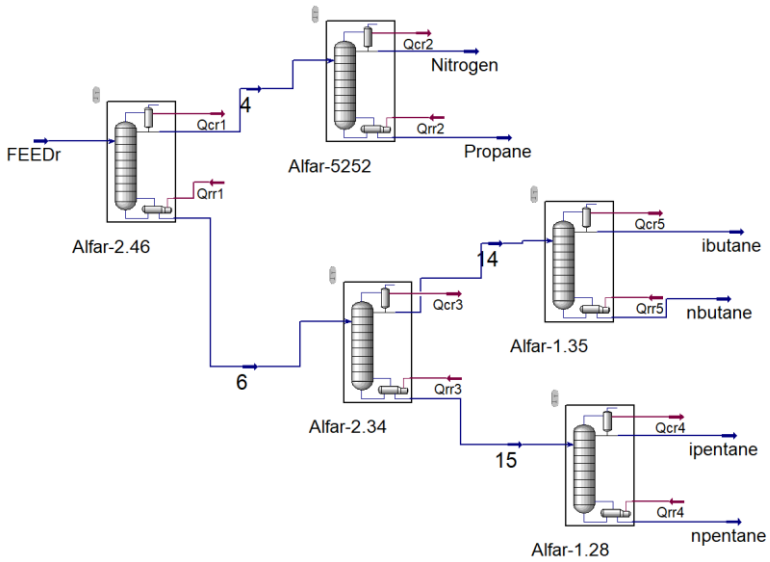

Figure 8. Simulation of rigorous distillation column network for Sequence-B design.

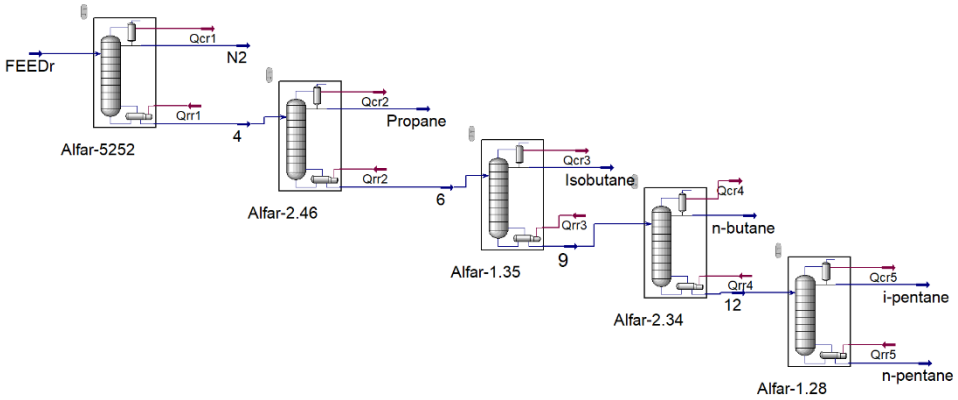

Figure 9. Simulation of rigorous distillation column network for Sequence-C design.

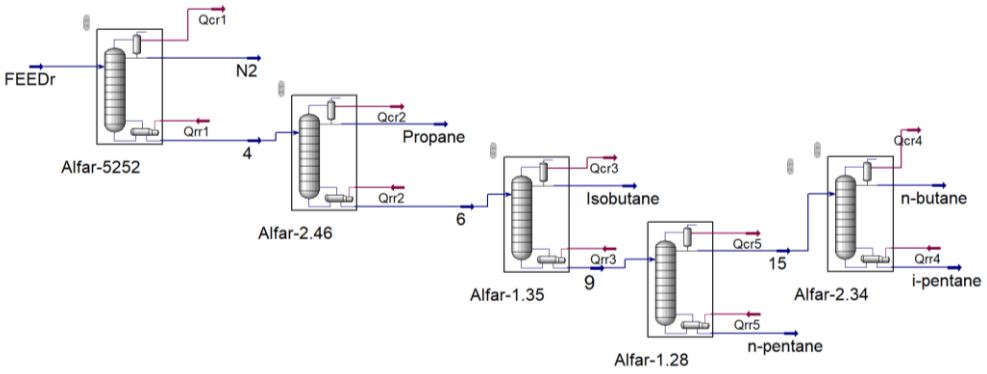

Figure 10. Simulation of rigorous distillation column network for Sequence-D design.

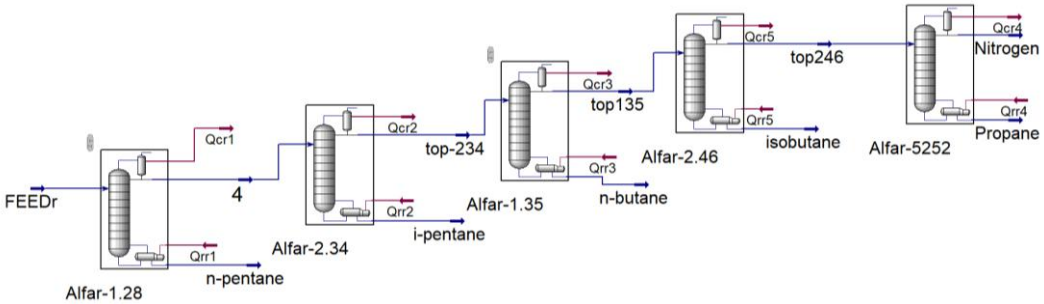

Figure 11. Simulation of rigorous distillation column network for Sequence-E design.

12. From all sequence designs, Sequence-A shows the lowest Total Net Energy (9,750,720.88 kJ/h), because of appropriateness of Sequence-A with the strategy/procedure for separation of multicomponent using distillation column network stated in Section 3.1. This finding is inline with finding of Nogaja *et al.* [16-18]. In the Sequence-A, following the rule of thumb, separation is sequentally started from the largest relative volatility ($\alpha_{i,i+1}$ = 5252) to the smallest one ($\alpha_{i,i+1}$ = 1.28). Sequence-B, Sequence-C, Sequence-D, and Sequence E do not follow the strategy/procedure for separation of multicomponent using distillation column network stated in Section 3.1. In contrary, the Sequence-E shows the largest Total Net Energy (13,237,692.57 kJ/h) meaning the most inappropriate to the separation strategy or the most energy consuming. Decreasing the relative volatility ($\alpha_{i,i+1}$) affects on increasing number of tray and recycle ratio required for distillation process and decreasing the Net Energy. From the Table 8 and Figure 12, it is clear that Total Net Energy order from lowest to highest one is: Sequence-A < Sequence-C < Sequence-D < Sequence-B < Sequence-E.

If we apply the sequence design which is not following the rule of thumb of separation process (Section 2.1 or Section 3.1), the separation may forces on the difficult separation factor (lower relative volatility or lower vapor pressure difference) which in turn needs higher energy [15]. Even for very high relative volatity ($\alpha_{i,i+1}$), a flash separator can be applied with appropriate operating conditions (temperature, pressure) which makes sure the dual phases (liquid and vapor) occurred. This case is inline with the proposed method by Tsirlin *et al.* [19] that selection of distillation sequence for which the total energy consumption in the cascade of columns reaches its minimum. This sequence is determined by values of thermal coefficients / efficiency. Coefficients themselves depend on temperatures in the reboiler and condenser. In several chemical separations by distillation, it is permissible for neighboring components to be present in the process products instead of pure product. For such multicomponent-product distillations, the energy requirements could be substantially lower than if each component is separated into its own pure product (unicomponent-product distillation) [20].

Table 8. Comparison of Total Net Energy of all sequence designs of distillation column network.

Sequence Design	Total Net Energy (kJ/h)	Mole Fraction of Product Component (from 0.999 recovery)					
		N_2	Propane	Isobutane	n-butane	i-pentane	n-pentane
Sequence-A	9,750,720.88	0.0771	0.3232	0.3796	0.4799	0.8737	0.9995
Sequence-B	12,753,267.11	0.7648	0.1990	0.2624	0.0713	0.7668	0.9996
Sequence-C	9,787,800.97	0.0771	0.4310	0.5326	0.6382	0.8766	0.9995
Sequence-D	9,888,102.35	0.0771	0.4310	0.5326	0.9995	0.9962	0.8302
Sequence-E	13,237,692.57	1.0000	0.9899	0.3729	0.6566	0.4828	0.9992

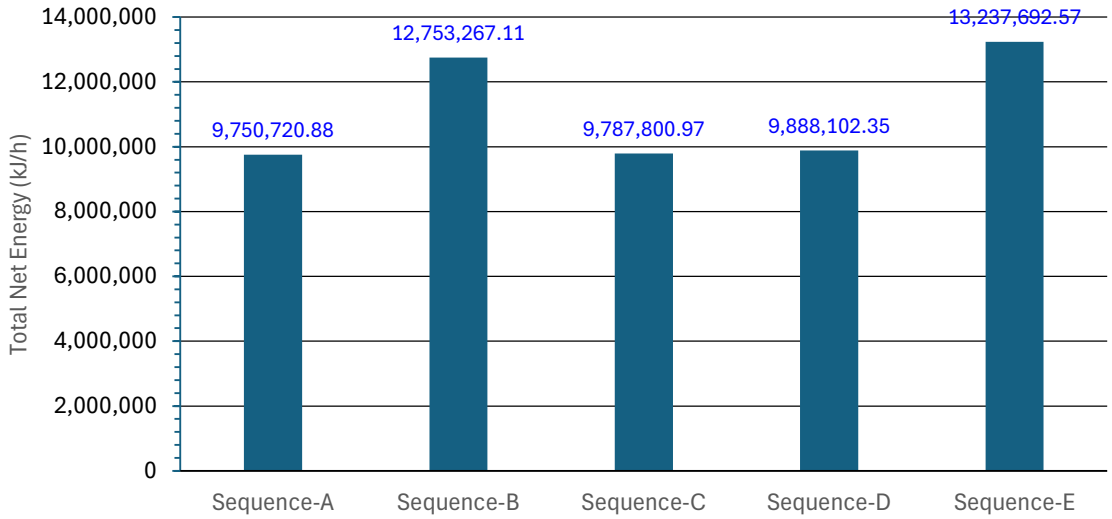

Figure 12. Comparison of Total Net Energy of all Sequence Designs of distillation column network.

4. Conclusion

Energy saving in separation systems, particularly in distillation systems, is a research field that has attracted considerable innovative approaches. A distillation system is an essential separation process yet it is inefficient in using thermal energy, and may operate with adverse environmental impact as it discharges a large amount of thermal energy into the environment. Applying the Rule of Thumb of Distillation Strategy (Section 2.1 and Section 3.1) for separating multicomponent mixtures is important by performing the easiest separation first (largest α_{12}), that is, the one least demanding of trays and reflux, and leaving the most difficult to the last. From all sequence designs, Sequence-A shows the lowest Total Net Energy (9,750,720.88 kJ/h), because of appropriateness of Sequence-A with the strategy/procedure for separation of multicomponent using distillation column network stated in Section 3.1 or Section 2.1. Decreasing the relative volatility ($\alpha_{i,i+1}$) affects on increasing number of tray and recycle ratio required for distillation process and decreasing the Net Energy. Total Net Energy order of five sequence designs from lowest to highest one is: Sequence-A < Sequence-C < Sequence-D < Sequence-B < Sequence-E.

Credit Author Statement

I. Istadi: Writing – review & editing, Writing – original draft, Supervision, Resources, Methodology, Formal analysis, Conceptualization, Validation Data curation, Investigation. **Teguh Riyanto:** Writing – review & editing, Writing – original draft, Resources, Project administration, Methodology, Formal analysis.

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