INTRODUCTION

Distillation is applied for nearly 95% of fluid separations in chemical industry, and approximately 3% of global energy is consumed in this Distillation units. The high rate of energy consumption in the distillation process prompted the researchers to develop new means to economize on energy and cost.

So far, extensive studies have been conducted on methods to reduce energy consumption in distillation towers. Using the thermal coupled structures in distillation towers is an essential factor in reducing energy consumption. A divided wall column has a vertical partition wall in the middle and can replace two or more conventional distillation towers or a Petlyuk tower. Previous research (WALTERMANN et al., 2019; GHALAVAND et al., 2021; FRANKE, 2017) In order to design a divided wall column with different complexities, the use of shortcut method based on a combination of equations (Fenske-Underwood - Gilliland-Kirkbride) has been investigated by (WALTERMANN et al., 2020; HIROYA SEKI, 2012; MA et al., 2019). (NEZHADFARD et al., 2018) A Semi Rigorous design based on a combination of equilibrium steps has been proposed. Previously, other authors have proposed a precise method for azeotropic distillation with an optimization approach to optimize operational and structural parameters in order to minimize the sum of annual costs (TULA et al., 2017; MURALIKRISHNA et al., 2002; SOTUDEH & SHAHRASI, 2007). (MURALIKRISHNA et al., 2002) Using shortcut methods and Vmin diagrams, the above parameters were calculated. Examining the articles, it can be concluded that the shortcut method is a suitable method for designing such towers. The use of this technology will lead to several results, including about 20% energy and capital savings, reduction of space required, reduction of thermal stress applied to temperature-sensitive compounds.

METHODS

Given the existence of the wall and the division of the tower into two parts, the Prefractionation and the main column and the ratio of liquid distribution on both sides of the wall, as a result, the design parameters of the divided wall column will be more than the simple tower. To calculate these parameters, shortcut and rigorous methods or a combination of the two can be deployed.

THE FIRST SHORTCUT METHOD FOR DESIGNING A DIVIDED WALL COLUMN

In this method (MURALIKRISHNA et al., 2002), a divided wall column is assumed to result from a combination of three ordinary towers (figure 1). The first part is called the prefractionator, the second part is called the second tower and the third part is called the third tower. In this method, the Underwood equations are used to acquire the minimum liquid returned for each part of the tower. Fenske Equation is used to calculate the minimum number of trays required (KIM et al., 2021), and Gilliland correction is used to calculate the actual liquid returned and the number of theoretical steps (MA et al., 2019). This method is known as the FUG (Fenske-Underwood-Gilliland) method. Next, the Kirkbride Equation is used to obtain the location of the feed tray (GHALAVAND et al., 2021).
**The second shortcut method for designing a divided wall column**

In this method (SOTUDEH, SHAHRAKI, 2007), as in the previous method, the divided wall column is assumed to be the result of a combination of three ordinary towers in Figure (2) and the current equations for all three parts of the tower are calculated. This method is presented using the shortcut method for designing distillation towers based on the Underwood equations. In the method that we will examine, the crucial factor of the ratio of liquid flow between the two parts of the middle wall of the tower is known as an effective parameter in the design of the tower.

**Source:** Search data.

**Figure 1.** Schematic of divided wall column

**Figure 2.** Parameters of a divided wall column

**Source:** Search data.
Comparison of shortcut methods for designing of divided wall columns for separating tertiary zeotropic mixtures

Figure 3. Change into a four-tower model

Information necessary for design

One of the essential points in simulating a divided wall column is how the ratio of liquid and steam flows is divided into both sides of the divided wall column’s wall. Making use of the four-tower model makes it possible to incorporate this vital parameter in the design. To achieve that aim, the lower product of the second part of the tower must be entered into the input of the flow divider in the software. And connect the two output products of this device to the first tray of the first and third towers. Likewise, for the lower part of the tower, we flow the upper product of the fourth tower into the input of the flow divider and connect the two output products to the lower tray of the first and third towers (Figure 4). The first tower has 3 input flows (input feed whose percentage and characteristics are known and output flows from the second and fourth towers) by connecting the flows mentioned above.

Figure 4. Four-tower model in ASPEN PLUS software

Source: Search data.
Calculation the initial values for the input flows to the first tower

The selected method for calculating the initial values is that in the ASPEN PLUS environment, a distillation tower with a condenser and a boiler, the input feed flow is divided into a wall tower that enters the tower with a certain percentage composition, at a certain temperature and pressure. To calculate the required parameters of the tower, the computational methods that we have explained in two shortcut methods are applied. After implementation, through determining the percentage composition of top and bottom products of the tower and all the trays of the tower, we write down the information about the percentage composition of liquid flow entering the first tray and steam flow entering the last tray. Then, we consider these values as the initial values in the design of a divided wall column.

Degrees of freedom

The design of a distillation tower comprises numerous parameters such as product composition and flow rate, operating pressure, total number of trays, feed tray location, return flow ratio, input heat to boiler, heat transfer rate in condenser, diameter and column height. Not all of these variables are independent, so analyzing the degree of freedom of the system will be useful to determine the exact number of independent variables that must be specified to define the whole system. Precise analysis of the degree of freedom necessitates counting the number of system variables and subtracting them from the number of equations that describe the system.

Several studies have been conducted to calculate the degrees of freedom of a divided wall column. Many researchers (LUYBEN, 2006; Becker et al., 2001; DEJANOVIC’ et al., 2010) have considered 5 degrees of freedom for a divided wall column, which are:

1. Return current ratio
2. The ratio of the return current from the boiler
3. The amount of by-product flow
4. Liquid flow on both sides of the wall
5. Steam flow on both sides of the wall

A realistic study was carried out by Ling and Leibniz (HAO LING et al., 2019) and reported that the amount of steam on both sides of the wall was proportionate to the cross-section of both sides of the wall. Thus, this parameter has been removed along with the pressure parameter and the degrees of freedom have been reduced to 4.

Parameters required for designing

Figure 4-8 illustrates the information necessary to design a divided wall column.
As demonstrated in Figure 4-8, the 11 parameters mentioned must be determined in order to simulate a divided wall column in software. Most of the needed information should be calculated utilizing the shortcut methods mentioned in Chapter 3 and the information received from each method should be transferred to the software and the output answer which is the percentage composition of tower products and other required information should be extracted from the software.

As a matter of fact, the software is applied to verify the shortcut methods examined.

Having Employed this method, known as the detailed method, the equations for each tower are calculated for each of the trays and the final result is reported. In addition, the balance information reports all trays, energy consumption, boiling and condensing heat load, and other information for each tower separately.

**Examination of the conditions and characteristics of the feed entering the tower**

In the prevailing study, to more precisely investigate the responses of the shortcut method, in both methods, three different feeds with differences in relative volatility characteristics in a way that:

1. The ratio of the relative volatility of light component to middle component and middle component to heavy component should be in the same order.
2. The ratio of the relative volatility of light component to middle component and middle component to heavy component should hold a higher rank.

3. We examined the ratio of the relative volatility of light component to middle component and middle component to the heavy component to have a lower order.

In each of the studied cases, the three-component feed was examined in the following 3 percentage composition:

**Table 1. Percentage compositions examined**

| Percentage composition 1 | A: 0.33 | B: 0.33 | C: 0.33 |
|--------------------------|----------|----------|----------|

| Percentage composition 2 | A: 0.01  | B: 0.45  | C: 0.045 |
|--------------------------|----------|----------|----------|

| Percentage composition 3 | A: 0.45  | B: 0.01  | C: 0.45  |
|--------------------------|----------|----------|----------|

| Percentage composition 4 | A: 0.45  | B: 0.45  | C: 0.1   |
|--------------------------|----------|----------|----------|

**Source:** Search data.

The input feeds are as follows:

**Table 2. Feeds examined and relative volatility ratios**

| Feed  | A   | B   | C   | A/B | B/C |
|-------|-----|-----|-----|-----|-----|
| Feed 1 | Benzene | Toluene | O-Xylene | 6.77 | 2.78 |
|       |       |       |       | 1.24 | 2.78 |
| Feed 2 | I-Butane | N-Butane | cycloButane | 1.76 | 1.34 |
|       |       |       |       | 1.3  | 1.3  |
| Feed 3 | Propylene | Butylene | Pentene | 7.64 | 1.99 |
|       |       |       |       | 3.82 | 1.99 |

**Source:** Search data.

All input feeds enter the tower at the same temperature and pressure, and the feed and product features are granted in Tables 3 and 4, respectively.

**Table 3. Feed Specifications**

| Feeds | Temperature (centigrade) | Kg/sqem Pressure | q | Feed flow Kmol/hr |
|-------|--------------------------|------------------|---|-------------------|
|       | 100                      | 0.75             | 0.557 | 30               |

**Source:** Search data.

**Table 4. Specifications of the requested product**

| Substance | Desired purity |
|-----------|----------------|
| Purity of substance A in the product above the tower | 0.95 |
| Purity of substance B in the middle product | 0.90 |
| Purity of substance C in the lower product | 0.95 |

**Source:** Search data.

**RESULTS**

Output information from the shortcut method in the first method (MATLAB software) and detailed method (ASPEN software)

In this section, it is first implemented separately for both methods. Then, after verifying the results obtained by matching the results presented in the previously examined articles, these methods were investigated for different feed states by combining different percentages. The results acquired from the shortcut methods are, in fact, the needed parameters for simulating a divided wall column in ASPEN software. The first method under examination is the method proposed by Morley Krishna (MURALIKRISHNA et al., 2002). The first feed entering the tower was benzene, toluene, and Ortho xylene, and the feed components enter the tower in equal moles. As can be observed in Table (6), the error rate of the lower product of the tower is less than other products, and on average, in this case, 6.3% error is observed.
Table 5. Results of the first method for feed mixture No. 1 percentage composition No. 1

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray | Feed tray | Middle product | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|-------------------------|---------------------------|--------------------------|---------------------------|-----------|-----------|--------------|-------------------------------------------|------------------------------------------|
| 12                      | 12                        | 12                       | 6                         | 10        | 7         | 3.3          | 1.82                                      |                                          |

Source: Search data.

Table 6. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 1 percentage composition No. 1

| Substance | Substance | Substance | flow Kmol/h | Error percentage | Average error |
|-----------|-----------|-----------|-------------|------------------|---------------|
| Upper     | 0.999     | 0.001     | 0           | 8.58             | 9.77          | 6.3          |
| Middle    | 0.13      | 0.82      | 0.05        | 10               | 8.89          |              |
| Lower     | 0         | 0.17      | 0.83        | 11.42            | 0.22          |              |

Source: Search data.

In the next case, the feed of benzene, toluene, and ortho-xylene with a combination of 10% benzene and 45% toluene and ortho-xylene enters the tower. The results of this case in Table (8) indicate a drastic increase in the average error of the tower.

Table 7. Results of the first method for feed mixture No. 1 percentage composition No. 2

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray | Feed tray | Middle product | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|-------------------------|---------------------------|--------------------------|---------------------------|-----------|-----------|--------------|-------------------------------------------|------------------------------------------|
| 7                       | 8                         | 7                        | 4                         | 5         | 4         | 22.13        | 4.77                                      |                                          |

Source: Search data.

Table 8. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 1 percentage composition No. 2

| Substance | Substance | Substance | flow Kmol/h | Error percentage | Average error |
|-----------|-----------|-----------|-------------|------------------|---------------|
| Upper     | 0.99      | 0.001     | 0           | 1.35             | 52.68         | 25.36        |
| Middle    | 0.1       | 0.76      | 0.12        | 13.5             | 15.56         |              |
| Lower     | 0         | 0.22      | 0.78        | 15.15            | 7.89          |              |

Source: Search data.

The next case is benzene, toluene, and ortho-xylene feed, with the difference that in the composition of feed percentage, toluene is only 10%, and benzene and ortho-xylene each constitute 45% of the input feed. As can be observed in Table (10), in this case, the middle product of the tower, is accompanied by a large error.
Table 9. Results of the first method for feed mixture No. 1 percentage composition No. 3

| Information obtained from the shortcut method in the first method for feed mixture No. 1 percentage composition No. 3 |
|---|---|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 18 | 10 | 18 | 6 | 16 | 6 | 1.35 | 0.34 |

Source: Search data.

Table 10. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 1 percentage composition No. 3

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 1 percentage composition No. 3 |
|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage |
| Upper product | 0.994 | 0.006 | 0 | 9.07 | 29.7 |
| Middle product | 0.48 | 0.25 | 0.27 | 3 | 72.22 |
| Lower product | 0.17 | 0.12 | 0.71 | 17.93 | 0.74 |

Source: Search data.

The next case is benzene, toluene, and ortho-xylene feed, with the difference that in the composition of feed percentage, ortho-xylene is only 10%, and benzene and toluene each constitute 45% of the input feed. As can be observed in Table (12), in this case, the separation of the component with a minimum percentage in the input feed, which is the lower product of the tower, is accompanied by a large error.

Table 11. Results of the first method for feed mixture No. 1 percentage composition No. 4

| Information obtained from the shortcut method in the first method for feed mixture No. 1 percentage composition No. 4 |
|---|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 12 | 15 | 12 | 8 | 11 | 9 | 2.1 | 2.82 |

Source: Search data.

Table 12. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 1 percentage composition No. 4

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 1 percentage composition No. 4 |
|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage |
| Upper product | 0.83 | 0.16 | 0 | 13.61 | 11.92 |
| Middle product | 0.17 | 0.76 | 0.33 | 13.5 |
| Lower product | 0 | 0.08 | 0.67 | 2.89 |

Source: Search data.

Normal hexane, normal heptane, and normal octane are the next feed to be studied. The characteristic of this feed is in the ratio equal to the ratio of the relative volatility of light component to middle component and middle component to heavy component.
The feed components enter the tower in equal moles.

In the case of feed with equal moles, the results indicate an increase in the error relative to the feed ratio of toluene benzene and ortho-xylene in the percentage composition. It should be noted that the upper product of the tower is associated with an error of only 0.39.

**Table 13.** Results of the first method for feed mixture No. 2 percentage composition No. 1

| Information obtained from the shortcut method in the first method for feed mixture No. 2 percentage composition No. 1 |
|---|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 12 | 11 | 12 | 6 | 10 | 7 | 3.9 | 2.5 |

**Source:** Search data.

**Table 14.** Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 2 percentage composition No. 1

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 2 percentage composition No. 1 |
|---|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
| Upper product | 0.82 | 0.18 | 0 | 11.63 | 0.39 | 16.43 |
| Middle product | 0.03 | 0.67 | 0.3 | 10 | 25.56 |
| Lower product | 0 | 0.13 | 0.87 | 8.37 | 23.35 |

**Source:** Search data.

The results of entering the normal hexane, normal heptane and normal octane feed with the second percentage composition, which normal hexane in the input feed is 10%, can be seen in Table (16). The simulation results show an average error of 3.35%.

**Table 15.** Results of the first method for feed mixture No. 2 percentage composition No. 2

| Information obtained from the shortcut method in the first method for feed mixture No. 2 percentage composition No. 2 |
|---|---|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 8 | 8 | 8 | 5 | 5 | 4 | 32.7 | 6.9 |

**Source:** Search data.

**Table 16.** Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 2 percentage composition No. 2

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 2 percentage composition No.2 |
|---|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
| Upper product | 0.8 | 0.2 | 0 | 3.68 | 3.30 | 3.35 |
| Middle product | 0 | 0.89 | 0.11 | 13.5 | 1.11 |
| Lower product | 0 | 0.056 | 0.994 | 12.82 | 5.64 |

**Source:** Search data.

Normal hexane, normal heptane and normal octane feed enter the tower by the third percentage composition, in which normal heptane is 10 in the input feed and the other two
component have equal moles. As in the previous feed in the same percentage composition, the simulation results of Table (18) demonstrates an insignificant amount of error.

Table 17. Results of the first method for feed mixture No. 2 percentage composition No. 3

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|--------------------|-------------------------------|-------------------------------------------|------------------------------------------|
| 19                       | 10                        | 19                       | 6                         | 16                 | 7                             | 1.6                                       | 0.63                                     |

Source: Search data.

Table 18. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 2 percentage composition No. 3

| Substance | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-----------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.85        | 0.13        | 0.02        | 15.5             | 2.73          | 36.52                      |
| Middle product | 0.14        | 0.08        | 0.78        | 3                | 91.11         |
| Lower product | 0           | 0.06        | 0.94        | 11.5             | 15.71         |

Source: Search data.

Normal hexane, normal heptane and normal octane feed enter the tower in the fourth percentage composition, which the heaviest component is minimum in the input feed (10%).

The results of the simulation, Table (20) shows an increase in the error of the lower product of the tower, and on average for all three products of the tower an error of 19.54% has been reported.

Table 19. Results of the first method for feed mixture No. 2 percentage composition No. 4

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|--------------------|-------------------------------|-------------------------------------------|------------------------------------------|
| 13                       | 10                        | 13                       | 9                         | 11                 | 9                             | 2.36                                       | 4.27                                     |

Source: Search data.

Table 20. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 2 percentage composition No. 4

| Substance | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-----------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.84        | 0.16        | 0           | 13.91            | 8.89          | 19.54                      |
| Middle product | 0.13        | 0.78        | 0.09        | 13.5             | 13.33         |
| Lower product | 0           | 0.3          | 0.7          | 2.59             | 36.38         |

Source: Search data.

The third feed under consideration is isobutane, normal butane, and cyclobutane. In this feed, as in the previous feed, the ratio of the relative volatility of the light component to the middle component and the middle component to the heavy component is equal, with the difference
that this ratio (1.3) is lower than the ratio of the previous feed (2.2). The ratio of light to heavy component volatility in this feed is (1.76), and the ratio of the middle component to heavy component volatility is (1.34). The proximity of these two numbers demonstrates that the mixture is difficult to separate. This method has an average error of 10.52%. It is worth mentioning that the number of steps required for this separation has increased substantially compared to previous feeds, with 33 trays on either side of the wall, 36 trays for the upper, and 12 trays for the bottom.

**Table 21.** Results of the first method for feed mixture No. 3 percentage composition No. 1

| Information obtained from the shortcut method in the first method for feed mixture No. 3 percentage composition No. 1 |
|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 33 | 36 | 33 | 12 | 27 | 20 | 12.86 | 12.98 |

**Table 22.** Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 1

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 1 |
|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage |
| Upper product | 0.807 | 0.193 | 0 | 11.82 | 0.41 |
| Middle product | 0.01 | 0.75 | 0.24 | 10 | 16.67 |
| Lower product | 0 | 0.007 | 0.993 | 8.18 | 14.5 |

**Source:** Search data.

Isobutane, normal butane, and cyclobutane enter the tower, this time in the second percentage composition. ISO butane in the input feed is merely 10%, and the other two components are 45% each.

The simulation results of Table (24) show a 5.02% error in the upper product of the tower, which is the minimum component in the input feed. While the two middle and lower products show only 2.2% and 4.28% error.

**Table 23.** Results of the first method for feed mixture No. 3 percentage composition No. 2

| Information obtained from the shortcut method in the first method for feed mixture No. 3 percentage composition No. 2 |
|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 20 | 25 | 20 | 10 | 15 | 10 | 99 | 26.7 |

**Source:** Search data.

**Table 24.** Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 2

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 2 |
|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage |
| Upper product | 0.73 | 0.27 | 0 | 4.1 | 5.02 | 3.84 |
| Middle product | 0 | 0.92 | 0.08 | 13.5 | 2.22 |
| Lower product | 0 | 0.01 | 0.99 | 12.4 | 4.28 |

**Source:** Search data.
The third percentage composition for isobutane, normal butane, and cyclo-butane feed, which is the minimum middle component (10%), is considered the tower’s input. In the results acquired from the simulation of Table (26) as in the previous two feeds, it can be observed a large error in this percentage composition and the number of steps required compared to the previously studied feeds for this separation is highly increased.

Table 25. Results of the first method for feed mixture No. 3 percentage composition No. 3

| Information obtained from the shortcut method in the first method for feed mixture No. 3 percentage composition No. 3 |
|---|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 50 | 32 | 50 | 14 | 45 | 20 | 5.89 | 5.3 |

Source: Search data.

Table 26. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 3

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 3 |
|---|---|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
| Upper product | 0.84 | 0.16 | 0 | 16.03 | 4.99 | 34.29 |
| Middle product | 0 | 0.15 | 0.85 | 3 | 83.33 |
| Lower product | 0 | 0.001 | 0.999 | 10.97 | 14.55 |

Source: Search data.

The feed of isobutane, normal butane, and cyclobutane are examined in the fourth percentage composition. In this case, the simulation results can be observed in Table (28). The average error obtained compared to the previous two feeds in this percentage composition indicates a reduction of the error to 13.97%. The increase in the number of tower steps is justified by the proximity of the relative volatility ratios.

Table 27. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 4

| Results obtained from the comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 3 percentage composition No. 4 |
|---|---|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
| Upper product | 0.84 | 0.16 | 0 | 13.96 | 8.57 | 13.97 |
| Middle product | 0.13 | 0.81 | 0.06 | 13.5 | 10 |
| Lower product | 0 | 0.14 | 0.86 | 2.54 | 23.35 |

Source: Search data.

Table 28. Results of the first method for feed mixture No. 4 percentage composition No. 1

formation obtained from the shortcut method in the first method for feed mixture No. 4 percentage composition No. 1

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|---|---|---|---|---|---|---|---|
| 9 | 5 | 9 | 5 | 4 | 3 | 10.37 | 8.36 |

Source: Search data.
The last feed under examination is propylene, butylene, and pentane. The characteristic of this feed is that the ratio of the volatility of the light to the heavy component is higher than that of the middle to the heavy component. The relative volatility of the light component to the heavy component is 7.64. The relative volatility of the middle component to the heavy component is 1.99, which is estimated to be more straightforward to separate than the previous cases. In the first state of this feed, in the percentage composition, the mole, too, enters the tower. The simulation results are illustrated in Table (30). Predictably, the simulation results for this state of input feed indicate only 3.45% error for the upper product of the tower, 2.22% error in the middle product, and 4.8% error in the bottom product.

**Table 29. Results of the first method for feed mixture No. 4 percentage composition No. 1**

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|-------------------------|---------------------------|--------------------------|---------------------------|-------------------|---------------------------------|---------------------------------------------|----------------------------------------|
| 9                       | 5                         | 9                        | 5                         | 4                 | 3                              | 10.37                                       | 8.36                                   |

Source: Search data.

**Table 30. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 4 percentage composition No. 1**

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.9        | 0.1         | 0           | 10.92            | 3.45          |
| Middle product | 0         | 0.88        | 0.12        | 10               | 2.22          |
| Lower product | 0          | 0.004       | 0.996       | 9.08             | 4.8           |

Source: Search data.

The percentage composition of the feed is propylene, butylene and pentene so that propylene constitutes only 10% of the input feed and the rest of the feed is equally distributed. The results, Table (32) shows an increase in error in the lower product of the tower. On average, 6.37% error is reported from the feed.

**Table 31. Results of the first method for feed mixture No. 4 percentage composition No. 2**

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|-------------------------|---------------------------|--------------------------|---------------------------|-------------------|---------------------------------|---------------------------------------------|----------------------------------------|
| 6                       | 4                         | 6                        | 5                         | 4                 | 2                              | 99                                         | 35.6                                   |

Source: Search data.

**Table 32. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 4 percentage composition No. 2**

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.6        | 0.4         | 0           | 4.92             | 3.58          |
| Middle product | 0         | 0.85        | 0.15        | 13.5             | 5.56          |
| Lower product | 0          | 0.003       | 0.997       | 11.58            | 9.98          |

Source: Search data.
The feed of propylene, butylene, and pentene comprises the third percentage composition so that the middle component in the input feed is only 10%, and the rest are equal to 45% each. Given the pattern generated in the previous three feeds, it is predicted that the simulation will be accompanied with a high amount of error in this percentage composition. The results are shown in Table (34) confirm this claim.

**Table 33. Results of the first method for feed mixture No. 4 percentage composition No. 3**

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|----------------------------|--------------------------|----------------------------|---------------------|-------------------------------|--------------------------------------------|------------------------------------------|
| 13                       | 5                          | 13                       | 4                          | 8                   | 4                             | 1.68                                       | 0.57                                     |

**Source:** Search data.

**Table 34. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 4 percentage composition No. 3**

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.84 | 0.15 | 0 | 15.77 | 4.52 | 31.74 |
| Middle product | 0.02 | 0.14 | 0.84 | 3 | 84.44 |
| Lower product | 0 | 0.025 | 0.975 | 12.33 | 6.26 |

**Source:** Search data.

The last case to be studied in the first method is the fourth percentage composition of the mixture of propylene, butylene, and pentene so that the heavier component has a minimum value (10 percent). The simulation results in Table (36) report an average of 9.99% error. This error is only 1.47% for the upper product of the tower, no error for the middle product, and 28.49% for the bottom product. Considering the difference in the relative volatility of the input components, the result obtained is justifiable.

**Table 35. Results of the first method for feed mixture No. 4 percentage composition No. 4**

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|----------------------------|--------------------------|----------------------------|---------------------|-------------------------------|--------------------------------------------|------------------------------------------|
| 10                       | 7                          | 10                       | 10                         | 5                   | 4                             | 2.26                                       | 4.88                                     |

**Source:** Search data.

**Table 36. Comparison of purity results obtained from MATLAB software with the first method for feed mixture No. 4 percentage composition No. 4**

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.9 | 0.1 | 0 | 14.46 | 1.47 | 9.99 |
| Middle product | 0.03 | 0.9 | 0.07 | 13.5 | 0 |
| Lower product | 0 | 0.001 | 0.999 | 2.04 | 28.49 |

**Source:** Search data.
Output information from the shortcut method in the second method (MATLAB software) and detailed method (ASPEN software):

In this method, the information obtained from the provided shortcut method is entered into ASPEN software. The output answer is presented in the form of purity percentage of the tower’s upper, middle and lower products. All three feeds studied in the first method are repeated for this method, and the results are presented in below Tables. The first feed to be studied is toluene benzene and ortho-xylene, which enter the tower as feed in equal moles. The results of this simulation are shown in Table (38). The average error, in this case, is almost equal to the average error of the first method, with the difference that the number of steps in this method is much less than the number of steps in the first method.

Table 37. Results of the second method for feed mixture No. 1 percentage composition No. 1

| Information obtained from the shortcut method in the second method for feed mixture No. 1 percentage composition No. 1 |
|---|---|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 8 | 5 | 8 | 4 | 4 | 4 | 3.53 | 4.16 |

Source: Search data.

Table 38. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 1 percentage composition No. 1

| Results obtained from the comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 1 percentage composition No. 1 |
|---|---|---|---|---|---|---|
| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
| Upper product | 0.84 | 0.16 | 0 | 11.5 | 1.68 | 8 |
| Middle product | 0 | 0.81 | 0.19 | 10 | 10 |
| Lower product | 0 | 0.02 | 0.98 | 8.5 | 13.32 |

Source: Search data.

In the second case, the toluene and ortho-xylene benzene feed enters the tower with a different percentage composition. So that benzene is present in the input feed only 10% and toluene and ortho-xylene with an equal portion of 45%.

As the results of this case can be seen in Table (40), in this method only the lower product of the tower has an error of 2.93% and the average reported error is only 2.98%. Compared to the first method (25.36% error), this method provides a better answer in this percentage composition.

Table 39. Results of the second method for feed mixture No. 1 percentage composition No. 2

| Information obtained from the shortcut method in the second method for feed mixture No. 1 percentage composition No. 2 |
|---|---|---|---|---|---|---|---|
| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
| 6 | 6 | 6 | 4 | 3 | 2 | 18.38 | 3.5 |

Source: Search data.
Table 40. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 1 percentage composition No. 2

| Substance A | Substance B | Substance C | flow (Kmol/h) | Error percentage | Average error |
|-------------|-------------|-------------|---------------|-----------------|--------------|
| Upper product | 0.95 | 0.05 | 0 | 2.82 | 6 |
| Middle product | 0.02 | 0.9 | 0.08 | 13.5 | 0 |
| Lower product | 0 | 0.09 | 0.91 | 13.68 | 2.93 |

Source: Search data.

In the third case, the feed of benzene, toluene, and ortho-xylene enters the tower with a combination of 10% toluene and 45% benzene and ortho-xylene. The results of this case are shown in Table (15) and, as in the previous method, indicate a large error in predicting the middle product of the tower.

Table 41. Results of the second method for feed mixture No. 1 percentage composition No. 3

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|-------------------------|---------------------------|--------------------------|---------------------------|-------------------|-------------------------------|------------------------------------------|----------------------------------------|
| 11                      | 2                         | 11                       | 2                         | 6                 | 6                            | 2.47                                     | 3.6                                    |

Source: Search data.

Table 42. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 1 percentage composition No. 3

| Substance A | Substance B | Substance C | flow (Kmol/h) | Error percentage | Average error |
|-------------|-------------|-------------|---------------|-----------------|--------------|
| Upper product | 0.84 | 0.16 | 0 | 15.82 | 3.6 |
| Middle product | 0 | 0.2 | 0.8 | 3 | 77.78 |
| Lower product | 0 | 0.003 | 0.997 | 11.18 | 13.088 |

Source: Search data.

The fourth case is the feed of benzene, toluene and ortho-xylene with a percentage composition of ortho-xylene of only 10% and benzene and toluene 45% each enters the tower. As shown in Table (44), this method has an average error of 25.27%. It should be noted that the lower product, which was considered a heavy component and was minimum in the input feed, is associated with 53.58% error. In the previous method, 32.06% error was reported.

Table 43. Results of the second method for feed mixture No. 1 percentage composition No. 4

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|-------------------------|---------------------------|--------------------------|---------------------------|-------------------|-------------------------------|------------------------------------------|----------------------------------------|
| 7                       | 7                         | 7                        | 5                         | 5                 | 6                            | 2                                        | 12.8                                   |

Source: Search data.
Table 44. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 1 percentage composition No. 4

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.79        | 0.21        | 0           | 15.15            | 6.68          | 25.27         |
| Middle product | 0.1         | 0.76        | 0.14        | 13.5             | 15.56         |               |
| Lower product | 0           | 0.02        | 0.98        | 1.35             | 53.58         |               |

Source: Search data.

Normal hexane, normal heptane and normal octane are the next feed to be studied. The characteristic of this feed is in the equal ratio of relative volatility of light component to middle component and middle component to heavy component.

In the first case, this feed enters the tower in a homogeneous way.

The results shown in Table (46) are associated with an average error of 18.78%.

The average error of the first method in these feed conditions was equal to 16.43%, with the difference that in this method the number of tower steps has been significantly reduced, so that the total number of tower steps in the previous method was 29 steps and in this method is 20 steps.

Table 45. Results of the second method for feed mixture No. 2 percentage composition No. 1

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|----------------------------|----------------------------|---------------------------|---------------------|----------------------------------|---------------------------------------------|----------------------------------------|
| 10                       | 5                          | 10                         | 5                         | 5                   | 5                                | 4.54                                        | 5.14                                   |

Source: Search data.

Table 46. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 2 percentage composition No. 1

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.075       | 0.25        | 0           | 13               | 2.63          | 18.78          |
| Middle product | 0.01        | 0.66        | 0.33        | 10               | 26.67         |               |
| Lower product | 0           | 0.01        | 0.99        | 7                | 27.05         |               |

Source: Search data.

The results for normal hexane, normal heptane and normal octane feed with the second percentage composition, that normal hexane in the input feed is 10% and the rest of the components are equal to 45%, are shown in Table (48). In this case, this method is associated with an average error of 6.08%, which is an increase compared to the previous method.
Table 47. Results of the second method for feed mixture No. 2 percentage composition No. 2

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|-------------------|-------------------------------|------------------------------------------|------------------------------------------|
| 8                        | 6                         | 8                        | 5                         | 3                 | 2                             | 22.77                                    | 4.3                                      |

Source: Search data.

Table 48. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 2 percentage composition No. 2

| Substance       | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-----------------|-------------|-------------|-------------|------------------|---------------|
| Upper product   | 0.775       | 0.225       | 0           | 3.65             | 0.75          |
| Middle product  | 0.01        | 0.84        | 0.15        | 13.5             | 6.67          |
| Lower product   | 0           | 0.11        | 0.89        | 12.58            | 10.83         |

Source: Search data.

Normal hexane, normal heptane and normal octane feed enter the tower in the third percentage composition, which normal heptane in the input feed is 10% and the other two components are homogeneous. As in the previous method in the same percentage composition, the simulation results of Table (50) report a very large error.

Table 49. Results of the second method for feed mixture No. 2 percentage composition No. 3

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|-------------------|-------------------------------|------------------------------------------|------------------------------------------|
| 13                       | 2                         | 13                       | 2                         | 7                 | 6                             | 3.14                                    | 4.3                                      |

Source: Search data.

Table 50. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 2 percentage composition No. 3

| Substance       | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-----------------|-------------|-------------|-------------|------------------|---------------|
| Upper product   | 0.78        | 0.13        | 0.09        | 17.3             | 5.22          |
| Middle product  | 0           | 0.21        | .79         | 3                | 76.67         |
| Lower product   | 0           | 0.005       | 0.995       | 9.7              | 24.74         |

Source: Search data.

Normal hexane, normal heptane and normal octane feed enter the tower in the third percentage composition, which normal heptane in the input feed is 10% and the other two components are homogeneous. As in the previous method in the same percentage composition, the simulation results of Table (50) report a very large error. It should be noted that in the second percentage composition, the more volatile product is minimal and the...
simulation answer is accompanied with a small error. In contrast, In this case, when the heavy component in the input feed is minimal, this method is associated with a large amount of error in the lower product of the tower.

Table 51. Results of the second method for feed mixture No. 2 percentage composition No. 4

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|-------------------|-------------------------------|------------------------------------------|----------------------------------------|
| 7                        | 6                         | 7                        | 6                         | 5                 | 5                             | 2.8                                      | 16.78                                  |

Source: Search data.

Table 52. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 2 percentage composition No. 4

| Substance A flow Kmol/h | Substance B flow Kmol/h | Substance C flow Kmol/h | Error percentage | Average error |
|-------------------------|-------------------------|-------------------------|------------------|---------------|
| Upper product           |                         |                         |                  |               |
| 0.82                    | 0.18                    | 0                       | 15.23            | 2.62          |
| Middle product          |                         |                         |                  |               |
| 0.07                    | 0.8                     | 0.13                    | 13.5             | 11.11         |
| Lower product           |                         |                         |                  |               |
| 0                       | 0.007                   | 0.993                   | 1.27             | 55.75         |

Source: Search data.

The third feed under consideration is isobutane, normal butane, and cyclobutane. Like the previous feed, this feed has a relative volatility ratio of the light component to middle component and middle component to heavy component. This ratio (1.3) is lower than the ratio of the previous feed (2.2). The volatility ratio of light to the heavy component in this feed is 1.76, and the volatility ratio of the medium component to heavy component is 1.34. The proximity of these two numbers indicates that the mixture is difficult to separate. The results of this method in Table (54) report an average error of 8.34%, which is a better response than the first method with an average error of 10.52%, in addition to a decrease in the number of tower steps.

Table 53. Results of the second method for feed mixture No. 3 percentage composition No. 1

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|-------------------|-------------------------------|------------------------------------------|----------------------------------------|
| 27                       | 14                        | 27                       | 10                        | 14                | 14                            | 18.51                                    | 18.67                                  |

Source: Search data.

Table 54. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 3 percentage composition No. 1

| Substance A flow Kmol/h | Substance B flow Kmol/h | Substance C flow Kmol/h | Error percentage | Average error |
|-------------------------|-------------------------|-------------------------|------------------|---------------|
| Upper product           |                         |                         |                  |               |
| 0.83                    | 0.17                    | 0                       | 11.47            | 0.21          |
| Middle product          |                         |                         |                  |               |
| 0.04                    | 0.78                    | 0.18                    | 10               | 13.33         |
| Lower product           |                         |                         |                  |               |
| 0                       | 0.014                   | 0.986                   | 8.53             | 11.47         |

Source: Search data.
Isobutane, normal butane and cyclobutane enter the tower this time in the second percent composition. ISO butane in input feed is only 10% and the other two components are 45% each.

The simulation results in Table (56) show the optimal response of this method in the percentage composition. The average error is only 2.4%, which is a better answer than the first method (error 3.84%), in addition to the fact that the total number of steps is also reduced.

### Table 55. Results of the second method for feed mixture No. 3 percentage composition No. 2

| steps of the first tower | steps of the second tower | steps of the third tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|--------------------|-------------------------------|--------------------------------------------|----------------------------------------|
| 20                       | 18                        | 20                       | 10                 | 8                            | 7                                          | 79.74                                  | 14.5                                   |

Source: Search data.

### Table 56. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 3 percentage composition No. 2

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.9        | 0.1         | 0           | 3.24             | 2.32          | 2.4          |
| Middle product | 0          | 0.9         | 0.1         | 13.5             | 0             | 0            |
| Lower product | 0          | 0.08        | 0.92        | 13.26            | 4.88          |              |

Source: Search data.

The third composition percentage for feed is isobutane, normal butane, and cyclobutane so that the middle component is minimal (10%), which are considered as the input of the tower. The results obtained from the simulation of Table (58) as other feeds in this percentage composition and as in the previous method do not provide an acceptable answer.

### Table 57. Results of the second method for feed mixture No. 3 percentage composition No. 3

| steps of the first tower | steps of the second tower | steps of the third tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|--------------------|-------------------------------|--------------------------------------------|----------------------------------------|
| 37                       | 6                         | 37                       | 3                  | 18                            | 20                                         | 12.99                                  | 14.16                                  |

Source: Search data.

### Table 58. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 3 percentage composition No. 3

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.85        | 0.15        | 0           | 15.87            | 5.18          | 29.87        |
| Middle product | 0          | 0.26        | 0.74        | 3                | 71.11         |
| Lower product | 0          | 0.001       | 0.999       | 11.13            | 13.3           |

Source: Search data.
The feed of isobutane, normal butane, and cyclobutane are examined in the fourth percent composition. In this case, the heavy component makes up only 10% of the input feed. The simulation results can be seen in Table (60). As we saw in the previous two feeds in this case of feed, for the present method, in this case, this method also provides a favorable answer. As observed in the previous two feeds, in this case, too, only 2.10 and 5.56% error is observed for the upper and middle products, respectively.

Table 59. Results of the second method for feed mixture No. 3 percentage composition No. 4

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|--------------------|---------------------------------|------------------------------------------|-----------------------------------------|
| 22                      | 15                        | 22                       | 14                        | 14                 | 15                              | 12.92                                    | 73.25                                   |

Source: Search data.

Table 60. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 3 percentage composition No. 4

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.86 | 0.14 | 0 | 14.6 | 2.10 | 13.71 |
| Middle product | 0.07 | 0.85 | 0.08 | 13.5 | 5.56 |
| Lower product | 0 | 0.002 | 0.998 | 1.9 | 33.47 |

Source: Search data.

The last feed studied is propylene, butylene, and pentane. The characteristic of this feed is that the ratio of the volatility of the light to the heavy component is higher than that of the middle to the heavy component. In the first case, the feed homogeneously enters the tower. The simulation results in this case in Table (62) indicate an increase in the mean error compared to the first method. In addition, the number of tower steps has increased in this way.

Table 61. Results of the second method for feed mixture No. 4 percentage composition No. 1

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product’s tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|--------------------|---------------------------------|------------------------------------------|-----------------------------------------|
| 12                      | 3                        | 12                       | 10                        | 6                  | 3                              | 3.54                                    | 4.16                                   |

Source: Search data.

Table 62. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 4 percentage composition No. 1

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|---------------|
| Upper product | 0.72 | 0.28 | 0 | 13.82 | 4.74 | 24.34 |
| Middle product | 0 | 0.6 | 0.4 | 10 | 33.33 |
| Lower product | 0 | 0 | 1 | 6.18 | 34.95 |

Source: Search data.
The second percentage composition of the feed is propylene, butylene and pentene so that propylene makes up only 10% of the input feed and the rest of the feed is evenly distributed. The results of this simulation in Table (64) show an average error of 6.78%, which is almost equal to the error of the first method (6.37%), but the number of tower steps has increased compared to the equal conditions in the first method.

**Table 63.** Results of the second method for feed mixture No. 4 percentage composition No. 2

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|--------------------|----------------------------------|------------------------------------------|------------------------------------------|
| 12                       | 4                         | 12                       | 12                        | 5                  | 2                               | 19.7                                     | 3.74                                     |

**Source:** Search data.

**Table 64.** Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 4 percentage composition No. 2

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|--------------|
| Upper product | 0.71        | 0.29        | 0           | 4.18             | 4.13         | 6.78         |
| Middle product | 0          | 0.85        | 0.15        | 13.5             | 5.56         |
| Lower product | 0           | 0.07        | 0.93        | 12.32            | 10.66        |

**Source:** Search data.

Propylene, butylene, and pentene feed make up the third percentage, which is only 10% of the middle component in the feed, and the rest is 45% each. The simulation results in Table (66) report a very large error of this state of the feed. Due to the division of the middle component in the prefractionator of the divided wall column, in case the middle component is minimal in the input feed, the shortcut method does not provide a favorable response.

**Table 65.** Results of the second method for feed mixture No. 4 percentage composition No. 3

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|--------------------|----------------------------------|------------------------------------------|------------------------------------------|
| 12                       | 2                         | 12                       | 3                         | 6                  | 4                               | 2.29                                     | 3.46                                     |

**Source:** Search data.

**Table 66.** Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 4 percentage composition No. 3

| Substance A | Substance B | Substance C | flow Kmol/h | Error percentage | Average error |
|-------------|-------------|-------------|-------------|------------------|--------------|
| Upper product | 0.74        | 0.26        | 0           | 18.14            | 4.67         | 43.34         |
| Middle product | 0          | 0.05        | 0.95        | 3                | 94.44        |
| Lower product | 0           | 0           | 1           | 8.86             | 30.92        |

**Source:** Search data.
The last case to be studied in the first method is the fourth percentage composition of the mixture of propylene, butylene, and pentene so that in the input feed, the heavier component is minimum (10 percent). The simulation results in Table (68) report an average of 26.5% error. As with previous feeds in this percentage combination, it provides an acceptable answer only for the upper and middle products of the tower.

**Table 67. Results of the second method for feed mixture No. 4 percentage composition No. 4**

| steps of the first tower | steps of the second tower | steps of the third tower | steps of the fourth tower | Feed tray location | Middle product's tray location | The rate of flow returned from the condenser | The rate of flow returned from the boiler |
|--------------------------|---------------------------|--------------------------|---------------------------|--------------------|-------------------------------|----------------------------------------|----------------------------------------|
| 7                        | 3                         | 7                        | 12                        | 4                  | 3                             | 2.07                                   | 12.75                                  |

Source: Search data.

**Table 68. Comparison of purity results obtained from MATLAB software with the second method for feed mixture No. 4 percentage composition No. 4**

| Substance | Upper product | Middle product | Lower product | Error percentage | Average error |
|-----------|---------------|----------------|---------------|------------------|---------------|
| Substance A | 0.84          | 0.02           | 0             | 15.6             | 2.18          |
| Substance B | 0.16          | 0.82           | 0             | 13.5             | 8.89          |
| Substance C | 0             | 0.16           | 1             | 0.9              | 68.42         |

Source: Search data.

**SUMMARY OF RESULTS OBTAINED**

Regarding the feed mixture number one of table (69), in case the feed enters the tower in the first and fourth percentages composition, the first method offers a better answer and in the third and fourth percentages composition, the second method offers a more appropriate answer. As can be observed from the results presented in Table (70), the average error percentage for the feed mixture No. 2 in the first method is lower than the average error percentage in the second method. Concerning the mixture number three, table (71), in all percentages combinations, the second method presents a more favorable answer. The application of the optimal Prefractionator parameter in the second method justifies the desired response of this method, provided the relative volatility ratios of the feed components are equal.

for mixture number four in Table (72), where the volatility ratio of the light component to heavy is higher than that of middle to heavy component, in all feed percentages combinations, the first method is associated with less error than the second method.

The primary characteristic of this feed is a large difference in the volatility of light and medium components compared to heavy components.

In all feeds studied and in all percentage compositions (except for two cases), the total number of tower steps in the second method is much lower than the total number of tower stages in the first method.

This point, along with the better answer of the second method, confirms the argument of the inefficiency of the Fenske method regarding the correct calculation of the number of steps of the divided wall column.

In the second method, a different method from the Fenske method is used to calculate the minimum required steps. It has been argued that the conditions of divided wall column trays are different simple towers, so the use of the Fenske method is not effective.
This difference is since the percentage composition of liquid flow returning to the main tower with the percentage composition of steam entering the tower in the divided wall column is not equal, while the Fenske method is correct by assuming the equality of these two parameters.

| Composition percentage | Average error percentage for mix number one | total number of tower steps |
|------------------------|-------------------------------------------|-----------------------------|
|                        | a B/C = 2.43 & a B/C = 2.78               |                             |
|                        | First method | Second method | First method | Second method |
| 1                      | 6.3           | 8              | 30           | 17            |
| 2                      | 25.36         | 2.98           | 19           | 16            |
| 3                      | 34.22         | 31.49          | 34           | 15            |
| 4                      | 19.84         | 25.27          | 35           | 19            |

Source: Search data.

Table 70. Average product error percentage and total number of tower steps for feed mix No. 2

| Composition percentage | Average error percentage for mix number two | total number of tower steps |
|------------------------|-------------------------------------------|-----------------------------|
|                        | a B/C = 2.2 & a B/C = 2.2                 |                             |
|                        | First method | Second method | First method | Second method |
| 1                      | 16.43        | 18.78         | 29           | 20            |
| 2                      | 3.35         | 6.08          | 21           | 19            |
| 3                      | 36.52        | 35.54         | 35           | 17            |
| 4                      | 19.54        | 23.16         | 37           | 19            |

Source: Search data.

Table 71. Average product error percentage and total number of tower steps for feed mix No. 3

| Composition percentage | Average error percentage for mix number three | total number of tower steps |
|------------------------|-------------------------------------------|-----------------------------|
|                        | a B/C = 1.3 & a B/C = 1.3                 |                             |
|                        | First method | Second method | First method | Second method |
| 1                      | 10.52        | 8.34          | 81           | 51            |
| 2                      | 3.84         | 2.4           | 55           | 48            |
| 3                      | 34.29        | 29.87         | 96           | 46            |
| 4                      | 13.97        | 13.71         | 94           | 51            |

Source: Search data.

Table 72. Average product error percentage and total number of tower steps for feed mix No. 4

| Composition percentage | Average error percentage for mix number four | total number of tower steps |
|------------------------|-------------------------------------------|-----------------------------|
|                        | a B/C = 3.82 & a B/C = 1.99               |                             |
|                        | First method | Second method | First method | Second method |
| 1                      | 3.49         | 24.34         | 19           | 25            |
| 2                      | 6.37         | 6.78          | 15           | 28            |
| 3                      | 31.74        | 43.34         | 22           | 17            |
| 4                      | 9.99         | 26.5          | 27           | 22            |

Source: Search data.

As can be observed, for the third percentage composition, which has a lower percentage of the middle component in the input feed, no acceptable result was obtained in any of the methods and in all cases. Therefore, by removing this percentage composition, we consider the average error of each method in the rest of the percentage compositions in Table (73):
Table 73. Comparison of average error in two methods

|                      | Mixture1 | Mixture2 | Mixture3 | Mixture4 |
|----------------------|----------|----------|----------|----------|
| Average error percentage of the first method | 17.17    | 13.11    | 9.44     | 6.62     |
| Average error percentage of the second method | 12.08    | 16.00    | 8.15     | 19.21    |

Source: Search data.

CONCLUSION

This paper first investigated the types of distillation tower arrangements and separation structures of mixtures and thermal coupled structures. Then we examined the shortcut method in designing divided wall columns. In order to compare the shortcut methods of designing distillation towers with the divided wall, the details of the two shortcut methods of Moralikrishna and Sotoudeh were examined. Then, different simulation modes of divided wall columns were analyzed using ASPEN PLUS software, and the method used in the present study was introduced and investigated.

According to the information obtained, the following results are inferred:

In case the ratio of the relative volatility of light component to middle component (α_A / B) is smaller than the ratio of the relative volatility of middle component to heavy component (α_B / C) (mixture 1), the second method offers a better answer.

If the ratio of relative volatility is equal, the second method offers a more acceptable answer. If the molar fraction of the volatility component is minimum, the second method offers a better answer. In case the molar fraction of the heavy component is minimal, the second method offers a better answer. If the feed percentage composition is equal, both methods provide an acceptable answer. If the percentage composition of input feed in the middle component is minimal, the answer of both methods is associated with a large error.

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Comparison of shortcut methods for designing of divided wall columns for separating tertiary zeotropic mixtures

Resumo
Recentemente, a coluna de parede dividida tem sido considerada como um dos tipos de torres termicamente acopladas para separação de misturas multicomponentes. Na estrutura desta torre, existe uma parede que divide a torre em duas partes, o Pré-fracionador e a Coluna Principal. A coluna de parede dividida é termodinamicamente equivalente à torre Petlyuk. Portanto, para obter os parâmetros de projeto e simulação da torre Petlyuk utilizando o software disponível, esta torre deve ser dividida em torres mais simples. O método de atalho é empregado para adquirir os parâmetros iniciais. Na presente pesquisa, inicialmente, o projeto de coluna de parede dividida foi conduzido usando métodos de atalho para separar misturas zeotrópicas de três componentes. Em seguida, o projeto e a simulação da coluna de parede dividida são realizados utilizando o software ASPEN PLUS e os resultados dos dois métodos são comparados de vários ângulos.

Palavras-chave: Coluna de parede dividida. Métodos de atalho. Destilação termicamente acoplada. Torre Petlyuk. Mistura zeotrópica.

Abstract
Recently, divided wall column has been considered as one of the types of thermally coupled towers for separating multicomponent mixtures. In the structure of this tower, there is a wall that divides the tower into two parts, the Prefractionator and the Main Column. The divided wall column is thermodynamically equivalent of the Petlyuk tower. Therefore, in order to obtain the design and simulation parameters of the Petlyuk tower utilizing the available software, this tower must be divided into simpler towers. The shortcut method is employed to acquire the initial parameters. In the present research, initially, the design of divided wall column has been conducted using shortcut methods to separate three-component zeotropic mixtures. Next, the design and simulation of the divided wall column is performed employing ASPEN PLUS software and the results of the two methods are compared from various angles.

Keywords: Divided wall column. Shortcut methods. Thermally coupled distillation. Petlyuk tower. Zeotropic mixture.

Resumen
Recientemente, la columna de pared dividida ha sido considerada como uno de los tipos de torres acopladas térmicamente para separar mezclas multicomponentes. En la estructura de esta torre, hay un muro que divide la torre en dos partes, el Prefraccionador y la Columna Principal. La columna de pared dividida es termodinámicamente equivalente a la torre Petlyuk. Por lo tanto, para obtener los parámetros de diseño y simulación de la torre Petlyuk utilizando el software disponible, esta torre debe dividirse en torres más simples. El método de acceso directo se emplea para adquirir los parámetros iniciales. En la presente investigación, inicialmente, el diseño de la columna de pared dividida se ha realizado utilizando métodos abreviados para separar mezclas zeotrópicas de tres componentes. A continuación, se realiza el diseño y la simulación de la columna de pared dividida empleando el software ASPEN PLUS y se comparan los resultados de los dos métodos desde varios ángulos.

Palabras-clave: Columna de pared dividida. Métodos de acceso directo. Destilación acoplada térmicamente. Torre Petlyuk. Mezcla zeotrópica.