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Research Paper

Effect of Operational and Structural Parameters in Dividing Wall Column Distillation Energy Efficiency for Separation of Methanol, Isopropanol, and N-Butanol

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Abstract: Although distillation is considered a mature process, it is associated with high energy consumption. Distillation is reported to consume 40 percent of the energy used in the chemical industries worldwide. In this paper, the steady-state simulation of two processes, including two conventional distillation columns and DWCD, is conducted. The influence of operational and structural parameters in the DWCD energy efficiency for separation methanol, isopropanol, and n-butanol is performed. In the conventional method, there are two distillation columns with two reboilers and two condensers, while in DWCD, there are one reboiler and one condenser. A model consisting of four columns including two absorbers, a rectifier, a stripper, and two vapor and liquid splitters are used to simulate the DWCD. The number of stages in the absorbers columns is indicating the wall height in DWCD. The various parameters have been optimized using sensitivity analysis to minimize heat duties of the reboilers and condensers with considering the limitations for the concentrations of methanol, isopropanol, and n-butanol in the products. The studied parameters can be divided into two categories of structural and process parameters. The structural parameters include the number of stages in each column, the feed stage number, and the side product stage number. The process parameters include the reflux ratio, the vapor split ratio, and the liquid split ratio. According to the results, the DWCD, in compared with the conventional distillation columns, saves energy 19.95% for the reboiler heat duty and 20.64% for the condenser heat duty for the investigated process.

keywords: Distillation, Energy Efficiency, Dividing Wall Column (DWC), Upgrading.

1. Introduction

Distillation is the most important separation process and has a significant contribution to energy consumption in chemical technologies. The cost of producing a product is directly related to the separation process used, because it determines the quality and quantity of the products. This indicates that the separation processes should be energy efficient and cost-effective. In the distillation process, to evaporate a liquid mixture at high temperature, the heat is transferred to the reboiler and leaves at the condenser at low temperature. This fact leads to the low energy efficiency of the distillation process. This subject has led researchers to develop and improve the energy efficiency of this process. The various methods have been proposed to increase the energy efficiency of the distillation process. These include a fully thermally coupled distillation column (Petlyuk column), a heat integrated distillation column (HIDiC), and dividing wall column distillation (DWCD). As one type of fully thermally coupled distillation column, DWCD is a very promising technology (Sun et al. 2015). The DWCD turns two or more distillation columns into a single unit by placing a dividing wall. The dividing wall divides a single column into two parts, a prefractionator, and the main column. This system has only one reboiler and one condenser (Nguyen, 2015). A large number of publications have been focused on the divided wall column. Szabo et al. (2008) investigated DWCD with the simulation of the process. They divided the column into four sections to simulate, and each

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section was simulated using a software model and analyzed the effects of the main parameters of DWCD. Errico et al. (2009) considered DWCD for the separation of a four-component mixture, including normal paraffins. The system had four products, and five different feed combinations were considered. Rangaiah et al. (2009) developed general procedures for the simulation of DWCD. They concluded that vapor and liquid splitters had significant effects on energy consumption. Barroso-Mnnoz et al. (2010) reported an experimental study on the hydrodynamic behavior of DWCD. They tested several different values for gas and liquid, including air and water velocities, to measure pressure drop. Niggemann et al. (2010) investigated the separation of a ternary mixture of n-hexanol, n-octanol, and n-decanol. The inner diameter of the column was 68 mm. Each of the four columns had a 980 mm height. The total height of the DWC was approximately 12 m. A welded wall was inserted in the middle. Kiss and Rewagad (2011) presented the simulation results of control and dynamics of a DWCD process. The case study considered was a ternary separation of a mixture including benzene, toluene, and xylene. Kaur (2012) performed the simulation study of DWCD for a ternary separation of mixture benzene-toluene-xylene (BTX). They concluded that the optimum value of liquid and vapor split ratios were 0.603 and 0.45, respectively. Landaeta et al. (2012) simulated the separation of aromatics using DWC and Kaibel distillation columns. They used Aspen Tech software to simulate rigorously and optimize designs. The results showed that designing based on two DWC systems reduced energy consumption by up to 7%, while combined design, including a conventional stripper and a Kaibel column, reduced energy consumption by up to 17%. Long and Lee (2012) used response surface methodology (RSM) for DWCD design and optimization. The process was acetic acid purification. They used a three-column distillation system for the design of DWCD. The feed was containing acetic acid, methanol, formic acid, water, and propionic acid. Their results showed that DWCD decreased total costs by 44.57% in comparison with the conventional distillation method. Sangal et al. (2012) presented the optimization of DWCD parameters for energy efficiency. The results showed that the process variables compared to structural variables had significant effects on energy efficiency. Sangal et al. (2013) simulated a DWCD process to study the effects of process parameters on product quality and to improve energy efficiency. The process was a C4-C6 normal paraffin ternary mixture. Wang et al. (2013) studied a DWCD process with a side rectifier to aniline distillation. Arora (2014) studied simulation of the separation of three ternary mixtures, including benzene-toluene-p-xylene, benzene-toluene-o-xylene, and methanol-water-glycerol in a DWCD. Ge et al. (2014) developed a method based on the combination of neural network (NN) and genetic algorithm (GA) to optimize a DWCD process. Three case studies including n-pentane/n-hexane/n-heptane, benzene/toluene/ethylbenzene and ethanol/n-propanol/n-butanol were analyzed. Khushalani et al. (2014) studied a benzene–toluene–xylene (BTX) process in a DWCD and evaluated the variation of product purities with the wall position. Wang (2014) presented steady-state simulation and analysis of benzene–toluene–xylene (BTX) separation in a DWCD. Fang et al. (2015) studied energy-saving effects of DWCD. They investigated the separation of n-hexane, n-heptane, and n-octane mixtures in the DWCD process by simulation and experiment. They considered two modes of DWCD process, including DWC with thermal insulation (HIDWC) and DWC with wall heat transfer (HTDWC). Illner and Othman (2015) studied DWCD for more efficient separation of fatty acid mixtures. Fatty acid separation in the industry is performed using two conventional distillation columns. Nguyen (2015) proposed a procedure for the design of DWCD based on the FUGK model. They used ProSim software for rigorous simulation and optimization of the process. The experimental results showed that the product concentration, composition profile, and temperature along the column were in a perfect agreement with the simulation results. Shojae et al. (2015) performed DWC simulations to separate dimethyl ether from a mixture of water and ethanol. Their results showed that the DWC structure resulted in a heat duty reduction of about 24% for the condenser and 7% for the reboiler. They used a three-column model to simulate the DWCD process. Sun et al. (2015) investigated experimental study and simulation of a CFD vapor splitter in a packed DWCD process. Yuqi et al. (2015) performed an optimization and experimental study of DWCD for separation of hexane-heptane-octane mixture and evaluated different parameters effects on the energy consumption. Khalili-Garakani et al. (2016) carried out a comparison between different configurations, including thermally coupled, thermodynamically equivalent, and DWC, for the separation of 3 different samples of three-component mixtures. Gor et al. (2017) performed a simulation of DWCD for the separation of a ternary system, including butane-pentane-hexane. A four-column model was applied to simulate DWC. The various parameters' effects on the purity of components and reboiler and condenser heat duties were investigated. The energy reduction by DWC was 34.74% for condenser and 31.28% for reboiler duties. Kim (2017) evaluated energy saving in a crude distillation unit with a DWCD. They concluded that the unit saved 37% of heat and 17% on cooling compared to the conventional process. Bernad-Serra et al. (2018) studied the vapor splitting device by CFD in a DWC. The system studied was a mixture of benzene, toluene, and xylene. The system was first studied through freedom analysis degrees to understand the effect of interconnecting flows on column performance. Filho et al. (2018) used the response surface method (RSM) to optimize DWC design. A central composite design is applied for validation of the response surface for an aromatic ternary separation. Shi et al. (2018) implemented heterogeneous azeotropic distillation in a DWC using chloroform as an entrainer for the separation of the mixtures of the components, including 2,2,3,3-tetra fluorine, 1-propanol, and water. Zhai et al. (2019) simulated a DWC using the rigorous model and studied the influences of liquid split ratio and vapor split ratio. It was shown that the heat duty was sensitive to variations of liquid and vapor split ratios. The model was validated for a ternary mixture system including benzene–toluene–xylene.

In the present paper, the simulation of two processes, including two conventional distillation columns and a DWCD system, is performed for separation of a ternary mixture. The optimization of various parameters is conducted by sensitivity analysis for both processes to reduce the reboilers and the condensers' heat duties with considering desired purities of the products. The feed contains three components of methanol, isopropanol, and n-butanol. The investigated parameters include the number of stages of the columns, the feed stage number of the columns, side product stage number, reflux ratio, and vapor and liquid split ratios. The results show that the DWCD process has 19.95% and 20.64% energy saving for the reboiler and the condenser heat duties, respectively. The DWCD process is one of the safest technologies to reduce the energy consumption of distillation towers. According to the studies, evaluation of structural and operational parameters effects and the optimization of DWCD for a ternary feed including methanol, isopropanol, and n-butanol and also the comparison of its energy consumption with the conventional method have been investigated for the first time in this research.

2. Materials and Methods

Aspen Plus software is used to model and simulate the conventional distillation columns and DWCD process. The shortcut and rigorous simulations are performed with DSTWU and RadFrac models, respectively. The thermodynamic model NRTL is used for modeling due to the high non-ideality of the chemical system. For a binary mixture, the equations for the NRTL model are as follows:

$$\begin{cases} \ln \gamma_1 = x_2^2 \left[\tau_{21} \left(\dfrac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \dfrac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right] \\ \ln \gamma_2 = x_1^2 \left[\tau_{12} \left(\dfrac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \dfrac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right] \end{cases}$$

$$\begin{cases} \ln G_{12} = -\alpha_{12}\tau_{12} \\ \ln G_{21} = -\alpha_{21}\tau_{21} \end{cases}$$

Here, γ_i is the activity coefficient of component i; x_i is the mole fraction of component i in the liquid phase. τ_{12} and τ_{21} are the dimensionless interaction parameters, which are related to the interaction energy parameters by the following equations:

$$\begin{cases} \tau_{12} = \dfrac{\Delta g_{12}}{RT} = \dfrac{U_{12} - U_{22}}{RT} \\ \tau_{21} = \dfrac{\Delta g_{21}}{RT} = \dfrac{U_{21} - U_{11}}{RT} \end{cases}$$

U_{ij} is the energy between molecular surface i and j. U_{ii} is the energy of evaporation. R is the gas constant, and T is the absolute temperature. U_{ij} has to be equal to U_{ji}. α_{12} and α_{21} are the so-called non-randomness parameters.

3. Results and Discussion

Table 1shows the feed specifications of the processes.

The criterion for optimization in this research is minimizing the heat duties of the reboilers and the condensers in the system with considering the following limitations for the concentrations:

a) The mass and molar fractions of methanol in the product stream ≥ 0.98

b) The mass and molar fractions of 2-propanol in the product stream ≥ 0.95

c) The mass and molar fractions of n-butanol in the product stream ≥ 0.98

Table 1 The feed specifications

Mass Frac (wt %)	
methanol	40
isopropanol	30
n- butanol	30
Mass Flow (kg/hr)	3
Temperature (C)	70
Pressure (atm)	1.1

3.1. The Conventional Distillation Process

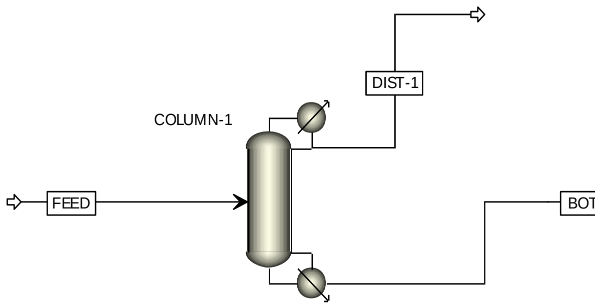


Fig. 1 shows the conventional distillation model for separating the three-component mixture, including methanol, isopropanol, and n-butanol. The system has two distillation columns. The feed enters the first column. With considering the boiling point of the components, methanol leaves the top of the first column, and the bottom product of the first column contains 2-propanol and n-butanol, which enters the second column. 2-propanol and n-butanol leaves the top and the bottom of the second column, respectively.

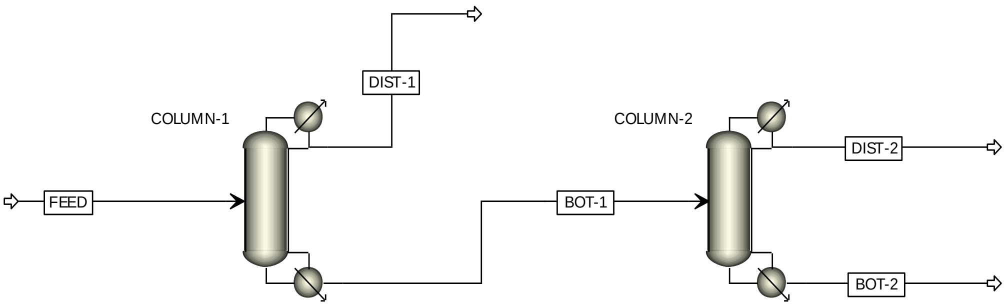


Fig. 1 The conventional distillation process for separating a ternary mixture

3.1.1. Simulation of the conventional distillation process

The flow specifications of the products of the distillation columns in the rigorous simulation results have been shown in **Table 2.** The input data for rigorous simulation is based on shortcut simulation results. Table 3 and Table **4** show the reboilers and the condensers' heat duties and the specifications of two columns in the simulation results, respectively.

3.1.2. Optimization for the conventional distillation process

3.1.2.1. The number of stages of the first column

The stages number effects of the first column on the output parameters have been illustrated in **Fig. 2** (a) to **Fig. 2** (d). (The data are indicated in details in Table A-1 in the supplementary data section). The other parameters have been considered constant.

Table 2 The flows specifications of input and output of distillation columns in the simulation results

	BOT-1	BOT-2	DIST-1	DIST-2	FEED
Mole Frac					
METHA-01	0.002	1.35E-08	**0.989**	0.003	0.580
ISOPR-01	0.545	0.002	0.011	**0.982**	0.232
N-BUT-01	0.454	**0.998**	TRACE	0.015	0.188
Total Flow (kmol/hr)	0.027	0.012	0.038	0.015	0.065
Mass Frac					
METHA-01	0.001	6 PPM	**0.980**	0.002	0.400
ISOPR-01	0.493	0.002	0.020	**0.980**	0.300
N-BUT-01	0.506	**0.998**	TRACE	0.019	0.300
Total Flow (kg/hr)	1.777	0.885	1.223	0.893	3.000

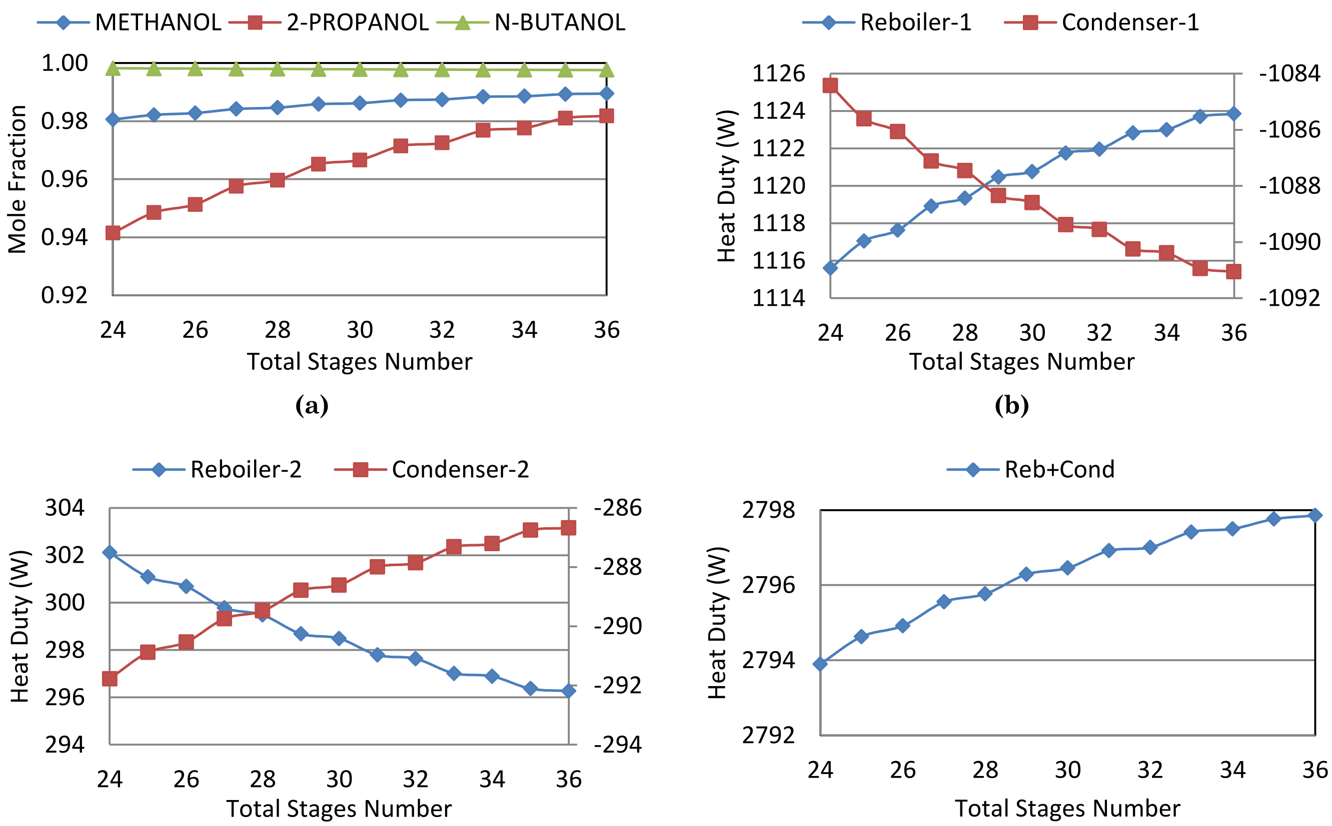
Table 3 The heat duties of the reboilers and the condensers in the conventional simulation results

Heat Duty (W)	Column-1	Column-2
Reboiler	1123.847	296.267
Condenser	-1091.056	-286.685

Table 4 The specifications of the columns in the simulation results

	Unit	Column-1	Column-2
No. of Stages	-	36	19
Distillate rate	kg/hr	1.2225	0.893
Feed Stage	-	20	10
Reflux Ratio	-	1.95	0.71
Condenser Pressure	atm	1	1
Pressure Drop	atm	0.1	0.1

Fig. 2 (a) depicts the influence of the number of stages of the first column on the mole fraction of the components in the products. It can be observed that by increasing the number of first column stages, the concentrations of all three components are increased. But the rate of increase for butanol as the heaviest component is the lowest, and for 2-propanol as the intermediate component is more significant than the other two components. NS is the number of the total stages, NF is the feed stage, RR is the reflux ratio. According to the results of **Fig. 2** (b), the heat duties of both the reboiler and the condenser of the first column increases with increasing the number of the first column stages. Its effect on the reboiler heat duty is more significant. It can be explained that by increasing the number of the first column stages, the height of the column increases, and owing to fixing the other parameters such as flowrates and refluxes, the required heat duties are increased. According to the results of **Fig. 2** (c), with the increasing number of the first column stages, the heat duties of the reboiler and the condenser of the second column decrease. It can be explained that with increasing the number of stages of the first column, the separation enhances in the first column, and owing to the fact that the other parameters are constant, the task of the second column reduces. So, the reboiler and the condenser heat duties of the second column are reduced. **Fig. 2** (d) depicts the effect of the number of stages of the first column on the sum of heat duties of the reboilers and the condensers of the two columns. It can be observed that with increasing the number of the first column stages, the total heat duties of two columns are increased. According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties by considering desired purities of the products, the number of 31 has opted for the first column stages.



(c) (d)

Fig. 2 The effect of stages number of the first column on the output parameters
(a) the molar fractions of the products (b) the heat duties of the reboiler and the condenser of the first column (c) the heat duties of the reboiler and the condenser of the second column (d) sum of heat duties of the reboilers and the condensers of the first and the second columns
(2 Columns, NS2=19, NF2=10, RR1=1.95, RR2=0.71)

3.1.2.2. The number of stages of the second column

The stages number effects of the second column on the output parameters have been illustrated in **Fig. 3** (a) to **Fig. 3** (d). (The data are indicated in details in Table A-2 in the supplementary data section). The other parameters have been considered constant. **Fig. 3** (a) depicts the influence of the number of stages of the second column on the mole fractions of the components in the products. It can be observed that since methanol has been separated in the first column, its concentration is constant with increasing the number of second column stages. However, increasing the number of second column stages results in a better separation of two other components, including isopropanol and butanol. **Fig. 3** (b) illustrates the effect of the number of second column stages on the heat duties of the reboiler and the condenser of the first column. According to the results of **Fig. 3** (b), there is no effect. As can be seen in **Fig. 3** (c), increasing the number of stages of the second column leads to an increase in the heat duty of the reboiler by 1.41 W and a decrease in the heat duty of the condenser by 0.44 W. As can be observed in **Fig. 3** (d), with increasing the number of second column stages, the sum of the reboilers and the condensers' duties of the two columns are increased. According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties by considering desired purities of the products, the number of 13 has opted for the second column stages.

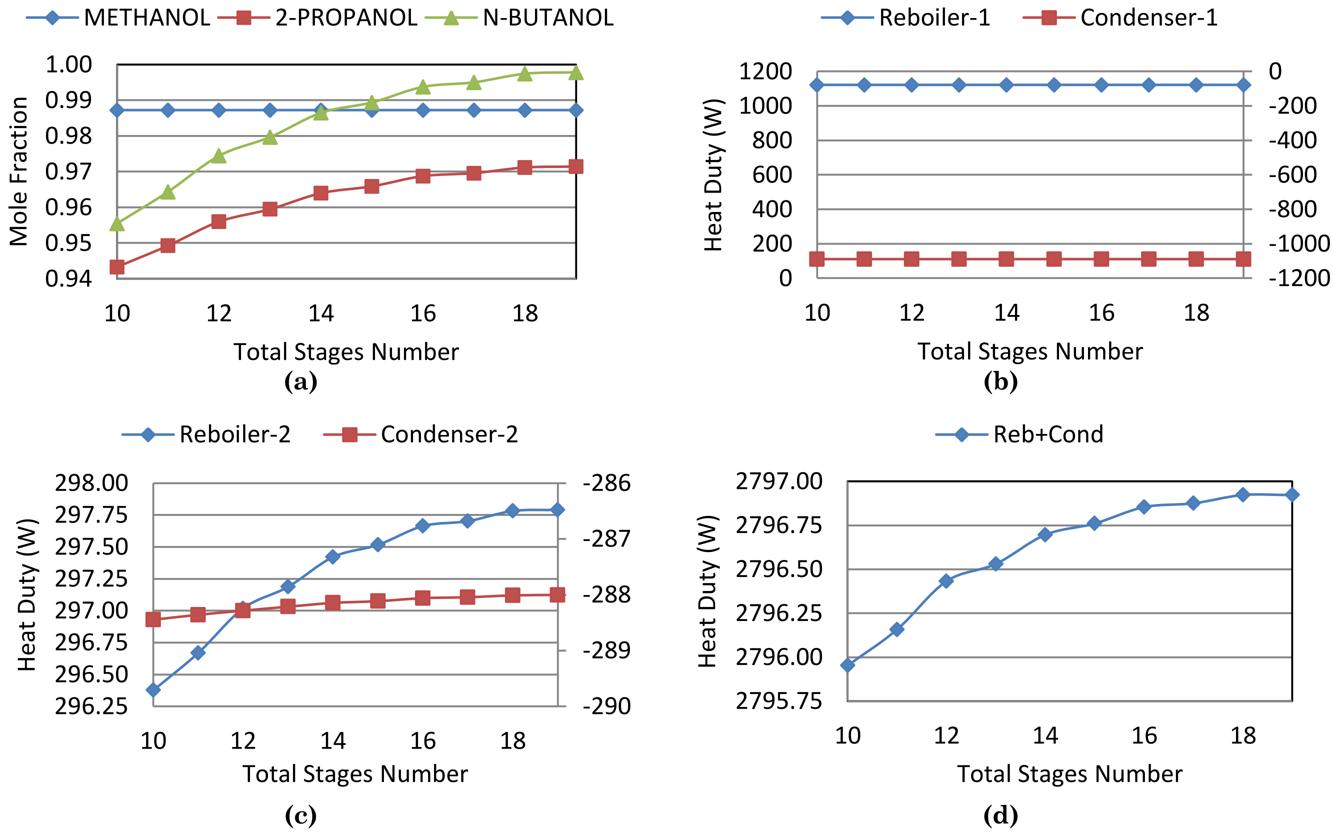


Fig. 3 The effect of the stages number of the second column on the output parameters
(a) the molar fractions of the products (b) the heat duties of the reboiler and the condenser of the first column (c) the heat duties of the reboiler and the condenser of the second column (d) sum of heat duties of the reboilers and the condensers of the first and the second columns
(2 Columns, NS1=31, NF1=18, RR1=1.95, RR2=0.71)

3.1.2.3 The Reflux ratio of the first column

The reflux ratio of the first column effects on the output parameters have been illustrated in **Fig. 4** (a) to **Fig. 4** (d). (The data are indicated in details in Table A-3 in the supplementary data section). The other parameters have been considered constant. It can be observed in **Fig. 4** (a) that by increasing the reflux ratio of the first column,

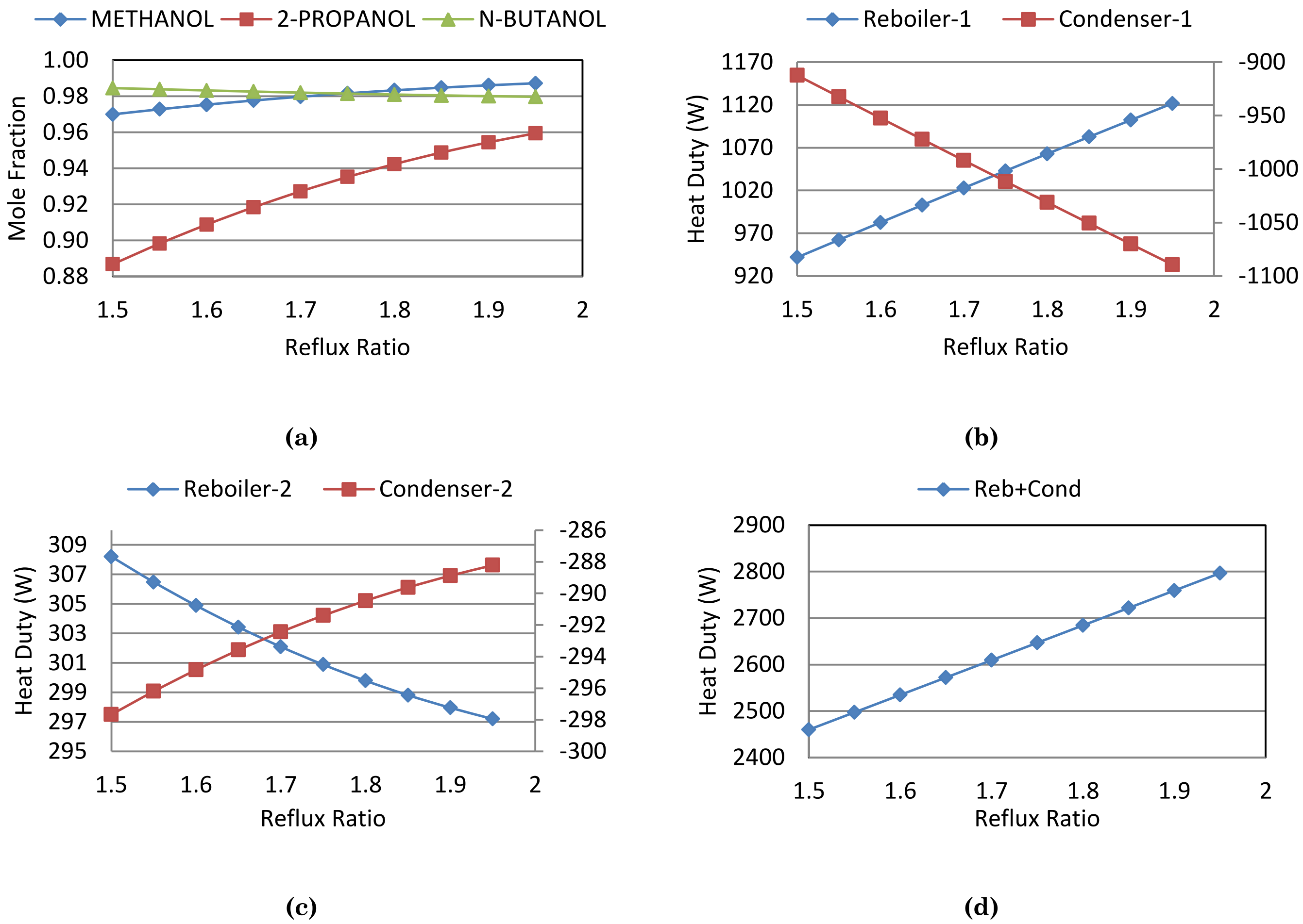


Fig. 4 The influence of the reflux ratio of the first column on the output parameters (a) the molar fractions of the products (b) the heat duties of the reboiler and the condenser of the first column (c) the heat duties of the reboiler and the condenser of the second column (d) sum of heat duties of the reboilers and the condensers of the first and the second columns (2 Columns, NS1=31, NF1=18, NS2=13, NF2=7, RR2=0.71)

the concentration of butanol as the heaviest component is almost constant, but the concentration of the other two components, including methanol and isopropanol, is enhanced. The effect of increasing the reflux ratio of the first column on the concentration of isopropanol as an intermediate component is more significant than the other components. It can be explained that by increasing the reflux ratio, the separation is increased, resulting in increasing the concentration of the components in the products.

According to the results of **Fig. 4** (b), by increasing the reflux ratio of the first column, the reboiler and the condenser heat duties of the first column increased. The increase in the heat duties is linear, which is perfectly logical. As can be observed in **Fig. 4** (c), increasing the reflux ratio of the first column results in decreasing the heat duties of the reboiler and condenser of the second column. The trend is almost linear. It can be explained that by increasing the reflux ratio of the first column, the separation in the first column has been increased. So, the role of the second column in the process decreases, leading to reducing the reboiler and the condenser heat duties of the second column. As can be observed in **Fig. 4** (d), with increasing the reflux ratio of the first column, the sum of the reboilers and the condensers' heat duties of two columns are increased. This increase is linear. According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties with considering desired purities of the products, 1.95 has opted for the reflux ratio of the first column.

3.1.2.4. The Reflux ratio of the second column

The reflux ratio of the second column effects on the output parameters have been illustrated in **Fig. 5** (a) to **Fig. 5** (d). (The data are indicated in details in Table A-4 in the supplementary data section). The other parameters have been considered constant. According to the results of **Fig. 5** (a), by increasing the reflux ratio of the second column, the concentration of methanol is constant, while the concentrations of two other components are increased. The comparison between the concentrations of the components increases due to the increase in the reflux ratio of two columns indicates that in the case of the first column, the concentration of the components is more increased.

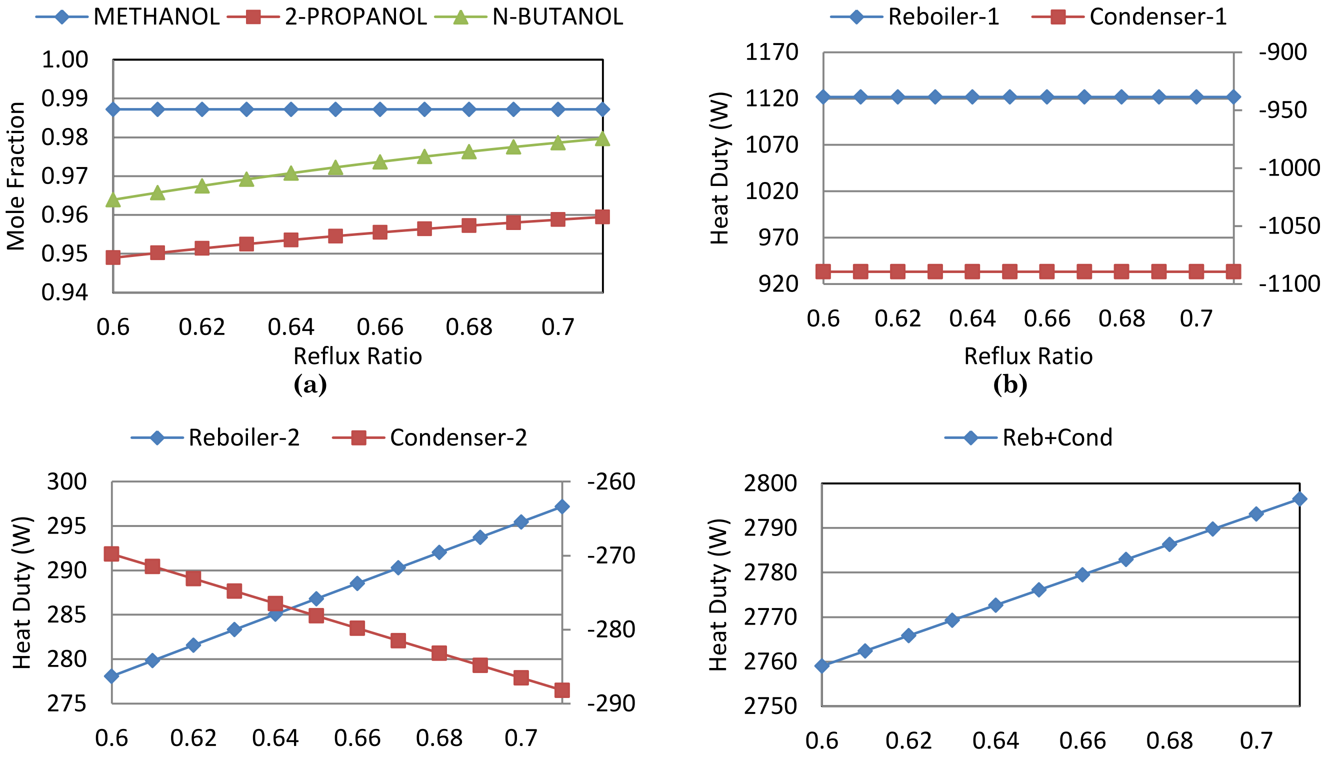


Fig. 5 The effect of the reflux ratio of the second column on the output parameters
(a) the molar fractions of the products (b) the heat duties of the reboiler and the condenser of the first column (c) the heat duties of the reboiler and the condenser of the second column (d) sum of heat duties of the reboilers and the condensers of the first and the second columns
(2 Columns, NS1=31, NF1=18, NS2=13, NF2=7, RR1=1.95)

Fig. 5 (b) illustrates the effect of the reflux ratio of the second column on the heat duties of the reboiler and the condenser of the first column. As can be observed, it has no effect. As can be observed in **Fig. 5** (c), increasing the reflux ratio of the second column, results in increasing both the reboiler and the condenser heat duties of the second column. This increase is linear, which is quite reasonable. As can be observed in **Fig. 5** (d), with increasing the reflux ratio of the second column, the sum of reboilers and condensers' heat duties of the two columns are increased. This increase is linear. Based on the results of **Fig. 5** (d) and **Fig. 4** (d), the effect of increasing the first column reflux ratio on the sum of heat duties of the reboilers and condensers of two columns is more in comparison with the effect of increasing the second column reflux ratio. This result can be explained by the feed flowrates of two columns. According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties by considering desired purities of the products, 0.67 has opted for the reflux ratio of the second column.

3.1.2.5. Feed stage of the first column

The feed stage number effects of the first column on the output parameters have been illustrated in **Fig. 6** (a) to **Fig. 6** (d). (The data are indicated in details in Table A-5 in the supplementary data section). The other parameters have been considered constant. According to the results of **Fig. 6** (a), with increasing the feed stage number of the first column, the concentration of butanol is increased, while the concentration of methanol and isopropanol as the lightest and the medium components at first increased and then decreased. As can be observed in **Fig. 6** (b), by increasing the feed stage number of the first column, the reboiler and the condenser heat duties of the first column, at first is somewhat increased and then decreased. As can be observed in **Fig. 6** (c), by increasing the feed stage number of the first column, the reboiler and the condenser heat duties of the second column first decreased and then increased. The comparison between the effect of the feed stage number of the first column on the reboiler and the condenser heat duties of the first and the second columns shows that its effect on the increase of the reboiler and the condenser heat duties of the first column is more significant than the decrease of the reboiler and the condenser heat duties of the second column. As can be observed in **Fig. 6** (d), by increasing the feed stage number of the first column, the sum of reboilers and the condensers' duties of two columns first increased with a gentle slope and then decreased with a steep slope. According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties with considering desired purities of the products, the number 17 has opted for the feed stage of the first column.

3.1.2.6. Feed stage of the second column

The feed stage number effects of the second column on the output parameters have been illustrated in **Fig. 7** (a) to Error! Reference source not found. (d). (The data are indicated in details in Table A-6 in the supplementary data section). The other parameters have been considered constant. According to the results of **Fig. 7** (a), with increasing the feed stage number of the second column, the concentrations of isopropanol and butanol as the key components of the top and bottom products of the second column are more affected, first increased and then decreased. By increasing the feed stage number of the second column, the concentration of methanol is constant, which is quite reasonable since methanol is separated in the first column.

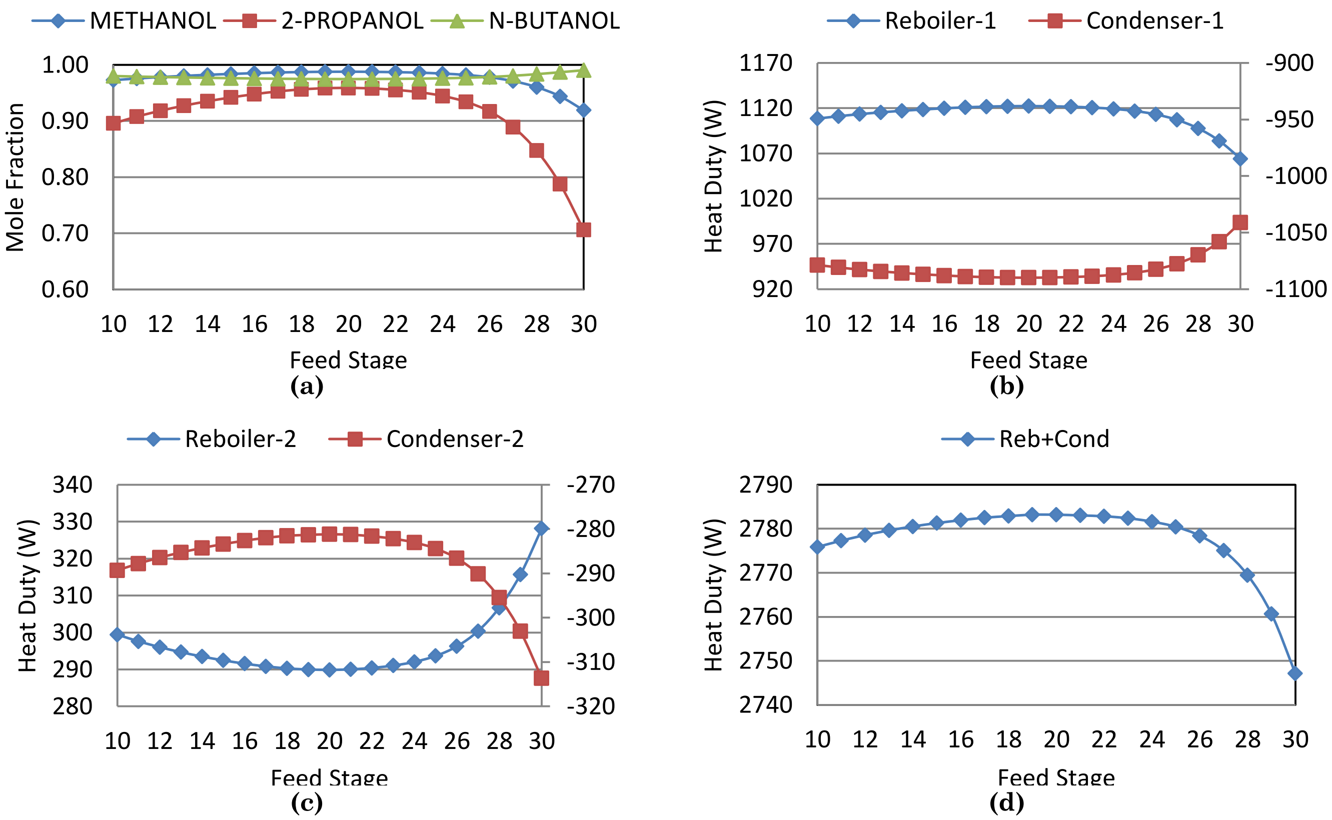


Fig. 6 The effect of the feed stage number of the first column on the output parameters (a) the molar fractions of the products (b) the heat duties of the reboiler and the condenser of the first column (c) the heat duties of the reboiler and the condenser of the second column (d) sum of heat duties of the reboilers and the condensers of the first and the second columns (2 Columns, NS1:31, NS2:13, NF2:7, RR1:1.95, RR2: 0.67)

Fig. 7 (b) illustrates the effect of the feed stage number of the second column on the heat duties of the reboiler and the condenser of the first column. It can be observed that there is no effect. As can be observed in **Fig. 7** (c), by increasing the feed stage number of the second column, the reboiler heat duty of the second column at first increases and then decreases, but it has little effect on the condenser heat duty of the second column. It can be observed in **Fig. 7** (d) that by increasing the feed stage number of the second column, the sum of the reboilers and the condensers' heat duties of the two columns first increases and then decreases. According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties with considering desired purities of the products, the number 7 has opted for the feed stage number of the second column.

3.1.3. The results of optimization in two conventional distillation columns

The optimum conditions of two conventional distillation columns have been shown in **Table 5**.

Table 6 shows the mole fractions of the components in the process products of two conventional distillation columns at the optimum conditions.

Table 7 shows the heat duties of the reboilers and the condensers of two conventional distillation columns at the optimum conditions.

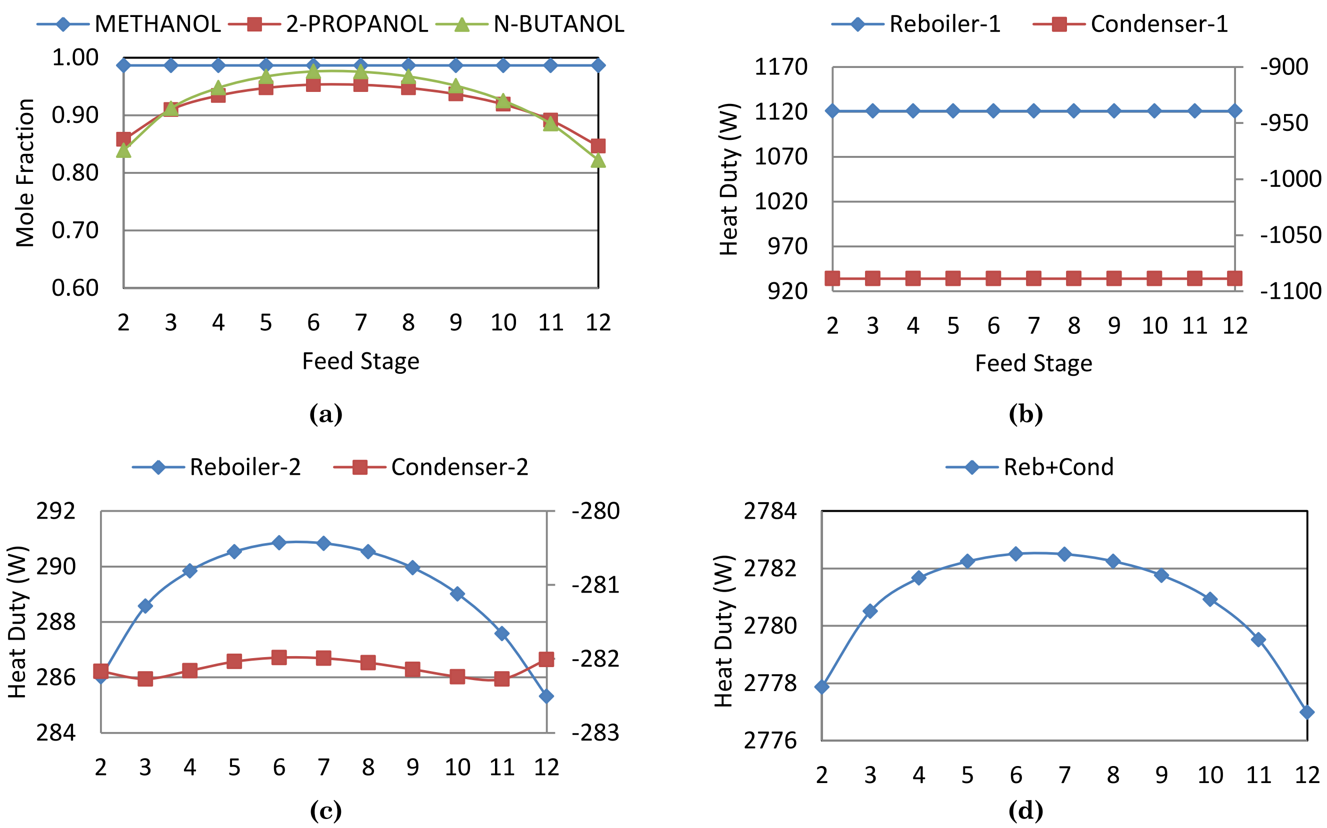


Fig. 7 The effect of the feed stage number of the second column on the output parameters (a) the molar fractions of the products (b) the heat duties of the reboiler and the condenser of the first column (c) the heat duties of the reboiler and the condenser of the second column (d) sum of heat duties of the reboilers and the condensers of the first and the second columns (2 Columns, NS1:31, NF1:17, NS2:13, RR1:1.95, RR2: 0.67)

Table 5 The optimum conditions of two conventional distillation columns

Column-1	Column-2	Column-1		Column-2	
RR	RR	NSTAGE	Feed Stage	NSTAGE	Feed Stage
1.95	0.67	31	17	13	7

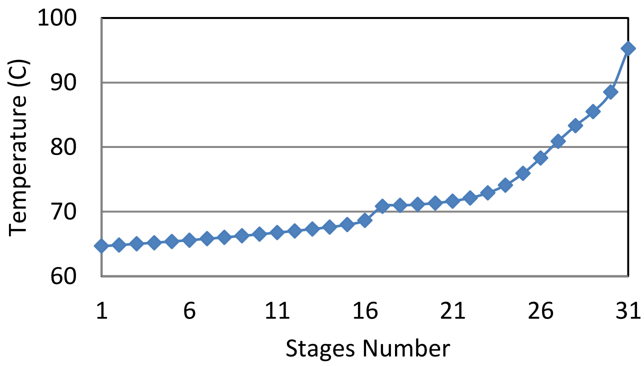
Table 6 The mole fractions of the components in the process products of two conventional distillation columns at the optimum conditions

	BOT-1	BOT-2	DIST-1	DIST-2	FEED
Mole Frac					
METHA-01	0.010	4.896E-06	0.986	0.018	0.580
ISOPR-01	0.538	0.025	0.014	0.953	0.232
N-BUT-01	0.452	0.975	1.426E-13	0.030	0.188
Mole Flow (kmol/hr)	0.027	0.012	0.038	0.015	0.065
Mass Frac					
METHA-01	0.005	2.126E-06	0.975	0.009	0.400
ISOPR-01	0.489	0.020	0.025	0.954	0.300
N-BUT-01	0.506	0.980	3.261E-13	0.037	0.300
Mass Flow (kg/hr)	1.777	0.885	1.223	0.893	3.000

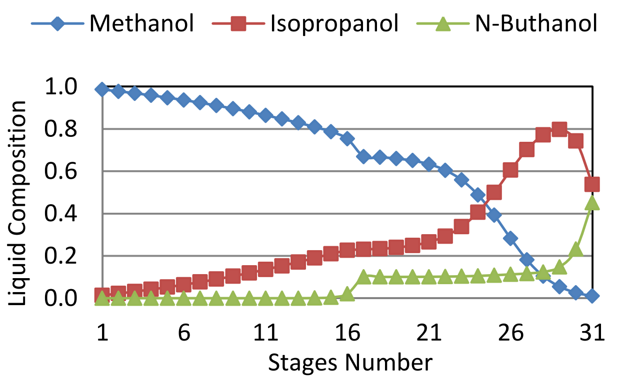
Table 7 The heat duties of the reboilers and the condensers of two conventional distillation columns at the optimum conditions

Heat Duty (W)	Column-1	Column-2
Reboiler	1120.94	290.84
Condenser	-1088.73	-281.99

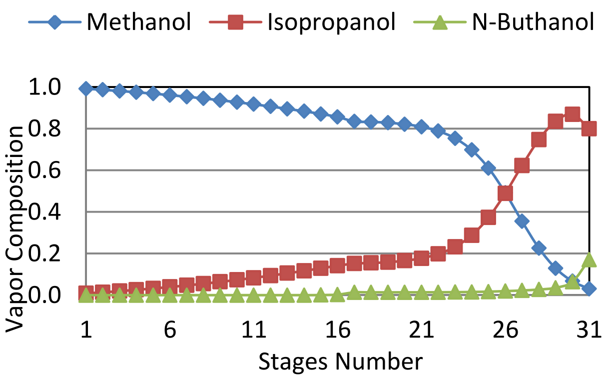
The profiles of two conventional distillation columns at the optimum conditions have been illustrated in **Fig. 8** (a) to **Fig. 8** (f). **Fig. 8** (a) shows the temperature profile of the first column at various stages at the optimum conditions. According to the results of **Fig. 8** (a), the temperature increases with increasing stage number. A breakpoint is observed at stage 17, which corresponds to the feed stage of the first column. Since the feed enters at a temperature of 70 °C and its temperature is higher than the feed stage temperature, an increase in temperature is observed. The temperature then rises with increasing stage number, which corresponds to the temperature changes in the distillation process. The first column involves the separation of methanol from the mixture of isopropanol and butanol. The top temperature of the column is 64.67 ^{0}C, which is similar to the methanol boiling point of 64.7 ^{0}C. The column bottom temperature is 95.27 ^{0}C, which is the temperature of isopropanol and butanol mixture. **Fig. 8** (b) depicts the concentration profiles of the components in the liquid phase at various stages for the first column at the optimum conditions. It can be observed that with increasing the number of the stages, butanol concentration increases as the heaviest component and the concentration of isopropanol as the intermediate component at first increases and then decreases, the concentration of methanol as the lightest component decreases. A breakpoint is observed in stage 17, which corresponds to the location of the feed stage of the first column. The composition difference between the feed and stage 17 leads to the changes in concentration profiles. The methanol concentration at the top of the column is 0.986, which leaves as the top product of the column. The concentrations of isopropanol and butanol in the bottom product are 0.538 and 0.452, respectively. **Fig. 8** (c) shows the concentration profile of the components in the vapor phase at various stages of the first column at the optimum conditions. According to this figure, the concentration profiles in the vapor phase are similar to those in the liquid phase. The comparison between **Fig. 8** (b) and **Fig. 8** (c) concerning the concentration profiles in liquid and vapor phases at different stages of the first column shows that the trend of changes in the vapor phase is more slowly. So there is no breakpoint at the feed stage (stage no. 17). It can be explained that the feed enters as the liquid phase on the stage. This column is concerned with the separation of isopropanol and butanol. The concentration of isopropanol in the top product of the column is 0.953. The concentrations of butanol and methanol in the top product of the column are 0.0297 and approximately zero, respectively. In the bottom product of the column, the concentrations of butanol and isopropanol are 0.975 and 0.025, respectively. The temperature profiles of the second column at the optimum conditions have been shown in **Fig. 8** (d). It can be observed that the temperature is increased with increasing stage number. This column corresponds to the separation of isopropanol and butanol. The top temperature of the column is 82.02 ^{0}C, which is similar to the boiling point of isopropanol (82.15 ^{0}C). The bottom temperature of the column is 118.86 ^{0}C, which is very close to the boiling point of butanol (118.75 ^{0}C). The concentration profiles of the components in the liquid phase of the second column at the optimal conditions have been illustrated in **Fig. 8** (e). According to the results, the concentration of methanol is almost zero at all stages and the concentration of butanol as the heaviest component increases with increasing stage number, and at stage 13, which leaves the column, is 0.975. The composition of isopropanol as the intermediate component decreases with increasing stage number and leaves the column at a concentration of 0.953. **Fig. 8** (f) depicts the concentration profiles in the vapor phase of the second column at the optimal conditions. The trends are quite similar to the liquid phase.



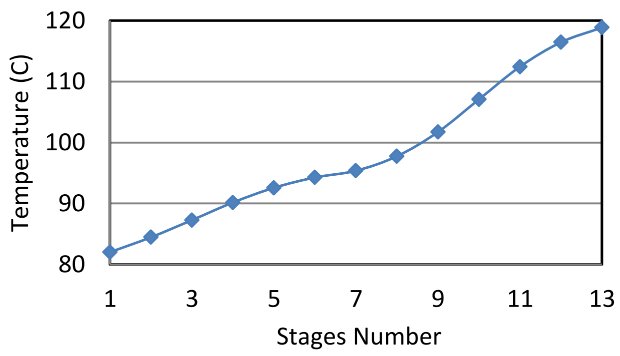
(a) Temperature profile of the first column



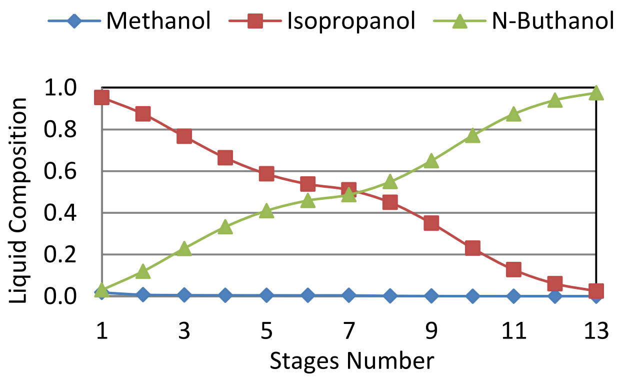
(b) The concentration profiles of the components in the liquid phase of the first column



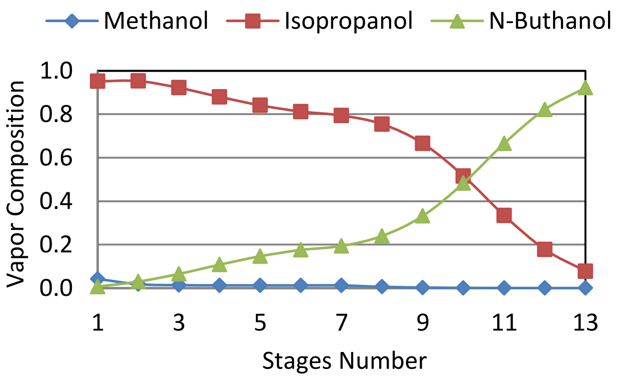
(c) The concentration profiles of the components in the vapor phase of the first column



(d) The temperature profiles of the second column



(e) The concentration profiles of the components in the liquid phase of the second column



(f) The concentration profiles of the components in the vapor phase of the second column

Fig. 8 The profiles at the optimal conditions

(2 Columns, NS1=31, NF1=17, NS2=13, NF2=7, RR1=1.95, RR2=0.67)

3.2. Dividing Wall Column Distillation (DWCD) Process

DWCD process is a technology that combines the required columns for the separation of a mixture in one column. In this technology, one or more dividing wall is located within a distillation column to upgrade separation efficiency. According to the literature, this technology can save up to 20-30% in energy costs due to high energy efficiency and reducing remixing effects. Some advantages of this technology include less required space, reducing energy and investment costs. Two reboilers and two condensers are required to separate the ternary mixture by the conventional methods, while the DWC just needs one column, including a reboiler and a condenser, resulting in saving on investment costs (Nguyen, 2015). The Julius Montz GmbH company claimed that by using DWC, the investment and the operating costs would be reduced by 30-30% and up to 25%, respectively (Illner and Othman, 2015). Kim (2017) evaluated DWC for crude oil. Economic analysis showed 9% investment savings and 26% cost reduction.

There is no standard model for simulation of the DWCD process in commercial software such as Aspen Plus. Four models have been presented for simulation of a DWC in the literature.

1) Pump around sequence
2) Two-column sequences including prefractionator
3) Two-column sequences including postfractionator
4) Four-column sequences

In this study, a four-column sequences model has been applied for simulation. The diagram used to simulate the DWCD process has been illustrated in Fig. 9.

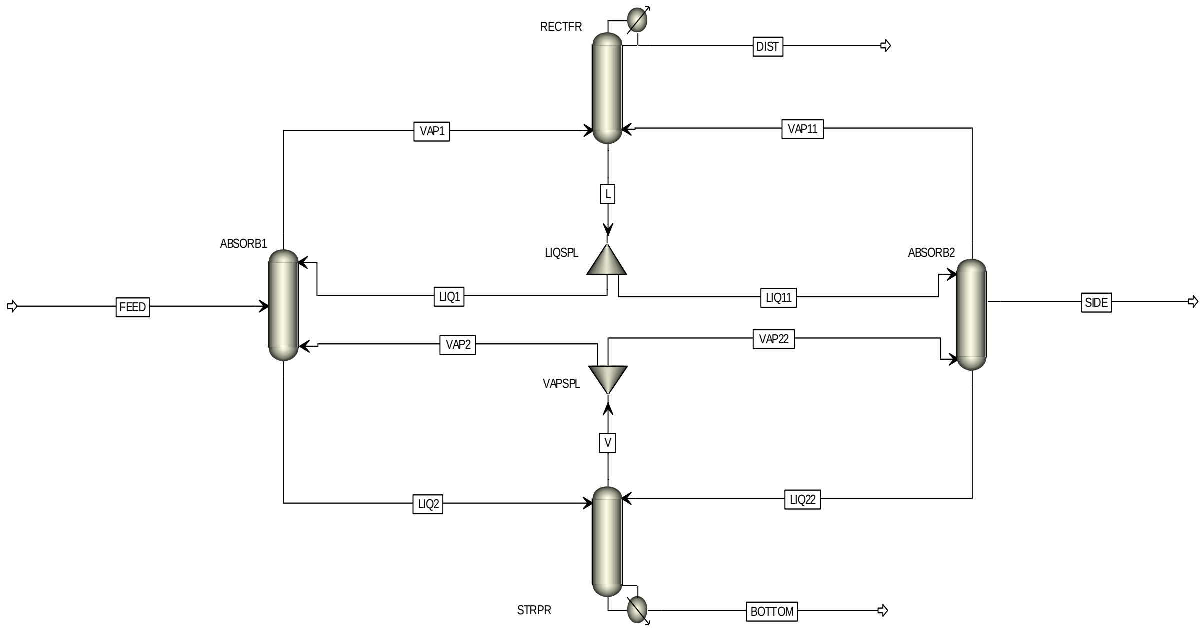


Fig. 9 Diagram of DWCD process simulation for separation of a ternary feed

The system contains four distillation columns and two vapor and liquid splitters. The four columns include two Absorbers, a Rectifier, and a Stripper. Feed enters Absorber-1. The top product of Absorber-1column comes into the Rectifier as a vapor phase. The bottom product enters the Stripper. The top product of the Rectifier is the final product of the system and includes the lightest component. The bottom product of the Rectifier is in the liquid phase and enters the liquid splitter. It is divided into two streams, one part of which enters Absorber-1 and the other part enters Absorber-2. The bottom product of Stripper is the final product of the process and contains the heaviest component. The top product of Stripper is in the form of vapor and enters the vapor splitter and is divided into two streams, one part of which enters Absorber-1 and the other part enters Absorber-2. The Absorber-2 column has two output products, the top of which is in the vapor phase and enters the Rectifier column. The lower product of the Absorber-2 column is liquid and enters the Stripper column. Its side product is the final product of the process and contains the intermediate component. The Absorber-2 column has two liquid and vapor inlets, which are liquid and vapor splitters outputs, respectively.

Table 8 shows the initial characteristics of the four columns and the liquid and vapor splitters in the DWCD process. Table 9 shows the characteristics of the products of the DWCD process.

Table 10 shows the reboiler and condenser heat duties in the DWCD process.

3.2.1. DWCD process optimization

3.2.1.1. The number of stages of Absorber-1

The number of stages effects of Absorber1 column on the output parameters has been illustrated in **Fig. 10** (a) to **Fig. 10** (c). (The data are indicated in details in Table A-7 in the supplementary data section). Abs is an absorber, Nside is side product stage number, NS is total stages number, Rect is rectifier, Strip is an stripper, VAPSPL is vapor split ratio, and LIQSPL is the liquid split ratio. The other parameters have been considered constant (number of stages of Absorber-2: 20, number of side product stage in Absorber-2: 14, number of stages of Rectifier: 20, number of stages of Stripper: 20, reflux ratio of the column: 2, vapor split ratio: 0.35, liquid split ratio: 0.65). **Fig. 10** (a) depicts the effect of the number of stages of the Absorber1 column on the mole fractions of the components in the products.

Table 8 The initial characteristics of the four columns and the liquid and vapor splitters in the DWCD process

	Unit	Absorber1	Absorber2	Rectifier	Stripper	LIQSPL	VAPSPL
Stage Number	-	20	20	20	20	-	-
Distillate Rate	Kg/h	-	-	-	-	-	-
Reflux Ratio	-	-	-	2	-	-	-
Feed Stage	-	10	-	-	-	-	-
Side Stage	-	-	14	-	-	-	-
Pressure (Stage 1)	atm	1.03	1.03	1	1.05	-	-
Pressure Drop	atm	0.02	0.03	0.03	0.02	-	-
Bottom Rate	Kg/h	-	-	-	0.9	-	-
Side Rate	Kg/h	-	0.9	-	-	-	-
Split Ratio	-	-	-	-	-	0.65	0.35

Table 9 The characteristics of the products of the DWCD process

	BOTTOM	DIST	SIDE	FEED
Mole Frac				
METHA-01	5.145E-14	**0.988**	0.053	0.580
ISOPR-01	2.851E-05	0.012	**0.947**	0.232
N-BUT-01	**1.000**	1.115E-20	1.832E-05	0.188
Mole Flow (kmol/hr)	0.012	0.037	0.015	0.065
Mass Frac				
METHA-01	2.224E-14	**0.978**	0.029	0.400
ISOPR-01	2.312E-05	0.022	**0.971**	0.300
N-BUT-01	**1.000**	2.554E-20	2.316E-05	0.300
Mass Flow (kg/hr)	0.900	1.200	0.900	3.000

Table 10 The reboiler and the condenser heat duties in the DWCD process

Heat Duty (W)	Absorber1	Absorber2	Rectifier	Stripper
Reboiler	_	_	_	1130.5401
Condenser	_	_	-1088.228	_

According to the results of **Fig. 10** (a), the concentration of butanol in the product remains constant with increasing the number of stages of Absorber1. However, the concentrations of methanol and 2-propanol are increased. It can be explained that separation is increased by increasing the number of column stages. **Fig. 10** (b) shows the effect of the number of stages of the Absorber1 column on the heat duties of the reboiler and the condenser of the system. It can be observed that with increasing the number of stages, both the reboiler and the condenser heat duties increase. The reason for this can be explained that as the number of stages of the Absorber1 column increases, the column height is increased, and more heat duty is required due to the stability of the other parameters. The effect of the number of stages of the Absorber1 column on the sum of heat duties of the reboiler and the condenser of the DWCD has been illustrated in **Fig. 10** (c). As can be observed, the sum of the reboiler and the condenser heat duties of the DWCD process are increased by increasing the number of stages of the Absorber-1 column. According to the sensitivity analysis of this section, to reduce the reboiler and condenser heat duties with considering desired purities of the products, the number of 16 has opted for the stages of the Absorber-1 column.

3.2.1.2. The number of stages of Absorber-2

The number of the stages effects of the Absorber2 column on the output parameters has been illustrated in **Fig. 11** (a) to **Fig. 11** (c). (The data are indicated in details in Table A-8 in the supplementary data section). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of feed stage in Absorber-1: 8, number of stages of Rectifier: 20, number of stages of Stripper: 20, reflux ratio of the column: 2, vapor split ratio: 0.35, liquid split ratio: 0.65). The effects of the number of stages of the Absorber-2 column on the mole fraction of the components in the DWC system products have been illustrated in **Fig. 11** (a). According to the results of **Fig. 11** (a), the concentration of butanol in the product is constant, and the concentration of methanol and 2-propanol increases with increasing the number of stages of the Absorber-2 column. It can be explained that by increasing the number of column stages, separation is enhanced. **Fig. 11** (b) shows the effect of the number of stages of the Absorber-2 column on the heat duties of the reboiler and the condenser of the system. As can be observed, both the reboiler and the condenser heat duties increase with increasing the number of stages. The reason for this can be explained that as the number of stages of Absorber-2 increases, the column height is increased, and more heat duty is required due to the stability of the other parameters. **Fig. 11** (c) depicts the effect of the number of stages of the Absorber-2 column on the sum of heat duties of the reboiler and the condenser of the DWC system. It can be observed that the sum of the reboiler and the condenser heat duties of the DWCD process are increased by increasing the number of stages of the Absorber-2 column. According to the sensitivity analysis of this section, to reduce the reboiler and condenser heat duties with considering desired purities of the products, the number of 16 has opted for the stages of Absorber-2.

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following item. Szabo et al. (2008) evaluated the effect of wall height, representing the number of stages of feed and side product sections in a DWC system. The wall had a central vertical position; the feed, and the side product stages were the same. They investigated the separation of benzene, toluene, and o-xylene. The reboiler heat duty decreased first and then slightly increased with increasing the wall height in DWC. There was an optimum stage number for wall height to minimize energy consumption.

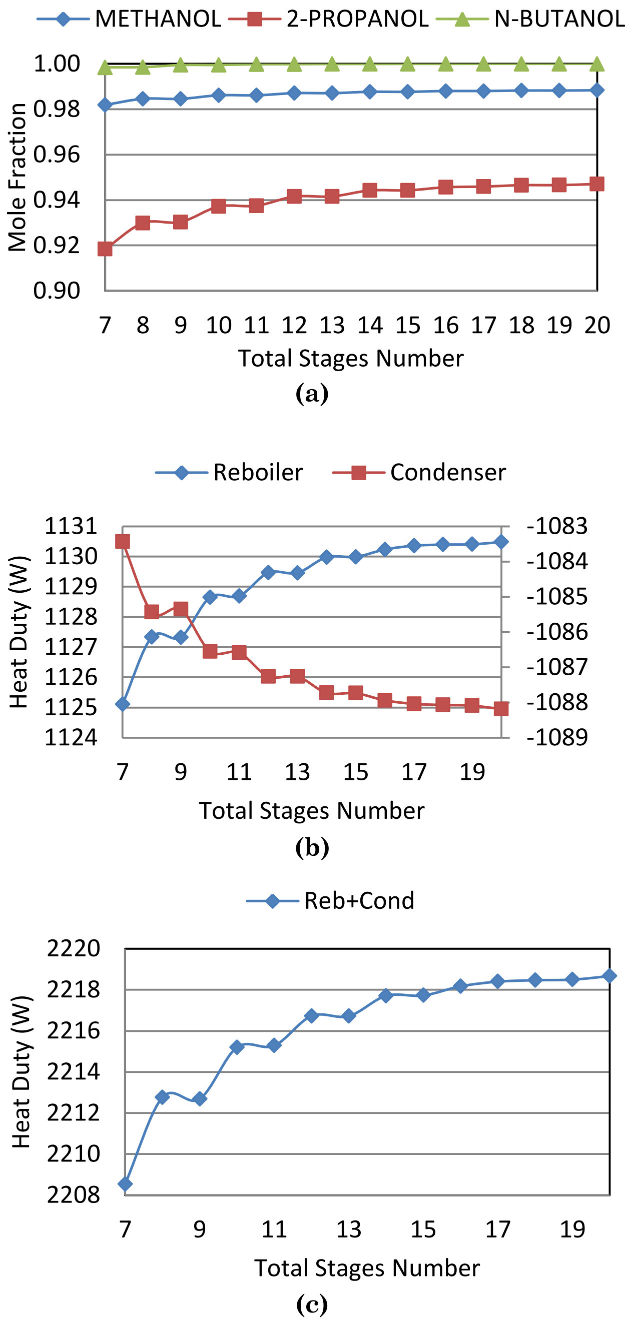


Fig. 10 The effect of the stages number of Absorber1 column on the output parameters (a) the mole fractions of the components in the DWC process products (b) the heat duties of the reboiler and the condenser of the system (c) the sum of heat duties of the reboiler and the condenser of the DWCD (NS(Abs2):20, NSide(Abs2):14, NS(Rect):20, NS(Strip):20, RR:2, VAPSPL:0.35, LIPSPL:0.65)

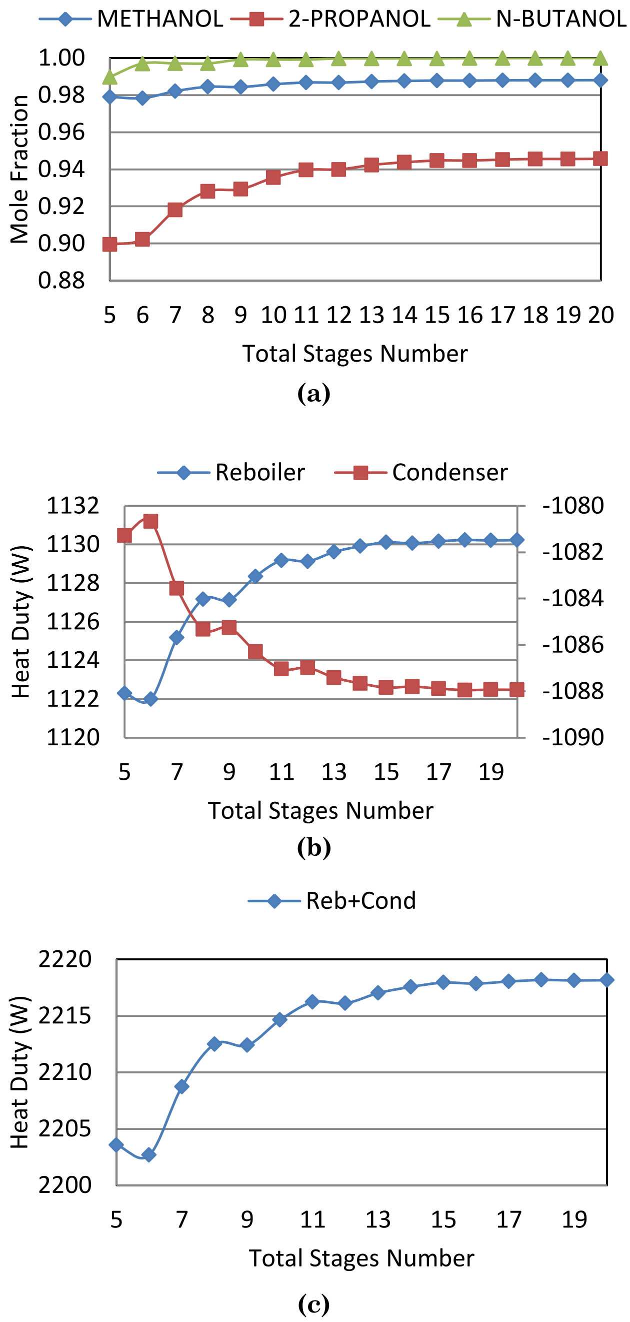


Fig. 11 The effect of the stages number of Absorber2 column on the output parameters (a) the mole fraction of the components in the DWC system products (b) heat duties of the reboiler and the condenser of the system (c) the sum of heat duties of the reboiler and the condenser of the DWC system (NS(Abs1):16, NF(Abs1):8, NS(Rect):20, NS(Strip):20, RR:2, VAPSPL:0.35, LIPSPL:0.65)

3.2.1.3. The number of stages of Rectifier

The number of the stages effects of Rectifier column on the output parameters has been illustrated in **Fig. 12** (a) to **Fig. 12** (c). (The data are indicated in details in Table A-9 in the supplementary data section). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of feed stage in Absorber-1: 8, number of stages of Absorber-2: 16, number of side product stage in Absorber-2: 11, number of stages of Stripper: 20, reflux ratio of the column: 2, vapor split ratio: 0.35, liquid split ratio: 0.65).

Fig. 12 (a) depicts the effect of the number of stages of the Rectifier column on the mole fraction of the components in the products. According to the results of **Fig. 12** (a), the concentration of butanol in the product remains constant, and the concentrations of methanol and 2-propanol increase by increasing the number of stages of the Rectifier column. It can be explained that by increasing the number of column stages, separation is increased. **Fig. 12**(b) shows the effect of the number of stages of the Rectifier column on the heat duties of the reboiler and the condenser of the system. As can be observed, both the reboiler and the condenser heat duties increase with an increase in the number of stages. The reason for this can be explained that as the number of stages of the Rectifier increases, the column height is increased, and more heat duty is required due to being constant the other parameters. It is also observed that the changes of the reboiler and the condenser heat duties are almost linear. **Fig. 12** (c) illustrates the effect of the number of stages of the Rectifier column on the sum of heat duties of the reboiler and the condenser of the DWC system. It is observed that the changes are almost linear. As can be observed, the sum of the reboiler and the condenser heat duties of the DWCD process increases by increasing the number of stages of the Rectifier column. According to the sensitivity analysis of this section, to reduce the reboiler and condenser heat duties, with considering desired purities of the products, the number of 20 has opted for the stages of the Rectifier.

3.2.1.4. The effect of the number of Stripper stages

The number of the stages effects of the Stripper column on the output parameters has been illustrated in **Fig. 13** (a) to **Fig. 13** (c). (The data are indicated in details in Table A-10 in the supplementary data section). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of feed stage in Absorber-1: 8, number of stages of Absorber-2: 16, number of side product stage in Absorber-2: 11, number of stages of Rectifier: 20, reflux ratio of the column: 2, vapor split ratio: 0.35, liquid split ratio: 0.65). **Fig. 13** (a) depicts the effect of the number of stages of the Stripper column on the mole fraction of the components in the DWC products. As can be observed by increasing the number of stages from 4 to 7, the concentration of propanol and butanol components somewhat increases and then remains constant, but the concentration of methanol is the same at all stages. The reason for this can be explained that the optimum number of stages for the Stripper is 7; since with its increasing, no separation is performed. **Fig. 13** (b) illustrates the effect of the number of stages of the Stripper column on the heat duties of the reboiler and the condenser of the DWCD process. According to the results of **Fig. 13** (b), a nonsignificant effect on the heat duty can be observed with increasing the number of column stages. **Fig. 13** (c) shows the effect of the number of stages of the Stripper column on the sum of heat duties of the reboiler and the condenser of the DWC. It can be observed by increasing the number of stages from 4 to 7, the total heat duties somewhat increase and then remain constant. According to the sensitivity analysis of this section, to reduce the reboilers and the condensers' heat duties with considering desired purities of the products, the number of 7 has opted for the stages of the Stripper.

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following item. Szabo et al. (2008) evaluated the effect of the relative position of the wall on the reboiler heat duty in a DWC system. The number of stages in the feed and the side product sections was equal, and the total number of stages was assumed to be constant. The height of the wall was nine stages. According to their results, the energy consumption was lower when the number of the stages above and below the wall has the same. They explained that one reason for this was that the components in the feed had a similar mass fraction. The feed was a mixture of benzene, toluene, o-xylene with the similar mass fraction.

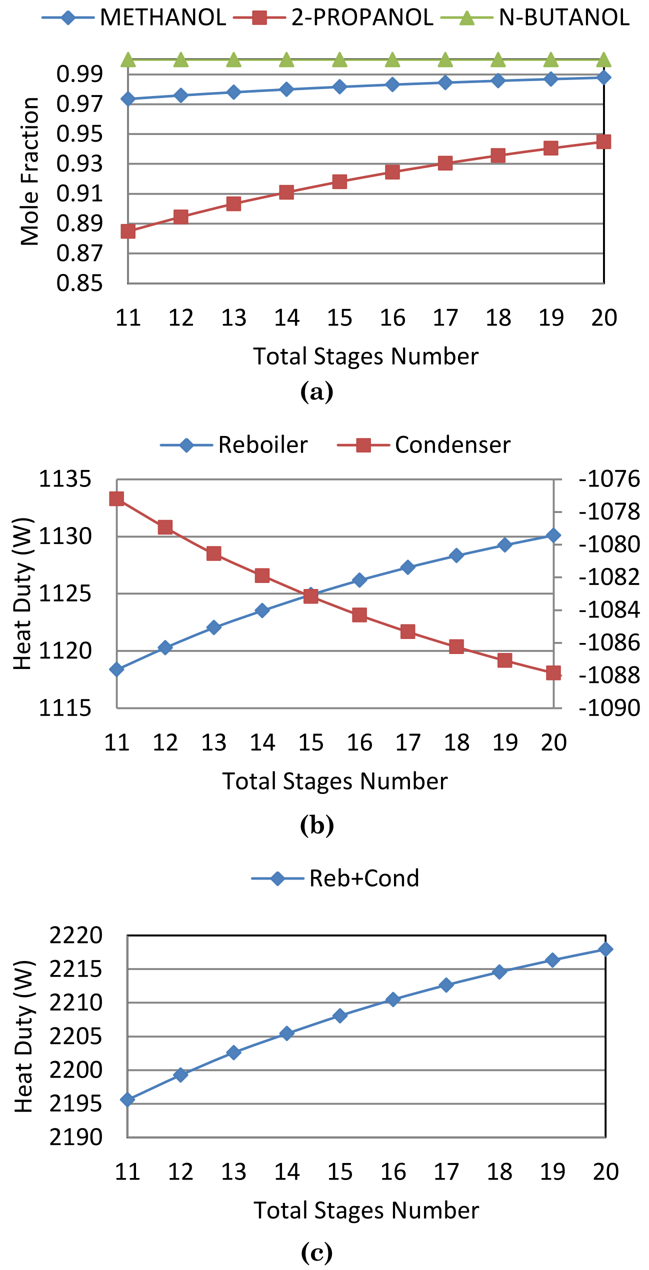


Fig. 12 The effect of the stages number of Rectifier column on the output parameters (a) the mole fraction of the components in DWC system products (b) the heat duties of the reboiler and the condenser of the system (c) the sum of heat duties of the reboiler and the condenser of the DWC system (NS(Abs1):16, NF(Abs1):8, NS(Abs2):16, NSide(Abs2):11, NS(Strip):20, RR:2, VAPSPL:0.35, LIPSPL:0.65)

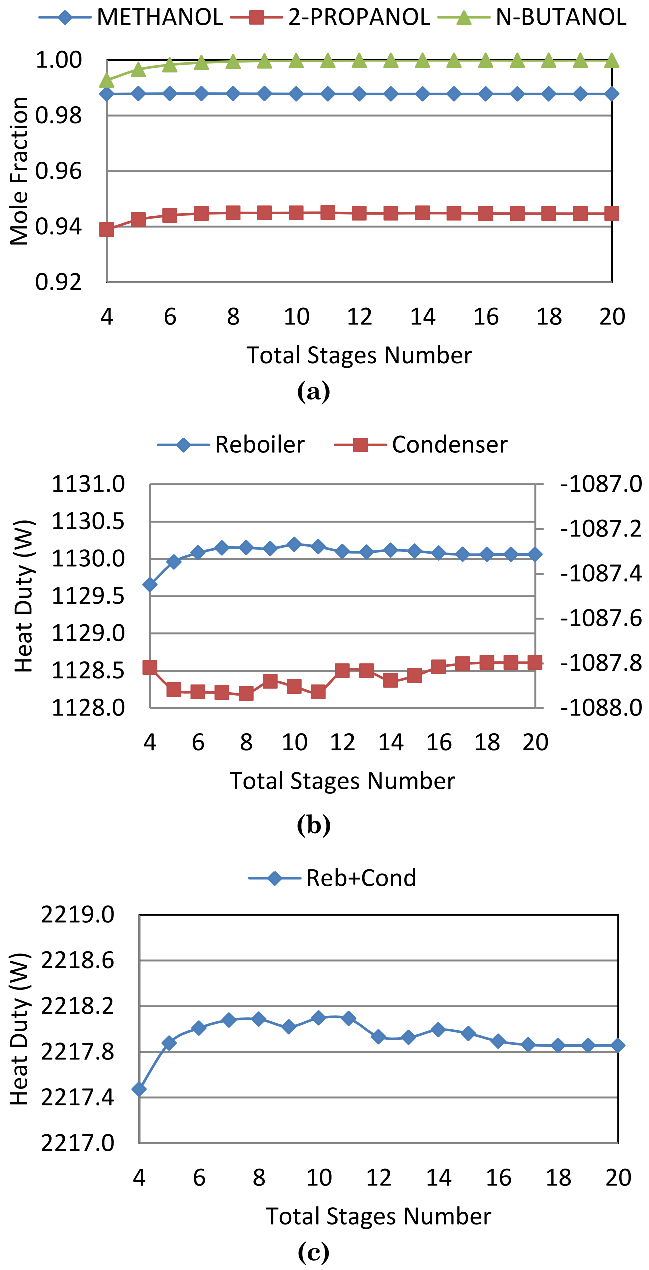


Fig. 13 The effect of the stages number of Stripper column on the output parameters (a) the mole fraction of the components in the DWC system products (b) the heat duties of the reboiler and the condenser of DWC system (c) the sum of heat duties of the reboiler and the condenser of the DWC system (NS(Abs1):16, NF(Abs1):8, NS(Abs2):16, NSide(Abs2):11, NS(Rect):20, RR:2, VAPSPL:0.35, LIPSPL:0.65)

3.2.1.5. The effect of reflux ratio

The effects of the reflux ratio on the output parameters have been illustrated in **Fig. 14** (a) to **Fig. 14** (c). (The data are indicated in details in Table A-11 in the supplementary data section). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of feed stage in Absorber-1: 8, number of stages of Absorber-2: 16, number of side product stage in Absorber-2: 11, number of stages of Rectifier: 20, number of stages of Stripper: 7, vapor split ratio: 0.35, liquid split ratio: 0.65).

The effects of the column reflux ratio on the mole fractions of the components in the DWC process products have been shown in **Fig. 14** (a). According to the results of **Fig. 14** (a), the concentrations of all the components in the products have increased by increasing the reflux ratio. This increase is more significant for the middle component.

The reflux ratio in distillation columns is an important parameter. With increasing it, more liquid rich in volatile compounds returns to the column. Therefore, the gradient of the operating line for the enrichment section of the distillation column moves toward a maximum value of one. So, the liquid flow rate in the column is increased, and separation is enhanced.

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following item. Arora (2014) investigated simulation of DWCD for three ternary mixtures containing benzene-toluene-p-xylene, benzene-toluene-o-xylene and methanol-water-glycerol. They concluded that with increasing RR, the purity of top product increased. Gor et al. (2017) evaluated the effect of the reflux ratio on the mole fraction of the components in DWC. The feed was a mixture of butane-pentane-hexane. They concluded that pentane and hexane mole fractions as the intermediate and the heaviest components increased with increasing reflux ratio, but butane mole fraction as the lightest component was almost constant.

Fig. 14 (b) depicts the effect of the reflux ratio on the reboiler and the condenser heat duties. According to the results of this section, both the reboiler and the condenser heat duties are increased with increasing the reflux ratio, and the profiles are linear.

The result is perfectly reasonable. By increasing the reflux ratio, owing to being constant the top product and the side product flow rates, the flow rate in all stages of the column increase, leads to increasing the heat duties of the reboiler and the condenser. The effect of increasing the reflux ratio on the sum of heat duties of the reboiler and the condenser of the DWC has been shown in **Fig. 14** (c). As can be observed, the sum of heat duties of the reboiler and the condenser linearly increases with increasing the reflux ratio. In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following items. Kaur (2012) investigated the simulation of DWCD for separation of BTX. They investigated the variation of reboiler duty with the reflux ratio. The reboiler duty increased as the reboiler duty increased. The trend of their profile confirmed our results. Gor et al. (2017) also investigated reboiler heat duty variations in terms of the reflux ratio in a DWC system. They concluded that with increasing column reflux ratio, the heat duty of the reboiler linearly increased.

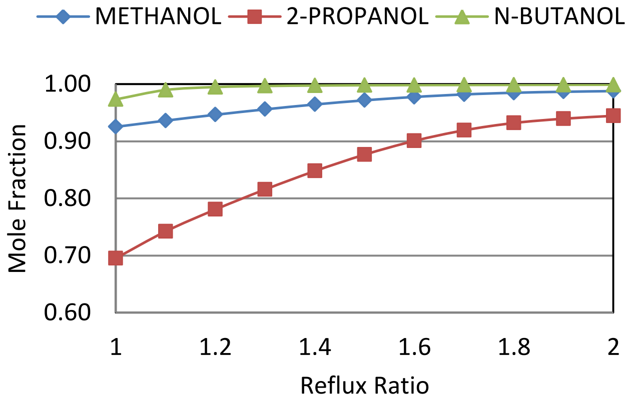
It can be concluded that the appropriate reflux ratio results in a better separation in different parts of the column and also reduces the heat duties of the reboiler and the condenser. According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties with considering desired purities of the products, the number of 2 has opted for the reflux ratio of the DWCD process.

3.2.1.6. The effect of vapor split ratio

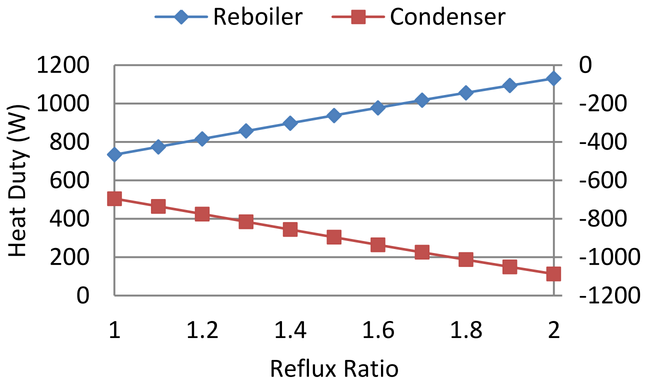
In this study, the vapor split ratio is the ratio of the vapor flow input into Absorber-2 to the total inlet vapor flow to vapor splitter at the bottom of the two parallel columns of Absorber-1 and Absorber-2. (The data are indicated in details in Table A-12 in the supplementary data section). The effect of vapor split ratio on the output parameters have been illustrated in **Fig. 15** (a) to **Fig. 15** (c). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of feed stage in Absorber-1: 8, number of stages of Absorber-2: 16, number of side product stage in Absorber-2: 11, number of stages of Rectifier: 20, number of stages of Stripper: 7, reflux ratio of the column: 2, liquid split ratio: 0.65).

The effect of the vapor split ratio on the mole fractions of the components in the process products is illustrated in **Fig. 15** (a). According to the results of **Fig. 15** (a), the mole fractions of the products are significantly dependent on the values of the vapor split ratio and so the interconnected flows of the process. With increasing the vapor split ratio, the mole fractions of all three components at first increase and then decrease. These changes are more significant for the intermediate component of isopropanol. The profiles of the ratio of the vapor split have a maximum value of 0.4.

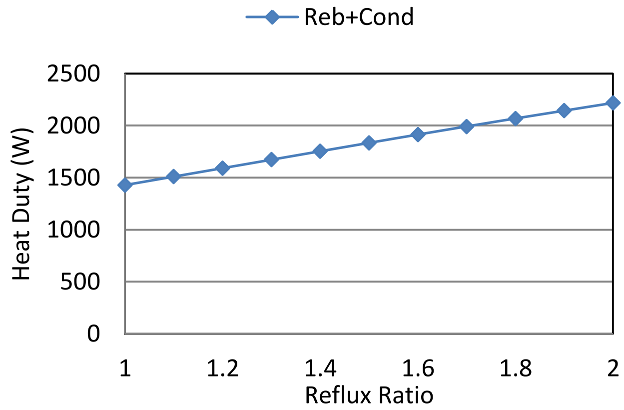
In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following items. Arora (2014) evaluated the separation process of ternary mixtures, including benzene-toluene-paraxylene, benzene-toluene-orthoxylene, and methanol-water-glycerol, in a DWC system and investigated the effect of the vapor split ratio on the purity of products. Based on their conclusions, the lowest effect of the vapor split ratio was on the concentration of the heaviest component in the bottom product of the column. The more significant influence of the vapor split ratio was on the concentration of the intermediate component in the side product. There was an optimum value for the vapor split ratio, where the concentration was optimum. Gor et al. (2017) also studied the effect of the vapor split ratio on the mole fractions of the components in a DWC system. There was a maximum point for all the components, according to their results.



(a)

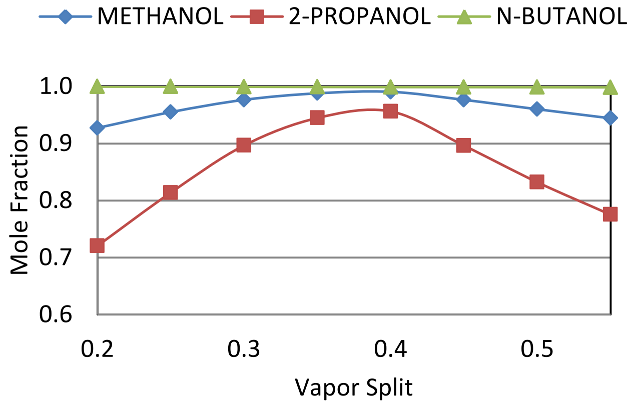


(b)

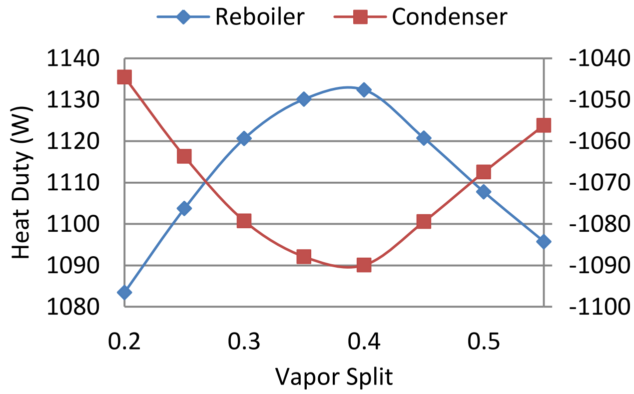


(c)

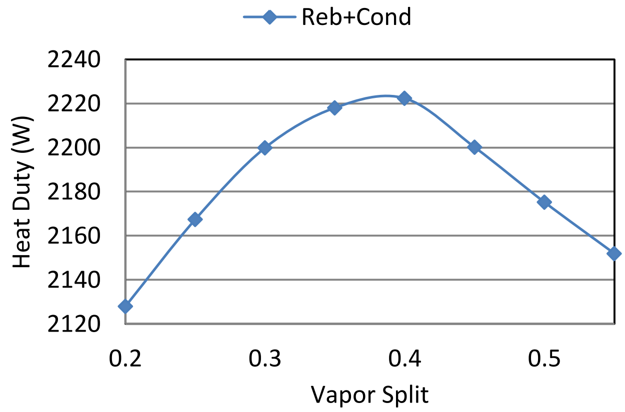
Fig. 14 The effect of the column reflux ratio on the output parameters (a) the mole fractions of the components in the DWC process products (b) the reboiler and the condenser heat duties of system (c) the sum of heat duties of the reboiler and the condenser of the DWC system (NS(Abs1):16, NF(Abs1):8, NS(Abs2):16, NSide(Abs2):11, NS(Rect):20, NS(Strip):7, VAPSPL:0.35, LIPSPL:0.65)



(a)



(b)



(c)

Fig. 15 The effect of the vapor split ratio on the output parameters (a) the mole fractions of the components of the products in DWC system (b) the heat duty of the reboiler and the condenser of the DWC system (c) the sum of heat duties of the reboiler and the condenser of the DWC system (NS(Abs1):16, NF(Abs1):8, NS(Abs2):16, NSide(Abs2):11, NS(Rect):20, NS(Strip):7, RR:2, LIPSPL:0.65)

Fig. 15 (b) illustrates the effect of the vapor split ratio on the heat duties of the reboiler and the condenser of the DWC process. It can be observed that the reboiler and the condenser heat duties are significantly dependent on the vapor split ratio. With increasing the vapor split ratio, the heat duty of both the reboiler and the condenser increases first and then decreases and has a maximum value in the vapor split ratio of 0.4.

The influence of the vapor split ratio on the sum of heat duties of the reboiler and the condenser of the DWC process has been shown in **Fig. 15** (c). As can be observed by increasing the vapor split ratio, the sum of the reboiler and the condenser duties is increased first and then is reduced and has a maximum value in the vapor split ratio of 0.4.

According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties with considering desired purities of the products, the value of 0.35 has opted for the vapor split ratio of the DWCD process.

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following items. Kaur (2012) evaluated the vapor split ratio effect on reboiler heat duty in a DWC system. They concluded that there was an optimum value of the vapor split ratio, at which the reboiler heat duty was minimal. Sangal (2012) studied DWCD process for separation BTX. They evaluated the effects of vapor split ratio on reboiler heat duty. According to their results, with increasing vapor split ratio, the heat duty first increased and then decreased and there was a maximum point. Yuqi et al. (2015) also evaluated the vapor split ratio influence on heat duty of the reboiler and the condenser in a DWC system. They investigated the separation of hexane-heptane-octane. According to their results, there was an optimum value of the vapor split ratio, at which the heat duty of the reboiler and the condenser was minimum.

3.2.1.7. The effect of liquid split ratio

In this study, the liquid split ratio is the ratio of liquid input into Absorber-2 to the total inlet liquid flow to liquid splitter at the top of the two parallel columns of Absorber-1 and Absorber-2. Based on the studies, the liquid and vapor split ratios are important parameters for obtaining the desired concentrations of the products in the DWCD process. The effect of the liquid split ratio on the output parameters have been illustrated in **Fig. 16** (a) to **Fig. 16** (c). (The data are indicated in details in Table A-13 in the supplementary data section). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of feed stage in Absorber-1: 8, number of stages of Absorber-2: 16, number of side product stage in Absorber-2: 11, number of stages of Rectifier: 20, number of stages of Stripper: 7, reflux ratio of the column: 2, vapor split ratio: 0.35).

The effect of the liquid split ratio on the mole fractions of the components in DWC products has been shown in **Fig. 16** (a). According to the results of **Fig. 16** (a), the mole fractions of the two components of methanol and isopropanol at first increase and then decrease as the liquid split ratio increases. The effect of the ratio of liquid split on the mole fraction of isopropanol is more significant.

Since the feed enters the Absorber-1, in order to maintain the liquid balance in both parts, it is reasonable that a lower percentage of liquid enters the Absorber-1 column. There is a maximum value of 0.6 for the liquid split ratio in the profiles.

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following item. Sangal (2012) studied DWCD process for separation BTX. They investigated the concentration profile of toluene in side stream with different liquid split ratios. They found out that there was a maximum point in their graph. Arora (2014) investigated simulation of DWCD. They investigated the liquid split fraction effect on product purity in BTX system. The effect of increasing the liquid split ratio from 0.2 to 0.9 was studied. It was seen that changing the liquid split ratio had no effect on the product purities of top and bottom product (benzene and o-xylene). The value of side stream purity initially increased with increasing liquid split ratio, and then started decreasing. The maximum value of the toluene purity in side stream was at 60% split.

Fig. 16 (b) shows the effect of the liquid split ratio on the reboiler and the condenser heat duties. According to the results, the heat duty of both the reboiler and the condenser first increases and then decreases by increasing the liquid split ratio. A maximum value of 0.6 for the ratio of the liquid split in the profiles can be observed. The effect of the liquid split ratio on the sum of heat duties of the reboiler and the condenser of the DWC process has been illustrated in **Fig. 16** (c). It can be observed that the sum of heat duties of the reboiler and the condenser first increase and then decrease with the increase of the liquid split ratio.

Sangal (2012) studied DWCD process for separation BTX. They reported the effect of liquid split on reboiler duty. There was a maximum point for reboiler duty.

According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties with considering desired purities of the products, a value of 0.65 is opted for the liquid split ratio of the DWCD process.

Fig. 15 and **Fig. 16** show the significant influences of the liquid and vapor split ratios on the mole fraction of the products and the heat duties of the reboiler and the condenser. It should be noted that the internal flows in Absorber-1 are increased by the feed flow, and the internal flows in Absorber-2 are reduced by the side product flow. For this reason, the optimum value of the vapor split ratio is less than 0.5, and the optimum value of the liquid split ratio is greater than 0.5.

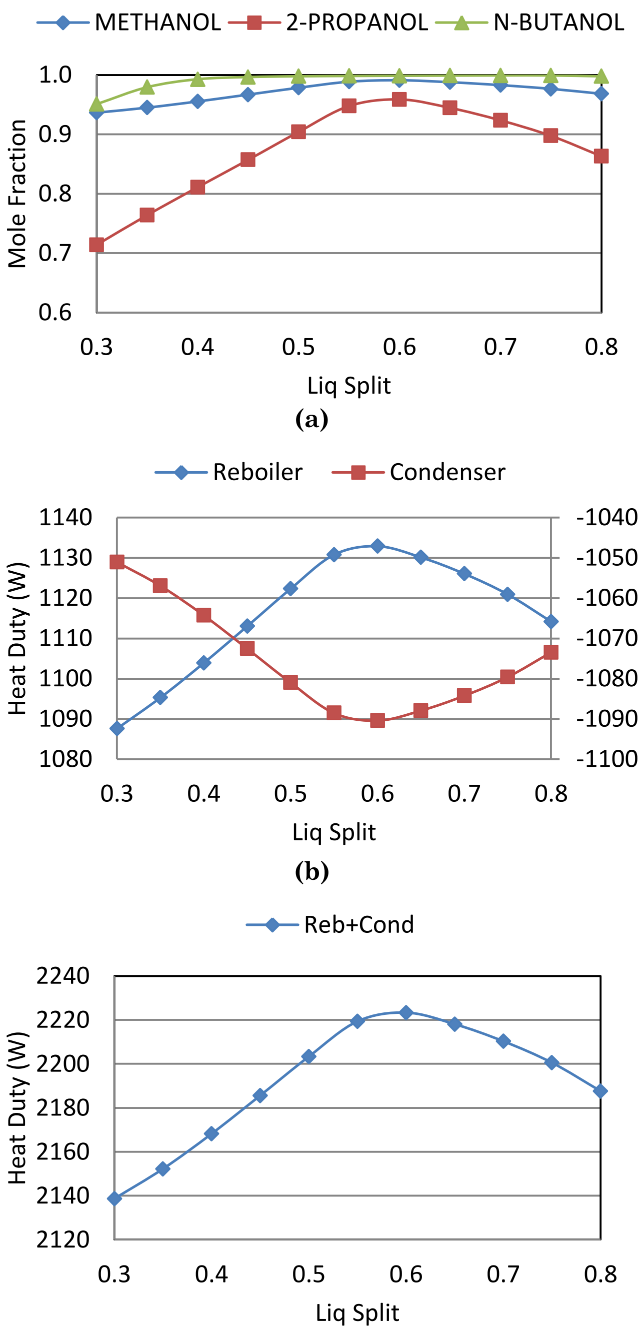
In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following items. Szabo et al. (2008) investigated that how the heat duty of the reboiler is changing with the split ratio. Their results showed that there was an optimum value which the energy consumption was minimal. The system was separation of BTX in DWCD. Rangaiah et al. (2009) studied DWCD for some systems at optimized column setting. There was an optimized vapor split fraction equal to 0.65 for separation BTX. For liquid split fraction also there was an optimum value equal to 0.45 for BTX system. They concluded that vapor and liquid splits in DWCD affect significantly the energy consumption. Kaur (2012) investigated the simulation of DWCD for separation of BTX. The simulations were performed by varying the operational parameters, while the structural variables were considered constant. Their results showed that there were optimum values of vapor split and liquid split for the minimum the reboiler duty. At steady state, the optimum liquid split was 0.603 and the optimum vapor split was found to be 0.45. Arora (2014) investigated simulation of DWCD in BTX mixture. They investigated the effect of vapor split fraction. Their results showed that with increasing vapor split from 0.3 to 0.5, the purity of benzene and toluene increased and attained a maximum. Then it gradually decreased. There was an optimum amount of vapor split ratio for obtaining the maximum concentrations of benzene and toluene in the products. Aurangzeb and Jana (2016) investigated DWCD for separation of a ternary system. The ternary mixture was included n-hexane/n-heptane/n-octane. They studied the effect of liquid and vapor splits. Based on their report, liquid and vapor splits played a vital role in obtaining the purity in side stream. According to their results, the best vapor and liquid splits were 31% and 57%. Its effect on the intermediate product was higher than that on the other products and there was an optimal point for liquid and vapor split ratios. Gor et al. (2017) evaluated the liquid split ratio effects on output parameters in a DWC system. They concluded that with increasing liquid split ratio, the reboiler heat duty first increased and then decreased. According to their results, pentane and hexane mole fractions as the intermediate and the heaviest components had a maximum value of mole fractions and changed with the liquid split ratio. However, there was no effect on butane mole fraction as the lightest component. Ehlers et al. (2018) simulated a DWCD for separation a ternary feed. They investigated the optimum vapor and liquid splits in different feed compositions. In the conditions of equal molar fractions in the feed, the optimum liquid and vapor splits are 0.24 and 0.55, respectively. They are comparable with our results, which is 0.65 and 0.35, respectively. Zhai et al. (2019) also investigated the liquid and vapor split ratios effects on the heat duties in a DWC system. The feed was a mixture of benzene, toluene, and xylene. Based on their results, the heat duties were dependent on the liquid and vapor split ratios, and there was an optimum value of the ratios to minimize the energy consumption.

3.2.1.8. The effect of feed stage number of Absorber-1

The effect of feed stage number of Absorber-1 on the output parameters have been illustrated in **Fig. 17** (a) to **Fig. 17** (c). (The data are indicated in details in Table A-14 in the supplementary data section). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of stages of Absorber-2: 16, number of side product stage in Absorber-2: 11, number of stages of Rectifier: 20, number of stages of Stripper: 7, reflux ratio of the column: 2, liquid split ratio: 0.65, vapor split ratio: 0.35).

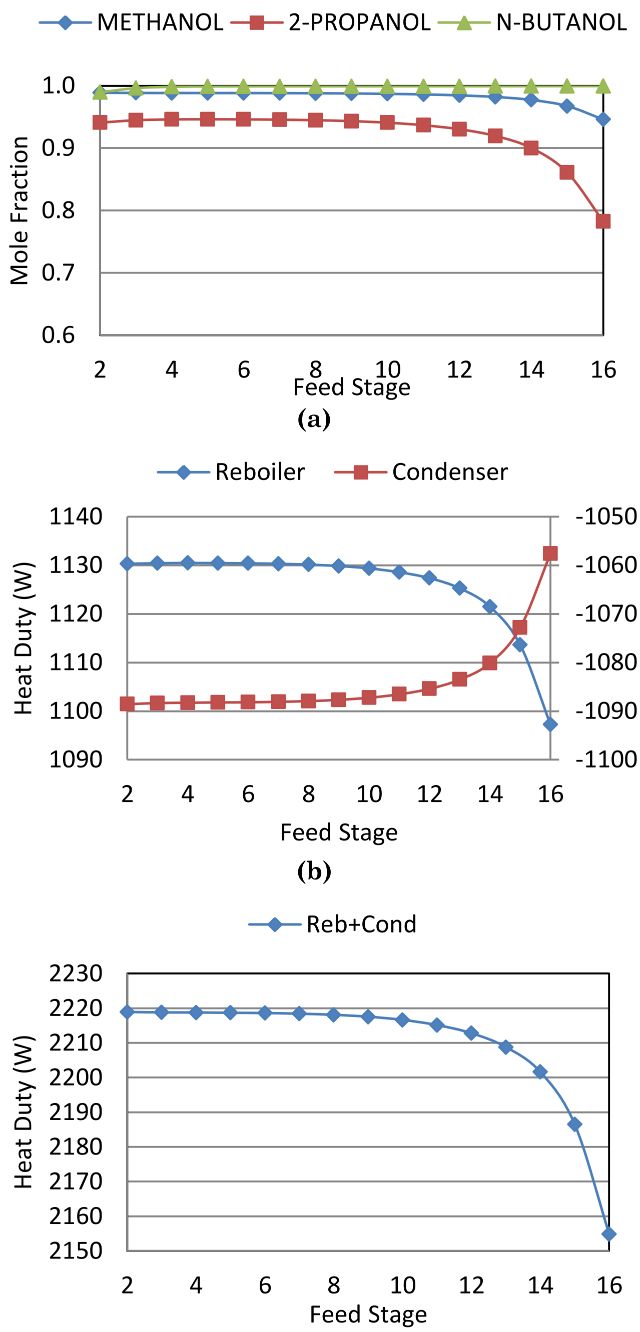
Fig. 17 (a) depicts the effect of feed stage number in the Absorber1 column on the mole fraction of the components in the products. According to the results of **Fig. 17** (a), for methanol and isopropanol components, increasing the feed stage number from 2 to 12 has no significant effect on the concentrations of the products and then reduces the concentrations. For butanol, changing the feed stage number does not affect the concentration of this component in the bottom product.

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following item. Arora (2014) evaluated the effect of feed stage number on the purity of products in a DWC system. According to their results, at the top of the column feed stage, it had no significant effect on product purities. **Fig. 17** (b) illustrates the effect of feed stage number in Absorber1 on the reboiler and the condenser heat duties. It can be observed, increasing the feed stage number results in reducing the heat duties of the reboiler and the condenser. The trends are initially slow and gradually followed by a steeper slope.



(c)

Fig. 16 The effect of the liquid split ratio on the output parameters (a) the mole fractions of the components in DWC products (b) the heat duties of the reboiler and the condenser of the system (c) sum of heat duties of the reboiler and the condenser of the DWC system (NS(Abs1):16, NF(Abs1):8, NS(Abs2):16, NSide(Abs2):11, NS(Rect):20, NS(Strip):7, RR:2, VAPSPL: 0.35)



(c)

Fig. 17 The effect of feed stage number in the Absorber1 column on the output parameters (a) the mole fractions of the components in the DWC system products (b) the reboiler and the condenser heat duties (c) sum of heat duties of the reboiler and the condenser of DWC (NS(Abs1):16, NS(Abs2):16, NSide(Abs2):11, NS(Rect):20, NS(Strip):7, RR:2, LIPSPL:0.65, VAPSPL: 0.35)

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following item. Yuqi et al. (2015) evaluated the effect of feed stage number on reboiler heat duty in a DWC. The reboiler heat duty increased with decreasing feed stage number.

The effect of feed stage number in Absorber1 on the sum of heat duties of the reboiler and the condenser of the DWC has been depicted in **Fig. 17** (c).

It can be observed that by increasing the feed stage number, the sum of heat duties of the reboiler and the condenser decreases. The profile trends are first slow and then faster.

According to the sensitivity analysis of this section, to reduce the reboilers and condensers' heat duties with considering desired purities of the products, the value of 8 is opted for the feed stage number of Absorber1 in the DWCD process.

3.2.1.9. The effect of side product stage number of Absorber-2

The effect of the side product stage number of Absorber-2 on the output parameters has been illustrated in **Fig. 18** (a) to **Fig. 18** (c). (The data are indicated in details in Table A-15 in the supplementary data section). The other parameters have been considered constant (number of stages of Absorber-1: 16, number of feed stage in Absorber-1: 8, number of stages of Absorber-2: 16, number of stages of Rectifier: 20, number of stages of Stripper: 7, reflux ratio of the column: 2, liquid split ratio: 0.65, vapor split ratio: 0.35).

The effect of side product stage number in Absorber2 on mole fractions of the components of products has been shown in **Fig. 18** (a). According to this figure, by increasing the stage number of the side product, the mole fractions of methanol and isopropanol components first increase and then remain constant. The effect of this parameter on the mole fraction of butanol is negligible. **Fig. 18** (b) depicts the effect of side product stage number in Absorber2 on the heat duties of the reboiler and the condenser of DWC. It can be observed by increasing the side product stage number; the reboiler and the condenser heat duties first increase and then remain constant. The influence of side product stage number in Absorber2 on the sum of heat duties of the reboiler and the condenser of DWC has been illustrated in **Fig. 18** (c). As can be observed, the sum of heat duties of the reboiler and the condenser is first increased and then remains constant by increasing the number of side product stage.

According to the sensitivity analysis of this section, to reduce the reboiler and condenser heat duties with considering desired purities of the products, the value of 11 is opted for the side product stage number of Absorber2 in the DWCD.

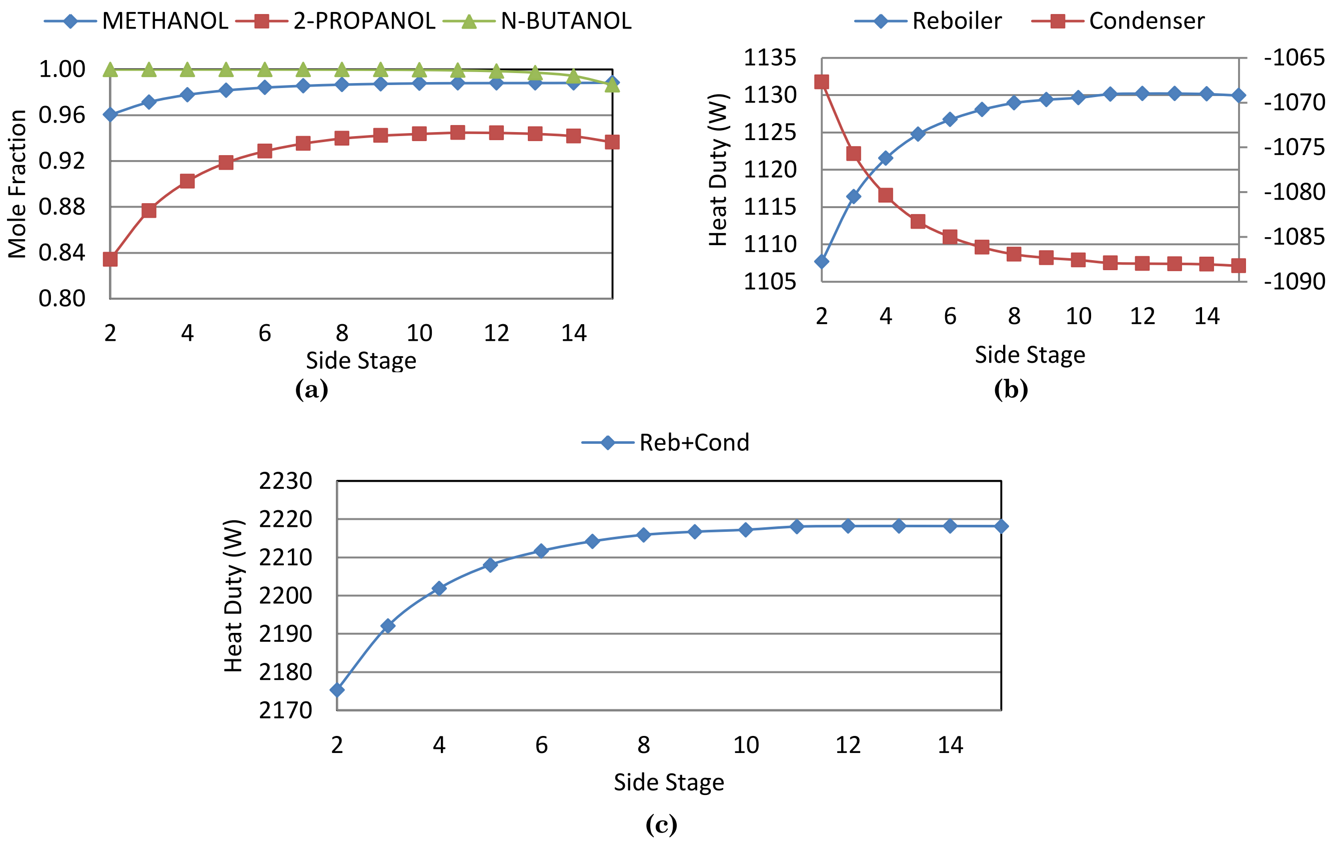


Fig. 18 The effect of side product stage number in Absorber2 on the output parameters (a) mole fractions of the components of products (b) heat duties of the reboiler and the condenser of DWC (c) sum of heat duties of the reboiler and the condenser of DWC
(NS(Abs1):16, NF(Abs1):8, NS(Abs2):16, NS(Rect):20, NS(Strip):7, RR:2, LIPSPL:0.65, VAPSPL: 0.35)

3.2.2. The optimum conditions of DWC

The profiles of DWC at optimum conditions have been shown in **Fig. 19** (a) to **Fig. 19** (g). The optimum parameters include number of stages of Absorber-1 (NS(Abs1)): 16, number of feed stage in Absorber-1 (NF(Abs1)): 8, number of stages of Absorber-2 (NS(Abs2)): 16, number of side product stage in Absorber-2 (NS(Side)): 11, number of stages of Rectifier (NS(Rect)): 20, number of stages of Stripper (NS(Strip)): 7, reflux ratio of the column (RR): 2, liquid split ratio (LIPSPL): 0.65, vapor split ratio (VAPSPL): 0.35.

Temperature profiles of four sections of the DWC, including Absorber-1, Absorber-2, Rectifier, and Stripper, at optimum conditions, have been illustrated in **Fig. 19** (a). According to the results of **Fig. 19** (a), the temperature increases with increasing stage number. An insignificant difference can be observed in the temperature profiles of the two parallel sections of the column, composing Absorber-1 and Absorber-2. It can be mentioned that the temperature profile is S-shaped. The upper part of the diagram is for the Stripper column, which is associated with the separation of isopropanol and butanol, and the lower part is for the Rectifier column, which is related to the separation of methanol and isopropanol and has a lower temperature. The top temperature of the column is 64.65 ^{0}C, which is similar to the boiling point of methanol (64.7 ^{0}C). The bottom temperature of the column is 119.6 ^{0}C, which is close to the boiling point of butanol (118.75 ^{0}C) as the bottom product of the column. The temperature at stage 31 of DWC (stage 11 of Absorber-2) corresponds to the isopropanol side product stage and equals 81.47 ^{0}C, which is similar to the isopropanol boiling point (82.15 ^{0}C). It can be observed with a detailed look at the figure that there are two intersections in the temperature profiles of the two columns of Absorber-1 and Absorber-2. The first is the feed stage of the Absorber1 column (step 8 of the Absorber1 column and step 28 of the entire DWC), and the second is the side product stage number of the Absorber-2 column (step 11 of the Absorber-2 column and step 31 of the whole DWC). The other significant note is that the maximum temperature difference between the two columns of Absorber-1 and Absorber-2 corresponds to stage 10 of the two columns (stage 30 of the whole DWC). At this stage, the temperature of Absorber-1 is 76.99 ^{0}C, and the temperature of Absorber-2 is 79.61 ^{0}C, and the difference is 2.62 ˚C. So, the effect of heat transfer across the dividing wall is negligible, as it is neglected in the simulation.

In order to compare the results of this section with the findings of the other researchers, it can be mentioned to the following items. Niggemann and Fieg (2011) investigated DWCD for separation of hexanol, octanol and decanol. They studied the temperature profiles for the DWCD. The trend of their profile confirmed our results. Kiss and Ignat (2012) investigated a DWCD for separation a ternary mixture including methanol-water-glycerol. They reported temperature and composition profiles in DWCD. The temperature difference between the two sides of the wall was very low. Landaeta et al. (2012) evaluated the temperature profile in a four-component mixture of aromatics using two DWC columns with different arrangements. The trend of temperature change with stage number in their work also followed the S-shape diagram. Kenig (2014) reported the temperature and mole fraction of components versus stage number for separation $C_6/C_7/C_8$ mixture in a DWCD. The temperature difference between two sides of the wall was very low.

Nguyen (2015) evaluated the effect of the concentration of components in the feed on the temperature difference on both sides of the wall in a DWC system. They concluded that the feed composition had a significant effect on DWC operation. According to their results, the two sides of the wall had a lower temperature difference when the concentration of the intermediate component was equal to or greater than the other components of the feed. When the intermediate component concentration in the feed was lower than the other components, the temperature difference was higher. Illner and Othman (2015) investigated simulation of a DWC for fractionation of fatty acid in oleochemical industries. They investigated the temperature profile of the DWCD. Their results showed that the temperature difference between the two sides was around 20 ^{0}C. They considered that it was negligible in comparison with the maximum temperature in the column (240 ^{0}C). Aurangzeb and Jana (2016) investigated DWCD for separation of a ternary system. The ternary mixture was included n-hexane/n-heptane/n-octane. They reported the temperature profile of DWCD at steady state. Their profile confirmed our results. The temperature in the right was higher than that in the left. Roach (2017) performed a design model for DWCD. The feed was n-hexanol, n-octanol, n-decanol. They reported the temperature profiles for different cases of feed compositions. The equimolar feed showed a larger temperature difference across the dividing wall section. The temperature of the right part was higher than that of the left part of the wall. Ehlers et al. (2018) simulated a DWCD for separation a ternary feed. They investigated the temperature profile of DWCD. The trend of their profile confirmed our results. Wu (2020) investigated separation of 1,2-propylene glycol, 1,3-butanediol and 1,4-butanediol in DWCD. They reported the temperature and composition profiles in DWCD. There was difference between temperatures of right and left of the dividing wall. The temperature of right of the wall was higher than that of left of the wall.

Fig. 19 (b) depicts the mole fractions profiles of methanol concentration in the liquid phase at various stages of the four sections of the DWC column under the optimum conditions. It can be observed that with increasing stage number, the methanol concentration decrease as the lightest component in the four sections of DWC. The comparison between the mole concentration of methanol in the liquid phase in two parallel columns containing Absorber-1 and Absorber-2 shows that the concentration of methanol in Absorber-1 is higher than that in Absorber-2. Methanol leaves the top of the column at a mole fraction of 0.988%, and its concentration is approximately zero at the bottom of the column.

The mole fractions profiles of isopropanol concentration in the liquid phase at various stages of the four sections of the DWC column under the optimum conditions have been illustrated in **Fig. 19** (c). According to the results of **Fig. 19** (c), with increasing stage number, the concentration of isopropanol in the liquid phase first increases and then decreases. The comparison between isopropanol mole fraction in the liquid phase in two parallel sections of the DWC, including Absorber-1 and Absorber-2, represents that the isopropanol concentration is more in the Absorber-2 column. Isopropanol mole fraction at the top of the column is 0.012 and at the bottom of the column is 0.001; its maximum is in stage 33 and equals 0.977%. The mole fraction profiles trend throughout the DWC is consistent with the results of the other researchers (Landaeta et al. 2012).

The Rectifier column, the upper part of the column, concerns the separation of methanol and isopropanol, and the lower part, Stripper, is related to the separation of isopropanol and butanol. In the middle part, the concentration of isopropanol reaches a maximum value that is obtained side product.

Fig. 19 (d) shows the profiles of butanol mole fraction in the liquid phase at various stages of the four sections of the DWC column under the optimum conditions. It can be observed that butanol concentration in the liquid phase in the Rectifier column is approximately zero, with increasing the number of stages. The concentration then increases towards the bottom of the Stripper column, reaching its maximum value and, then leaves as the bottom product. The comparison between the butanol mole fractions in the liquid phase in two parallel columns, containing Absorber-1 and Absorber-2 shows that butanol concentration in the Absorber-1 is more significant. The graph is S-shaped. The butanol mole fraction at the top of the column is approximately zero and is 0.999 at the bottom of the column, from which the butanol product leaves. This result is consistent with the findings of the other researchers (Landaeta et al. 2012).

The profiles of three components, including methanol, isopropanol, and butanol in the vapor phase at various stages of the four sections of DWCD under the optimum conditions, have been depicted in **Fig. 19** (e) through **Fig. 19** (g).

According to the results of **Fig. 19** (e) through **Fig. 19** (g), the mole fraction trend of the components in the vapor and liquid phases are similar. Evaluation of the diagrams in the vapor and liquid phases represents that there is a breakpoint at the feed stage of the Absorber-1 column (stage 8 of the Absorber-1 and stage 28 of the entire DWCD process column).

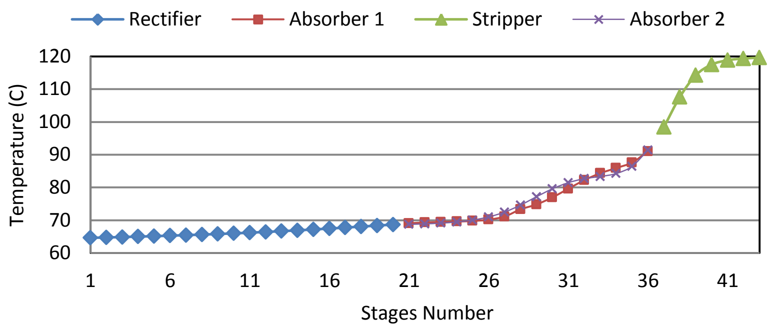
3.2.3. The results of optimization of DWCD process

The products specifications of the DWCD process after optimization have been presented in **Table 11**.

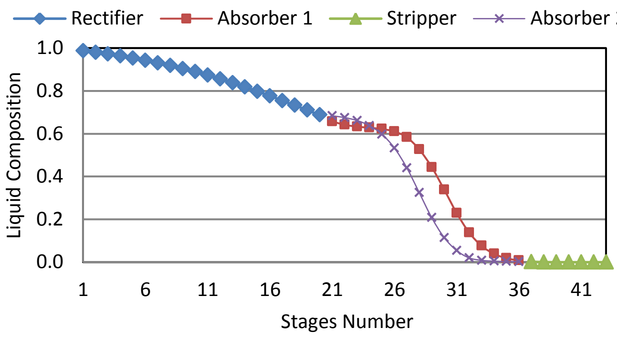
The reboiler and the condenser heat duties in the results of DWCD process simulation after optimization have been shown in **Table 12**.

3.3. The comparison between the results of DWCD and the conventional processes

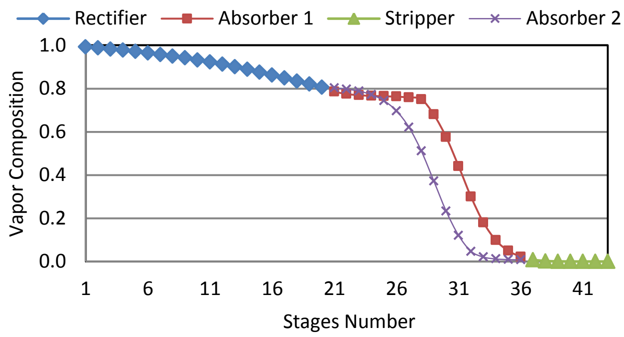
The comparison between the heat duties of the condensers and the reboilers of DWCD and the conventional processes has been presented in **Table 13**.



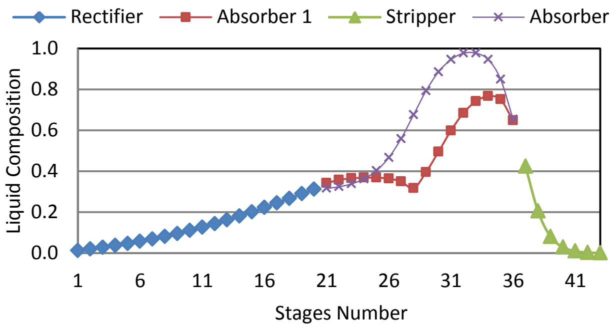
(a) Temperature profile of four sections of DWC



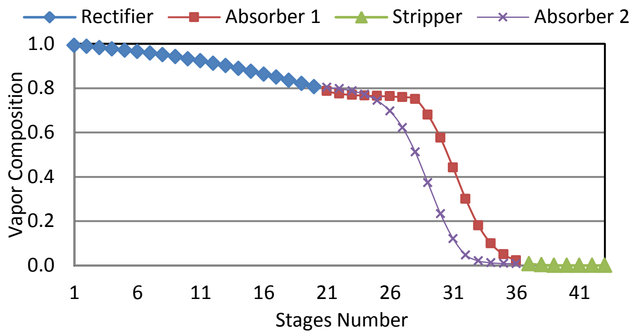
(b) The mole fractions profile of methanol in the liquid phase



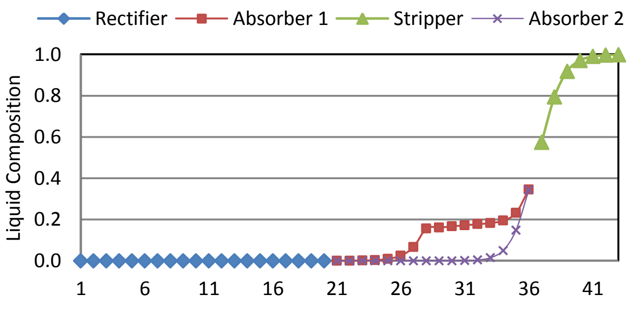
(e) The mole fractions profile of methanol in the vapor phase



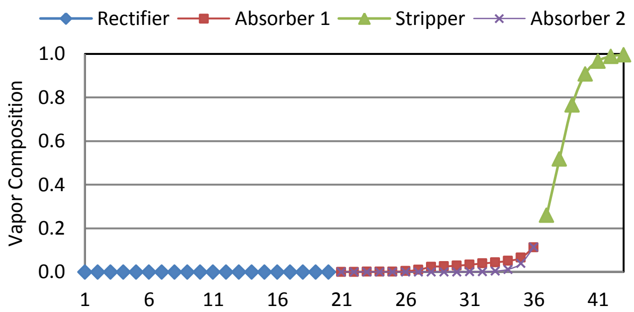
(c) The mole fractions profile of isopropanol in the liquid phase



(f) The mole fractions profile of isopropanol in the vapor phase



(d) The mole fractions profile of butanol in the liquid phase



(g) The mole fractions profile of butanol in the vapor phase

Fig. 19 profiles of DWC at the optimum conditions
(NS(Abs1):16, NF(Abs1):8, NS(Abs2):16, NS(Side):11, NS(Rect):20, NS(Strip):7, RR:2, LIPSPL:0.65, VAPSPL: 0.35)

Table 11 The products specifications in the DWCD process (after optimization)

	BOTTOM	DIST	SIDE	FEED
Mole Frac				
METHA-01	1.635E-07	**0.988**	0.055	0.580
ISOPR-01	0.001	0.012	**0.945**	0.232
N-BUT-01	**0.999**	9.125E-20	0.001	0.188
Mole Flow (kmol/hr)	0.012	0.037	0.015	0.065
Mass Frac				
METHA-01	7.07E-08	**0.978**	0.030	0.4
ISOPR-01	0.001	0.022	**0.969**	0.3
N-BUT-01	**0.999**	2.089E-19	0.001	0.3
Mass Flow (kg/hr)	0.9	1.200	0.9	3

Table 12 The reboiler and the condenser heat duties in DWCD process simulation (after optimization)

Heat Duty (W)	Absorber1	Absorber2	Rectifier	Stripper
Reboiler	_	_	_	1130.1465
Condenser	_	_	-1087.931	_

Table 13 The comparison between the condensers and the reboilers heat duties in DWCD and the conventional processes

Number	Column-1		Column-2		Sum		DWC Energy Saving (%)		
	Reboiler	Condenser	Reboiler	Condenser	Reboiler	Condenser	Reboiler	Condenser	Reb+Cond
1	1120.939	1088.929	290.84	-281.99	1411.78	-1370.93	19.95	20.64	40.59
2	1130.14	-1087.91	-	-	1130.14	-1087.91	-	-	-

The results show that the DWCD process has 19.95% and 20.64% energy saving for the reboiler and the condenser heat duties, respectively, compared to the conventional process composed of two distillation columns. To compare the obtained results in this research with those in the other studies, the following items can be mentioned. Kiss and Ignat (2012) investigated a DWCD for separation a ternary mixture including methanol-water-glycerol and compared the amounts of required energy with a conventional direct sequence. The results showed that the proposed DWCD requires 27% less energy. Landaeta et al. (2012) simulated the separation of aromatics using DWC and Kaibel distillation columns. The results showed that designing based on two DWC systems reduced energy consumption by up to 7%, while combined design, including a conventional stripper and a Kaibel column, reduced energy consumption by up to 17%. Gupta (2013) performed simulation studies of a EWDC (Extractive Divided Wall Distillation Columns) for the separation of water-ethanol mixture. Their results showed that in the optimum conditions, EDWC had a saving 20.6% for reboiler duty in comparison with the conventional extraction distillation. Shojae et al. (2015) performed DWC distillation simulations to separate dimethyl ether from a mixture of water and ethanol. Their results showed that the DWC structure resulted in a duties reduction at about 24% for the condenser and 7% for the reboiler. They used a three-column model to simulate the DWCD process. Aurangzeb and Jana (2016) investigated DWCD for separation of a ternary system. The ternary mixture was included n-hexane/n-heptane/n-octane. They resulted that DWCD could save a 22.6% saving in energy consumption. Gor et al. (2017) simulated the separation of the butane, pentane, and hexane mixture in a DWCD process. The effect of different parameters on the purity of the components and the duties of the reboiler and the condenser was investigated. The results showed that the energy reduction by DWC was 34.74% for the condenser and 31.28% for the reboiler. They used a 4-column model to simulate DWC using Aspen Plus. Kim (2017) investigated a DWCD process simulation for a crude oil distillation unit. The results showed that DWC resulted in reduced remixing in the feed stage and increasing the thermodynamic efficiency of the CDU. The unit performance evaluation showed that the DWC unit had a 37% energy saving in heat duty consumed and 17% in condenser duty compared to conventional distillation. Filho et al. (2018) optimized the performance of a DWCD process for separation aromatic mixtures using RSM. The DWC application resulted in energy savings of up to 44% compared to the conventional 2-column arrangement. The design parameters for the DWC included the number of stages in the upper, lower, and prefractionator sections and the internal vapor and liquid flows to the prefractionator.

In addition, it should be noted that the advantages of using DWCD are not a general result. It depends on the feed specifications, especially the relative volatilities and percentages of the components present in the feed. Khalili-Garakani et al. (2016) carried out a comparison between different configurations, including thermally coupled, thermodynamically equivalent, and DWC for separation of ternary feeds. Based on their results, the occurrence frequency as the best configuration for DWC, thermodynamically equivalent, thermally coupled, and the conventional sequences are 36%, 28%, 25%, and 11%, respectively.

In summary, the investigated parameters in this study can be divided into two categories, including structural and process parameters. The structural parameters include the number of stages of the Absorber-1 column, number of stages of the Absorber2 column, number of Rectifier column stages, and the number of stages of the Stripper column, feed stage number of Absorber-1, and side product stage number of Absorber-2. The process parameters include the reflux ratio of the rectifier column, vapor split ratio, and liquid split ratio. The present study showed the application of DWCD for separating a ternary mixture. The separating of four or more components and azeotropic mixtures with DWCD, extractive dividing wall column (EDWC), and RDWC (reactive dividing wall column) will be the options for future researches.

Conclusions

Distillation accounts for more than 95% of liquid separation in chemical industries. The energy consumption of distillation is estimated at 3% of the world's energy consumption (Rangaiah et al., 2009). The application of complex distillation column arrangements can substantially save energy. DWC process is one of the most attractive methods for separating three or more component mixtures because this method can leads to significant savings in both energy consumption and investment cost. In this study, the effect of operational and structural parameters in dividing wall column distillation energy consumption has been investigated. The feed contains three components of methanol, 2-propanol, and n-butanol. In order to compare the energy consumption of DWC and conventional method, at first, the simulation of two conventional distillation columns is performed, and the optimization of different parameters is conducted by sensitivity analysis to reduce the heat duties of the reboiler and the condenser. The parameters studied can be divided into two categories of structural and process parameters. Structural parameters include the number of stages of the columns, feed stage number, and side product stage. Process parameters include the reflux ratio, the vapor split ratio, and the liquid split ratio. At optimal conditions for the first case, including two distillation columns, first column specifications are the number of stages: 31, feed stage: 17, reflux ratio: 1.95, and second column specifications are steps number: 13, feed stage: 7, reflux ratio: 0.67. To simulate the DWC process, a four-column model consisting of two absorbers, a rectifier and a stripper and two vapor and liquid splitters were used. In optimal conditions, Absorber1 specifications are the number of stages: 16, feed stage number: 8, Absorber2 specifications are the number of stages: 16, side product stage number: 11, Rectifier specifications are the number of stages: 20, reflux ratio: 2, specifications of the Stripper are the number of stages: 6, liquid split ratio: 0.65 and vapor split ratio: 0.35. The results show that the DWC process, in comparison with the conventional system consisting of two distillation columns, has 19.95% energy savings for reboiler heat duty and 20.64% energy saving for condenser heat duty.

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Nomenclatures

ABS: absorber
BOT: bottom

Cond: condenser
DIST: distillate
DWCD: dividing wall column distillation
Frac: fraction
FUGK: Fenske-Underwood-Gilliland-Kirkbride
ISOPR: isopropanol
LIPSPL: liquid split ratio
LIQ: liquid
METHA: methanol
N-BUT: n-butanol
NF: feed stage
NRTL: non-random two liquid
NS: total stages number
NSide: side product stage number
NSTAGE: total stages number
R: gas constant
Reb: reboiler
Rect: rectifier
RECTFR: rectifier
RR: reflux ratio
Side: side product
Strip: stripper
STRPR: stripper
T: temperature
U_{ij}: Energy between surfaces i and j
VAP-vapor
VAPSPL: vapor split ratio
x_i: mole fraction of component i

Greek
α_{ij}: non-randomness parameters
γ_i: activity coefficient
Δg_{ij}: interaction energy parameters
τ_{ij} = dimensionless interaction parameter

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