Iranian Journal of Chemical Engineering
Vol. 12, No. 1 (Winter 2015), IAChE

Research note

Modeling and Simulation of a Divided Wall Column for 1,3 Butadiene Purification

R. Rahimi*[*], *M. H. Soodmand, M. Zivdar, A. Alborzi, M. Rahmanian

Chemical Engineering Department, Sistan and Balouchestan University, Zahedan, Iran

Abstract

The distillation process remains as the most common method of separation in chemical process industries. The energy used from this process accounts for an estimated 3% of the world energy consumption. The Dividing-Wall Column (DWC) for separation of multi-component mixtures has recently become a major concern of industries. The design of DWC is based on Thermally Coupled Distillation System (TCDS) eliminating some of the operational equipment. This paper presents the results of simulation of a DWC by using 3-simple sequence column model based on shortcut method by a commercial chemical Engineering software for purification of 1,3 butadiene unit.
From the results, it is shown, by using a DWC instead of two conventional sequential column, the heat duties of both the condenser and the reboiler are reduced about 28.5% and also desirable purity of the key-components for the case of study have been achieved.

Keywords: *Distillation, Dividing Wall Column, Modeling, Simulation, Thermally Coupled*

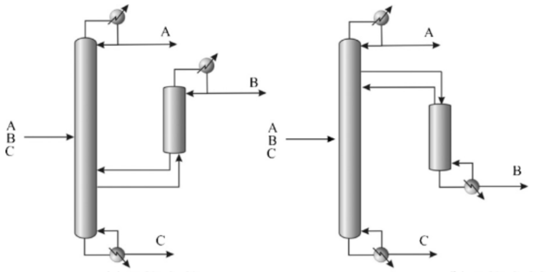
1. Introduction

Distillation is the most popular separation technology in the chemical and petrochemical industry. Distillation units use about 3% of the world's total energy consumption [1]. One of the methods for integrated process is thermal coupling of the distillation column for separation of multi-component mixtures. In this arrangement, one condenser or reboiler is often eliminated from the system. In the thermally coupling portion of the system, heat transfer is provided by direct contact of liquid and vapor flows. The proper sequences of thermally coupled columns for multi-component mixtures are illustrated in Fig. 1.

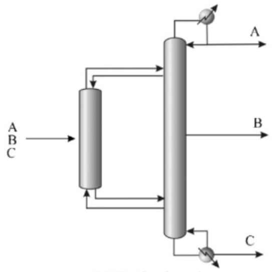
According to Fig. 1-c, there are two counter current streams between prefractionator and main column in Petlyuk tower. For example, a ternary mixture ABC in prefractionator is divided into two binary mixtures, AB in the top and BC in the bottom of the column. The vapor is related to AB's mixtures and liquid BC's mixtures respectively as the top and the bottom feed enter to the main column. On the other hand, at the same stage, liquid AB and vapor BC return to the prefractionator. Therefore,

---

∗ Corresponding author: rahimi@hamoon.usb.ac.ir interlinking of two streams leads to elimination of condenser and reboiler of the prefractionator [2]. Thus, these towers consist of two columns, the first column of which is a prefractionator and the other one is a main column. By housing both a prefractionator and a main column in a single shell and implantation of a dividing wall, it has been introduced as DWC. (Fig. 2)



(a) TCDS-SR (b) TCDS-SS



(c) Petlyuk column

Figure 1. Thermally coupled distillation options for ternary separations: (a) direct thermally coupled distillation sequence (TCDS-SR), (b) indirect thermally coupled distillation sequence (TCDS-SS), and (c) Petlyuk distillation column [3].

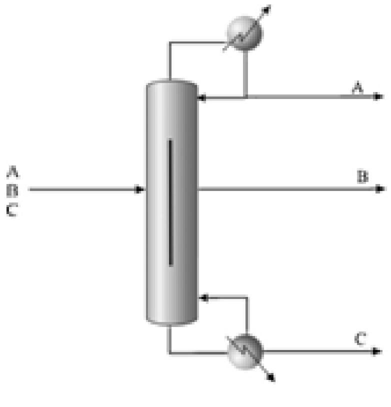


Figure 2. Dividing wall distillation column [3].

The idea of the DWC was introduced by Wright in 1949 [1]. The controlling and operating difficulties as well as the lack of design procedures caused the first industrial application to be installed only by BASF after about 36 years from the introduction of DWC.

The improvement of the efficiency in the DWC is mostly due to the least mixing in the feed stage and remixing of the middle component in a prefractionator [4]. A dividing or divided wall distillation column can reduce energy consumption 30-50% more than conventional distillation sequence. Therefore resulting in savings of about 25% in capital and 35% in operating costs for some mixtures [3,5].

Nowadays, over 100 DWCs have been installed all over the world [6]. According to Schultz [7] the dividing wall column will be converted into standard distillation equipment in the next 50 years.

In this work, feasibility study of a DWC for 1,3 butadiene purification process is presented. The results have been compared in terms of energy requirements and concentrations of key components.

2. Modeling and simulation

There is no designed model for DWC as a standard model in commercial software packages such as ASPEN Plus, so it cannot be designed directly. Since the configuration of a DWC can be imagined as a unit consisting of various simple columns, we have to divide it into simple columns to be able to simulate and survey a DWC.

Presently, there are several ways to simulate a dividing- wall column, each of which has its advantages and disadvantages.

2-1. Pump- around model

As shown in Fig. 3, in this model, a DWC is shown as a single column in which various sections of DWC are placed vertically one above the other. The liquid pumps and vapor bypass cause similarity of vapor and liquid traffic to a DWC [8].

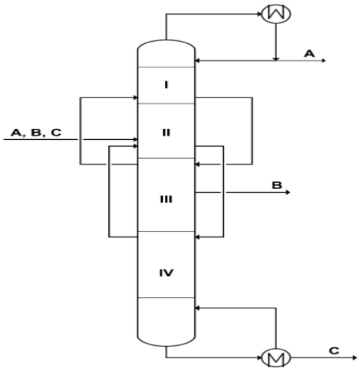


Figure 3. Pump-around model [9].

2-2. Two column sequence model

Two column arrangements model is more flexible than pump- around model and also thermodynamically is equivalent to DWC.

To simulate Petlyuk column in this method (Fig. 4) the column should be divided to three sections. Section one is a prefractionator and sections two and three are main separation column. It is known as 3-simple columns sequence [10].

2-3. Four column sequence model

Although it is difficult in this model to initialize all interconnecting streams and it also has slow convergence, this configuration allows more flexibility in the simulation than other configurations available in the software. Therefore, it is the best model for dynamic simulations and the most suitable to survey vapor and liquid split [12] (Fig. 5).

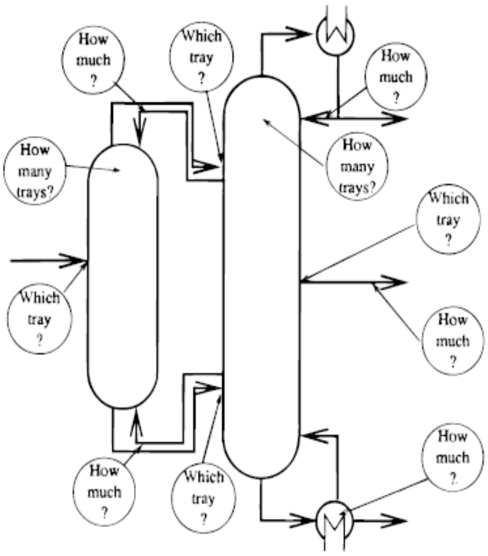


Figure 4. Design specifications for Petlyuk column [11].

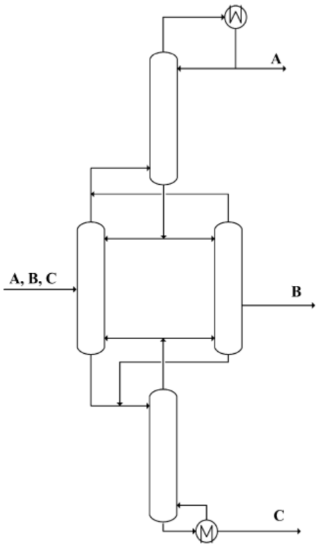


Figure 5. Four-column model [9].

In this paper, shortcut method has been used to obtain approximate required parameters for 3-simple column sequence model.

The shortcut method is based on Fenske–Underwood–Gilliland equations, where Fenske equation denote minimum equilibrium stages and Underwood and Gilliland equations have been used to estimate minimum reflux ratio and actual stage in finite reflux ratio respectively [13].

The following restriction must be employed for the 3-column to convert it into a dividing wall column.

$$\overline{V}_2 = V_3 \qquad (1)$$

This means that the vapor flow in the stripping section of column II is equal to the vapor flow in the rectifying section of column III.

3. Case study

First, the conventional column distillation sequence of 1,3 butadiene purification plant as the case study was simulated in order to compare the results with DWC in key components and energy consumption. Table 1 provides required data for simulating of C2C and it is illustrated in Fig. 6.

The initial design of the 3-simple column model made use of shortcut distillation design in process simulator software.

In this case of study, there are 3-key components, the light key component is methyl acetylene, the middle component is 1,3 butadiene and the heavy key component is 1,2 butadiene. In the first column from 3-simple column model, using shortcut method two selected key components are methyl acetylene as light key and 1,2 butadiene as heavy key components.

Table 1

General data for the conventional distillation system.

Parameters and operating condition		**Column C1**	**Column C2**
Feed flow rate (kg/h)		6553.88	6528.5
Feed composition (mass flow)	1,3 Butadiene	6485	6474.16
	1,2 Butadiene	13.1	13.1
	Methyl Acetylene	7.8	0
	Cis-2-Butene	28.1	28.1
	Trans-2-Butene	1.3	1.3
	C5+	9.1	9.1
	Water	6.88	0.14
	i-butene	2.6	2.6
Number of trays		60	68

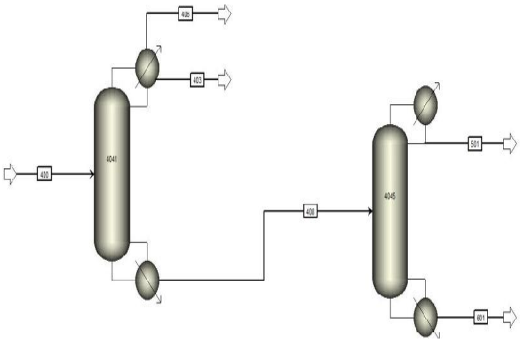


Figure 6. Conventional column distillation sequence.

In the column II, the light key component is still methyl acetylene and heavy key is 1,3 butadiene and finally in column III, 1,3 butadiene is light key and 1,2 butadiene is heavy key component.

The shortcut method results were shown in Table 2 to obtain an estimation of rigorous simulation of 3-simple column.

Further, the initial design was adjusted by Rigorous simulation. The Rigorous simulation has been done by appropriate model in the software simulator. In this simulation, the required parameters such as number of tray in each section of DWC, feed tray, side and the position of interlinking vapor and liquid stream are obtained as shown in Fig. 7.

Table 2

Results from Shortcut distillation design.

	Prefractionator	**Column II**	**Column III**
Light key component recovery	methyl acetylene (0.99)	methyl acetylene (0.98)	1,3 butadiene (0.995)
Heavy key component recovery	1,2 butadiene (0.001)	1,3 butadiene (0.019)	1,2 butadiene (0.01)
Minimum reflux ratio	2.079	13.36	1.94
Minimum stages	11.05	11.34	23.60
Number of trays	29.17	17.57	37.76
Feed tray position	13.36	9.13	18.58

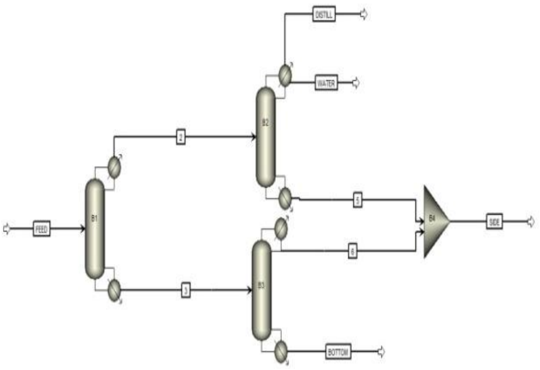


Figure 7. Rigorous simulation of 3-simple column.

It is important to know that these available parameters cannot satisfy the merging column II and III to one main column, so the necessary restriction (1) should be employed.

In order to facilitate the column structure, the number of stages on either side of the wall must be equal.

$$N_1 = N_{a,2} + N_{r,2} \tag{2}$$

Table 3 represents the results of rigorous simulation of 3-simple column in order to achieve variable required parameters of Petlyuk column such as number of trays and stage location for interlinking streams.

Table 3

General data for the DWC design.

Parameters and operating condition		**Value**
Feed flow rate (kg/h)		6554.21
Feed composition (mass flow)	1,3 Butadiene	6485
	1,2 Butadiene	13.1
	Methyl Acetylene	7.8
	Cis-2-Butene	28.1
	Trans-2-Butene	1.3
	C5+	9.1
	Water	6.88
	i-butene	2.6
Number of trays in prefractionator		27
Number of trays in column II		18
Number of trays in column III		40
Feed tray position		14
Side tray position		19
Upper interlinking stage		10
Lower interlinking stage		37

Fig. 8 shows the Petlyuk column was simulated by appropriate model in the simulator in order to achieve purity specification and minimum energy consumption.

4. Result and discussion

The main goal of this paper is to present a feasibility study of the use of thermally coupled distillation column such as DWC in 1,3 butadiene purification. The case study of purification of 1,3 butadiene in a conventional system and in a DWC were analyzed and compared in terms of desirable key-components purity and energy requirement. Table 4 shows the results obtained.

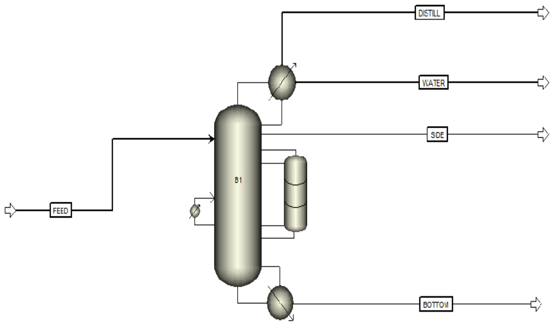


Figure 8. Petlyuk column

Table 4
Purity comparison of key–components.

Desirable component purity (Mole Fraction)	Conventional distillation sequence	DWC
Methyl acetylene	0.48	0.44
1,3 butadiene	0.997	0.997
1,2 butadiene	0.22	0.20

Table 5 shows the results of condenser and reboiler heat duties. From Table 5, DWC can lead to about 28.5% energy saving in reboiler and condenser. Moreover, DWC needs only one condenser and one reboiler comparable to the conventional distillation sequence.

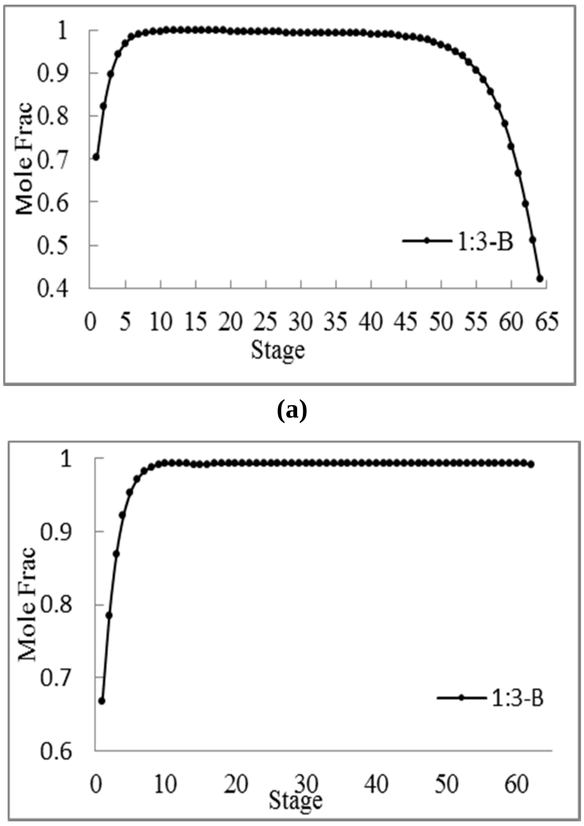
Composition profile of the key components for the Petlyuk column and direct sequence are shown in Fig. 9 and Fig. 10.

Fig. 9-a shows the composition profile in the main column of the Petlyuk tower. It shows that the side product is taken out of the location of the maximum concentration of the middle components belonging to stages between the upper and the lower interlinking stages.

Table 5
Energy consumption comparison.

	Heat duty condenser (KW)	Heat duty reboiler (KW)
Conventional distillation sequence	3003	2976
DWC	2145	2126
Energy saving%	28.57	28.56

Fig. 9-b shows the composition profile in the first column of the direct sequence. Concentration of the middle component 1-3 butadiene in the middle region of the column reaches the maximum value.

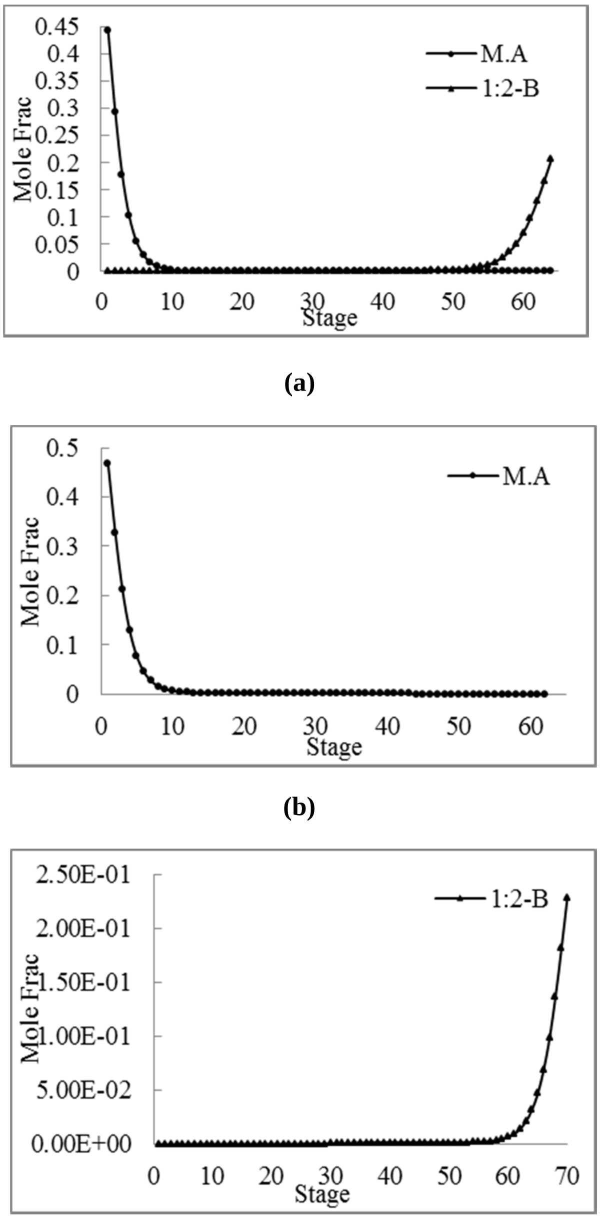


(a)

(b)

Figure 9. Composition profile of 1,3 butadiene for (a) the main Petlyuk column and (b) the first column of the direct sequence.

Fig. 10-a shows the composition profiles of methyl acetylene and 1,2 butadiene in the main column demonstrating methyl acetylene as the light key component with high volatility ratio moves the top of the column and low concentration of methyl acetylene remains in the middle and bottom of the column. Also 1,2 butadiene, because of low volatility ratio moves down and makes the top product free of 1,2 butadiene. Fig. 10-b and 10-c show that of profile of methyl acetylene of the first column and composition profile of 1,2 butadiene of the second column conventional 2 columns, respectively. They have the same behavior with composition profile of Fig. 10-a.



(a)

(b)

(c)

Figure 10. Composition profile of (a). Methyl Acetylene and 1,2 Butadiene for the main Petlyuk column (b). Methyl Acetylene for the first column of the direct sequence (c). 1,2 Butadiene for the second column of the direct sequence.

5. Conclusions

In this paper, the DWC column has been simulated using shortcut design method as a basis. The simulation results indicate savings of about 28.5% in condenser and reboiler heat duties comparable to conventional two column in direct sequence. The desirable purity of products for the case of studies was achieved using DWC column.

Acknowledgment

The authors would like to thank the R&D department and also Operation and Process department of 1,3 Butadiene plant of Amir Kabir Petrochemical Company, www.akpc.ir.

Nomenclature

V_i	Vapor flow rate in the rectifying section of column i , (kmol/h)
$\overline{V}_i$	Vapor flow rate in the stripping section of column i , (kmol/h)
N_i	Total number of trays for column i
$N_{s,i}$	Number of stages in the stripping section of column i
$N_{r,i}$	Number of stages in the rectifying section of column i

References

[1] Laszlo, S., Miklos B. and Sandor Nemeth., “Analysing Divided Wall Column”, *Clean Techn. Environ. Policy.*, **13**, 633, (2011).

[2] Yildirim, O., “Dividing wall columns in chemical process industry: A review on current activities”, *Sep. Purif. Tech.*, **80** (3), 403 (2011).

[3] Fabricio, O., Barroso-Munoza., S., Hernandez., H., Hernandez-Escotoa., J., Segovia-Hernandez.,G., Rico-Ramirez.,V. and Chavezc., R. H. “Experimental Study on Pressure Drop in a Dividing Wall Distillation Column”, *Chem. Eng. Process.*, **49** (2), 177 (2010).

[4] Young Han Kim., “Structural design and operation of a fully thermally coupled distillation column”, *Chem. Eng.*, **85**, 289 (2002).

[5] Premkumar, R. and Rangaiah, G. P., “Retrofitting conventional column systems to Dividing-Wall Columns”, *Chem. Eng. Res. Des.*, **87** (1), 47 (2009).

[6] Harmsen, J., “Process intensification in the petrochemicals industry: Drivers and hurdles for commercial implementation”, *Chem. Eng. Process.*, **49** (1), 70 (2010).

[7] Schultz, M. A., Stewart, D. G., Harris, J. M., Rosenblum, S. P. and O'Brien, D. E., “Reduce costs with dividing-wall columns”, *Chem. Eng. Prog.*, **98** (5), 64 (2002).

[8] Becker, H., Godorr, S., Kreis, H. and Vaughan, J., “Partitioned distillation columns-why, when & how”, *Chem. Eng.*, **108** (1), 68 (2001).

[9] Dejanovic, Lj., Matijasevic, Z. Olujic., “Review Dividing Wall Column-A breakthrough towards sustainable distilling”, *Chem. Eng. Process.*, **49** (6) 559, (2010).

[10] Ramírez-Coronaa, N. B., Jimenez-Gutierreza., A., Castro-Agueroc., A. and Rico-Ramíreza., V., “Optimum design of Petlyuk and divided-wall distillation systems using a shortcut model”, *Chem. Eng. Res. Des.*, **88**, 1405 (2010).

[11] Dunnebier., G. and Pantelides., C. C. “Optimal Design of Thermally Coupled Distillation Columns”, *Ind. Eng. Chem. Res.*, **38** (1), 162 (1999).

[12] Ling, H. and Luyben, W. L., “New control structure for divided-wall columns”, *Ind. Eng. Chem. Res.*, **48**, 6034 (2009).

[13] Seider, W. D., Seader, J. D. and Lewin, D. R., “Product & Process Design Principles: Synthesis, Analysis and Evaluation”, 2nd ed., John Wiley, New York, (2003).