



Process Systems Engineering and Process Safety

A comparative study of different arrangements for methanol distillation process

Davood Hajavi¹, Norollah Kasiri^{2,*}, Javad Ivakpour³¹ Department of Energy, College of Environment and Energy, Tehran Science and Research Branch, Islamic Azad University, Tehran, Iran² CAPE Lab, School of Chemical Engineering, Iran University of Science & Technology, Narmak, Tehran, Iran³ Research Institute of Petroleum Industry, Olympic Sq., Tehran, Iran

ARTICLE INFO

Article history:

Received 22 June 2014

Received in revised form 26 December 2014

Accepted 17 February 2016

Available online 11 June 2016

Keywords:

Methanol distillation

Heat integration

 $V_{\min}$ diagram

Energy saving

Optimization

ABSTRACT

The current study presents an effective method of determining and optimizing distilled methanol alternative arrangements. To complement the information required to run the rigorous simulation, $V_{\min}$ method is used as a base for the selection of the optimum arrangement among different alternatives. Results obtained from $V_{\min}$ diagram and shortcut simulation are utilized, by means of the simulator, for the precise simulation of alternative arrangements of methanol distillation under optimum conditions. Taking into account target function profit and the process parameters and conditions, the most optimum parameter value for reaching maximum profit was obtained, based on which all the arrangements with or without their heat integration were compared to each other. Technical and economic analysis results indicate, that increased profit by Prefractionator with heat integration arrangement is 4.79% compared to the base arrangement, while the three-column, four-column and five-column arrangements have benefits increase by 3.61%, 3.55% and 3.46%, respectively.

© 2016 The Chemical Industry and Engineering Society of China, and Chemical Industry Press. All rights reserved.

1. Introduction

Distillation is widely used as the separation process in the chemical industries accounting for up to 3% of total world energy consumption [1]. Separation processes and their efficiency aimed to obtain a pure product at lowest cost and energy consumption play a significant role in the chemical industries. Demands for decrease in capital costs, energy consumption, operating and maintenance costs lead to continued re-examination of current separation process. Moreover, the emergence of new distillation arrangements with higher energy efficiency which decrease intensity of liquid and vapor flow inside the tower, turns it into more compact distillation units with smaller diameter and consequently reduction of capital costs, has encouraged designers [2]. The first solution for the reduction of energy consumption in methanol distillation process is for the heat integration to be introduced. Therefore, different arrangements with or without heat integration were presented [3]. In methanol production distillation method is used in order to separate the product with the intended purity. In the methanol production process, the first introduced distillation arrangement consisted of two-columns (Fig. 1), which had been utilized to separate the pure product from water and organic materials. But as the energy costs increased, reduction of energy consumption turned into a necessity

forcing designers to focus their attention on replacing the two-column arrangement. So, they presented alternative arrangements for the reduction of energy consumption which are explained in recent studies [4–6]. Three-column double-effect arrangement.

Developed by Lurgi was the only one from among other arrangements that reached industrialization phase (Fig. 2) [7].

Then most of researchers have focused on improving product purity and reducing energy consumption. For example, Chu *et al.* presented a four-column arrangement for the reduction of impurities and increasing methanol purity (Fig. 3) [8]. But, Zhang *et al.* expanded this arrangement, by adding another column, known as the five-column arrangement (Fig. 4), also increasing number of heat integrations between columns, and leading to further reduction in energy consumption in methanol distillation [9]. As the literature shows, all the suggested and expanded arrangements for the improvement of methanol distillation are among direct sequence arrangements.

In order to minimize energy consumption and also achieve maximum benefit, recognition of different distillation arrangements is required. The variety of column arrangements from simple ones such as direct, indirect and distribution sequence arrangements [10] to complex ones like Prefractionator [11] and Petlyuk [12], led the authors to a comparison of a more comprehensive set of sequences using energy consumption as the criterion. In direct-sequence, the lightest component is separated in the first column and the heavier components are removed in the following columns, with the heaviest component being left for the last column for separation [Fig. 5(a)].

* Corresponding author.

E-mail address: capepub@cape.iut.ac.ir (N. Kasiri).

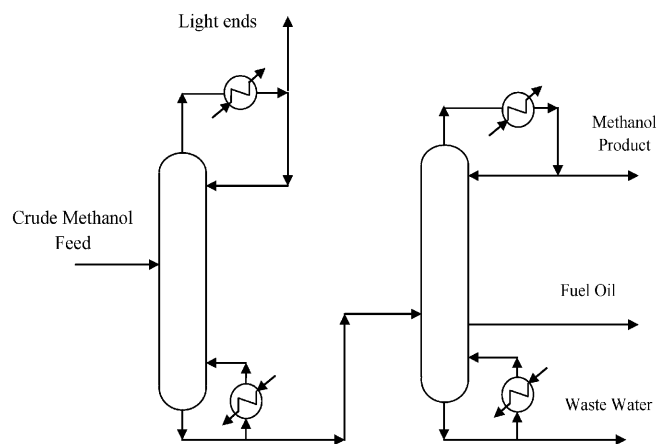


Fig. 1. Schematic diagram of the traditional two-column methanol distillation.

In indirect-sequence, the heaviest component is removed first with the lighter components being removed in the following columns, leaving the separation of the lightest component for the last column [Fig. 5(b)]. In distributed sequences, the separations of the

lightest and heaviest components are carried out in consecutive columns [Fig. 5(c)] [10]. A Prefractionator sequence is an arrangement with partial thermal coupling using a partial condenser in the first column. This arrangement is preferred when the separation between the components is very difficult, or an intermediate component is high in composition [Fig. 6(a)] [11]. In a Petlyuk column, flows of vapor and liquid are exchanged between the two columns. The first column, which is similar to Prefractionator, with no reboiler and condenser, provides the feeds to the second with part of it returning to the initial column [Fig. 6(b)]. DWC is thermodynamically equivalent to the Petlyuk, with the advantage of all being confined to only one column [13]. With the presence of complex arrangements, there is a need to compare these with simple ones. In this paper, different arrangements for methanol distillation with or without heat integration using the $V_{\min}$ diagram and rigorous simulation are compared with each other (Figs. 5–7). This comparison is then used for the selection of the basic arrangement for methanol distillation. The basic arrangement will show the development path of methanol distillation arrangements. The selected basic sequence is the optimal arrangement. Then the optimal arrangement thus obtained is compared with existing already developed arrangements for methanol distillation (Figs. 2–4). In this way, we can choose the development path for distillation arrangements, and analyze whether the

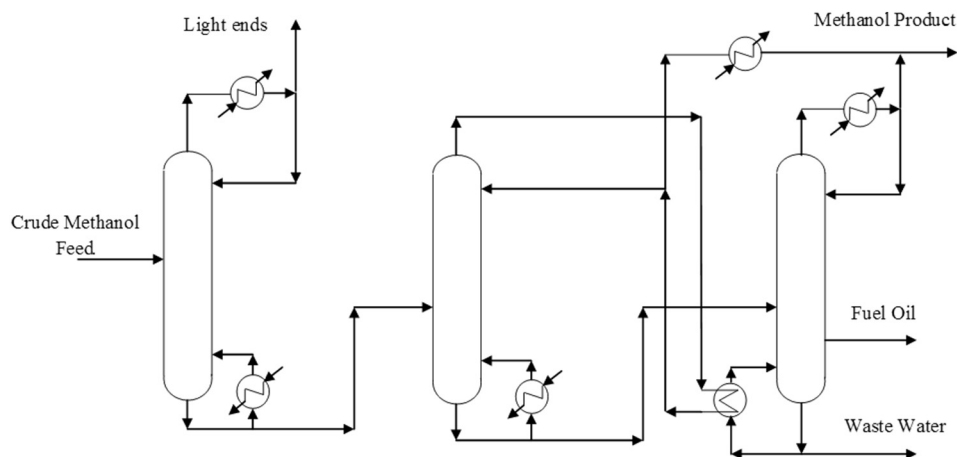


Fig. 2. Schematic diagram of three-column double-effect arrangement.

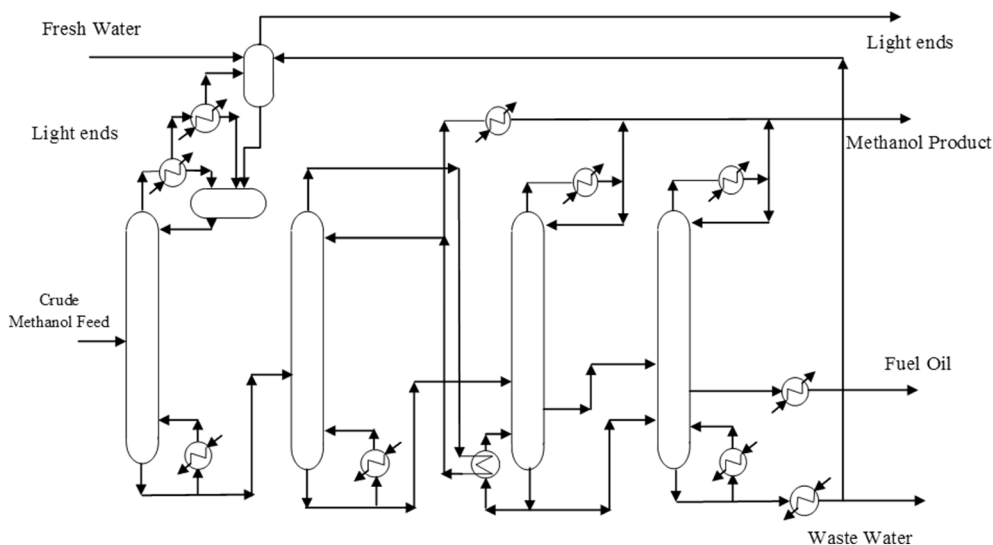


Fig. 3. Schematic diagram of four-column arrangement.

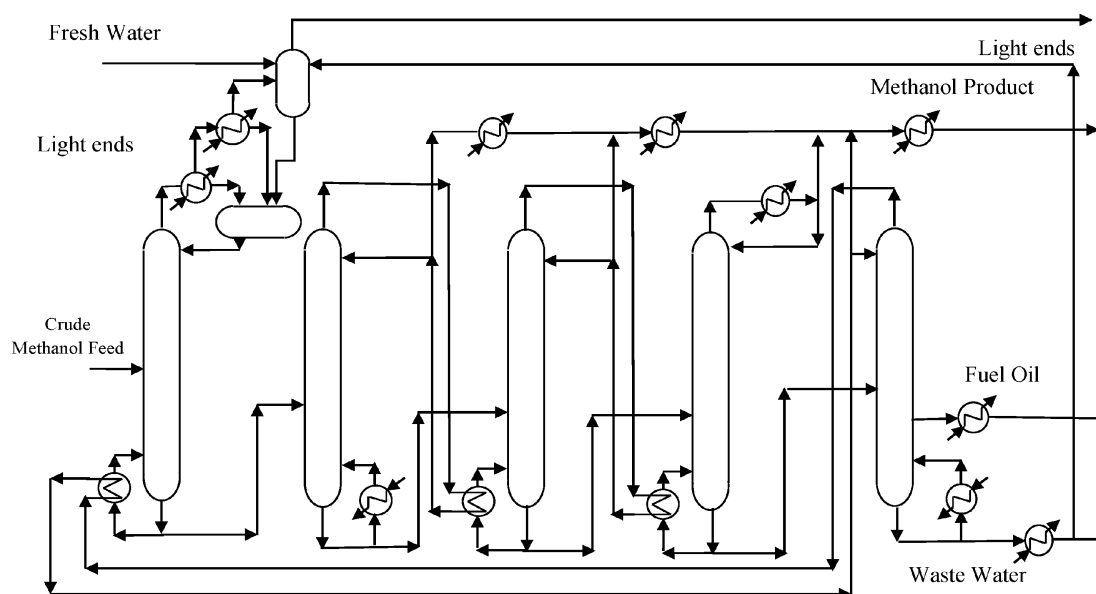


Fig. 4. Schematic diagram of five-column arrangement.

new complex arrangements can replace current arrangements in methanol distillation. It should be noted that today's complex arrangements, such as direct-sequence, which has been developed to 4- and 5-columns, may be further developed and optimized. Each sequence is simulated using a short cut method and $V_{\min}$ method which is then optimized using a cost function as criterion. The optimum conditions of all different sequences were then compared on their financial merits for the selection of the best.

2. Case Study

Here the case study, is the methanol distillation unit. In doing so we are seeking an arrangement which can produce pure methanol by reducing energy consumption and costs. Initially using $V_{\min}$ diagram method, different arrangements are compared in terms of energy consumption, before each is generated in a simulation environment. The most efficient arrangement in terms of energy consumption and economic costs is

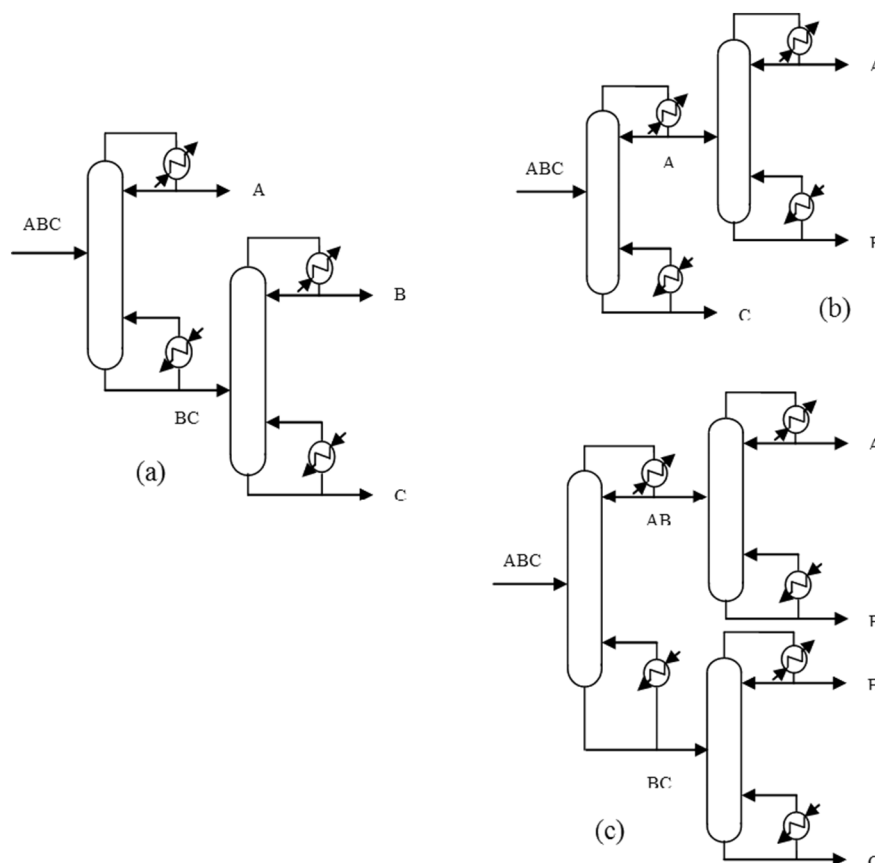


Fig. 5. Simplex arrangements: direct-sequence arrangement (a), indirect-sequence arrangement (b), distributed sequences arrangement (c).

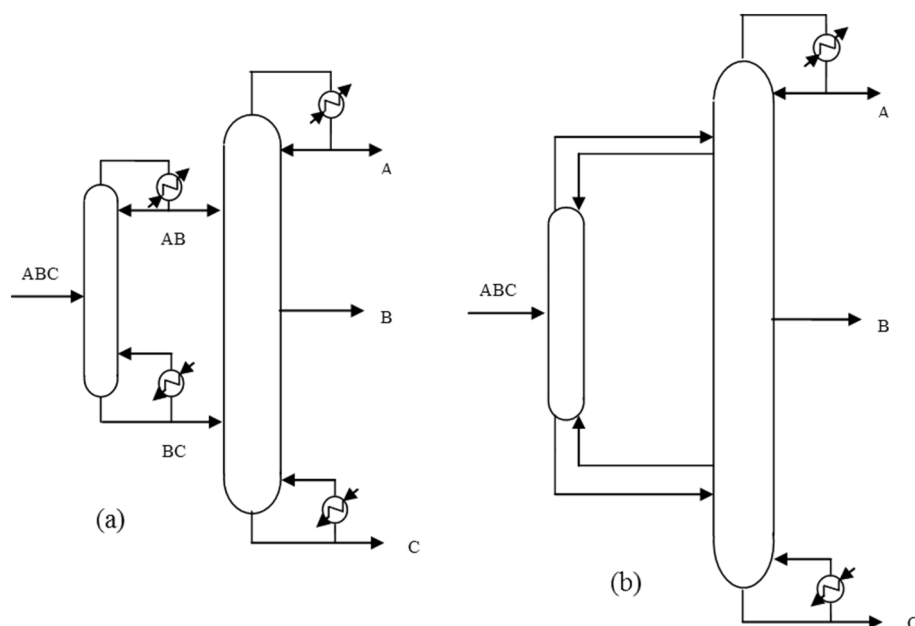


Fig. 6. Complex arrangements: Prefractionator arrangement (a), Petlyuk arrangement (b).

then selected and presented as the best arrangement capable of producing pure methanol. Table 1 presents the specifications of crude methanol.

Here, low boilers entail compounds with a boiling point lower than methanol which are separated as light ends such as: dimethyl ether (DME), methyl formate, and acetone. High boilers are compounds with a boiling point higher than methanol and lower than water such as ethanol, propanol, 1-butanol, butanol, 2-pentanol, and octane. They are also separated as a lateral flow, with a heating value. The aim of methanol distillation is to produce AA degree methanol based on American Standards. The intended methanol needs to have special characteristics in order to reach AA degree. Table 2 presents these characteristics.

3. $V_{\min}$ Diagram

$V_{\min}$ diagram was for the first time presented by Halvorsen [14]. It is devised by means of Underwood equations, and is used for the ideal and non-ideal compounds. Due to recent developments, the method of $V_{\min}$ diagram, may be used as an engineering tool capable of accurate and complete assessment of the potential to minimize the energy required for distillation columns. $V_{\min}$ diagram contains all the information necessary to calculate the minimum energy required, also showing internal flows needed for an optimal operation of various arrangements for a multi-component feed with each of the products [15]. This graph consists of information about intensity of vapor flow and distillation only based on the feed data. Multicomponent separation in this graph is only based on data feedstock, and it can be seen from the graph that the amount of energy required for any separation is only based on vapor flow to feed. The old column data is not required for the design of the new column [16]. This simple graphical method provides a direct insight into the proper separation behavior for different arrangements. It may be changed into an analytical form and implemented within process simulators. In this paper, the results of the $V_{\min}$ diagram based on Underwood and King equations [17] have been used as the initial data required for the more accurate rigorous simulations. Halvorsen and Skogestad present details of the analytical method [18]. As a simplification, the $V_{\min}$ diagrams have been plotted based on only three components namely methanol, (B), as the main component, acetone, (A), as the heaviest component lighter than methanol and ethanol, (C), as the lightest component heavier than methanol. It is noted that this simplification of the components is to select only the basic arrangement among

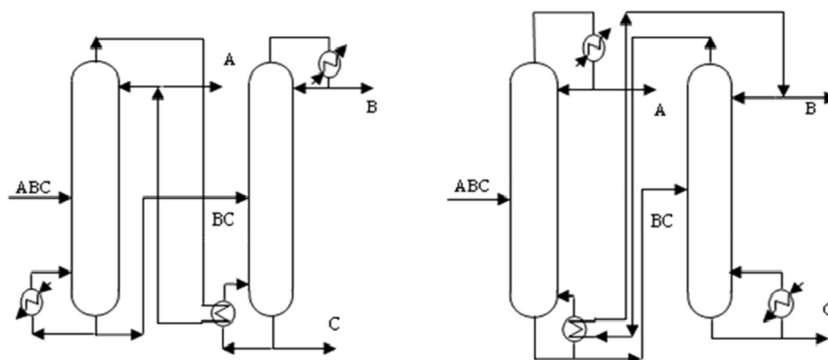
different arrangements, then selected optimal arrangement compared with the current arrangements of methanol distillation. This compares to is that the author to see whether the selected optimal arrangement ability to compete with the current arrangements of methanol distillation? K value and relative volatility of key components to the heavier ones are shown in Table 3. The optimum operating conditions were set at the minimum energy required to produce products with a fixed purity. The $V_{\min}$ values obtained using the Underwood and King equations were then plotted. Method to obtain the $V_{\min}$ diagram and how to use it is similar to work for Engelen and Skogestad in 2004 [17]. Results for $V_{\min}$ diagram are used as a graphical tool for the rapid determination of the multi-effect distillation used in this work. The data needed to plot the $V_{\min}$ diagram are, feed compositions, mole fraction, and the relative volatility of the components. Recovery values for key components, and the vapor and distillate flow rates are obtained from $V_{\min}$ diagram, and the minimum number of trays and feed tray location are obtained from the short-cut method. The number of trays can be considered $4N_{\min}$ in the rigorous simulation as proposed by Halvorsen [14].

$V_{\min}$ diagram can also be used to find the minimum vapor flow of multi-effect arrangements with heat integration (Fig. 7). This is presented by Fig. 8 for the multi-effect arrangements. The mentioned graph here is used for the analysis of a mixture containing acetone, methanol and ethanol.

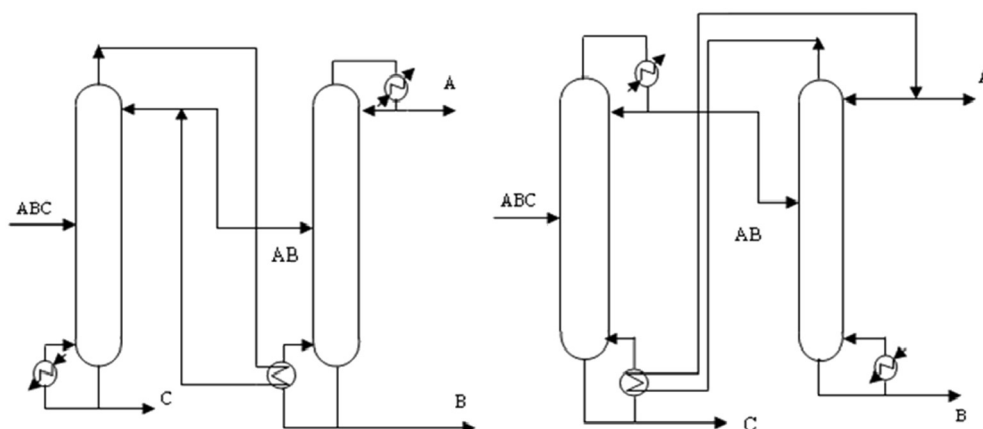
Here, relative volatility is taken into account at two different pressures. As the diagram indicates, the lowest vapor flow rate exists in the Prefractionator arrangement, indicating a less energy consumption for this arrangement. Values obtained can be used as the initial estimate of rigorous simulation under efficient conditions [19]. It should be noted that in this diagram Direct, Indirect, Prefractionator arrangements with heat integration and Petlyuk arrangement are compared to each other, among which the Prefractionator has the minimum vapor flow rate.

Here, it is probable that Prefractionator, due to its lower vapor flow rate, can be selected as the efficient arrangement from among different alternatives (Table 4). The highest energy savings (minimum vapor flow rate) for the Prefractionator with integration occur because there is a high concentration of the middle component (methanol) and as well as small amounts of the light component (acetone) in the feed [15]. There is generally a large difference between the Prefractionator with integration arrangement and the Petlyuk arrangement, which is

Direct split arrangements with heat integration



Indirect split arrangements with heat integration



Prefractionator arrangements with heat integration

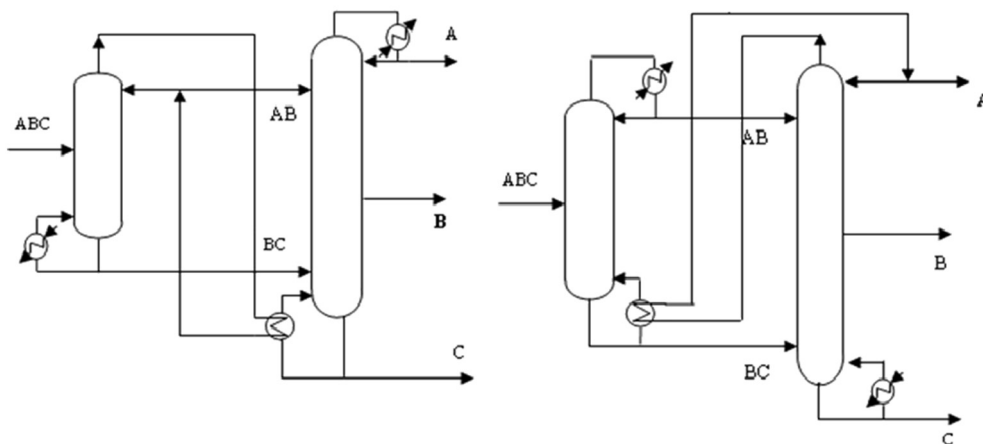


Fig. 7. Multi-effect arrangements with heat integration.

the best non-integrated arrangement. Results obtained from $V_{\min}$ diagram is used for simulating alternative arrangements under optimum conditions to select the most efficient arrangement more precisely by taking energy costs into consideration.

4. Simulation of Different Arrangements Under Steady-state Conditions

$V_{\min}$ diagram is initially used to examine all possible modes of column arrangements, followed by the Short cut model to provide the total number of trays as well as the feed tray location, eventually using the HYSIM Inside-Out method in a simulation environment to

carry out the rigorous simulations. The NRTL model has been used for thermodynamic predictions. A quasi Newton method is then used to optimize the profit function for each simulation.

Hot utility used is saturated steam at 0.5 MPa pressure. Inlet and outlet temperatures of water cooling in condensers are 30 and 40 °C, respectively. According to American Standard AA grade methanol must have 99.8% purification which is the fixed specification used through. The methanol composition in waste water should also not exceed 0.005 wt%.

To optimize arrangements suggested by profit function, the utility, feed and product costs should be determined. Table 5 [20] and Table 6 [21,22] show the utility, feed and product costs, respectively.

Table 1
Crude methanol specifications

Mole composition/%	
CO ₂	0.0073
CO	0.0001
H ₂	0.0002
CH ₄	0.0005
N ₂	0.0001
N ₂ O	0.1849
CH ₃ OH	0.8061
Low boilers	0.0003
High boilers	0.0006
Total	1
Temperature/°C	67
Pressure/Pa	9×10^5
Flow rate/kg h ⁻¹	239405

Table 2
Characteristics of AA degree methanol

Comp	Spec/% (by mole)
Acetone	≤0.003
CH ₃ OH	≥99.8
Ethanol	≤0.005
H ₂ O	≤0.1

Table 3
Values of relative volatility of key components in two different pressures

Tag	Component	K-value	α
9×10^5 Pa			
A	0.0085	0.3648	4.3636
B	0.806	0.1422	1.7009
C	0.1855	0.0836	1
3×10^5 Pa			
A	0.0085	0.9731	4.3636
B	0.806	0.3792	1.7004
C	0.1855	0.223	1

Procedures concerning with evaluation of costs of installation and commissioning of columns and exchangers are provided in Appendix A.

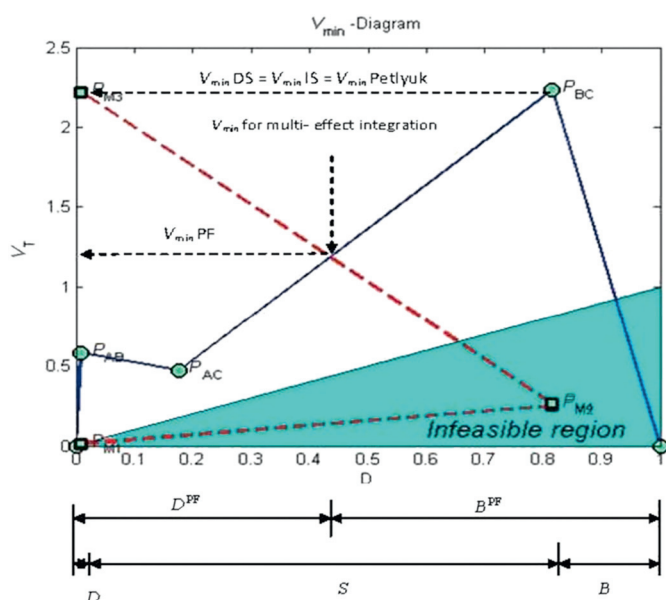


Fig. 8. $V_{\min}$ diagram of multi-effect arrangements with heat integration.

Table 4
Energy required for different arrangements

Distillation arrangement	V/F for first column	V/F for second column	Total
Direct sequence	0.5837	2.2306	2.8143
Indirect sequence	2.2201	0.5934	2.8135
Prefractionator	0.4738	2.2306	2.7044
Petlyuk or Kaibel	–	–	2.2306
Direct sequence with integration	–	–	2.2306
Indirect sequence with integration	–	–	2.2216
Prefractionator with integration	–	–	1.1859

Table 5
Price of utility units

Utility	Temperature/°C	Price/USD·t ⁻¹
LP steam	160	17
Cooling water	30	0.0202

Table 6
Price of feed materials and products

Material	Price/USD·t ⁻¹
Methanol product	4700
Distillation cost	27
Bottom cost	0.42
Feed cost	470

5. Results and Discussions

5.1. Analysis of energy consumption

Tables 7, 8 and 9 show the operating conditions and calculated results of every column for non-heat integration, heat integration and current arrangements used in methanol distillation.

It should be noted that the current arrangements described in Table 9, are developed in direct sequence arrangement. Here the $V_{\min}$ diagram is used for the selected arrangement with minimum energy consumption. The simple and complex arrangements are compared in Tables 7 and 8. The results obtained here are compared with the conventional arrangements in Table 9.

As the results show, direct column sequence arrangement compared to arrangements without heat integration has the lowest energy consumption value of 138.67 MW, while among heat integrated arrangements indirect split with integration, which produces less methanol, has the lowest energy consumption value of 113.6 MW. In an overall comparison among all arrangements it appears that heat integrated Prefractionator with an energy consumption value of 117.5 MW and methanol production of 211600 kg·h⁻¹ is the most favorable. As the results obtained from simulation in Table 9 show, among conventional proposed arrangements of methanol distillation, five-column arrangement (which has not been applied industrially), with 75.87 MW has the lowest energy consumption.

Therefore, Prefractionator with heat integration is the only arrangement demonstrating some advantages over all other arrangements proposed so far, in terms of energy consumption, methanol production etc. What is obtained from $V_{\min}$ diagram for multi-effect arrangements also shows that among alternative arrangements of methanol distillation, Prefractionator has the lowest $V_{\min}/F$, that is the lowest energy consumption among alternative arrangements. This arrangement of lower energy consumption has been compared with simple and complex arrangements. Although when compared to the five-column arrangement it utilizes more energy, as more methanol is also produced from this method, it is more economically beneficial. It may also be added that there is still potential for further development of the arrangement

Table 7

Calculated results of methanol distillation of every column in arrangement without integration

Items	Direct column sequence		Indirect column sequence		Distributed column sequence			Prefractionator	
	C1	C2	C1	C2	C1	C2	C3	C1	C2
Top pressure $\times 10^{-5}$ /Pa	8.1	1.2	2.2	1.5	8.3	1.7	2	8.3	1.7
Top temperature/ $^{\circ}$ C	117.2	68.86	85.57	73.07	129.1	77.58	82.84	133.9	77.76
Bottom temperature/ $^{\circ}$ C	133.6	104.2	128.7	79.84	134	82.82	121.7	128.6	118.6
Reflux ratio	2.63	1.13	3.43	5.94	2.3	2.7	2.44	1.42	2.63
Number of theoretical stage	21	70	55	26	25	70	47	25	119
Rectifying section	20	62	49	6	24	12	19	24	91
Stripping section	1	8	6	20	1	58	28	1	28
Duty of condenser/MW	−2.119	−71.37	−212.9	−9.543	−38.91	−31.22	−106	−13.48	−223.4
Duty of reboiler/MW	19.87	118.8	280.1	18.99	72.82	23.9	140.3	39.71	263.9
Total heat requirement/MW	138.67		299.09		237.02			303.61	
Consumption of cooling Water $\times 10^{-3}$ /kg $\cdot$ h $^{-1}$	6274.9		18994.9		15035			20231	
Consumption of Steam $\times 10^{-3}$ /kg $\cdot$ h $^{-1}$	235.21		507.31		402.04			447.6	
Flow rate of product Methanol/kg $\cdot$ h $^{-1}$	209800		206800		209500			208400	
Purified methanol yield/%	99.8		99.8		99.8			99.8	

Table 8

Calculated results of methanol distillation of every column in arrangements with integration

Items	Direct split with integration		Indirect split with integration		Prefractionator with integration		Petlyuk	
	C1	C2	C1	C2	C1	C2	C1	C2
Top pressure $\times 10^{-5}$ /Pa	8.1	1.8	2.2	1.5	8.3	2.2	8.3	2.2
Top temperature/ $^{\circ}$ C	90.95	79.84	86.1	73.16	129.2	84.58	87.1	85.2
Bottom temperature/ $^{\circ}$ C	132.6	121.4	105.7	80.05	133.9	113.4	79.01	133.6
Reflux ratio	2.9	1.64	0.75	0.7	3.75	7.5	–	12.54
Number of theoretical stage	21	70	55	26	36	171	18	155
Rectifying section	20	62	49	6	29	117	16	145
Stripping section	1	8	6	20	7	54	2	10
Duty of condenser/MW	0.2907	−101.4	−47.1	−67.66	−79.49	−44.44	–	−692.5
Duty of reboiler/MW	17.76	150.1	113.6	0.01415	117.5	79.49	–	768.3
Total heat requirement/MW	167.86		113.6		117.5		768.3	
Consumption of cooling water $\times 10^{-3}$ /kg $\cdot$ h $^{-1}$	8646		5777		3794		59130	
Consumption of steam $\times 10^{-3}$ /kg $\cdot$ h $^{-1}$	284.23		192.9		199.4		1303	
Flow rate of product methanol/kg $\cdot$ h $^{-1}$	209700		201400		211600		208300	
Purified methanol yield/%	99.8		99.8		99.8		99.8	

proposed here. But, arrangements should be compared to each other on the basis of energy consumption as well as economic costs so that a more precise comparison for efficient selection is made.

5.2. Temperature difference of heat transfer

Tables 10 and 11 show the temperature difference on both sides of condenser/reboiler for every double-effect arrangement and for

conventional arrangements of methanol distillation respectively. As Table 10 shows, temperature difference in indirect split with integration is higher than that of other arrangements. It is even higher than the temperature difference on both sides of each condenser/re-boiler for conventional arrangements shown in Table 11.

As all the temperature differences are higher than 9 $^{\circ}$ C which are appropriate for the required heat transfer and therefore support the possibilities of new processes.

Table 9

Calculated results of methanol distillation of every column in current arrangements

Items	Three-column scheme			Four-column scheme				Five-column scheme				
	C1	C2	C3	C1	C2	C3	C4	C1	C2	C3	C4	C5
Top pressure $\times 10^{-5}$ /Pa	2.1	7.1	1.2	1.413	9.013	1.413	1.313	1.413	9.713	4.613	1.413	3.213
Top temperature/ $^{\circ}$ C	45.38	129.2	71.02	60.35	132.8	73.17	71.24	66.67	135.5	108.7	73.19	97.74
Bottom temperature/ $^{\circ}$ C	67.42	123.7	106.1	81.21	138.9	87.75	113.6	81.31	141	118.4	96.09	140
Reflux ratio	0.2654	3.1231	1	1.04	2.8139	4.31	1.41	1.2	2.4482	2.2258	1.55	1.5255
Number of theoretical stage	40	85	85	22	28	72	36	22	27	32	40	84
Rectifying section	30	10	26	4	27	52	25	4	26	30	38	74
Stripping section	10	75	59	18	1	20	11	18	1	2	2	10
Duty of condenser/MW	−0.2	−71.38	−82	−0.9357	−44.23	−53.3	−54.5	−1.592	−49.71	−55.33	−60.29	−5.519
Duty of reboiler/MW	4.426	91.05	71.38	4.4	73.59	44.23	54.33	5.519	65.37	49.71	55.33	10.5
Total heat requirement/MW	95.476			132.32				75.87				
Consumption of cooling water $\times 10^{-3}$ /kg $\cdot$ h $^{-1}$	7036.02			9290.89				5283.9				
Consumption of steam $\times 10^{-3}$ /kg $\cdot$ h $^{-1}$	161.908			224.433				128.71				
Flow rate of product methanol/kg $\cdot$ h $^{-1}$	207400			209000				208800				
Purified methanol yield/%	99.8			99.8				99.8				

Table 10

Temperature difference on both sides of condenser/reboiler for double-effect distillation

Items	Direct split with integration	Indirect split with integration	Prefractionator with integration
	C1/C2	C1/C2	C1/C2
Inlet temperature at hot side/°C	126.8	131.6	130.1
Outlet temperature at hot side/°C	126.7	130.9	128
Inlet temperature at cool side/°C	117.6	81.06	114.8
Outlet temperature at cool side/°C	117.6	82.6	121.5
LMTD/°C	9.15	49.42	10.74

Table 11

Temperature differences on both sides of condenser/reboiler for current methanol distillation arrangements

Items	Three-column scheme	Four-column scheme	Five-column scheme		
	C2/C3	C2/C3	C2/C3	C3/C4	C5/C1
Inlet temperature at hot side/°C	127.6	132.6	135.5	108.7	97.74
Outlet temperature at hot side/°C	127.6	132.2	135	107.8	96.51
Inlet temperature at cool side/°C	116.9	87.09	118.4	96.08	81.31
Outlet temperature at cool side/°C	117	90	119.1	101.3	85.5
LMTD/°C	10.65	43.84	16.5	9.40	13.67

Table 12 shows the temperature difference from every double-effect arrangement, which uses the saturated steam at 0.5 MPa as the heat resource.

One of the flaws of temperature difference reduction in reboiler for various arrangements is the increase in heat transfer level of that arrangement. The latter leads to increase in capital cost of the arrangement. C1 column in double-effect arrangements is the high pressure column. As Table 12 shows, temperature difference of indirect split with integration is lower than that of other arrangements. That is, heat transfer level of the arrangement is increased. In current methanol distillation arrangements, C2 is the high pressure column.

According to Table 13, compared to other arrangements, five-column one has the lowest temperature difference, therefore one of its defects is the increase in heat transfer level and consequently, rise in capital cost.

Table 12

Temperature differences on both sides of vapor-heated reboilers in double-effect arrangements

Items	Direct split with integration	Indirect split with integration	Prefractionator with integration
	C1	C1	C1
Inlet temperature at hot side/°C	160	160	160
Outlet temperature at hot side/°C	152	152	152
Inlet temperature at cool side/°C	131.8	138.3	134.4
Outlet temperature at cool side/°C	134.6	145.4	135.7
LMTD/°C	22.70	14.15	20.77

Table 13

Temperature difference on both sides of steam-heated reboilers in current methanol arrangements

Items	Three-column scheme		Four-column scheme			Five-column scheme	
	C1	C2	C1	C2	C4	C2	C5
Inlet temperature at hot side/°C	160	160	160	160	160	160	160
Outlet temperature at hot side/°C	152	152	152	152	152	152	152
Inlet temperature at cool side/°C	90.66	134.3	81.21	138.9	113.6	141	140
Outlet temperature at cool side/°C	91.06	136.3	81.3	141	113.6	142.3	140
LMTD/°C	65.07	20.55	74.68	15.87	42.27	14.09	15.66

5.3. Technical economic analysis

Tables 14, 15 and 16 show the economic calculations regarding alternative methanol distillation arrangements. In these tables, profit and total profit are calculated as:

$$\text{profit} = \text{product cost} - \text{operating cost}$$

$$\text{total profit} = \text{product cost} - \text{operating cost} - (\text{total capital cost} / \text{plant life time})$$

Here, the basis of arrangement comparison for technical economic analysis is two-column direct column sequence arrangement, against which all other arrangements with or without heat integration and also conventional methanol distillation arrangements are compared. As it is shown in the tables, although Prefractionator with heat integration, whose benefit increase is 4.79%, compared to the basic arrangement is the only one capable of competing with conventional arrangements of methanol distillation, three-column, four-column and five-column arrangements have benefit increases by 3.61%, 3.55% and 3.46%, respectively. In fact, the profit increase depends on reducing the cost and increasing the income. Here, it can be seen that operating costs of Prefractionator with heat integration is low, compared to two and three-column arrangements, but higher than that of four and five-column arrangements. Increase in income obtained from production of pure product leads to the increase in Prefractionator with heat integration profit. This arrangement with heat integration saved the operating costs by 28.03% and increased the capital cost by 8.87%. The degree of saving of operating costs in Prefractionator with heat integration is almost equal to that of four-column and more than that of three-column arrangements. Compared to five-column arrangement, Prefractionator has lower saving of operating costs. It is obvious that due to the number of columns in conventional methanol distillation arrangements, these arrangements have higher capital cost compared to Prefractionator.

As it is shown, the value of saving for three-column, four-column and five column arrangements is 27.78%, 28.85 and 29.28, respectively. According to results, the operating cost is two orders of magnitude larger than capital costs. Consequently, it can be said that as far as possible in arrangement designs, the number of heat integrations and heat exchange volume should be increased because the degree of operating costs reduction is far higher compared to degree of increase in capital costs. So, according to feed compositions, those arrangements should be preferred which provide more heat integration potentials. It is also apparently clear from the results that water cooling costs of condensers is one order of magnitude smaller than steam costs for reboilers and hence more attention should be paid to temperature reduction and reboilers' heat consumption in the columns optimization process.

Table 14

Results of economic costs of methanol distillation alternative arrangements without heat integration

Items	Direct column sequence	Indirect column sequence	Distributed column sequence	Prefractionator
Feed cost/USD·a ⁻¹	9.0014 × 10 ⁸	9.0014 × 10 ⁸	9.0014 × 10 ⁸	9.0014 × 10 ⁸
Steam cost/USD·a ⁻¹	2.8682 × 10 ⁸	6.9401 × 10 ⁷	5.2918 × 10 ⁷	3.3102 × 10 ⁷
Cooling cost/USD·a ⁻¹	8.1184 × 10 ⁵	4.0578 × 10 ⁶	1.0442 × 10 ⁶	1.0599 × 10 ⁶
Operating cost	1.1878 × 10 ⁹	9.7360 × 10 ⁸	9.5410 × 10 ⁸	9.3430 × 10 ⁸
Product cost	7.8880 × 10 ⁹	7.7760 × 10 ⁹	7.8910 × 10 ⁹	7.8380 × 10 ⁹
Capital cost	4.0430 × 10 ⁵	2.0260 × 10 ⁶	8.4010 × 10 ⁵	6.0270 × 10 ⁵
Total capital cost	1.9113 × 10 ⁶	2.2451 × 10 ⁶	2.0369 × 10 ⁶	2.4477 × 10 ⁶
Profit	6.7002 × 10 ⁹	6.8024 × 10 ⁹	6.9369 × 10 ⁹	6.9037 × 10 ⁹
Plant life time	10.00	10.00	10.00	10.00
Total annual cost	1.1880 × 10 ⁹	9.7382 × 10 ⁸	9.5431 × 10 ⁸	9.3455 × 10 ⁸
Total profit	6.7000 × 10 ⁹	6.8022 × 10 ⁹	6.9367 × 10 ⁹	6.9035 × 10 ⁹
Operating cost saving/%	0	22.00	24.49	27.13
Total capital cost saving/%	0	−14.87	−6.17	−21.91
TAC saving/%	0	21.99	24.48	27.12
Profit increase/%	0	1.52	3.53	3.04

According to other results, it may be concluded that in order for the capital cost to reduce, it is better to keep the minimum temperature difference in condensers of columns, to enable the use of cooler hot utility.

Fig. 9 shows the comparison of calculated values of total profit for four arrangements which are normalized and obtained according to the largest value. As the Prefractionator with integration is a two-column arrangement; according to the comparison with a conventional two column process provided in Table 15 has a lower operating cost and thus is more profitable. Hence compared to the base state, this arrangement is better than the other arrangements. In comparison to the Prefractionator with the conventional three-column distillation of methanol, it has a lower operating cost, more product income, higher capital cost, lower total annual cost and hence is more profitable. When comparing the proposed Prefractionator arrangement with the conventional 4 and 5 column processes, it has a higher operating cost, more product income, lower capital cost, higher total annual cost and is therefore more profitable. The reason behind the presentation of 4 and 5 column arrangements is to reduce costs and methanol waste at the same time. The propose Prefractionator arrangement with heat integration also has potentials for more development to further reduce costs and methanol wastage. Tables 15 and 16 show that total capital cost of Prefractionator arrangement with heat integration (2.0974×10^6) is lower than of three-column (1.7302×10^7), four-column (2.7800×10^6) and five-column (2.4646×10^6). Not only is the operating cost of Prefractionator with heat integration higher than those of four- and five-column arrangements, but also the amount of product cost is also higher than those of the mentioned arrangements.

It should be noted however, that total capital cost of Prefractionator is lower than that of four- and five-column arrangements leading to higher total profit of Prefractionator. Considering life time of 1, 10 and 20 years, this comparison is shown in Fig. 8 for all four arrangements. It is obvious that the value of total profit of Prefractionator with heat integration is higher than the value of other arrangements. So, it can be said that Prefractionator with heat integration is the most economical arrangement for methanol distillation.

6. Conclusions

- (1) A comparative study of different arrangements for methanol distillation process is presented in this paper.
- (2) Shortcut equation for minimum vapor flow rate and $V_{\min}$ diagram in distillation systems, presents an appropriate target for comparing energy consumption in different arrangements.
- (3) Prefractionator arrangement has the lowest $V_{\min}/F$, that is the lowest energy consumption among alternative arrangements. Also this arrangement has an appropriate temperature difference for heat transfer in condenser and reboiler.
- (4) It has been shown that the Prefractionator with heat integration arrangement exhibits significant benefit increase compared to conventional arrangements of methanol distillation.
- (5) Utilization of an economic equation demonstrating the profit instead of total annual cost leads not only to a more flexible combination of operating, capital, feed costs and product benefits in our equations, but also better decisions are made for selecting efficient arrangements.

Table 15

Results of economic costs of methanol distillation alternative arrangements with heat integration

Items	Direct split with integration	Indirect split with integration	Prefractionator with integration	Petlyuk
feed cost/USD·a ⁻¹	9.0014 × 10 ⁸	9.0014 × 10 ⁸	9.0014 × 10 ⁸	9.0014 × 10 ⁸
steam cost/USD·a ⁻¹	4.0542 × 10 ⁷	1.8197 × 10 ⁷	2.6928 × 10 ⁷	1.7734 × 10 ⁷
cooling cost/USD·a ⁻¹	1.5102 × 10 ⁶	2.8664 × 10 ⁵	6.6544 × 10 ⁵	9.6782 × 10 ⁶
operating cost	9.4219 × 10 ⁸	9.1862 × 10 ⁸	9.2773 × 10 ⁸	1.0872 × 10 ⁹
product cost	7.8780 × 10 ⁹	7.5560 × 10 ⁹	7.9490 × 10 ⁹	7.8560 × 10 ⁹
capital cost	4.3300 × 10 ⁵	1.2510 × 10 ⁶	9.3540 × 10 ⁵	1.4550 × 10 ⁵
total capital cost	1.2028 × 10 ⁶	1.4892 × 10 ⁶	2.0974 × 10 ⁶	4.1145 × 10 ⁶
profit	6.9358 × 10 ⁹	6.6374 × 10 ⁹	7.0213 × 10 ⁹	6.7688 × 10 ⁹
plant life time	10.00	10.00	10.00	10.00
total annual cost	9.4231 × 10 ⁸	9.1877 × 10 ⁸	9.2794 × 10 ⁸	1.0876 × 10 ⁹
total profit	6.9357 × 10 ⁹	6.6372 × 10 ⁹	7.0211 × 10 ⁹	6.7684 × 10 ⁹
operating cost saving/%	26.07	29.30	28.03	9.25
total capital cost saving/%	58.90	28.34	−8.87	−53.55
TAC saving/%	26.07	29.30	28.02	9.23
profit increase/%	3.52	0.94	4.79	1.02

Table 16

Results of economic costs of current methanol distillation arrangements

Items	Three-column scheme	Four-column scheme	Five-column scheme
feed cost/USD·a ⁻¹	9.0014 × 10 ⁸	9.0014 × 10 ⁸	9.0014 × 10 ⁸
steam cost/USD·a ⁻¹	2.7894 × 10 ⁷	2.0400 × 10 ⁷	1.7503 × 10 ⁷
cooling cost/USD·a ⁻¹	1.5205 × 10 ⁶	1.3069 × 10 ⁶	1.1280 × 10 ⁶
operating cost	9.2955 × 10 ⁸	9.2185 × 10 ⁸	9.1877 × 10 ⁸
product cost	7.8730 × 10 ⁹	7.8600 × 10 ⁹	7.8510 × 10 ⁹
capital cost	2.4220 × 10 ⁵	2.2260 × 10 ⁵	1.4950 × 10 ⁵
	1.1300 × 10 ⁶	8.7160 × 10 ⁵	7.8550 × 10 ⁵
	1.5930 × 10 ⁷	7.1530 × 10 ⁵	2.3140 × 10 ⁵
		9.7050 × 10 ⁵	6.1140 × 10 ⁵
			6.8680 × 10 ⁵
total capital cost	1.7302 × 10 ⁷	2.7800 × 10 ⁶	2.4646 × 10 ⁶
profit	6.9434 × 10 ⁹	6.9382 × 10 ⁹	6.9322 × 10 ⁹
plant life time	10.00	10.00	10.00
total annual cost	9.3128 × 10 ⁸	9.2212 × 10 ⁸	9.1902 × 10 ⁸
total profit	6.9417 × 10 ⁹	6.9379 × 10 ⁹	6.9320 × 10 ⁹
operating cost saving/%	27.78	28.85	29.28
total capital cost saving/%	—8895	—31.25	—22.45
TAC saving/%	27.56	28.83	29.26
Profit increase/%	3.61	3.55	3.46

Nomenclature

<i>B</i>	bottom product flow rate, kmol·h ⁻¹
<i>D</i>	distillate flow rate, kmol·h ⁻¹
<i>S</i>	side product flow rate, kmol·h ⁻¹
<i>V</i>	vapor flow rate, kmol·h ⁻¹
<i>V_B</i>	bottom vapor flow rate, kmol·h ⁻¹
<i>V_{min}</i>	minimum vapor flow rate, kmol·h ⁻¹
<i>V_T</i>	top vapor flow rate, kmol·h ⁻¹

Appendix A

Here, profit is calculated through subtraction of Income and costs:

$$\text{profit} = \text{product cost} - \text{feed cost} - \text{utility cost}$$

Income obtained from product sale is calculated by:

$$\begin{aligned} \text{product cost (USD} \cdot \text{a}^{-1}) &= [\text{dist stream (t} \cdot \text{h}^{-1}) \times \text{dist cost (USD} \cdot \text{t}^{-1}) \\ &\quad + \text{bottom stream (t} \cdot \text{h}^{-1}) \times \text{bottom cost (USD} \cdot \text{t}^{-1}) \\ &\quad + \text{side stream (t} \cdot \text{h}^{-1}) \times \text{side cost (USD} \cdot \text{a}^{-1})] \\ &\quad \times 8000 (\text{h} \cdot \text{a}^{-1}) \end{aligned}$$

Cost of inlet feed to arrangements is calculated through:

$$\text{feed cost (USD} \cdot \text{a}^{-1}) = [\text{feed stream (t} \cdot \text{h}^{-1}) \times \text{feed cost (USD} \cdot \text{a}^{-1})] \times 8000 (\text{h} \cdot \text{a}^{-1})$$

Utility cost is obtained by this equation:

$$\begin{aligned} \text{utility cost (USD} \cdot \text{a}^{-1}) &= [\text{steam stream (t} \cdot \text{h}^{-1}) \times \text{steam cost (USD} \cdot \text{t}^{-1}) \\ &\quad + \text{cooling water stream (t} \cdot \text{h}^{-1}) \\ &\quad \times \text{cooling water cost (USD} \cdot \text{t}^{-1})] \times 8000 (\text{h} \cdot \text{a}^{-1}) \end{aligned}$$

In many of articles, for optimization the minimization of total annual cost is used, which is calculated as such:

$$\text{TAC} = \text{capital cost}/10 + \text{utility cost}$$

Number 10 in above formula is considered with plant lifetime. Calculation of arrangements costs includes parts below:

1. Capital cost
 - (1) Cost of column purchase, which it itself involves cost of column body, tray and installation.
 - (2) Costs concerning purchase and installation of heat exchangers including condensers and reboilers.
2. Operating cost.
3. Costs regarding utility parts.

Calculation of cost of column purchase requires column height and diameter. The latter is obtained by simulator software and the former is a function of number of trays. For a certain number of trays the theory is identified. That is, after running, the software determines the diameter of distillation column having Valve tray and Weir height of about 50.8 mm. For estimating real number of trays, column total efficiency is calculated by:

$$\lg(E_0) = 1.67 - 0.25 \lg(\mu_{\text{avg}} \alpha_{\text{avg}}) + 0.3 \lg(L_m/V_m) + 0.3(h_1) \quad (\text{A1})$$

In this equation, μ_{avg} is the average feed viscosity, which is calculated by total multiplication of mole feed components fraction at components viscosity. α_{avg} is the relative volatility of average key feed components. L_m/V_m differ in rectifying and stripping parts whose average is calculated and used in the following formula:

$$N_{\text{actual}} = N_{\text{theoretical}}/E_0 \quad (\text{A2})$$

Considering distance between trays being 0.6 and disengagement being 6 m, column height is calculated by:

$$H = h + 6.0 \quad (\text{A3})$$

When tray stack height equals:

$$H = (N_{\text{actual}} - 1) \times 0.6 \quad (\text{A4})$$

Costs of distillation columns (assuming that carbon steel material is used in column production) can be calculated through below formula, which is updated by CEPICI (Chemical Engineering Plant Cost Index). Cost concerning installation of column body:

$$C_{\text{cb}}(\text{USD}) = (\text{PCI}/113.6) \times 937.61 \times d^{1.066} \times H^{0.802} \quad (\text{A5})$$

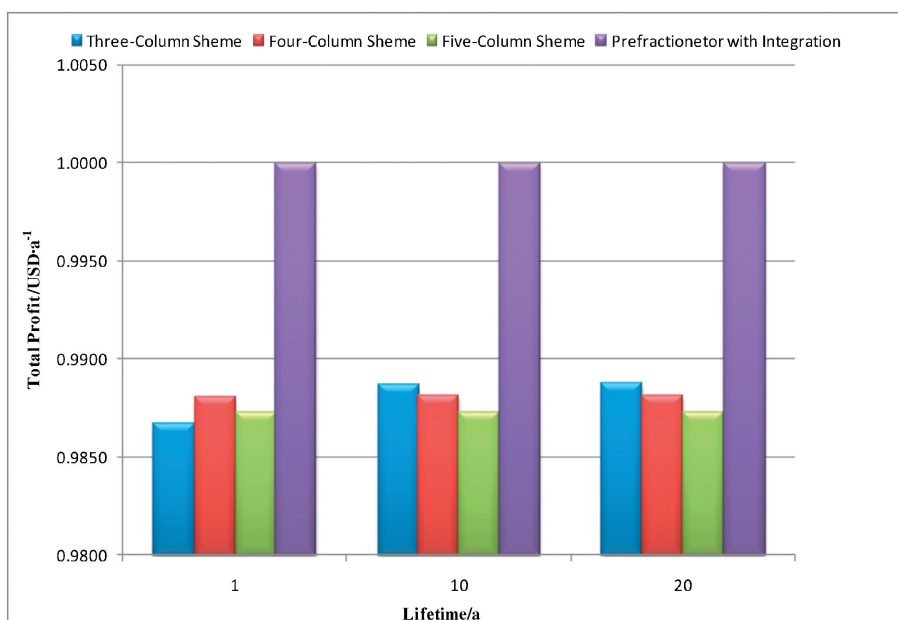


Fig. 9. Values of total profit for four arrangements.

If the design pressure is more than 345 kPa, a correction factor will be used:

$$a = \left[1 + 1.45 \times 10^{-4} (P - 345) \right] \quad (A6)$$

Costs concerning column tray installation:

$$C_{ct}(\text{USD}) = (\text{PCI}/113.6) \times (136.14) \times d^{1.55} \times h \quad (A7)$$

Total column cost equals total column body installation cost plus column tray installation cost which can be obtained through following equations. According to its heat transfer level, exchanger cost is calculated by this equation:

$$A = Q/U\Delta T_{LM} \quad (A8)$$

In the above equation, A represents heat transfer level, Q exchanger heat load, U the average heat transfer coefficient, ΔT_{LM} logarithmic average temperature. Heat transfer coefficients [21] for this system are calculated by:

$$\begin{aligned} U_{\text{reboiler}} &= 3400 \text{ kJ} \cdot \text{m}^{-2} \cdot \text{h}^{-1} \cdot ^\circ\text{C}^{-1}, \\ U_{\text{condenser}} &= 2800 \text{ kJ} \cdot \text{m}^{-2} \cdot \text{h}^{-1} \cdot ^\circ\text{C}^{-1}, \\ U_{\text{exchanger}} &= 2100 \text{ kJ} \cdot \text{m}^{-2} \cdot \text{h}^{-1} \cdot ^\circ\text{C}^{-1}, \end{aligned}$$

Assuming that exchangers are shell and tube, floating head and carbon steel, exchanger cost will be obtained by:

$$C_e(\text{USD}) = (\text{PCI}/113.6) \times (474.67) \times A^{0.65} \quad (A9)$$

Above relationship is true for $18.6 < A < 464.5$ and pressure higher than 1034.2 kPa. Below equation leads to the utility costs:

$$C_{\text{Utility}} = W \times C \times H_y \quad (A10)$$

Here W is the water or steam flow in terms of $\text{t} \cdot \text{h}^{-1}$ (ton per hour), C represents water or steam price in terms of $\text{USD} \cdot \text{t}^{-1}$, H_y is the total work hour in a year equaling 8000 h per year.

All the costs are based on mid-1968 and mid-2013 updates, which itself is based on CEPCI cost index [23].

References

- [1] K. Engelen, S. Skogestad, Selecting appropriate control variables for a heat integrated distillation system with prefractionator, *Comput. Chem. Eng.* 28 (2004) 683–691.
- [2] R. Agrawal, Separations: Perspective of a process developer/designer, *AIChE J.* 47 (2001) 967–971.
- [3] A.K. Jana, Heat integrated distillation operation, *Appl. Energy* 87 (2010) 1477–1494.
- [4] J. Wu, L. Chen, Simulation of novel process of distillation with heat integration and water integration for purification of synthetic methanol, *J. Chem. Ind. Eng. (China)* 56 (2005) 477–481 (in Chinese).
- [5] Z.C. Zhou, J. Wu, Novel purification process of synthetic methanol with full integration of heat and water, *J. Chem. Ind. Eng. (China)* 58 (2007) 3210–3214 (in Chinese).
- [6] B.Z. Liu, Y.C. Zhang, P. Chen, K.J. Yao, Research on energy-saving process of methanol distillation, *Chem. Ind. Eng. Prog. (China)* 26 (2007) 739–742 (in Chinese).
- [7] R.A. Meyers, Handbook of synfuels technology, McGraw-Hill, New York, 1984.
- [8] Y.Z. Chu, L.P. Qin, S.L. Wang, Y. Huang, S.P. Zhou, Optimum design of methanol distillation process and columns, *Chem. Ind. Eng. Prog. (China)* 27 (2008) 1659–1662 (in Chinese).
- [9] J. Zhang, S. Liang, X. Feng, A novel multi-effect methanol distillation process, *Chem. Eng. Process.* 49 (2010) 1031–1037.
- [10] R. Premkumar, Retrofitting industrial, conventional column systems to Petlyuk/Divided Wall columns, A thesis submitted for the degree of master of engineering, Department of Chemical and Bio-molecular Engineering, National University of Singapore, 2007.
- [11] H. Seki, M. Shamsuzzoha, Process design and control of dividing wall columns, KFUPM Dhahran, Saudi Arabia, 2012 25–26.
- [12] I. Dejanovic, L. Matijasevic, I.J. Halvorsen, S. Skogestad, H. Jansen, B. Kaibel, Z. Olujic, Designing four-product dividing wall columns for separation of a multi component aromatics mixture, *Chem. Eng. Res. Des.* 89 (2011) 1155–1167.
- [13] I.J. Halvorsen, S. Skogestad, Energy efficient distillation, *J. Nat. Gas Sci. Eng.* (2011) 1–10.
- [14] I.J. Halvorsen, Minimum energy requirements in complex distillation arrangements NTNU PhD Thesis 2001.
- [15] I.J. Halvorsen, S. Skogestad, Minimum energy consumption in multi-component distillation. 3. More than three products and generalized Petlyuk arrangements, *Ind. Eng. Chem. Res.* 42 (2003) 616–629.
- [16] I.J. Halvorsen, S. Skogestad, Minimum energy consumption in multi-component distillation. 2. Three-product Petlyuk arrangements, *Ind. Eng. Chem. Res.* 42 (2003) 605–615.
- [17] H.K. Engelen, S. Skogestad, Graphical Visualisation of Minimum Energy Requirements for Multi-Effect Distillation Arrangements, 2003 submitted to the AIChE Journal, (February 2003).
- [18] I.J. Halvorsen, S. Skogestad, Minimum energy for the four-product Kaibel column, AIChE annual meeting, AIChE, San Francisco, Paper 216d, 2006.
- [19] I. Dejanovic, L. Matijasevic, Z. Olujic, An effective method for establishing the stage and reflux requirement of three-product Dividing Wall columns, *Chem. Biochem. Eng. Q.* 25 (2) (2011) 147–157.

- [20] S. Lee, N.V.D. Long, M. Lee, Design and optimization of natural gas liquefaction and recovery processes for offshore floating liquefied natural gas plants, *Ind. Eng. Chem. Res.* 51 (2012) 10021–10030.
- [21] S.k. Almeland, K.A. Meland, D.G. Edvardsen, S. Skogestad, M. Panahi, Process design and economical assessment of a methanol plant, NTNU Norwegian University of Science and Technololy, Faculty of Natural Sciences and Technology, Department of Chemical Engineering, 2009.
- [22] E. Rev, M. Emtir, Z. Sztikai, P. Mizsey, Z. Fonyo, Energy saving of integrated and coupled distillation systems, *Comput. Chem. Eng.* 25 (2001) 119–140.
- [23] <http://www.chemengonline.com/pci>.