ВЫБОР ОПТИМАЛЬНОЙ ПОСЛЕДОВАТЕЛЬНОСТИ РАЗДЕЛЕНИЯ ДЛЯ МНОГОКОМПОНЕНТНОЙ ПЕРЕГОНКИ С ИСПОЛЬЗОВАНИЕМ МЕТОДА НА ОСНОВЕ ЗАДАЧИ РАЗДЕЛЕНИЯ ПО ПРЕДЕЛЬНОЙ СКОРОСТИ ПАРОВ (MVR МЕТОД)

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В области химической обработки одной из трудностей, которая привлекает наибольшее внимание исследователей, является разработка эффективных последовательностей разделения. Многокомпонентная смесь может быть разделена на составляющие ее элементы перегонкой в ряде различных последовательностей, однако затраты, связанные с каждой из этих последовательностей, различны. В этой статье мы предлагаем количественный подход для определения идеальной последовательности колонн с помощью задачи разделения на основе предельной скорости пара (MVR) неключевых компонентов, присутствующих в жидкой смеси. Отбор потенциальных возможностей проектирования осуществляется внутри структуры, что позволяет разбить последовательности разделения на отдельные задачи. Объем работы, необходимой для вычислений, значительно сокращается при использовании задачного подхода. MVR рассчитывается для каждой задачи разделения перед применением к самим последовательностям. Затем MVR используется для ранжирования каждой последовательности. Последовательность с наименьшим MVR размещается первой и считается лучшей последовательностью. Согласно полученным данным были оценены оптимальные последовательности для четырехкомпонентной смеси изобутана, н-бутана, изопентана и н-пентана и пятикомпонентной смеси пропана, изобутана, н-бутана, изопентана и н-пентана.

Ключевые слова: синтез последовательностей, многокомпонентное разделение, надстройка, задача разделения

SELECTION OF OPTIMAL SEPARATION SEQUENCE FOR MULTICOMPONENT DISTILLATION USING A SEPARATION TASK BASED MARGINAL VAPOR RATE (MVR) METHOD

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In the field of chemical processing, one of the difficulties that receives the greatest attention from researchers is the development of efficient separation sequences. A multicomponent mixture may be separated into its constituent elements by distillation in a number of different sequences; however, the costs associated with each of these sequences are different. In this article, we provide

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a quantitative approach for identifying the ideal column sequence by separation task based marginal vapour rate (MVR) of non-key components present in a liquid mixture. The screening of potential design possibilities is carried out inside a framework, which makes it possible to break down the separation sequences into individual tasks. The amount of work required for computation is significantly reduced when using the task approach. The MVR is calculated for each separation task before being applied to the sequences themselves; the MVR is then used to give ranks to each sequence. The sequence with the lowest MVR is placed first and is considered to be the best sequence. According to the findings, the optimal sequences for the four-component mixture of ibutane, n-butane, i-pentane, and n-pentane, and a five-component mixture of propane, i-butane, n-butane, i-pentane, and n-pentane were evaluated.

Key words: sequence synthesis, multicomponent separation, superstructure, separation task

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INTRODUCTION

Separation techniques are responsible for a substantial amount of the operating expenditures as well as the overall capital investment made by chemical industries. As a result, there has been a lot of interest in the development of systematic methods that can identify the most efficient separation sequences. There has been a significant increase in the focus placed on the development of systematic methods for identifying the most effective separation sequences [1-4]. As the number of components increases, so does the number of potential sequences [5]. Thorough evaluation of all potential sequences is computationally intensive, particularly for more component mixtures, and is unsuited for the early phases of flow sheet design and development. Short-cut strategies for evaluating process alternatives are thus required, and they can recommend a few potential sequences for further detailed analysis [1,6-9].

In multicomponent distillation synthesis, the separation of multicomponent mixtures is possible in a number of distinct column sequences. Despite the fact that all of these column sequences result in the identical products, the capital and operational expenses associated with each sequence are unique. It is possible that a choice of separation sequence that is not ideal may result in significant additional expenses throughout the operation. Among the research that has been done on column sequencing, a number of different approaches have been proposed in the literature [10-19]. All these approaches reported in the literature are categorised into three broad groups by Nishida et al. (1981) [20]:

(a) Heuristic techniques.(b) Adaptive strategies.

(c) Algorithmic techniques.

The concept of the separation task was presented by Hendry and Hughes. This concept divides the distillation superstructure into distinct separation tasks, and these distinct separation tasks are evaluated with the help of the ideal thermodynamically orientated Underwood-Fenske-Gilliland algorithm. In their expansion of this idea, Shah and Kokossis considered complex distillation processes [21]. Along with the state task network, Sargent and Gaminibandara established the idea of a superstructure for distillation column networks [22]. Thong and Jobson (2004) [23] devised a sequential technique for azeotropic mixture synthesis.

Heuristic techniques, which have the advantage of being rapid and need just a little amount of data, have created a far more fundamental basis for an assessment that is both straightforward and quick. The fundamental drawback of these methods is that they frequently only provide access to a single dominant heuristic rule, which can result in significant miscalculations; alternatively, they may provide a collection of contradictory heuristic rules that need to be evaluated against one another in a very specific manner. As a direct consequence of this, it might be difficult (though not impossible) to use heuristic rule-based techniques in an organized way [24-26].

By continually making small adjustments to the configurations that have been created in the past, adaptive approaches work toward the objective of achieving the best possible separation arrangement. It

includes the evolutionary criteria that will explain how the system will develop to a sequence of configurations that are progressively superior to the previous ones. There are two distinct varieties of algorithmic methodologies, namely mathematical programming methods, and parametric research. The primary objective of parametric studies is to identify the critical aspects and evaluate how those aspects influence the optimal separation arrangement. These parametric assessments have limited applications since there are many elements that impact the cost of the separation arrangement. Their primary discoveries consist of a set of heuristic principles that may be used to make estimates in a rapid and simple manner [10,27-29]. The establishment of the optimal separation structure may be accomplished via the application of mathematical programming approaches, which use a variety of mathematically based optimization procedures. The rigor of these processes, in addition to the fact that only these approaches can guarantee the most accurate response, is the primary advantage of using these methods. On the other hand, the most significant limitation of these methods is that they can only be used to problems that can be easily simplified [30-33].

The huge number of possible sequences in column sequencing is the key reason to be concerned. This number grows at an exponential rate corresponding to the quantity of product being processed. This work outlines a technique consisting of a series of steps for selecting the best sequence of distillation columns for separating the multicomponent mixture. In the first step, the design options are produced with the help of a separation superstructure. After that, feasible separation tasks are generated. At the second step of the process, the marginal vapor rate method is used to do an analysis of the design alternatives [26]. As contrast to mathematical modeling or optimization methods, shortcut techniques provide a quick evaluation of a single separation activity without the need for extensive specification of the distillation column. The current work involves the establishment of a quantitative method for determining the optimal distillation sequence from task-based calculated MVR values without taking into account distillation columns with heat integration. This method has been effectively used to determine the optimal sequence of distillations.

METHODOLOGY

A. Distillation column sequencing and generation of separation tasks

Figure illustrates all of the possible separation sequences into individual components that may be carried out on a mixture consisting of four different components, under the assumption that sharp splits and simple two-product splits can be carried out. The number of subgroups, separation tasks, and alternative sequences associated with the distillation method for separating components of multicomponent mixtures are outlined in Table 1. There are several possible configurations in which the same separation steps might occur, which would result in the same feed and product compositions. This is seen in Fig. 1, where the first and second sequences both begin with the same initial separation. This characteristic is used in a superstructure, which is known as a state task network, to decrease the complexity of multicomponent mixture separation [34]. Every potential composition that may be obtained in this superstructure is referred to as a state. The states indicate the feed, and separation sequence products.

The number of sequences grows exponentially as the number of components increases. This is a wellknown [35] phenomenon that may be characterized by equation (1)

$$N_{s} = \frac{[2(N-1)]!}{N!(N-1)!}$$
(1)

where N is the number of components and N_S is the number of sequences.



Figure. All possible configurations for the sharp separation of the four component mixture by distillation Рисунок. Все возможные конфигурации для резкого разделения четырехкомпонентной смеси путем перегонки

Table 1

The number of subgroups, separation tasks, and sequences related to multicomponent mixture separation *Таблица 1*. Количество подгрупп, задач разделения и последовательностей, связанных с разделением многокомпонентных смесей

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Number of components (N)	Number of subgroups (S _B)	Number of tasks (T_N)	Number of sequences (N _S)			
2	3	1	1			
3	6	4	2			
4	10	10	5			
5	15	20	14			
6	21	35	42			
7	28	56	132			
8	36	84	429			
9	45	120	1430			
10	55	165	4862			

A task is described as an operation that connects three separate states: the feed state, the distillate state, and the bottom state [36-39]. The number of tasks (T_N) can be developed automatically by separating all potential state compositions into intermediate products or products and estimated by equation (2). Each separation sequence can be viewed as a viable task combination. A task combination is admissible if it begins with the feed state and concludes with the product states. The fundamental benefit of superstructure is that, in contrast to the exponential rise of the number of sequences (Table 1), the number of tasks only grows with the third power of the number of products [40].

$$T_{N} = \frac{(N-1)(N)(N+1)}{6},$$
 (2)

B. Marginal vapour rate based on separation tasks

It is preferable to use sequencing methods that rely on column design and, in certain circumstances, total annual cost calculation when the implementation of heuristics strategies for sequencing ordinary distillation columns is either imprecise or results in contradictory findings. There are methods that are expedient and less rigorous than others that may provide sequences that are acceptable, nevertheless they aren't necessarily the best. There are a great number of approaches, many of which are identical, that can be found in the literature that aim to restrict the search space [41-44]. The marginal vapor rate (MVR) approach that Modi and Westerberg (1992) developed is superior to the other methods and may be used without the need for extensive column designs and cost estimations.

The marginal annualized cost (MAC) was described by Modi and Westerberg (1992) as the cost difference between separation in the absence of nonkey elements and separation with the nonkey constituents. They demonstrate that the MVR, which is the equivalent change in molar vapor rate moving up the column, is an accurate approximation of the MAC. The sequence that has the lowest total column MVRs is the one that is selected as the optimal sequence. Since vapor rate is a significant factor in calculating column diameter, reboiler and condenser areas, and reboiler and condenser jobs, it is a good cost measure. This is the reason that the excellent estimate may be attributed to the fact that vapor rate is a good cost metric.

The equations by Underwood [45] are used to compute the minimum reflux ratio in an appropriate method for estimating the molar vapor rate in a simple distillation column separating a nearly ideal system. A material balance is used to estimate the molar vapor rate, V, entering the condenser in a conventional distillation column separating a nearly ideal system. If the liquid being fed into the column is already saturated, then the molar vapor rate will be almost constant at this value of V as it travels through the column. Since the minimal reflux ratio is unaffected by the product purities that are selected, the choice of product purities is not an essential factor in MVR calculations. In order to make the analysis of the material balance more straightforward, assume that the separations were approximately ideal, with the key constituents that were lighter than light key (LK) remaining in the top and the key constituents that were heavier than heavy key (HK) remaining in the residue.

The estimation of the marginal vapor rates for each separator as well as for the overall sequence enables comparisons to be made across different distillation sequences. The marginal vapor rate for each key split in a separation may be estimated with the use of equation (3).

$$MVR = \sum_{\text{nonkey}i} V_i = \sum_{\text{nonkey}i} \left| \frac{\alpha_{ik}}{\alpha_{ik} - \frac{\alpha_{ik,k} + \alpha_{hk,k}}{2}} f_i \right| \quad (3)$$

L

L

Where the vapor rate, the relative volatility, and the feed flow rate of the nonkey component *i* associated with each key split in a separation network are denoted by V_i , α_{ik} and f_i , respectively. MVR is a metric that illustrates the influence in which the presence of other species has on the results of carrying out a split between the key elements of the column. The sum of these terms for every *i* indicates the magnitude of the rise in MVR that can be attributed to the existence of these columns' nonkey elements. If there is a larger gap between the relative volatility of nonkey elements and the volatility of key elements, then the denominator will be larger, and the MVR will be lower. After calculating the MVR for each column, the MVR for the sequence is computed by adding up the MVRs for each column in the sequence. This results in the MVR of a sequence. With a given feed flow rate and the relative volatilities of components, the sequence that has the lowest overall MVR is the best option.

CASE STUDIES

For the work reported in this article, a fourcomponent and a five-component mixture reported in the literature were explored for the step by step analysis presented in methodology. In the first case study, a zeotropic mixture of *i*-Butane, *n*-Butane, *i*-Pentane, and *n*-Pentane is assumed to be separated into pure components at 1.013 bar pressure and 1000 kmol/s total flow rate, as stated in Table 2 [7,46,47]. In the next section, the components *i*-Butane, *n*-Butane, *i*-Pentane, and *n*-Pentane are denoted by the letters A, B, C, and D, respectively. There are five alternative sequences (Figure and Table 3), each with ten distinct separation tasks. According to the labeling in Table 3, the sequences are numbered one through five.

Table 2 Data of the problem specification for a four component mixture

Таблица 2. Данные технического задания для четырехкомпонентной смеси

No	Component	Feed flow rate (kmol/h)	Relative volatility	Adjacent relative volatility
1	<i>i</i> -Butane	126	2.0	
				1.12
2	<i>n</i> -Butane	292	1.8	
				1.50
3	<i>i</i> -Pentane	186	1.2	
				1.20
4	<i>n</i> -Pentane	396	1.0	

Table 3

Possible sequences for sharp separation of four component mixture *Таблица 3*. Возможные последовательности для резкого разделения четырехкомпонентной смеси

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Sequence	Column 1	Column 2	Column 3
1	A/BCD	B/CD	C/D
2	A/BCD	BC/D	B/C
3	AB/CD	A/B	C/D
4	ABC/D	A/BC	B/C
5	ABC/D	AB/C	A/B

Table 4
Data of the problem specification for a five component
mixture

Таблица 4. Данные технического з	вадания
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S. No.	Component	Feed flow rate (kmol/h)	Relative volatility	Adjacent relative volatility
1	Propane	50.0	9.70	
				2.00
2	<i>i</i> -Butane	150.0	4.85	
				1.33
3	<i>n</i> -Butane	250.0	3.65	
				2.40
4	<i>i</i> -Pentane	200.0	1.52	
				1.52
5	<i>n</i> -Pentane	350.0	1.00	

As indicated in Table 4, the second case study comprises the separation of Propane, *i*-Butane, *n*-Butane, *i*-Pentane, and *n*-Pentane into pure components at a pressure of 1.013 bar and a total flow rate of 1000 kmol/s [7,26]. The letters A, B, C, D, and E represent propane, *i*-Butane, *n*-Butane, *i*-Pentane, and *n*-Pentane in the next section, respectively. There are fourteen alternative sequences (Table 8), each with twenty distinct separation tasks. According to the labeling in Table 5, the sequences are numbered one through fourteen.

Possible sequences for sharp separation of five component mixture

Таблица 5. Возможные последовательности для региого разделения пятикомпонентной смеси

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Sequence	Column 1	Column 2	Column 3	Column 4
1	ABCD/E	ABC/D	AB/C	A/B
2	ABCD/E	ABC/D	A/BC	B/C
3	ABCD/E	AB/CD	A/B	C/D
4	ABCD/E	A/BCD	B/CD	C/D
5	ABCD/E	A/BCD	BC/D	B/C
6	ABC/DE	A/BC	B/C	D/E
7	ABC/DE	AB/C	A/B	D/E
8	AB/CDE	A/B	CD/E	C/D
9	AB/CDE	A/B	C/DE	D/E
10	A/BCDE	BCD/E	BC/D	B/C
11	A/BCDE	BCD/E	B/CD	C/D
12	A/BCDE	BC/DE	B/C	D/E
13	A/BCDE	B/CDE	CD/E	C/D
14	A/BCDE	B/CDE	C/DE	D/E

RESULTS AND DISCUSSION

Based on separation tasks, MVRs for four and five component systems were determined in this study. The optimal sequence, which is rated first, was discovered by comparing the total MVRs of all the sequences for a given feed composition. The remaining sequences are similarly sorted in ascending order based on the values of their MVRs. The sequence with the highest MVR value is ranked last. All of the following sequences are ranked in the middle.

Table 6

Key splits for the four component system *Таблица 6*. Ключевые расщепления лля четырехкомпонентной системы

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S. No.	Key Split (LK/HK)	Arithmetic Average of RV	VA	VB	VC	VD
1	A/B	1.9	-	-	318.86	440.00
2	B/C	1.5	504.00	-	-	792.00
3	C/D	1.1	280.00	750.86	-	-

Table 6 shows the key splits for the preceding section's four component system. The MVR is computed for each component in each key split, allowing the marginal vapor rates for every specific column in a sequence to be calculated. Table 7 displays the ten distinct separation tasks and the estimated MVR values for nonkey constituents in each task. Table 8 lists all active tasks in each sequence, as well as the total of MVR values in the presence of non-key components for that sequence.

Table 7

Ten distinct separation tasks and the estimated MVR values for five component mixture

Таблица 7. Десять отдельных задач разделения и оцененные значения MVR для пятикомпонентной смеси

Task #	Feed	Тор	Bottom	MVR
1	ABCD	А	BCD	758.86
2	BCD	В	CD	792.00
3	CD	С	D	0
4	BCD	BC	D	750.86
5	BC	В	С	0
6	ABCD	AB	CD	1296.00
7	AB	А	В	0
8	ABCD	ABC	D	1030.86
9	ABC	А	BC	318.86
10	ABC	AB	С	504.00

Table 8

All active tasks in each sequence and the total of MVR for four component mixture

Таблица 8. Все активные задачи в каждой последовательности и общее количество MVR для четырехкомпонентной смеси

Sequence #	Active tasks			Total MVR	Rank
1	1	2	3	1550.86	5
2	1	4	5	1509.71	3
3	6	7	3	1296.00	1
4	8	9	5	1349.71	2
5	8	10	7	1534.86	4

There are four key splits in a five component mixture as opposed to three in a four component mixture, shown in Table 9. The MVR is computed for each component in each key split, whereas Table 10 displays the twenty separate separation tasks as well as the computed MVR values for nonkey constituents in each task. Table 11 lists all active tasks in each sequence, as well as the total of MVR values in the presence of nonkey components for that sequence.

Separation task analysis was used to find the sequence with the lowest MVR in each of the case studies provided. The study began with finding separation stages (identical feed and end compositions) in that separation superstructure. Once tasks have been created, active tasks from each sequence are represented,

Table 9

Key splits for the five component system *Таблица* 9. Ключевые расщепления для пятикомпонентной системы

S. No.	Key Split (LK/H K)	Arithmetic Average of RV	VA	VB	VC	VD	VE
1	A/B	7.275	-	-	251.72	52.82	55.78
2	B/C	4.25	88.99	1	-	111.36	107.69
3	C/D	2.585	68.17	321.19	-	I	220.82
4	D/E	1.26	57.46	202.65	381.80	-	-

Table 10

Twenty distinct separation tasks and the estimated MVR values for five component

тиолица го. двадцать	различных задач разделения
и оценочные значения	MVR для пяти компонентов

Task #	Feed	Тор	Bottom	Total
1	ABCDE	ABCD	Е	641.91
2	ABCD	ABC	D	389.36
3	ABC	AB	С	88.99
4	AB	А	В	0.00
5	ABC	А	BC	251.72
6	BC	В	C	0.00
7	ABCD	AB	CD	200.35
8	CD	С	D	0.00
9	ABCD	А	BCD	304.55
10	BCD	В	CD	111.36
11	BCD	BC	D	321.19
12	ABCDE	ABC	DE	610.18
13	DE	D	Е	0.00
14	ABCDE	AB	CDE	308.04
15	CDE	CD	E	381.80
16	CDE	С	DE	220.82
17	ABCDE	A	BCDE	360.32
18	BCDE	BCD	Е	584.45
19	BCDE	BC	DE	542.01
20	BCDE	В	CDE	219.05

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Table 11

All active tasks in each sequence and the total of MVR for five component mixture

Таблица 11. Все активные задачи

в каждой последовательности и общее количество MVR для пятикомпонентной смеси

Sequence #	Active tasks			Total	Rank	
1	1	2	3	4	1120.26	11
2	1	2	5	6	1282.99	14
3	1	7	4	8	842.26	5
4	1	9	10	8	1057.81	10
5	1	9	11	6	1267.65	13
6	12	5	6	13	861.90	6
7	12	3	4	13	699.17	3
8	14	4	15	8	689.84	2
9	14	4	16	13	528.86	1
10	17	18	11	6	1265.96	12
11	17	18	10	8	1056.13	9
12	17	19	6	13	902.34	7
13	17	20	15	8	961.17	8
14	17	20	16	13	800.19	4

and the overall MVR value for each sequence is determined. By comparing the total value of MVRs, all sequences are sorted, and the best sequence is determined by the lowest value of MVR, which is rated first. Sequence three, which corresponds to the direct sequence, is shown to be best for the first case study. In the second case study, however, sequence nine is revealed to be the best sequence. Obviously, the best sequence depends on the composition of feed.

CONCLUSION

The aim of this contribution is to find the best sequence for a distillation column network. The column sequencing approach provided here is built on concepts from prior contributions discussed in the introduction. The use of a superstructure enables the disintegration of sequences into independent separation tasks, considerably reducing computing labour. According to the case studies described in this article, separation task development and assessment of MVR for each task is a beneficial technique in distillation network design since it allows for a fast examination of design alternatives. In the case study with a mixture of *i*-Butane, *n*-Butane, *i*-Pentane, and *n*-Pentane, the optimal sequence was determined to be sequence-3 with the lowest MVR. In the second case study of Propane, i-Butane, n-Butane, i-Pentane, and n-Pentane, sequence-9 was shown to be the optimal sequence. The outcomes of this approach is consistent with other methods as well as established algorithms from the literature and it offers the designer the ability to choose a few near-optimal sequences out of a large pool of potential sequences, which may then be studied further.

By comparing the marginal vapour rates of all the active tasks engaged in that sequence, an ideal sequence of distillation columns for a specific feed flow rate and relative volatilities was obtained. The sequence with the lowest total MVR is the ideal sequence, and it is a measure of separation cost.

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