THEORETICAL BASES OF CHEMICAL TECHNOLOGY ТЕОРЕТИЧЕСКИЕ ОСНОВЫ ХИМИЧЕСКОЙ ТЕХНОЛОГИИ

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RESEARCH ARTICLE

Application of diabatic extractive distillation schemes with preliminary separation of azeotropic components for separation of acetone-toluene-*n*-butanol mixture

Pavel S. Klauzner $^{\mathackineq}$, Danila G. Rudakov, Elena A. Anokhina, Andrey V. Timoshenko

MIREA – Russian Technological University (M.V. Lomonosov Institute of Fine Chemical Technologies), Moscow, 119571 Russia ©Corresponding author, e-mail: klauzner@mirea.ru

Abstract

Objectives. The study aims to investigate the effectiveness of the use of various options for organizing the process of diabatic distillation in the separation of a mixture of acetone-toluenen-butanol by extractive distillation using dimethylformamide as an entrainer in a scheme with preliminary separation of azeotropic components.

Methods. As the main research method, mathematical modeling in the Aspen Plus V. 12 software package was used. As a model for describing vapor-liquid equilibrium, the local composition Non-Random Two Liquid equation model was used. Parametric optimization of diabatic schemes was carried out according to the criterion of reduced energy costs.

Results. Based on the scheme for extractive distillation of an acetone-toluene-n-butanol mixture with preliminary separation of azeotropic components, five options for organizing diabatic distillation schemes were considered, both with and without use of a compressor to reach a required flows temperature.

Conclusion. It is shown that the use of diabatic schemes in the extractive distillation of a acetone-toluene-n-butanol mixture with dimethylformamide makes it possible to diminish the reduced energy costs by 8.9–43.5%. Meanwhile the maximum reduction in energy consumption is achieved in a scheme where upper vapor flows of two other columns are used to heat the azeotropic components separating column.

Keywords: extractive distillation, heat integration, diabatic distillation, energy saving

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НАУЧНАЯ СТАТЬЯ

Применение схем неадиабатической экстрактивной ректификации с предварительным отделением азеотропообразующих компонентов для разделения смеси ацетон–толуол–*н*-бутанол

П.С. Клаузнер[⊠], Д.Г. Рудаков, Е.А. Анохина, А.В. Тимошенко

МИРЭА – Российский технологический университет (Институт тонких химических технологий им. М. В. Ломоносова), Москва, 119571 Россия ⊠Автор для переписки, e-mail: klauzner@mirea.ru

Аннотация

Цели. Исследование энергетической эффективности применения неадиабатической экстрактивной ректификации при разделении смеси ацетон-толуол-н-бутанол с диметилформамидом в качестве разделяющего агента в схеме с предварительным отделением азеотропообразующих компонентов.

Методы. В качестве основного метода исследования применялось математическое моделирование с использованием программного комплекса Aspen Plus V. 12. Моделирование парожидкостного равновесия производилось по уравнению локальных составов Non-Random Two Liquid. Параметрическая оптимизация неадиабатических схем проводилась по критерию приведенных энергетических затрат.

Результаты. На основе схемы экстрактивной ректификации смеси ацетон-толуол-н-бутанол с предварительным отделением азеотропообразующих компанентов было рассмотрено пять вариантов организации схем неадиабатической ректификации, как с использованием компрессора для достижения необходимой температуры потоков, так и без него. **Выводы.** Показано, что применение неадиабатической экстрактивной ректификации в схеме разделения смеси ацетон-толуол-н-бутанол с диметилформамидом с предварительным отделением азеотропообразующих компонентов позволяет снизить приведенные энергетические затраты на 8.9–43.5%, при этом максимальное снижение энергозатрат достигается в схеме с использованием для обогрева колонны отделения азеотропообразующих компонентов верхних паровых потоков двух других колонн.

Ключевые слова: экстрактивная ректификация, теплоинтеграция, недиабатическая ректификация, энергосбережение

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INTRODUCTION

The extractive distillation (ED) method is used in the basic organic and petrochemical synthesis industries separate non-ideal to mixtures. However, the use of ED in large-tonnage processes is associated with significant energy consumption, which makes reducing energy costs for its implementation an important task. As in the case of conventional distillation, various methods can be used for this, including internal [1-3] and external [4-6] thermal integration, as well as a combination of these approaches [7-9].

One approach to reducing energy costs in the ED process involves the use of diabatic distillation schemes, in which the external supply (or removal) of heat to the column plates is carried out by means of integrating heat flows between different scheme devices. Although distillation schemes offer numerous diabatic advantages over other thermal integration approaches the specific [10], features and patterns of their application in ED have as vet been little studied.

In a previous work [11], we evaluated the efficiency of the use of diabatic energy distillation in the ED scheme of a mixture of acetone-toluene-n-butanol with dimethylformamide (DMF), in which the entrainer is used in the first column of the scheme. Based on this scheme, four diabatic distillation schemes were proposed, two of which proved to be workable without increasing the pressure of steam flows in compressors, while in the other two, compression of flows in the compressor was necessary to ensure the temperature difference necessary for heat exchange. It was shown that, due to this organization of the diabatic process, the applicable energy costs can be reduced by 11-17%; however, in this case, diabatic distillation schemes with a compressor do not offer significant energy efficiency advantages as compared to schemes without a compressor.

The work set out to synthesize diabatic distillation schemes based on another variant of the conventional ED scheme of a mixture of acetone-toluene-*n*-butanol with DMF involving preliminary isolation of azeotrope-forming components (Fig. 1) and evaluate their energy efficiency.

CALCULATION SECTION

Modeling and determination of optimal scheme parameters were performed in the *Aspen Plus v.12.1*



Fig. 1. Scheme of extractive distillation of the acetone–toluene–*n*-butanol mixture with dimethylformamide as the entrainer with preliminary separation of azeotropic components. Hereinafter: C1 – extractive distillation column, C2 – acetone–toluene separation column, C3 – entrainer regeneration column;
1 – entrainer (DMF); 2 – feed; 3 – acetone; 4 – toluene, 5 – *n*-butanol.

software package (*Aspen Technology*, USA). As initial data for the development of diabatic distillation schemes, the results of optimizing the conventional ED scheme of the studied mixture set out in the dissertation of E.A. Anokhina¹ were used (Fig. 1). In order to describe the vapor–liquid equilibrium in the acetone–toluene–*n*-butanol system with DMF, the Non-Random Two Liquid equation of local compositions of, whose parameters were also published by E.A. Anokhina, was used.

As in our previous work [11], the calculations of the schemes were carried out on 1000 kg/h of the initial mixture containing 71.3 wt % acetone, 14.7 wt % toluene, and 14.0 wt % *n*-butanol. The temperature of the feed stream was 61.8°C; the pressure was 101.3 kPa. The pressure of the top of the columns was assumed to be 101.3 kPa; columns with theoretical plates were considered. The calculations were carried out in the design-verification variant having a fixed product flow quality, which was set to be the same as in the work [11] and the dissertation of E.A. Anokhina-namely, at a 99.5 wt % concentration of acetone and *n*-butanol, a toluene concentration of 99.6 wt %, and a DMF concentration of 99.99 wt %. The optimal operating parameters of the conventional scheme are given in Table 1.

¹ Anokhina E.A. *Extractive distillation in complexes with partially coupled heat and material flows*. Dr. Sci. Thesis (Eng.). Moscow; 2020. 549 p. (in Russ.)

For the practical implementation of diabatic distillation schemes, it is necessary to ensure that the temperature difference of the flow, whose heat is intended for use (i.e., the heat source), as well as the temperature on the plates of the distillation section of the columns into which this heat is directed (the heat receiver), is sufficient to provide the driving force of heat exchange. As in our previous work [11], when modeling schemes, the temperature difference ΔT between the heat source and receiver was assumed to be at least 10°C. To assess the feasibility of implementing diabatic ED schemes with specified heat transfer parameters and preliminary

selection of the required compression ratio $E_{\rm comp}$ in the compressor, an analysis of the temperature profiles of all columns of the conventional scheme was carried out as shown in Fig. 2.

As can be seen, the highest temperatures are observed on the plates of the rectifying sections of columns C1 and C3. Since the temperature on the plates of the rectifying section of column C2 is much lower, only the upper steam flows of columns C1 and C3 were considered for the purposes of ensuring heat transfer in diabatic schemes. Thus, based on the analysis of profiles, five variants of diabatic distillation schemes can be proposed (Fig. 3).

 Table 1. Optimal operating parameters of extractive distillation scheme with preliminary separation of azeotropic components (Footnote 1)

Parameters	C1	C2	С3
N _{total}	45	18	44
N _F	35	10	9
N _s	20	_	_
Q _{reb} , kW	92.3	153.1	107.1
$Q_{\rm cond}, { m kW}$	78.3	146.3	107.1
R	4.4	0.44	3.7
$T_{\rm cond}, ^{\circ}{ m C}$	110.3	56.2	117.8
T _{reb} , °C	142.0	105.9	151.8
S, kg/h	395.3	_	_
T _s , °C	100	_	_
Q _{total} , kW		352.6	

Note: C1 is the extractive distillation column; C2 is the acetone separation column; C3 is the entrainer regeneration column; N_{total} is the total number of plates in a column; N_{F} is the feed plate number in a column; N_{s} is the number of the plate with the entrainer in a column; Q_{reb} is the reboiler heat duty; Q_{cond} is the condenser heat duty; R is the reflux ratio; T_{cond} is the condenser temperature; T_{reb} is the reboiler temperature; S is the entrainer flow rate; T_{s} is the entrainer temperature; Q_{total} is the total heat duty.



Fig. 2. Temperature profiles of columns of conventional extractive distillation scheme: (a) column C1, (b) column C2, (c) column C3.

Scheme I (Fig. 3a). The upper steam flow of the C3 column is used to heat the C2 column. In this case, the flow temperature is sufficient to provide heat supply to any plate of the distillation section of the C2 column without additional compression.

Scheme II (Fig. 3b). Heating of the C2 column is provided using the upper steam flow of the C1 column. In this case, heat supply without the use of a compressor is possible on plates from the 11th to the 14th.

Scheme III (Fig. 3c). Heating of the C2 column is carried out simultaneously with the use of steam flows of the C1 and C3 columns.

Scheme IV (Fig. 3d). The upper steam flow of column C1 is used to heat column C3. In this case, in order to ensure a given temperature difference ΔT between the heat source and receiver, it is necessary to use a compressor with a compression ratio of at least 2.4.

Scheme V (Fig. 3e). To heat the column C1, the upper steam flow of the column C3 is used. In this case, in order to provide the driving force of heat exchange, it is also necessary to compress the flow with compression ratio $1.6 \le E_{\rm comp} \le 2.2$. When $E_{\rm comp} > 2.2$ it is possible to supply heat to the reboiler of the column C1 and, thus, the implementation of an adiabatic scheme with a heat pump.

Note that in the schemes using a compressor, a preheater is installed in front of it to prevent possible cavitation. The thermal duty on the preheater is designated by $Q_{\rm PH}$.

A comparison of diabatic distillation schemes with the conventional ED scheme was carried out according to the criterion of reduced energy costs (Q_{cons}) , which were calculated according to the formula proposed by the authors [12]:

$$Q_{\rm cons} = Q_{\rm total} + 3W_{\rm comp},\tag{1}$$

where Q_{total} is the total energy costs in the column reboilers, kW; W_{comp} is the power consumed by the compressor, kW.

The correct relative evaluation of schemes involves comparing their energy consumption with an optimal set of operating parameters for each of them. The optimal parameters of the conventional ED scheme, which are defined in the dissertation of E.A. Anokhina (Footnote 1), are presented in Table 1.

The criterion for optimizing diabatic schemes was the given energy costs, $Q_{\rm cons}$. The optimization parameters were the position of the heat supply plate to the stripping section of the column, $N_{\rm HE}$; the amount of heat supplied, $Q_{\rm HE}$; and the compression ratio in the compressor, $E_{\rm comp}$, necessary to ensure the accepted value ΔT . At the same time, the optimization procedure had some features for each of the schemes under consideration.

As already mentioned, the temperature of the flow coming out of the top of the column C3 $(T_{cond} = 117.8^{\circ}C)$ in Scheme I is sufficient









Fig. 3. Diabatic extractive distillation schemes: (a) Scheme I, (b) Scheme II, (c) Scheme III, (d) Scheme IV, (e) Scheme V.

to provide heat supply to any of the plates of the stripping section of the column C2. At the same time, all the heat given off by this flow at full condensation, 107.2 kW, can be used. Thus, for this scheme, the only optimization parameter is the position of the heat supply plate $N_{\rm HE}$. The results reflecting the search for the optimal position of $N_{\rm HE}$ are presented in Table 2.

It can be seen that, the closer the heat supply plate $N_{\rm HE}$ is located to the reboiler, the lower the

reflux ratio and the duty on the column reboiler. The most effective variant is the heat supply to the lower (17th) plate of the column. The optimal operating parameters of Scheme I are presented in Table 3.

The optimization of Scheme II was carried out similarly, the only difference being that here the temperature of the upper steam flow of column C1 ($T_{\rm cond} = 110.3^{\circ}$ C) is sufficient only to supply heat to the plates of the distillation section of column C2 from the 11th to the 14th. The results

$N_{_{ m HE}}$	${\it Q}_{_{ m HE}},$ kW	${\it Q}_{ m reb}{}^{ m C2}$, kW	R ^{C2}
11	107.2	57.18	0.56
12	107.2	53.38	0.52
13	107.2	51.16	0.52
14	107.2	49.52	0.48
15	107.2	48.20	0.47
16	107.2	47.16	0.46
17	107.2	46.39	0.45

Table 2. Dependence of the parameters of column C2 for diabatic Scheme I on the position of the heat supply stage $N_{\rm HE}$

Note: N_{HE} is the heat supply plate number in the heat exchanger; Q_{HE} is the exchanger heat duty; C2 is the acetone separation column; Q_{reb}^{C2} is the reboiler heat duty in C2; R^{C2} is the reflux ratio in C2.

Table 3. Optimal operation parameters for diabatic Scheme I

Parameters	C1	C2	С3
$N_{ m total}$	45	18	44
N _{he}	_	17	_
$Q_{\rm reb}$, kW	92.3	46.4	107.1
R	4.4	0.45	3.7
Q _{he} , kW	_	107.2	-
$Q_{\rm cons}$, kW		245.8	

Note: N_{total} is the total number of plates in the column; N_{HE} is the heat supply plate number in the heat exchanger; Q_{reb} is the reboiler heat duty; R is the reflux ratio; Q_{HE} is the exchanger heat duty; Q_{cons} is the reduced energy consumption in the scheme with thermal integration.

of determining the optimal position of $N_{\rm HE}$ in the C2 column of Scheme II are presented in Table 4, and the optimal operating parameters for the diabatic Scheme II are shown in Table 5.

For Scheme III, it is necessary to determine the optimal positions of two heat supply

plates— $N_{\rm HE}^{-1}$ (from column C1) and $N_{\rm HE}^{-2}$ (from column C3)—into column C2, as well as the amount of heat supplied transferred from the steam flow of column C1 ($Q_{\rm HE}^{-1}$) and the steam flow of column C3 ($Q_{\rm HE}^{-2}$). The optimization results are shown in Table 6.

$N_{ m HE}$	${\cal Q}_{_{ m HE}},{ m kW}$	${\it Q}_{ m reb}{}^{ m C2}$, kW	R ^{C2}
11	78.3	80.27	0.50
12	78.3	77.95	0.48
13	78.3	76.93	0.47
14	78.3	76.29	0.46

Table 4. Dependence of the	parameters of column	C2 for diabatic Scheme	II on the position of	f the heat supply stage $N_{\rm u}$
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Note: N_{HE} is the heat supply plate number in the heat exchanger; Q_{HE} is the exchanger heat duty; C2 is the acetone separation column; Q_{reb}^{C2} is the reboiler heat duty in C2; R^{C2} is the reflux ratio in C2.

Parameters	C1	C2	С3
$N_{ m total}$	45	18	44
$N_{ m HE}$	_	14	_
$Q_{ m reb}, m kW$	92.3	76.3	107.1
R	4.4	0.46	3.7
$Q_{\rm HE}$, kW	_	78.3	_
$Q_{\rm cons}$, kW		275.7	

Table 5. (Optimal	operation	parameters for	or diabatic	Scheme II
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Note: N_{total} is the total number of plates in the column; N_{HE} is the heat supply plate number in the heat exchanger; Q_{reb} is the reboiler heat duty; R is the reflux ratio; Q_{HE} is the exchanger heat duty; Q_{cons} is the reduced energy consumption in the scheme with thermal integration.

It can be seen that the amount of heat released during the complete condensation of steam flows at the position $N_{\rm HE}^2 = 16$ or $N_{\rm HE}^2 = 17$ is excessive; when implementing such a scheme, additional heat supply to the reboiler of the C2 column is not required. At the same time, the lowest values of the reflux ratio in the C2 column are observed at $N_{\rm HE}^{-1} = 13$ and $N_{\rm HE}^{-2} = 17$. The optimal operating parameters of Scheme III are presented in Table 7.

In Scheme IV (Fig. 3d), the temperature of the upper steam flow of column C1 ($T_{cond} = 110.3^{\circ}$ C)

insufficient to provide heating of the is distillation section of column C3. To achieve the necessary temperature difference, it is necessary to increase the flow pressure in the compressor. Thus, for this scheme it is necessary to determine both the optimal position of the plate $N_{\rm HE}$ and the optimal value of the compression ratio in the compressor $E_{\rm comp}$. It follows from Eq. (1) that the minimum value of the reduced energy costs (Q_{cons}) will be achieved with a minimum W_{comp} , and, accordingly, with a minimum E_{comp} , at which the difference necessary temperature

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$N_{ m HE}^{-1}$	$N_{ m HE}^{2}$	$Q_{\rm HE}^{1}$, kW	$Q_{\rm HE}^{2}$, kW	R ^{C2}	$Q_{ m reb}^{ m C2}$, kW
	11	78.3	107.2	0.92	27.91
	12	78.3	107.2	0.87	22.80
	13	78.3	107.2	0.82	17.67
11	14	78.3	107.2	0.76	11.95
	15	78.3	107.2	0.70	5.25
	16	68.6	107.2	0.59	0.00
	17	54.0	107.2	0.47	0.00
	11	78.3	107.2	0.87	23.25
	12	78.3	107.2	0.86	22.17
	13	78.3	107.2	0.81	17.04
12	14	78.3	107.2	0.76	11.29
	15	78.3	107.2	0.69	4.49
	16	66.0	107.2	0.57	0.00
	17	52.6	107.2	0.46	0.00
	11	78.3	107.2	0.83	18.55
	12	78.3	107.2	0.82	17.45
	13	78.3	107.2	0.81	16.47
13	14	78.3	107.2	0.75	10.70
	15	78.3	107.2	0.68	3.80
	16	64.7	107.2	0.56	0.00
	17	51.9	107.2	0.45	0.00
	11	78.3	107.2	0.78	13.32
	12	78.3	107.2	0.76	12.15
	13	78.3	107.2	0.75	11.11
14	14	78.3	107.2	0.74	10.15
	15	78.3	107.2	0.68	3.13
	16	63.2	107.2	0.54	0.00
	17	51.3	107.2	0.49	0.00

Table 6. Results of the search for optimal operating parameters of the diabatic Scheme III

Note: N_{HE}^{-1} is the heat supply plate number in the heat exchanger to column C2 from column C1; N_{HE}^{-2} is the heat supply plate number in the heat exchanger to column C2 from column C3; Q_{HE}^{-1} is the exchanger heat duty from the steam flow of column C1; Q_{HE}^{-2} is the exchanger heat duty from the steam flow of column C3; C2 is the acetone separation column; $Q_{\text{reb}}^{-\text{C2}}$ is the reboiler heat duty in C2; R^{C2} is the reflux ratio in C2.

Parameters	C1	C2	С3
$N_{ m total}$	45	18	44
$N_{\rm HE}^{-1}$	_	13	_
N _{HE} ²	_	17	_
$Q_{ m reb}, m kW$	92.3	0	107.1
R	4.4	0.45	3.7
$Q_{\rm HE}^{\ \ l}, {\rm kW}$	_	51.9	_
$Q_{\rm HE}^{2}$, kW	_	107.2	_
$Q_{\rm cons}$, kW		199.4	·

Table 7. Optimal	operation	parameters fo	r diabatic	Scheme	III
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Note: N_{total} is the total number of plates in the column; N_{HE}^{-1} is the heat supply plate number in the heat exchanger to column C2 from column C1; N_{HE}^{-2} is the heat supply plate number in the heat exchanger to column C2 from column C3; Q_{reb} is the reboiler heat duty; *R* is the reflux ratio; Q_{HE}^{-1} is the exchanger heat duty from the steam flow of column C1; Q_{HE}^{-2} is the exchanger heat duty in the preheater; E_{comp} is the compressor compression ratio; W_{comp} is the compressor power consumption; Q_{cons} is the reduced energy consumption in the scheme with heat integration.

Table 8. Results of the search for optimal operating parameters of the diabatic Scheme IV

$E_{_{ m comp}}$	W _{comp} , kW	$N_{_{ m HE}}$	$Q_{_{ m HE}},{ m kW}$	$Q_{\rm reb}^{\rm C3}$, kW	$Q_{_{ m PH}}$, kW	${\it Q}_{ m cons}, { m kW}$
2.4	9.0	10	71.4	99.7	4.5	131.2
2.5	9.5	12	71.3	96.2	4.5	129.2
2.6	9.9	14	71.0	92.9	4.5	127.1
2.7	10.3	15	70.9	91.3	4.9	127.1
2.8	10.8	43	70.9	36.8	5.2	74.4

Note: E_{comp} is the compressor compression ratio; W_{comp} is the compressor power consumption; N_{HE} is the heat supply plate number in the heat exchanger; Q_{HE} is the exchanger heat duty; C3 is the extractive distillation column; $Q_{\text{reb}}^{\text{C3}}$ is the reboiler heat duty in C3; Q_{PH} is the heat duty in the preheater; Q_{cons} is the reduced energy consumption in the scheme with thermal integration.

between the heat source and receiver is provided. At the same time, the minimum value of $E_{\rm comp}$ depends on the position of the heat supply plate. The results of optimization of Scheme IV are shown in Table 8.

It is interesting to note that, with an increase in Ecomp from 2.4 to 2.7, the range of plates in the exhaustive section, to which heat supply in the C3 column is possible, increases smoothly; with $E_{\rm comp} = 2.8$, there is a sharp jump, and heat supply becomes possible to any plate of the stripping section of the column. This is probably due to the characteristics of the temperature profile along the height of the column C3 (Fig. 2c), in the stripping section of which there is a zone where the temperature along the height of the column practically does not change. The optimal operating parameters of Scheme IV are presented in Table 9.

The optimization of Scheme V was carried out in a similar way. The results are presented in Tables 10 and 11.

Table 9. Optimal operation parameters for diabatic Scheme IV

RESULTS AND DISCUSSION

Table 12 shows the values of the reduced energy consumption for the conventional two-column ED scheme and the diabatic ED schemes obtained on its basis. The decrease of the reduced energy consumption $\Delta Q_{\rm cons}$ was calculated by Eq. (2):

$$\Delta Q_{\rm cons} = (Q_{\rm total} - Q_{\rm cons}) / Q_{\rm total} \times 100\%, \tag{2}$$

where $Q_{\rm total}$ is the total energy costs in the reboilers of the columns of the conventional ED scheme, and $Q_{\rm cons}$ is the reduced energy costs of the diabatic distillation scheme.

Table 12 shows that the greatest reduction in energy consumption compared to the conventional scheme is provided by diabatic Schemes I, II, and III, in which there are no compressors.

Parameters	C1	C2	С3	
$N_{ m total}$	45	18	44	
N _{HE}	_	_	43	
$Q_{\rm reb}$, kW	92.3	153.1	36.8	
R	4.4	0.44	3.7	
$Q_{\rm HE}$, kW	_	_	70.9	
$Q_{_{\mathrm{PH}}}$, kW	5.2	_	_	
E _{comp}	2.8	_	_	
W _{comp} , kW	10.8	_	_	
$Q_{\rm cons}$, kW	319.8			

Note: N_{total} is the total number of plates in the column; N_{HE} is the heat supply plate number in the heat exchanger; Q_{reb} is the reboiler heat duty; R is the reflux ratio; Q_{HE} is the exchanger heat duty; Q_{pH} is the heat duty in the preheater; E_{comp} is the compressor compression ratio; W_{comp} is the compressor power consumption; Q_{cons} is the reduced energy consumption in the scheme with thermal integration.

E _{comp}	W _{comp} , kW	$N_{_{ m HE}}$	$Q_{_{ m HE}}$, kW	$Q_{\rm reb}^{\rm C1}$, kW	$Q_{_{ m PH}}$, kW	${\it Q}_{ m cons},$ kW
1.6	1.1	37	10.8	89.3	0.2	92.8
1.7	1.3	38	12.4	87.4	0.3	91.6
1.8	1.4	39	14.4	85.4	0.3	89.9
1.9	2.0	42	27.9	71.7	0.5	78.2
2.0	3.1	43	40.1	59.6	0.7	69.6
2.2	4.0	44	44.3	50.1	0.9	63.0

Note: E_{comp} is the compressor compression ratio; W_{comp} is the compressor power consumption; N_{HE} is the heat supply plate number in the heat exchanger; Q_{HE} is the exchanger heat duty; C1 is the extractive distillation column; $Q_{\text{reb}}^{\text{C1}}$ is the reboiler heat duty in C1; Q_{PH} is the heat duty in the preheater; Q_{cons} is the reduced energy consumption in the scheme with thermal integration.

Table 11. Optimal operation parameters for diabatic Scheme V

Parameters	C1	C2	С3	
N _{total}	45	18	44	
N _{HE}	44	_	_	
$Q_{\rm reb}$, kW	50.1	153.1	107.1	
R	4.4	0.44	3.7	
Q _{HE} , kW	44.3	_	_	
$Q_{\rm PH}$, kW	_	_	0.9	
E _{comp}	_	_	2.2	
W _{comp} , kW	_	_	4.0	
$Q_{\rm cons}$, kW		323.2	<u>.</u>	

Note: N_{total} is the total number of plates in the column; N_{HE} is the heat supply plate number in the heat exchanger; Q_{reb} is the reboiler heat duty; R is the reflux ratio; Q_{HE} is the exchanger heat duty; Q_{PH} is the heat duty in the preheater; E_{comp} is the compressor compression ratio; W_{comp} is the compressor power consumption; Q_{cons} is the reduced energy consumption in the scheme with thermal integration.

Davamatana	Scheme							
rarameters	Convent.	I	П	III	IV	V		
$Q_{ m total}, { m kW}$	352.6	245.8	275.7	199.4	282.2	304.5		
W _{comp} , kW	0	0	0	0	10.8	4.0		
$Q_{\rm cons}$, kW	352.6	245.8	275.7	199.4	319.8	323.2		
$\Delta Q_{\rm cons}, \%$	0	30.3	21.8	43.5	9.3	8.9		

 Table 12. Energy efficiency of various variants of extractive distillation schemes

Note: Q_{total} is total energy costs in reboilers of the columns in the conventional scheme; W_{comp} is the compressor power consumption; Q_{cons} is the reduced energy consumption in the heat integration scheme; ΔQ_{cons} is the decrease in the reduced energy consumption in the heat integration scheme.

At the same time, the energy efficiency of Scheme I is higher than Scheme II, since more heat is released during condensation of the steam flow of column C3 than during condensation of the steam flow of column C1; as a result, the energy consumption in the reboiler of column C2 in Scheme I is reduced by 3.3 times, while in Scheme II, consumption is reduced by only 2 times compared to the conventional scheme. The maximum decrease of the reduced energy consumption is achieved in Scheme III: in this scheme, additional heat supply to the reboiler of column C2 ($Q_{reb}^{C2} = 0$) is not required, since steam flows coming out from above columns C1 and C3 adequately provide its heating, while compression of steam flows using a compressor to increase their temperature is also not required. The energy efficiency of Schemes IV and V is significantly lower than that of Schemes I-III, although the energy consumption in the reboiler of the column C3 of Scheme IV is reduced by 2.9 times, while in the reboiler of the column C1 of Scheme V, energy consumption is reduced by 1.8 times compared with the energy consumption of the corresponding columns of the conventional scheme. This is due both to the presence of compressors in Schemes IV and V, as well as to the fact that the share of column C1 and column C3 in the total energy consumption of the conventional Scheme 2 is 26.2 and 30.4%, respectively, and the share of column C2 is 43.4%; therefore, reducing energy consumption in the

reboilers of these columns makes a smaller contribution to reducing the energy consumption of the Scheme 2 than the reduction of energy consumption in the reboiler of the C2 column.

CONCLUSIONS

Thus, five variants of schemes with thermal integration of columns due to diabatic distillation were synthesized based on the conventional ED scheme of an acetone-toluene-n-butanol mixture with preliminary separation of azeotropeforming components. The optimal parameters of these schemes are determined by the criterion of reduced energy costs. The schemes of diabatic ED are shown to be characterized by 8.9-43.5% lower reduced energy consumption than the conventional two-column scheme. At the same time, the greatest reduction in energy consumption is achieved in the scheme of diabatic distillation, in which steam flows coming from above two other columns are used to heat the separation column of azeotrope-forming components: ED columns and DMF regeneration columns.

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Authors' contributions

P.S. *Klauzner* – planning and conducting research, analyzing research materials, writing the manuscript;

D.G. Rudakov – conducting research, analyzing research materials;

E.A. Anokhina – management and scientific consulting;
 A.V. Timoshenko – formulation of the scientific concept, general management.

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About the authors:

Pavel S. Klauzner, Cand. Sci. (Eng.), Assistant, Department of Chemistry and Technology of Basic Organic Synthesis, M.V. Lomonosov Institute of Fine Chemical Technologies, MIREA – Russian Technological University (86, Vernadskogo pr., Moscow, 119571, Russia). E-mail: klauzner@mirea.ru. ResearcherID AAJ-7842-2021, RSCI SPIN-code 6922-6509, https://orcid. org/0000-0001-5844-549X

Danila G. Rudakov, Cand. Sci. (Eng.), Associate Professor, Department of Chemistry and Technology of Basic Organic Synthesis, M.V. Lomonosov Institute of Fine Chemical Technologies, MIREA – Russian Technological University (86, Vernadskogo pr., Moscow, 119571, Russia). E-mail: rudakov@mirea.ru. Scopus Author ID 37018548000, ResearcherID M-5241-2014, RSCI SPIN-code 2366-9449, https://orcid.org/0000-0002-9892-7909

Elena A. Anokhina, Dr. Sci. (Eng.), Professor, Department of Chemistry and Technology of Basic Organic Synthesis, M.V. Lomonosov Institute of Fine Chemical Technologies, MIREA – Russian Technological University (86, Vernadskogo pr., Moscow, 119571, Russia). E-mail: anokhina.ea@mail.ru. Scopus Author ID 6701718055, ResearcherID E-5022-2016, RSCI SPIN-code 8161-7762

Andrey V. Timoshenko, Dr. Sci. (Eng.), Professor, Department of Chemistry and Technology of Basic Organic Synthesis, M.V. Lomonosov Institute of Fine Chemical Technologies, MIREA – Russian Technological University (86, Vernadskogo pr., Moscow, 119571, Russia). E-mail: timoshenko@mirea.ru. Scopus Author ID 56576076700, ResearcherID Y-8709-2018, RSCI SPIN-code 5687-7930, https://orcid.org/0000-0002-6511-7440

Об авторах:

Клаузнер Павел Сергеевич, к.т.н., ассистент кафедры химии и технологии основного органического синтеза Института тонких химических технологий им. М.В. Ломоносова ФГБОУ ВО «МИРЭА – Российский технологический университет» (119571, Россия, Москва, пр-т Вернадского, д. 86). E-mail: klauzner@mirea.ru. ResearcherID AAJ-7842-2021, SPIN-код РИНЦ 6922-6509, https://orcid.org/0000-0001-5844-549X

Рудаков Данила Григорьевич, к.т.н., доцент кафедры химии и технологии основного органического синтеза Института тонких химических технологий им. М.В. Ломоносова ФГБОУ ВО «МИРЭА – Российский технологический университет» (119571, Россия, Москва, пр-т Вернадского, д. 86). Е-mail: rudakov@mirea.ru. Scopus Author ID 37018548000, ResearcherID M-5241-2014, SPIN-код РИНЦ 2366-9449, https://orcid.org/0000-0002-9892-7909

Анохина Елена Анатольевна, д.т.н., профессор кафедры химии и технологии основного органического синтеза Института тонких химических технологий им. М.В. Ломоносова ФГБОУ ВО «МИРЭА – Российский технологический университет» (119571, Россия, Москва, пр-т Вернадского, д. 86). E-mail: anokhina.ea@mail.ru. Scopus Author ID 6701718055, ResearcherID E-5022-2016, SPIN-код РИНЦ 8161-7762

Тимошенко Андрей Всеволодович, д.т.н., профессор кафедры химии и технологии основного органического синтеза Института тонких химических технологий им. М.В. Ломоносова ФГБОУ ВО «МИРЭА – Российский технологический университет» (119571, Россия, Москва, пр-т Вернадского, д. 86). E-mail: timoshenko@mirea.ru. Scopus Author ID 56576076700, ResearcherID Y-8709-2018, SPIN-код РИНЦ 5687-7930, https://orcid.org/0000-0002-6511-7440

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