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RESEARCH ARTICLE

Energy saving in the extractive distillation of isobutyl alcohol–isobutyl acetate with *n*-butyl propionate

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Objectives. *Determination of the effectiveness of using various types of heat pumps in the extractive distillation of an isobutyl alcohol–isobutyl acetate mixture with n-butyl propionate as the entrainer.*
Methods. *As the main research method, mathematical modeling was performed using the Aspen Plus V. 9 software package. As a model for describing the vapor–liquid equilibrium, the local composition equation-based UNIQUAC model was employed, and the Redlich–Kwong model was adopted to examine the non-ideal vapor phase. When modeling the conventional scheme of extractive distillation, parametric optimization was carried out according to the criterion of total energy costs in the reboilers of the columns. For economical evaluation, Aspen Process Economic Analyzer V10.1 tools were employed.*
Results. *In comparison with the conventional extractive distillation scheme, three variants of schemes with vapor-recompression heat pumps were considered: with a heat pump placed on an extractive distillation column, on an extractive agent regeneration column, and with two heat pumps placed on both columns of the scheme. A scheme with an internal heat pump was also proposed, in which the heat pump compressor is located between sections of the extractive column that operate at different pressures: 506.6 kPa in the top sections and 101.3 in the bottom section. An economic analysis was conducted for all the considered schemes to calculate the total annual costs. It was shown that schemes with vapor-recompression heat pumps can significantly reduce the energy costs of extractive distillation by up to 39.6%; however, a significant reduction in the total annual costs is achieved only with sufficiently long operation periods of the plants. The reduction in the energy costs in the scheme with an internal heat pump was 44%, and the total annual costs were in the range of 20.2–30.1%, depending on the operating time of the plant.*
Conclusions. *It was shown that using heat pumps in the extractive distillation of the mixture of isobutyl alcohol–isobutyl acetate with n-butyl propionate as the entrainer can significantly reduce energy costs. The scheme with an internal heat pump is the most economical of all the considered schemes.*

Keywords: *extractive distillation, heat pump, energy saving.*

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ОРИГИНАЛЬНАЯ СТАТЬЯ

Энергосбережение в экстрактивной ректификации смеси изобутиловый спирт–изобутилацетат с бутилпропионатом

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Цели. *Определение эффективности применения тепловых насосов различного типа в экстрактивной ректификации смеси изобутиловый спирт–изобутилацетат с н-бутилпропионатом в качестве разделяющего агента.*
Методы. *Основной метод исследования – математическое моделирование в программном комплексе Aspen Plus V. 9. В качестве модели описания парожидкостного равновесия применялась основанная на уравнении локальных составов модель UNIQUAC, для учета неидеальности паровой фазы – модель Редлиха–Квонга. При моделировании традиционной схемы экстрактивной ректификации производилась параметрическая оптимизация по критерию суммарных энергетических затрат в кипятильниках колонн. Для экономической оценки применялись инструменты Aspen Process Economic Analyzer V10.1.*
Результаты. *В сравнении с традиционной схемой экстрактивной ректификации рассмотрено три варианта схемы с применением тепловых насосов открытого типа – с размещением теплового насоса на колонне экстрактивной ректификации, на колонне регенерации разделяющего агента и с размещением двух тепловых насосов на обоих колоннах схемы. Также предложена схема с внутренним тепловым насосом, в которой компрессор теплового насоса расположен между секциями экстрактивной колонны, которые работают при различных давлениях – 506.6 кПа в укрепляющей и экстрактивной секциях и 101.3 в отгонной. Была произведена экономическая оценка всех рассмотренных схем и вычисление полных приведенных затрат. Показано, что применение схем с тепловыми насосами открытого типа позволяет значительно, вплоть до 39.6%, снизить энергетические затраты на экстрактивную ректификацию, однако значительное снижение полных приведенных затрат достигается только при достаточно большом сроке функционирования установок. Снижение энергетических затрат в схеме с внутренним тепловым насосом составило 44%, а полных приведенных затрат – 20.2–30.1% в зависимости от времени функционирования установки.*
Выводы. *Показано, что применение тепловых насосов в процессе экстрактивной ректификации смеси изобутиловый спирт–изобутилацетат с бутилпропионатом в качестве разделяющего агента позволяет значительно снизить энергетические затраты. Наиболее экономичной из рассмотренных является схема с применением внутреннего теплового насоса.*

Ключевые слова: *экстрактивная ректификация, тепловой насос, энергосбережение.*

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INTRODUCTION[1]

Distillation is one of the main industrial processes for purifying and separating mixtures of different chemical components, and it is characterized by high specific energy costs [1]. This process consumes a significant amount of energy due to its low thermodynamic efficiency; consequently, researchers are constantly searching for strategies to reduce energy consumption. Currently, the main strategies for improving individual processes and technological schemes include internal [2] and external heat integration [3], as well as the use of heat pumps [4, 5].

Extractive distillation (ED), a process based on the application of a special additional entrainer that changes (increases, circulates) the relative volatility of the components of the initial mixture, is used for the separation of azeotrope mixtures and mixtures of components with relative volatility close to one. In the chemical industry, it is used to isolate benzene from pyrolysis and reforming fractions [6], as well as butadiene and isoprene from the pyrolysis and dehydrogenation products of C_4–C_5 fractions [7]. Even though ED, in some cases, is characterized by significantly lower energy consumption than that of azeotropic distillation [8, 9] and that the separation method is based on pressure variation [10–13], reducing the energy costs associated with its operation is an urgent task due to the multi-tonnage technologies of basic organic and petrochemical syntheses, for which it is mainly used [14]. The aforementioned approaches for improving conventional distillation have been employed to improve the ED process. A significant difference is that the use of external heat pumps for conventional distillation is already widespread, e.g., the technology for the distillation of propane–propylene fraction, while the incorporation of this approach in ED is still at the beginning stages [15].

The purpose of this work is to study the methods of applying heat pumps of various types to increase the energy efficiency of ED.

The technological schemes of the ED of an azeotropic mixture of isobutyl alcohol (IBA)–isobutyl acetate (IBAC) with *n*-butylpropionate (BP) as an entrainer were selected as the object of research. Since the mathematical modeling of chemical and technological processes is a powerful modern method for developing new technologies and improving traditional approaches [16], the Aspen Plus software package version 9.0 was used to solve the problem of increasing the separation efficiency of the above mixture.

Modeling of the conventional ED scheme

To simulate the vapor–liquid equilibrium, the UNIQUAC model was adopted, the parameters of which are shown in Table 1. We used both the binary interaction parameters built-in Aspen Plus for the IBA–IBAC system, which provide a more accurate description of the vapor–liquid equilibrium compared to [11], and the data [11] for the IBA–entrainer and IBAC–entrainer systems, since there are no built-in parameters for them. The average relative errors for each binary pair, when described by parameters from different sources, are shown in Table 2. To account for the imperfection of the vapor phase, the Redlich–Kwong equation of state was used.

To separate the mixture under consideration, both a conventional ED system with a heavy-boiling entrainer (Fig. 1) and systems using external and internal vapor-recompression heat pumps can be used. Since the ED of a binary mixture is conducted using a two-column system, heat pumps can be used separately for each of the columns or simultaneously for the two columns.

For all variants of the schemes, we considered the separation of the initial IBA–IBAC mixture with

Table 1. Binary coefficients of the UNIQUAC model

Component	Source			
	Liter.	DB	Liter.	Liter.
Component i	IBA	IBA	IBA	IBAC
Component j	IBAC	IBAC	BP	BP
a_{ij}	0.26671	0	0	0
a_{ji}	0.22675	0	0	0
b_{ij}	−58.459	1.3501	−17.787	−65.929
b_{ji}	−182.110	−45.3251	−24.770	64.567

[1] See the list of abbreviations at the end of the article for the introduced designations.

Table 2. Relative errors of the vapor–liquid equilibrium (VLE) modeling

Source	Component i	Component j	ΔY^R, %	ΔT^R, %
Liter.	IBA	IBA	1.58	0.44
DB	IBA	IBA	1.37	0.36
Liter.	IBA	BP	1.82	0.11
Liter.	IBAC	BP	1.88	0.26

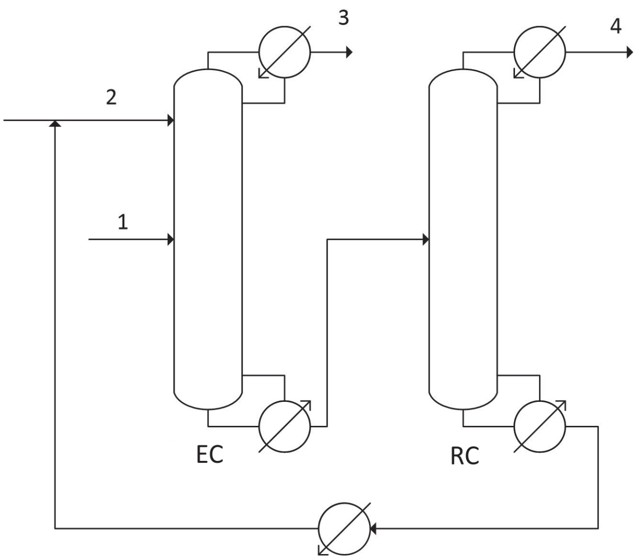

Fig. 1. Conventional scheme of the ED of mixture IBA–IBAC with BP as the entrainer. EC is the ED column, and RC is the entrainer regeneration column. (1) Feed, (2) entrainer, (3) IBA, (4) IBAC.

a concentration of 41 wt % isobutyl alcohol, a feed rate of 1500 kg/h, a temperature of 100°C, and a pressure of 108 kPa. The concentrations of IBA and IBAC in the product streams were maintained constant and equal to 99.5 mass %.

For the conventional ED (Fig. 1), the optimal operating parameters were selected according to the algorithm proposed in [17].

The pressure at the top of the columns was fixed at 101.3 kPa, and theoretical plates (TPs) with a pressure drop of 0.1013 kPa across the plates were considered. Calculations were performed in the design and verification version with the fixed quality of product flows. During the optimization process, the total number of plates in both columns, feed plates in the EC and RC columns, feed plate of the entrainer in the EC column, flow rate of the entrainer, and temperature of the entrainer were determined. The optimization criterion was the total heat duty on the reboilers Q_{total}. For optimization, we used the built-in tools of the Aspen Plus software package, such as the NQ curve, Sensitivity Analysis, and SQP optimization. The optimization procedure included several stages.

At the first stage, the total number of TPs in the columns was determined using the NQ curve tool with a fixed flow rate of the entrainer equal to 3000 kg/h: 66 and 48 in the EC and RC, respectively.

Further, the dependence of the operating parameters of the EC on the temperature of the entrainer feeding into it was studied. The data are shown in Table 3.

Table 3 shows that the energy consumption in the EC reboiler is almost independent on the entrainer supply temperature. The reflux ratio and steam flow in the upper part of the column increase by about 1.15 times when the $T_{entrainer}$ is increased from 110 to 146°C. As noted by M.K. Zakharov [20], an increase in the reflux ratio results in an increase in the internal energy savings during distillation, and an increase in the steam flow causes an increase in the efficiency of the heat pump application. Considering the above, we selected the entrainer supply temperature in the EC, equal to 146°C. In addition, the entrainer supply at this temperature allows you not to complicate the system with additional heat exchange on the recycling line of the separating agent.

Table 3. Dependence of the EC parameters on the entrainer temperature

T_S, °C	N_S/N_F	R	Q_{cond}, kW	Q_{reb}, kW
110	13/52	4.58	−533.7	611.7
120	13/52	4.78	−552.4	611.6
130	13/52	4.97	−571.2	610.9
140	13/52	5.17	−590.4	610.8
146	13/52	5.29	−601.4	610.6

To determine the limits of variation in the flow of entrainer, the minimum required amount of the entrainer, at which it is still possible to obtain products of a given quality for different positions of the NF and NS feed plates, is determined. The optimal entrainer feed rate at which the Q_{reb}^{EC} reaches the minimum value is determined. The results are presented in Table 4.

Based on these results, 2450 kg/h and 3300 kg/h were selected as the limits of variation of the entrainer feed rate for the subsequent optimization procedure of the two-column ED scheme. Further, within the established limits of variation of the entrainer feed rate, it is shown, by computational experiments, that this parameter does not affect the optimal position of the feed plate in the RC. The results are presented in Table 5.

The minimum energy consumption is observed when the feed flow to the RC is located on the 22nd TP. In the future, when determining the optimal parameters of the ED scheme as a whole, this feed plate should be fixed in the regeneration column.

Using the Sensitivity Analysis and SQP Optimization tools simultaneously, the optimal position of the feed plates and the entrainer in the EC and the optimal flow rate of the entrainer for the two-column ED complex were determined. In this case, the Sensitivity Analysis tool varied the positions of the feed plates and the entrainer, and using SQP for each fixed position NS/NF, the optimal flow of the entrainer was selected, at which value the total duty on the column boilers ($Q_{\text{total}} = Q_{\text{reb}}^{\text{EC}} + Q_{\text{reb}}^{\text{RC}}$) reaches the minimum value. The results are presented in Table 6.

The final operating parameters of the conventional ED scheme are presented in Table 7. The optimal amount of the entrainer supplied is 2671 kg/h, and the entrainer temperature is 146°C.

Modeling schemes with vapor-recompression heat pumps

Plesu *et al.* [18] proposed a method for the preliminary assessment of the feasibility of using heat pumps in distillation based on the efficiency coefficient (C_{ef})

$$C_{ef} = \frac{Q_{\text{reb}}}{A} = \frac{T_{\text{reb}}}{\left(T_{\text{reb}} - T_{\text{cond}}\right)} \,, \qquad (1)$$

Table 4. The minimal and optimal (for EC) entrainer rate depending on the position of N_S/N_F

N_S/N_F	S_{min}, kg/h	S_{opt}, kg/h	Q_{reb} at S_{min}, kW	Q_{reb} at S_{opt}, kW
12/51	2390	3000	721.2	603.3
12/52	2360	3050	710.3	601.3
12/53	2340	3100	715.2	604.6
13/51	2400	3050	738.1	603.2
13/52	2370	3100	708.5	605.5
13/53	2350	3150	721.1	608.9
14/51	2450	3200	730.9	605.7
14/52	2420	3250	702.2	607.3
14/53	2400	3300	725.5	610.5

Table 5. The optimal feed stage in the entrainer regeneration column at various entrainer amounts

S, kg/h	N_F	Q_{reb}, kW	Q_{cond}, kW	*R*
2450	22	358.9	−354.5	3.6
2600	22	378	−373.5	3.9
2800	22	397.7	−393.1	4.1
3000	22	417.4	−412.8	4.4
3300	22	437.2	−432.5	4.6

Table 6. Determination of the optimal operation parameters of the conventional ED scheme

N_S	N_F	*S*, kg/h	Q^{EC}_{reb}, kW	Q^{EC}_{cond}, kW	R^{EC}	Q^{RC}_{reb}, kW	Q^{RC}_{cond}, kW	R^{RC}	Q_{total}, kW
12	51	2732	630.8	−623.5	5.52	391.1	−386.5	4.04	1021.9
	52	2733	628.8	−621.5	5.50	391.0	−386.5	4.04	1019.8
	53	2635	635.3	−627.9	5.57	381.5	−377.0	3.91	1016.8
	54	2638	639.1	−631.8	5.61	382.0	−377.5	3.92	1021.2
13	51	2747	623.8	−616.5	5.45	392.6	−388.0	4.06	1016.3
	52	2747	620.5	−613.3	5.41	392.2	−387.7	4.05	1012.8
	53	2671	627.3	−620.0	5.48	385.2	−380.7	3.96	1012.5
	54	2672	632.3	−625.0	5.54	385.4	−380.9	3.96	1017.7
14	51	2842	618.8	−611.6	5.40	401.5	−396.9	4.17	1020.3
	52	2690	628.6	−621.4	5.50	386.6	−382.0	3.98	1015.2
	53	2657	632.3	−625.0	5.54	383.4	−378.9	3.94	1015.7
	54	2643	639.1	−631.8	5.61	381.9	−377.4	3.92	1021.0

Table 7. Optimal operating parameters of the conventional ED scheme

Columns	EC	RC
N_{total}	66	48
N_F	53	22
N_S	13	–
Q_{reb}, kW	618.2	394.3
Q_{cond}, kW	−515.2	−389.8
R	5.39	4.08
T_{cond}, °C	107.7	116.2
T_{reb}, °C	137.5	146.5
P_{cond}, kPa	101.3	101.3
P_{reb}, kPa	107.9	106.1

where Q_{reb} is the duty on the boiler of the column, *A* is the thermodynamic operation, and T_{cond} and T_{reb} are the absolute temperatures in the condenser and boiler of the distillation column, respectively.

Equation (1) was obtained by Plesu *et al.* [18], based on the equation for calculating the heat required for separation and the expression for the efficiency of the Carnot heat engine. According to Plesu, with a $C_{ef} > 10$, the use of heat pumps is economically feasible in most cases. With $10 > C_{ef} > 5$, the use of heat pumps is only appropriate under certain conditions, and with a $C_{ef} < 5$, heat pumps are not practical. Notably, this approach was proposed to evaluate the effectiveness of heat pumps in the distillation of zeotropic mixtures. However, in [21–24], it was used to evaluate the effectiveness of heat pumps in the ED of azeotropic mixtures. We decided to test the validity of this approach in the separation of the IBS–IBA mixture by ED with BP.

Based on the data from Table 7, the C_{ef} is 12.76 for the EC and 12.83 for the regeneration column. High C_{ef}

values imply a significant effect attributed to the heat pumps on both columns. Moreover, literature data [4] indicate that the maximum efficiency of the heat pump is achieved with the minimum possible temperature difference in the heat exchanger. Based on these data, the temperature difference, ΔT = 25 K, was set to determine the output pressure of the compressor. At the same time, the compressor provides the design pressure for the distillate of the extractive column, P_{comp}^{EC} = 506.6 kPa, and the distillate of the regeneration column, P_{comp}^{RC} = 456.0 kPa.

Based on the conventional scheme of ED and the above assumptions about the effectiveness of heat pumps, three variants of schemes including vapor-recompression heat pumps were modeled (Fig. 2). In all cases, the heat pump installed on the column introduced in the scheme fully utilizes the steam flow coming from the top of the column. After compression in the compressor with the W_{comp} power input to the P_{comp} pressure and adiabatic heating, the steam flow is directed to the heat exchanger, partially heating the column cube (the amount of heat transferred in this heat exchanger is indicated by Q_{HE}). Thereafter, the flow of the vapor–liquid mixture is directed to the throttle, where the pressure is reduced to 101.3 kPa. An auxiliary capacitor is used for the complete condensation of the flow, after which the flow is divided into the product and reflux.

Since the replacement of the standard heat exchange equipment of distillation columns with a binding, which would allow the use of a heat pump, does not have significant effects on the heat and mass

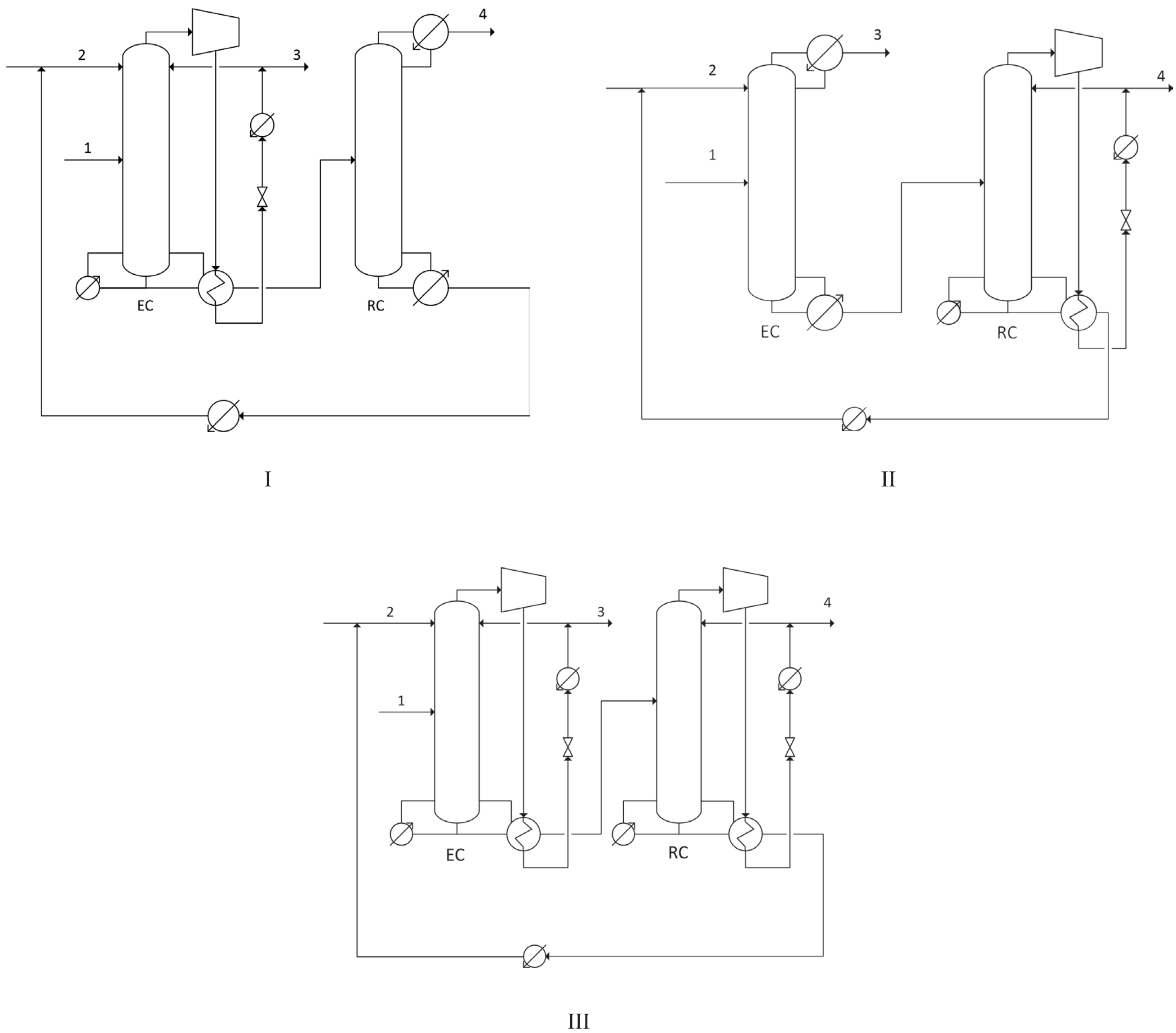

Fig. 2. Schemes of ED including vapor-recompression heat pumps.
The compressor installed on the vapor streams of (I) EC, (II) RC, and (III) both columns.
EC is the ED column, RC is the entrainer regeneration column. (1) Feed, (2) entrainer, (3) IBA, (4) IBAC.

exchange processes inside the columns, the repeated optimization of the structural parameters of the columns is not required. It should be noted that for all three variants of the process organization for the columns with heat pumps, additional reboilers and condensers are used, the duties of which are designated as Q_{reb} and Q_{cond}, respectively. This is because in these schemes the additional supply or removal of heat was not prevented, despite that the relevant heat duty and, consequently, the costs of heating steam and cooling water, as shown below, significantly reduced compared with those of the conventional scheme.

The calculated parameters of the three variants of schemes with heat pumps are shown below (Table 8).

In comparison with the conventional scheme, significant changes have been made to the technological schemes (Fig. 2) by including additional expensive equipment, such as "hot" compressors that consume electricity when compressing steam flows. At the same time, the application of the energy consumption criterion for choosing the optimal technological scheme is incorrect. Furthermore, for the optimization process of each technological scheme, this criterion is acceptable and appropriate. To compare the options for organizing a process that includes heterogeneous technological equipment, it is customary to use the criterion of the total annual costs (TAC).

$$\mathrm{TAC} = \mathrm{OC} + \frac{\mathrm{CC}}{\mathrm{OT}}, \qquad (2)$$

where OT is the lifetime of the installation in years; CC is the capital costs in USD; OC is the operating costs in USD per year.

Table 8. Operating parameters of the schemes with vapor-recompression heat pumps

Scheme I (Fig. 2)		
Columns	**EC**	**RC**
Q_{reb}, kW	64.83	394.32
Q_{HE}, kW	568.82	–
Q_{cond}, kW	−163.51	−389.81
Equipment	The compressor was installed on the vapor streams of EC	–
W_{comp}, kW	106.18	–
P_{comp}, kPa	506.63	–
Scheme II (Fig. 2)		
Columns	**EC**	**RC**
Q_{reb}, kW	618.16	91.54
Q_{HE}, kW	–	299.24
Q_{cond}, kW	−515.25	−150.15
Equipment	–	The compressor was installed on the vapor streams of RC
W_{comp}, kW	–	65.89
P_{comp}, kPa	–	455.96
Scheme III (Fig. 2)		
Columns	**EC**	**RC**
Q_{reb}, kW	64.83	91.54
Q_{HE}, kW	568.82	299.24
Q_{cond}, kW	−163.51	−150.15
Equipment	The compressor was installed on the vapor streams of both colomns	
W_{comp}, kW	106.18	65.89
P_{comp}, kPa	506.63	455.96

Since the change in the service life significantly affects the TAC, the criteria were calculated for 10- and 20-year periods. Aspen Process Economic Analyzer v10.1 (APEA) was used to calculate the capital and operating costs. The main economic parameters are shown in Tables 9 and 10, and the results of the economic assessment are shown in Table 11.

As can be observed, in a 10-year operation period, the use of technological schemes with heat pumps has very little economic impact, and practically, these technological solutions are on the verge of economic feasibility. It can also be observed that for the ED system, the most effective technical solutions are those that provide for the installation of a compressor on the steam stream of the distillate of the ED column. The use of a heat pump only on the recovery column of an entrainer is impractical. The scheme with two heat pumps is the most energy-efficient. According to the TAC criterion, the scheme with a heat pump on an extractive column is more profitable over 10 years; however, as noted above, the economic effect is insignificant. Conversely, for 20 years, the scheme with two heat pumps is more profitable.

Simulation of a circuit with an internal heat pump

The heat pump for ED can be placed not only on the steam flows of distillates of columns, but also on the steam flows between separate sections of columns.

Table 9. Utility costs (USD)

Energy resource	Cost, USD per unit
Electricity, kW	0.0775
Cooling water, t	0.03
Steam, kg	0.017

Table 10. Equipment costs (USD)

Equipment	General		Conventional scheme	
	Tower	Reflux pump	Main condenser	Main reboiler
EC	862500	4500	23600	21400
RC	404000	5200	20400	18400
Equipment	**Heat pump**			
	Compressor	**Heat exchanger**	**Support condenser**	**Support reboiler**
EC	707400	15100	8600	18400
RC	671000	11000	8500	12300

Table 11. Economical evaluation

Economic parameters	Conventional scheme (Fig. 1)	Scheme I	Scheme II	Scheme III
		Fig. 2		
Energy costs, USD per year	334155	248718	291574	201721
Energy saving, %	0	25.6	12.7	39.6
Capital costs, USD	1363800	2061400	2027100	2555800
TAC10, USD per year	470535	454858	494284	457301
TAC20, USD per year	402345	351788	392929	329511
TAC10 saving, %	0	3.3	−5.1	2.8
TAC20 saving, %	0	12.6	2.3	18.1

This solution was first proposed by Batista *et al.* [19], although it has not yet been compared with other options for organizing the process. The scheme with an internal heat pump is shown in Fig. 3.

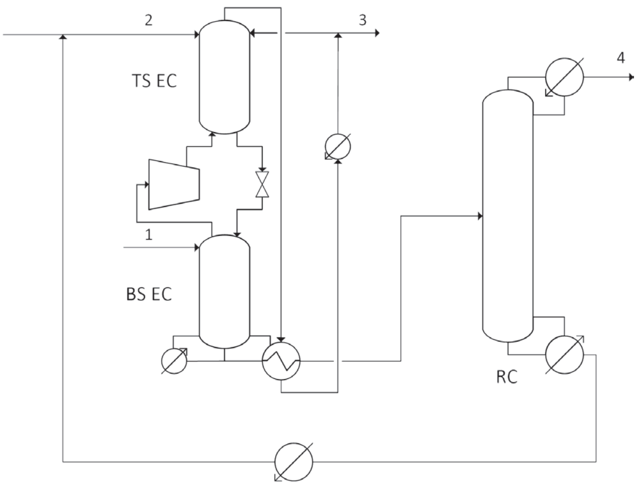

Fig. 3. Scheme of ED including an "internal" heat pump. TS EC denotes the top section of the ED column, BS EC denotes the bottom section of the ED column, and RC denotes the entrainer regeneration column. (1) Feed, (2) entrainer, (3) IBA, (4) IBAC.

In this scheme, the ED column is divided into two parts working at different pressures: 101.3 kPa in the exhaust section (bottom section – BS) and 506.64 kPa in the upper refining and extractive sections (top section – TS), with the feed being supplied to the first plate of the lower section. Partial heating of the boiler in the lower section is conducted by the steam flow of the distillate of the upper section.

When the operating pressure in the system changes, the view of the vapor–liquid equilibrium diagram changes as well. In this case, when the pressure increases, the composition of the azeotrope shifts in the direction of increasing concentration of the light-boiling component in it, up to the degeneration of azeotropy into tangential at a pressure of 506.64 kPa. Figure 4 (I) shows diagrams of the relative volatility lines (α_{12}) of the IBA (1)–IBAC (2) pair at 101.3 kPa, while Figure 4 (II) displays the same at a pressure of 506.64 kPa.

As shown, with increasing pressure in the presence of the entrainer in the system under consideration, the relative volatility of α_{12} of the IBA–IBAC pair increases; therefore, separation at increased pressure is facilitated and requires a relatively small amount of entrainer. Our calculated data on the increase in the relative volatility of the IBA–IBAC pair with increasing pressure are consistent with the data of the full-scale experiment of Monton *et al.* [25].

To model the scheme with an "internal" heat pump, it was necessary to determine the optimal operating parameters of the conventional ED scheme, in which the EC column operates at high pressure. In this case, there are additional heat costs for heating the feedstock and a heat exchanger for heating. This scheme was modeled and optimized using the previously mentioned algorithm [17]. The optimal operating parameters of this scheme are presented in Table 12. The optimal flow of entrainer is 1312 kg/h, and the entrainer temperature is 146°C.

Based on the parameters of the EC scheme operating at a pressure of 506.64 kPa and the conventional scheme (at a pressure of 101.3 kPa), the scheme with an "internal" heat pump was simulated. The parameters of the TS EC: the total number of plates, number of the entrainer feed plate, and the flow rate of the entrainer, correspond to the parameters of the refining and extractive sections of the EC in the scheme, operating at elevated pressures, and the parameters of the BS EC, i.e., the parameters of the lower section of the EC of schemes, operating at

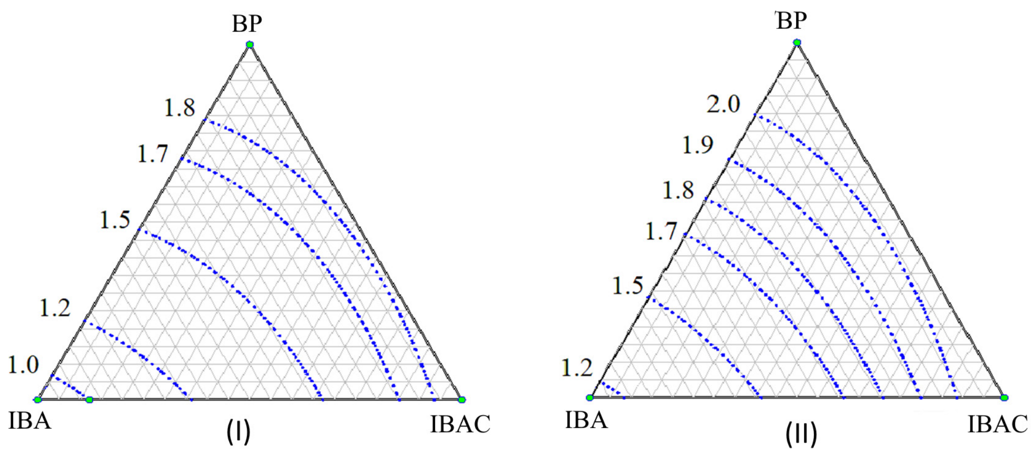

Fig. 4. Relative volatility diagrams (α_{12}) for IBA–IBAC with an entrainer at 101.3 kPa (I) and 506.64 kPa (II).

atmospheric pressure. The parameters of the scheme with an "internal" heat pump are shown in Table 13. The optimal flow of entrainer is 1312 kg/h, and the entrainer temperature is 146°C.

From the results shown, it is clear that an internal heat pump prevents additional heat supply to the reboiler of the EC column and excludes the support reboiler.

For the scheme with an internal heat pump, an economic assessment was also carried out, and the TAC value was determined. The equipment costs are shown in Table 14, and the economic analysis results in comparison with the conventional scheme are presented in Table 15.

As shown, using an internal heat pump can significantly reduce the energy costs and TACs.

Table 12. Operating parameters of the scheme of ED with EC, at 506.64 kPa

Columns	EC	RC
Total number of stages, N_{total}	56	50
Feed stage, N_F	44	23
EA, N_S	13	–
Q_{reb}, kW	473.8	214.2
Q_{cond}, kW	−408.9	−311.4
R	4.2	3.1
T_{cond}, °C	160.4	116.2
T_{reb}, °C	197.9	146.6
P_{cond}, kPa	506.6	101.3
P_{reb}, kPa	512.2	106.3
$Q_{additional\ feed\ heating}$, kW	76.6	–

Table 13. Operating parameters of the scheme with the "internal" heat pump

Columns	EC	RC
N_{total}	56	50
$N^{TS\ EC}$	43	–
$N^{BS\ EC}$	13	–
N_F	44 (1)	23
N_S	13	–
Q_{reb}, kW	0	214.2
Q_{HE}, kW	403.9	–
Q_{cond}, kW	−84.3	−311.4
R	4.2	3.1
T_{cond}, °C	160.4	116.2
T_{reb}, °C	130.8	146.5
P_{cond}, kPa	506.6	101.3
P_{reb}, kPa	102.5	106.1
Equipment	**EC**	**RC**
W_{comp}, kW	123.6	–
P_{comp}, kPa	511	–

Table 14. Equipment costs for the scheme with the "internal" heat pump

Equipment	Tower	Reflux pump	Main condenser	Main reboiler
TS EC	414000	5100	–	–
BS EC	68800	–	–	–
RC	605200	4500	21500	14600
Equipment	**Compressor**	**Heat exchanger**	**Support condenser**	
TS EC	727100	–	8300	
BS EC	–	12600	–	

Table 15. Economical evaluation

Economic parameters	Conventional scheme	Scheme with the "internal" heat pump
Energy costs, USD per year	334155	187266
Energy saving, %	0	44.0
Capital costs, USD	1363800	1881700
TAC10, USD per year	470535	375436
TAC20, USD per year	402345	281351
TAC10 saving, %	0	20.2
TAC20 saving, %	0	30.1

CONCLUSIONS

In this study, it is demonstrated that the use of heat pumps in the scheme of the ED of a mixture of isobutyl alcohol–isobutyl acetate with *n*-butylpropionate as an entrainer can be economically justified. Among the considered schemes with an external vapor-recompression heat pump, the scheme in which heat pumps are fixed on both columns has the highest energy efficiency. This scheme reduces the energy costs by 39.6% compared to the conventional ED scheme. According to the TAC criterion, when calculating based on the operating time of the installation of 10 years, the lowest value of TAC10 is achieved in the scheme with a heat pump attached to the ED column. This scheme provides a reduction of TAC10 by 3.3% compared to the conventional scheme. With a lifetime of 20 years, the lowest TACs are provided by the scheme including two heat pumps. The TAC20 of this scheme is lower by 18.1% compared to that of the conventional scheme. The proposed scheme including an internal heat pump is the most economical scheme considered in this paper, despite its somewhat non-standard configuration. This scheme provides a 44% reduction in energy costs, a 20.2% reduction in TACs with a 10-year operating life, and a 30.1% reduction over 20 years.

Thus, the incorporation of heat pumps into ED systems results in a significant reduction in energy consumption and significant economic impacts.

Key

A – thermodynamic work;
a, b – parameters of the UNIQUAC equation;
C_{ef} – efficiency coefficient;
CC – capital costs;
N – plate number;
OC – operating costs;
OT – operating time;
P – absolute pressure;

Q – heat duty;
R – reflux ratio;
S – flow rate of the extractive agent;
T – temperature;
TP – theoretical plates;
TAC – total annual costs;
TAC10 – total annual costs with a 10-year operating life;
TAC20 – total annual costs with a 20-year operating life;
W – power consumption;
Y – component concentration in the vapor phase;
DB – database of the software package;
BP – *n*-butylpropionate;
TS – top section;
IBAC – isobutyl acetate;
IBA – isobutyl alcohol;
Liter. – data from a literary source;
BS – bottom section;
VLE – vapor–liquid equilibrium;
RC – entrainer regeneration column;
EA – separating (extractive) agent;
EC – extractive distillation column;
ED – extractive distillation;

Indexes
comp – compressor;
cond – condenser;
i,j – numbers of the components;
F – feed;
HE – heat exchanger;
min – the minimum value;
opt – optimal value;
reb – reboiler;
S – extractive agent.

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