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RESEARCH ARTICLE

Optimal modes of side-section flow in heat-pump-assisted extractive distillation systems for separating allyl alcohol–allyl acetate mixtures with butyl propionate

Pavel S. Klauzner[@], 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. *To investigate the influence of side-section flow modes on the energy efficiency of a partially thermally coupled distillation sequence (PTCDS) with a vapor recompression heat pump for the extractive distillation of an allyl alcohol–allyl acetate mixture with n-butyl propionate and identify modes under which the combined use of a PTCDS and heat pump are the most efficient.*
Methods. *Mathematical modeling in the Aspen Plus V10 software package was used as the main research method. The local composition equation of the non-random two-liquid model was used as a model for describing the vapor–liquid equilibrium, while the Redlich–Kwong model was used to consider the non-ideal vapor phase. When modeling the conventional extractive distillation scheme and PTCDS, parametric optimization was carried out according to the criterion of the total energy costs in the column reboilers. For the economical evaluation, Aspen Process Economic Analyzer V10.1 tools were used.*
Results. *For extractive distillation of a mixture of allyl alcohol (30 wt %) and allyl acetate (70 wt %) with n-butyl propionate as an entrainer, the minimum energy consumption was achieved at the same side-section flow mode for the variants of a PTCDS with and without a heat pump. The reduction in energy costs relative to the conventional scheme was 20% for the sequence without a heat pump and 38% for that with a heat pump. An economic assessment was made of the best options in comparison with the conventional extractive distillation scheme. The PTCDS with a heat pump had an advantage over the sequence without a heat pump only for long periods of operation.*
Conclusions. *For the extractive distillation of an allyl alcohol–allyl acetate mixture, the optimal modes for the combined use of a PTCDS with a vapor recompression heat pump coincide with the optimal modes for a PTCDS without a heat pump.*

Keywords: *extractive distillation, heat pump, partially thermally coupled distillation sequence, energy saving*

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НАУЧНАЯ СТАТЬЯ

Оптимальные режимы бокового отбора в системах экстрактивной ректификации с тепловым насосом при разделении смеси аллиловый спирт–аллилацетат с бутилпропионатом

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. *Исследовать влияние режимов бокового отбора на энергетическую эффективность комплекса с частично связанными тепловыми и материальными потоками (ЧСТМП) с тепловым насосом (ТН) открытого типа в экстрактивной ректификации смеси аллиловый спирт–аллилацетат с н-бутилпропионатом и выявить условия, при которых совместное применение комплекса с ЧСТМП совместно с ТН наиболее эффективно.*
Методы. *Математическое моделирование в программном комплексе Aspen Plus V10. Для моделирования парожидкостного равновесия применяли уравнение локальных составов модель Non-Random Two Liquid, а для учета неидеальности паровой фазы – модель Редлиха-Квонга. При моделировании традиционной схемы экстрактивной ректификации и комплекса с ЧСТМП проводили параметрическую оптимизацию по критерию суммарных энергетических затрат в кипятильниках колонн. Для экономической оценки применяли инструменты Aspen Process Economic Analyzer V10.1.*
Результаты. *Для экстрактивной ректификации смеси 30 мас. % аллилового спирта и 70 мас. % аллилацетата с н-бутилпропионатом в качестве разделяющего агента показано, что минимум энергозатрат достигается при одинаковом уровне и количестве бокового отбора как для варианта комплекса с ЧСТМП с ТН, так и без него. Снижение энергетических затрат относительно традиционной схемы для комплекса без ТН составляет 20%, а с ТН – 38%. Была произведена экономическая оценка наилучших вариантов по сравнению с традиционной схемой экстрактивной ректификации. Показано, что применение комплекса с ЧСТМП с ТН имеет преимущество только при длительных сроках эксплуатации.*

Выводы. *Показано, что для экстрактивной ректификации смеси аллиловый спирт–аллилацетат оптимальные режимы бокового отбора при совместном применении комплекса с ЧСТМП с ТН открытого типа и комплекса с ЧСТМП без ТН совпадают.*

Ключевые слова: *экстрактивная ректификация, тепловой насос, комплекс с частично связанными тепловыми и материальными потоками, энергосбережение*

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INTRODUCTION

Allyl alcohol (AAL) is a key product of the chemical technology of basic organic synthesis. It is used for the synthesis of glycidol, glycerol, allyl, glycidyl, and several other esters used in the production of fibers, paints and varnishes, sealants, molded products, fiberglass-reinforced plastics, polymers, food products, medicines, and perfumery products. There are several industrial methods for obtaining AAL from allyl acetate (AAC)—saponification, hydrolysis, alcoholysis [1], and a combined reaction–distillation process [2]. Regardless of the preparation method, during the preliminary separation of the reaction products, an AAL–AAC mixture is formed; it has an azeotrope with a minimum boiling point and an AAL content of 0.63 wt. fract. (0.75 mol. fract.). To separate this mixture, the authors in [3] have proposed using extractive distillation (ED) with ethylene glycol as an entrainer; this entrainer is distinguished by a sufficiently high selectivity, and in its presence, the relative volatilities are reversed. As an alternative, we propose n-butyl propionate (BP) as an entrainer in [4]. The maximum difference in boiling points is 100°C when using EG and 48°C when using BP.

In several cases, ED is characterized by a significantly lower energy consumption than that of other special separation methods. Despite this, the search for ways to reduce the energy cost of its implementation remains urgent since it is used in large-tonnage technologies of basic organic and petrochemical synthesis. Conventional ways to reduce energy costs in ED include using selective entrainers and parametric and structural scheme optimization. As with conventional distillation, heat integration [5–8] and methods based on the approach of distillation to thermodynamically reversible [9] can be used to improve the ED process, e.g., schemes with a completely [10] or partially thermally coupled distillation sequence (PTCDS) [11, 12]. Many works have been devoted to PTCDS schemes. The use of such schemes in the ED of various mixtures [13–15] has been investigated, and an empirical criterion for a preliminary assessment of the energy efficiency of PTCDS schemes in ED [16] and an optimization algorithm for such schemes [17] have been proposed. Another promising [18] method for improving the ED process is the use of various heat pumps (HPs). At present, few works have been devoted to this topic [19–22]. Since the use of HPs and PTCDS schemes is based on different principles, it is advisable to consider the possibility of their joint use and evaluate the effectiveness of this approach.

Previously, in [4], we have considered the use of HPs in the ED of an azeotropic AAL–AAC mixture with a BP entrainer in conjunction with a PTCDS scheme. Relative to the conventional scheme, the reduction in energy costs of the combined scheme reached 50%. Since the energy efficiency and even the structure of the optimal technological scheme are a function of the initial composition of the food due to the process's irreversible nature, in this work, research is carried out on the initial composition with an AAL content of 30 wt %, significantly different from the previous study. It is known that the side-section flow mode, i.e., the position of the side-section tray (N_V) and the amount of side-section flow (V), has a significant effect on the energy efficiency of PTCDS schemes. Thus, the purpose of this work is to study the influence of these parameters on the energy efficiency of a PTCDS scheme with a vapor recompression HP and identify the conditions required for their joint use.

CALCULATIONS

All calculations were performed using Aspen Plus V10. As in [4], the non-random two-liquid equation was used to simulate the vapor–liquid equilibrium in this

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

study, and the Redlich–Kwong equation was used to consider the imperfections of the vapor phase arising during vapor compression.

For all variants of the schemes, the separation of the initial mixture with an AAL–AAC feed rate of 1000 kg/h, temperature of 97°C, and pressure of 105.0 kPa was considered [3].

The pressure of the top of the columns was taken as equal to 101.3 kPa [3], and real trays with an efficiency of 0.65 and a pressure drop of 0.1013 kPa on each were considered. The calculations were carried out in the design and verification mode, with a fixed quality of the product flows. The concentration of AAL and AAC in the product flows was set as constant and equal to 99.5 wt %; the BP concentration was equal to 99.9 wt %.

The optimization criterion was the minimum total heat duty on Q_{total} reboilers. In general terms, it could be written as (1):

$$Q_{total} = \Sigma_{i=1}^{K} Q_{reb}^{i}, \quad (1)$$

where K is the total number of distillation columns, i is the column number in the scheme, and Q_{reb}^{i} is the reboiler duty of the i column..

Technological schemes with HPs differ significantly from conventional ones since they contain "hot" compressors and additional heat exchange equipment. The compressors can be driven using both steam and electricity. To compare the energy costs in technological systems with dissimilar equipment, the consumption of equivalent fuel or an economic assessment of operating costs can be applied. In the case of using HPs in distillation processes, the authors of [23] proposed a simple formula (2) for assessing energy efficiency through reduced energy costs (Q_{red}):

$$Q_{red} = Q_{total} + 3W_{comp}, \quad (2)$$

where Q_{total} is the total energy consumption in the column reboilers (kW) and W_{comp} is the compressor power consumption (kW).

To compare the options for organizing a process that includes dissimilar technological equipment, the total annual cost (*TAC*) criterion is usually used (3):

$$TAC = OC + \frac{CC}{OT}, \quad (3)$$

where *OT* is the operating time of the unit in years; *CC* is the capital costs, USD; and *OC* is the operating costs, USD/year.

Since changes in the service life significantly affect the *TAC* value, the criterion calculations were carried out for 10- and 20-year periods.

Aspen Process Economic Analyzer V10.1 was used to calculate the capital and operating costs. The energy prices are given in Table 1.

Table 1. Utility costs (USD)

Utility	Cost, USD
Electricity, kW	0.0775
Cooling water, t	0.03
Steam, kg	0.017

Modeling and optimization of the conventional ED scheme

The conventional ED scheme (Scheme I) is shown in Fig. 1 and consisted of two columns—an ED column (EC) and an entrainer regeneration column (RC).

For the conventional version of the ED organization according to the algorithm proposed in [17], the optimal operating parameters were determined. In the optimization process, the total number of trays in both columns, the position of the feed plates to the EC and RC columns, the position of the entrainer feed plate to the EC, and the amount of entrainer flow were determined. For the optimization,

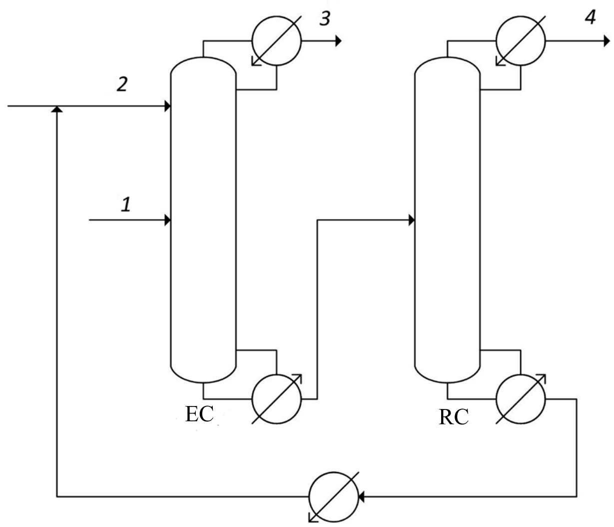

Fig. 1. Conventional ED scheme of AAL–AAC mixture with BP as the entrainer. EC is ED column, RC is entrainer regeneration column. Hereinafter: (1) feed, (2) entrainer, (3) AAL, (4) AAC.

the built-in tools of the Aspen Plus software package were used, which implemented the sequential enumeration of parameters and optimization via sequential quadratic programming (SQP).

The final operating parameters of the conventional ED scheme at a given composition (30-wt % AAC) of the initial mixture are presented in Table 2.

Modeling and optimization of a PTCDS scheme

The authors of [16] proposed a rule of thumb by which the use of PTCDS schemes is inappropriate when the reflux ratio in the RC is much lower than one. In this case, the value of RRC was 4.0, implying the achievement of a significant energy effect. Based on the conventional ED scheme, we simulated the scheme with a PTCDS (Scheme II), as shown in Fig. 2.

Table 2. Operating parameters of conventional ED scheme

Operating parameters	Columns	
	EC	RC
N_{total}	46	28
N_F	35	17
N_S	12	–
Q_{reb}, kW	299	375
Q_{cond}, kW	−275	−357
R	3.7	4.0
T_{cond}, °C	96.81	104.0
T_{reb}, °C	128.4	145.9
P_{cond}, kPa	101.3	101.3
P_{reb}, kPa	105.8	104.0
S, kg/h	2450	–
T_S, °C	120.0	–

The diagram in Fig. 2 was obtained by transforming the conventional scheme (Fig. 1) according to different algorithms [11, 12, 24]; it is a single complex column with a reinforcing side section. In the next stage, according to the algorithm proposed in [17],

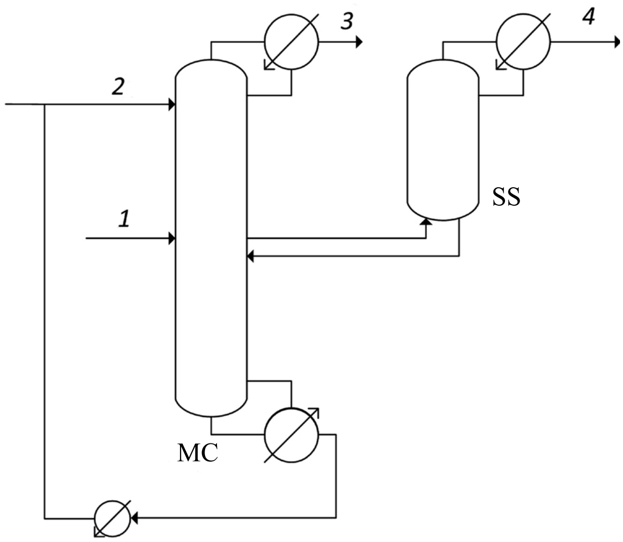

Fig. 2. PTCDS scheme: MC – main column, SS – side section.

the values of the flow and supply level of the side-section flow were determined. According to several studies, the optimal values of other variables, e.g., the number of feed plates, the entrainer feed plate, and the entrainer flow, in PTCDS schemes either do not differ or differ insignificantly from the corresponding parameters of the conventional scheme [12, 24]. Therefore, the optimization of PTCDS schemes to reduce the dimension tasks on these parameters may not have to be carried out. For several of the side-section trays, the SQP Optimization tool was used to determine the value corresponding to the minimum duty on the Q_{reb} reboiler. The data obtained at this stage are shown in Table 3.

The minimum lateral withdrawal flow was observed at $N_V = 47$, and the minimum energy consumption in the reboiler was observed at $N_V = 48$. The optimal operating parameters of the PTCDS scheme are presented in Table 4.

Combined use of a PTCDS scheme and HP

Based on the PTCDS scheme considered above, a scheme for the joint use of a PTCDS with a vapor recompression HP (Scheme III) was synthesized, as shown in Fig. 3.

For a preliminary assessment of the efficiency of using HPs based on the expression of the efficiency of a Carnot heat engine and an equation for calculating the heat required for separation, the authors of [25] proposed the efficiency factor of HPs, C_{ef}:

$$C_{ef} = \frac{Q_{reb}}{A} = \frac{T_{reb}}{\left(T_{reb} - T_{cond}\right)}, \tag{4}$$

Table 3. Operation parameters optimization of PTCDS. Q units are [kW]

N_V	V, kg/h	Q^{MC}_{reb}	Q^{SS}_{cond}	R^{MC}	Q^{SS}_{cond}	R^{SS}
44	1721	611	−337	4.4	−162	1.4
45	1645	569	−335	4.2	−157	1.4
46	1622	532	−339	3.9	−154	1.4
47	1612	522	−327	3.7	−156	1.2
48	**1692**	**521**	**−318**	**3.6**	**−161**	**1.3**
49	1858	528	−311	3.4	−176	1.5
50	2214	560	−313	3.4	−206	1.9
51	2901	608	−305	3.4	−262	2.8

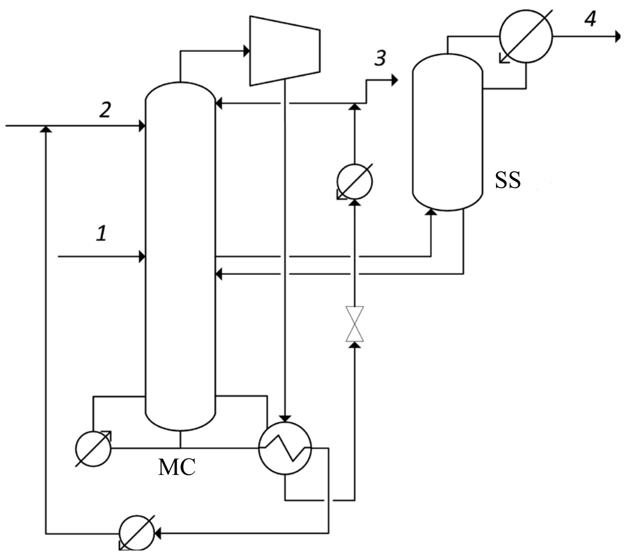

Fig. 3. PTCDS scheme with open type:
MC – main column, SS – side section.

where Q_{reb} is the column reboiler duty, A is the thermodynamic work, and T_{cond} and T_{reb} are the absolute temperatures in the condenser and reboiler of the EC, respectively.

Based on the data in Table 4, for the PTCDS scheme, C_{ef} equaled 8.3. In [25], it was noted that the use of HPs may be advisable at values of $C_{ef} > 5$.

It should be noted that when deriving Eq. (4), several assumptions were initially made to assess the applicability of HPs in the separation of zeotropic mixtures. Despite this, in several works, the criterion has also been used for PTCDS schemes with HPs in the separation of azeotropic mixtures, including ED [20, 26, 27].

Table 4. Optimal operating parameters of PTCDS

Operating parameters	Columns	
	MC	SS
N_{total}	57	17
N_F	35	–
N_V	48	–
N_S	12	–
V, kg/h	1692	–
Q_{reb}, kW	521	–
Q_{cond}, kW	−318	−161
R	3.6	1.3
T_{cond}, °C	96.8	104.9
T_{reb}, °C	147.0	–
P_{cond}, kPa	101.3	104.0
P_{reb}, kPa	107.5	–
S, kg/h	2450	–
T_S, °C	120.0	–

The steam flow of the main column was chosen as the working fluid for the HP since its heat content was higher than that of the upper steam flow of the side section. Simultaneously, the temperature of the steam flow required for effective heating of the column bottom was provided at a compression ratio in the compressor equal to 5.2. It is known that high economic efficiency from the use of HPs is achieved when this ratio is less than three [28, 29]. Thus, for an accurate comparison of the considered schemes, the following economic assessment was required.

For several positions of the side-section tray, N_V, and the corresponding optimal amount of side-section flow, V, considered when optimizing the PTCDS scheme, the operating parameters of an open-type HP were selected. The results are presented in Table 5.

In this case, $Q_{\text{reb}}^{\text{MC}}$ и $Q_{\text{cond}}^{\text{MC}}$ were duties on the auxiliary reboiler and condenser, respectively, W_{comp} was the compressor power consumption, Q_{HE} was the heat transferred in the heat exchanger of the HP, and Q_{HE} was the heat transferred in the heat exchanger of the HP, and $Q_{\text{red}}^{\text{HP}}$ was the reduced energy cost determined by Eq. (2).

RESULTS AND DISCUSSION

According to the calculated data (Tables 3 and 5), the final dependences of the duty on the reboiler of the PTCDS scheme and the reduced energy consumption when using a PTCDS with an HP on the position and amount of side-section flow are shown in Fig. 4.

Table 5 and Fig. 4 show that as the N_V increased, the efficiency of the HP decreased; however, the minimum reduced energy costs, $Q_{\text{red}}^{\text{HP}}$, were observed at the same N_V and V values as the minimum energy costs of the PTCDS scheme without an HP. The comparison of the energy costs of the conventional scheme and the best options for the complex with PTCDS and the combined use of a PTCDS and HP are presented in Table 6.

As already indicated, for an accurate comparison of the considered solutions, it was necessary to perform an economic assessment. To do this, we evaluated several design parameters of the distillation columns, i.e., the diameter of the column (D) and the height of the trayed (packed) section (H), and selected the types of contact device. This assessment was made using the Aspen Plus software package; the results are presented in Table 7.

The general results of the economic assessment carried out with the Aspen Process Economic Analyzer and the *TAC* values calculated according to Eq. (3) based on these results are shown in Table 8.

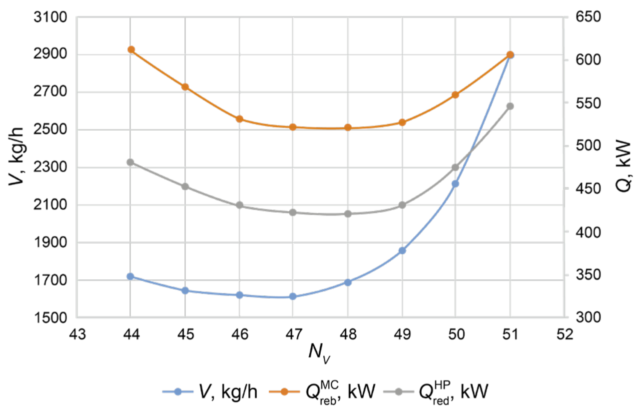

Fig. 4. PTCDS heat duty ($Q_{\text{reb}}^{\text{MC}}$, kW), PTCDS with HP reduced heat duty ($Q_{\text{red}}^{\text{HP}}$, kW) and V, kg/h dependence on side-stream stage (N_V).

Table 5. Operation parameters' dependence on N_V and V for HP schemes. Q and W units are [kW]

N_V	V, kg/h	$Q_{\text{reb}}^{\text{MC}}$	$Q_{\text{cond}}^{\text{SS}}$	R^{MS}	W_{comp}	Q_{HE}	$Q_{\text{red}}^{\text{HP}}$
44	1721	295	−86	4.4	62	331	481
45	1645	273	−81	4.2	60	302	453
46	1622	269	−74	3.9	54	276	431
47	1612	267	−71	3.7	52	263	423
48	**1692**	**274**	**−68**	**3.6**	**49**	**248**	**421**
49	1858	287	−66	3.4	48	240	431
50	2214	335	−66	3.4	47	230	476
51	2901	409	−65	3.4	46	224	547

Table 6. Energy duties of optimal PTCDS (II) and PTCDS with HP (III) schemes in comparison with conventional ED scheme (I)

Energy duties	Scheme		
	I	II	III
Q_{total}, kW	674	521	274
W_{comp}, kW	0	0	49
Q_{red}, kW	674	521	421
ΔQ_{red}, %	0	22	38

Table 7. Construction parameters of columns

Column	EC	RC	MC	SS
***D*, м**	0.6	0.75	0.7	0.45
***H*, м**	19	11	23	3
Tray/pack type	Valve trays	Valve trays	Valve trays	Raschig rings

Table 8. Economical evaluation

Economic parameters	Scheme		
	I	II	III
OC, USD/year	222420	179493	132675
Δ*OC*, %	0	19.3	40.3
CC, USD	502400	368000	1077100
*TAC*10	272660	216293	240385
*TAC*20	247540	197893	186530
Δ*TAC*10, %	0	20.7	11.8
Δ*TAC*20, %	0	20.1	24.7

CONCLUSIONS

The study showed that for the ED process of a mixture of AAL (30 wt %) and AAC (70 wt %) with BP, the use of a PTCDS scheme and that same scheme with an HP can significantly reduce energy expenses. Moreover, it was found that the change in the main variables (the level of the supply and the value of the lateral withdrawal flow), which affects the energy efficiency of the PTCDS scheme, also affects the efficiency of the HPs in the complex. However, in the case considered, the minimum energy costs were achieved under the same conditions in the PTCDS schemes both with and without an HP. A decrease in the concentration in the initial mixture of the component released in the distillate of the EC led to a decrease in the energy and economic efficiency of using the HP. According to the results of the economic assessment performed based on the *TAC* criterion with a unit operation time of 10 years, it would be more expedient to use a PTCDS scheme without an HP. However, with an operation time of 20 years, a *TAC* reduction of 24% would be provided by the scheme with an HP, and a reduction of 20.1% would be provided by the PTCDS scheme without an HP.

Abbreviations

A – hermodynamic work;
C_{ef} – efficiency factor;
CC – capital costs;
D – diameter;
H – height;
N – plate number;
K – total number of columns;
OC – operating costs;
OT – operating time;
P – absolute pressure;
Q – heat duty;
R – reflux ratio;
S – flow rate of an entrainer;
T – temperature;
TAC – total annual costs;
*TAC*10 – total annual costs with a 10-year operating life;
*TAC*20 – total annual costs with a 20-year operating life;
V – side flow;
W – power consumption;
AAL – allyl alcohol;
AAC – allyl acetate;
SS – side section;
BP – *n*-butyl propionate;
MC – main column;
RC – entrainer regeneration column;
HP – heat pump;
PTCDS – partially thermally coupled distillation sequence;
EC – extractive distillation column;
ED – extractive distillation.

Indices

comp – compressor;
cond – condenser;
i – numbers of the column;
F – feed;
HE – heat exchanger;
HP – heat pump;
min – the minimum value;
opt – optimal value;
reb – reboiler;
red – reduced;
S – entrainer.

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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.

The authors declare no conflicts of interest.

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About the authors:

Pavel S. Klauzner, 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, 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@mitht.ru. Scopus Author ID 37018548000, ResearcherID M-5241-2014, https://orcid.org/0000-0002-9892-7909

Elena A. Anokhina, 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: anokhina.ea@mail.ru. Scopus Author ID 6701718055, ResearcherID E-5022-2016.

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@mitht.ru. Scopus Author ID 56576076700, ResearcherID Y-8709-2018.

Об авторах:

Клаузнер Павел Сергеевич, 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. Вернадского, д. 86). E-mail: klauzner@mirea.ru. ResearcherID AAJ-7842-2021, 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. Вернадского, д. 86). E-mail: rudakov@mitht.ru. Scopus Author ID 37018548000, ResearcherID M-5241-2014, https://orcid.org/0000-0002-9892-7909

Анохина Елена Анатольевна, 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. Вернадского, д. 86). E-mail: anokhina.ea@mail.ru. Scopus Author ID 6701718055, ResearcherID E-5022-2016.

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. Вернадского, д. 86). E-mail: timoshenko@mitht.ru. Scopus Author ID 56576076700, ResearcherID Y-8709-2018.

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