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RESEARCH ARTICLE

Application of columns with side withdrawal in schemes for benzene recovery from benzene-containing fractions of various compositions

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Abstract

Objectives. The work set out to evaluate the energy and economic efficiency of applying complex columns with side withdrawal in extractive distillation schemes of benzene–cyclohexane–toluene mixtures of various compositions using *N*-methylpyrrolidone as the entrainer.

Methods. A method based on the transformation of graphs representing flowsheets was used for the synthesis of extractive distillation schemes incorporating columns with side withdrawal. Determination of optimal scheme parameters was performed by scanning the range of variable changes with a specified step according to the criterion of minimizing total energy consumption in the column reboilers. The Non-Random Two Liquid local composition equation was used for modeling vapor–liquid equilibrium. The computational experiment was carried out using the Aspen Plus v.10 software package.

Results. Six flowsheets incorporating columns with side withdrawal (flowsheets of subset I) were generated using the graph method based on five flowsheets for extractive distillation of the benzene–cyclohexane–toluene mixture incorporating columns with a side section (flowsheets of subset Θ). Optimal parameters of the synthesized flowsheets were determined for separating the studied mixture of two initial compositions according to the criterion of total energy consumption. These compositions are simplified analogs of fractions produced in the processes of catalytic hydrotreating-hydrocracking of pyrolysis gasoline (Composition 1) and during catalytic steam dealkylation of pyrolysis gasoline (Composition 2). Columns with side withdrawal in each flowsheet of subset I were calculated with both vapor-phase and liquid-phase side streams. Extractive distillation schemes of different structures were compared according to the criteria of total energy consumption in column reboilers ($\sum Q_{reb}$) and total annual cost (TAC).

Conclusions. It is established that the energy and economic efficiency of flowsheets incorporating columns with side withdrawal does not significantly depend on the phase state of the side stream. When separating the benzene–cyclohexane–toluene mixture of both considered compositions, the minimum $\sum Q_{reb}$ value was found to correspond to Flowsheet I2.2-V. This flowsheet consists of an extractive distillation column, an *N*-methylpyrrolidone regeneration column with a side withdrawal of a vapor-phase stream above the feed plate, and a distillation column for the benzene–toluene mixture. The minimum TAC value is characteristic of Flowsheet I1.1, which includes an extractive column with a side withdrawal of a stream below the feed plate in the vapor phase (for Composition 1) or in the liquid phase (for Composition 2). For separating the studied mixture of both considered compositions, it is advisable to use Flowsheet I1.1 with a liquid-phase side withdrawal stream from the extractive column, as in this case, withdrawing the side stream is simpler and regulating its flow rate and composition is easier.

Keywords

benzene, extractive distillation, columns with side draw, energy saving, optimization

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НАУЧНАЯ СТАТЬЯ

Применение колонн с боковым отбором в схемах выделения бензола из бензолсодержащих фракций различного состава

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Аннотация

Цели. Оценка энергетической и экономической эффективности применения сложных колонн с боковым отбором в схемах экстрактивной ректификации смеси бензол–циклогексан–толуол различного состава с *N*-метилпирролидоном в качестве разделяющего агента.

Методы. Для синтеза схем экстрактивной ректификации, включающих колонны с боковым отбором, использован метод трансформации графов, отображающих технологические схемы. Определение оптимальных параметров схем по критерию минимума суммарных энергетических затрат в кипятильниках колонн проводили методом сканирования области изменения переменных с заданным шагом. Для моделирования равновесия жидкость–пар использовано уравнение локальных составов Non-Random Two Liquid. Вычислительный эксперимент выполнен с применением программного комплекса Aspen Plus v.10.

Результаты. На базе пяти схем экстрактивной ректификации смеси бензол–циклогексан–толуол, включающих колонны с боковой секцией (схемы подмножества Θ), с применением метода графов сгенерировано шесть схем, включающих колонны с боковым отбором (схемы подмножества I). Определены оптимальные по критерию суммарных энергетических затрат параметры синтезированных схем при разделении исследуемой смеси двух исходных составов, которые являются упрощенными аналогами фракций, образующихся в процессах каталитической гидроочистки-гидрокрекинга бензинов пиролиза (состав 1) и при каталитическом деалкилировании бензинов пиролиза с водяным паром (состав 2). Колонны с боковым отбором в каждой схеме подмножества I рассчитаны как с парофазным, так и с жидкофазным боковым потоком. Проведено сравнение схем экстрактивной ректификации различной структуры по критериям суммарных энергетических затрат в кипятильниках колонн (ΣQ_{reb}) и полных годовых затрат (total annual cost, TAC).

Выводы. Установлено, что энергетическая и экономическая эффективность схем, включающих колонны с боковым отбором, практически не зависит от агрегатного состояния бокового потока. Выявлено, что при разделении смеси бензол–циклогексан–толуол обоих рассмотренных составов минимальное значение ΣQ_{reb} отвечает схеме I2.2-пар, которая состоит из колонны экстрактивной ректификации, колонны регенерации *N*-метилпирролидона с боковым отбором потока в паровой фазе выше тарелки питания и колонны ректификации смеси бензол–толуол. Минимальной величиной TAC характеризуется схема I1.1, включающая экстрактивную колонну с боковым отбором потока ниже тарелки питания в паровой фазе (в случае состава 1) или в жидкой фазе (в случае состава 2). Для разделения исследуемой смеси обоих рассмотренных составов целесообразно использовать схему I1.1 с жидкофазным потоком бокового отбора из экстрактивной колонны, поскольку в этом случае проще осуществить отбор бокового потока и легче регулировать его расход и состав.

Ключевые слова

бензол, экстрактивная ректификация, колонны с боковым отбором, энергосбережение, оптимизация

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INTRODUCTION

Benzene is a key raw material for the primary organic and petrochemical synthesis industries. It is used to produce alkylbenzenes, phenol, styrene, cyclohexane, maleic anhydride, and others. Benzene production in Russia in 2024 amounted to approximately 1.3 million tons [1]. The main sources of benzene are benzene-containing fractions formed during the pyrolysis and reforming of petroleum feedstocks, the hydrodealkylation of aromatic hydrocarbons, and coke production [2]. However, these fractions are multicomponent mixtures of aromatic and non-aromatic hydrocarbons containing azeotropes, which significantly complicates the isolation of benzene that meets GOST R 58415-2019[1] requirements, necessitating the use of special separation methods—extraction or extractive distillation (ED) with high-boiling entrainers [3].

Given the high demand for benzene in various industrial sectors and the large-scale nature of its production, the development of energy-efficient benzene recovery processes is an urgent challenge. This is addressed both through the search for new highly selective entrainers[2] [4–6] and by using systems having partially thermally coupled distillation columns (PTCDC) [7–10]. Structurally, the latter can either be implemented as complex columns with a side section [7–10] or as a dividing-wall column[3].

The authors of [7, 8] conducted a comparative analysis of ED flowsheets with different structures based on the criterion of total energy consumption in column boilers during the separation of benzene-containing fractions formed in the coking of coal [7], as well as in the catalytic hydrotreating and hydrocracking of pyrolysis gasoline and the catalytic dealkylation of pyrolysis gasoline with steam [8] (entrainer—*N*-methylpyrrolidone, NMP). To reduce the complexity of the problem, a simplified analogue of these fractions was considered, namely, a ternary mixture of benzene (B)–cyclohexane (CH)–toluene (T). It has been shown that among flowsheets consisting of two-outlet columns, when separating the B–CH–T mixture with a low toluene content (10 wt %), the scheme characterized by the lowest energy consumption is one in which NMP is applied in the first column and recovered in the last, whereas a scheme in which this component is separated in the bottom stream of the first column is used for the separation of mixtures having a high toluene concentration (40 and 45 wt %). Among the flowsheets involving a complex column with a single side section, the most energy-efficient for separating all mixtures considered in [7, 8] is one consisting of an ED column and an NMP regeneration column with a side-stripper. In this case, the use of a distillation column with a side section reduces the total energy consumption in the column boilers by 20–28% as compared to flowsheets with two-outlet columns.

When used in combination with a PTCDC, the main column is connected to the side section via counter-current flows of steam and liquid (thermal coupling). This necessitates the use of complex control systems to regulate the plant's operating parameters [9, 10]. One of the current trends in the development of energy-saving ED flowsheets involves the integration of side-draw columns into their structure. These units are simpler to operate than systems with PTCDC, yet they also reduce energy, capital, and total annual costs compared to traditional flowsheets using two-outlet columns [11–16]. For example, a two-column ED flowsheet for a toluene–methanol–water mixture (entrainer—glycerin), incorporating a side-draw column, is characterized by 65.7% lower energy costs and 62.3% lower total annual costs than an ED flowsheet consisting of three two-outlet columns [14].

The aim of this study is to evaluate the energy and economic efficiency of using complex columns with side withdrawal in ED flowsheets for B–CH–T mixtures of varying compositions.

CALCULATION

Synthesis of circuits incorporating columns with a side draw

The B–CH–T system has a B–CH binary azeotrope with a minimum boiling point at a benzene concentration of 54 mol % [17]. The separation of this mixture into pure components can be carried out by ED using high-boiling entrainers such as dimethylformamide, NMP, *N*-formylmorpholine, and others [3]. Similar to previous studies [7, 8], we selected NMP as the entrainer; in its presence, the relative volatility of the azeotrope-forming components is inverted, leading to the recovery of cyclohexane in the distillate of the extractive column.

1 GOST R 58415-2019. National Standard of the Russian Federation. Petrochemical benzene. Specifications. Moscow: Standartinform; 2019 (in Russ.).

2 Solovykh I.A. Extraction of benzene, toluene, and xylenes from reforming catalyst fractions using extraction and extractive distillation with selective solvent mixtures: Cand. Sci. Thesis. St. Petersburg: 2015, 19 p. (In Russ.).

3 thyssenkrupp Uhde. URL: https://www.thyssenkrupp-uhde.com. Accessed December 04, 2025.

The phase diagram of the B–CH–T mixture (Fig. 1) belongs to class 3.1.0-1a according to the classification proposed by L.A. Serafimov [18].

The authors of [19] tested the applicability of ED flowsheets for subset P consisting of two-outlet columns used to separate ternary azeotropic systems having different vapor–liquid equilibrium diagram structures. The investigation confirmed that, in the case of mixtures having a phase portrait of 3.1.0-1a with straight distillation lines, three flowsheets—P1, P2, and P5—are viable (Fig. 2).

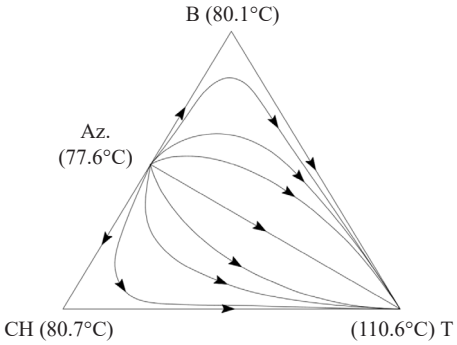

Fig. 1. Phase equilibrium diagram of the B–CH–T system. Az.—azeotrope

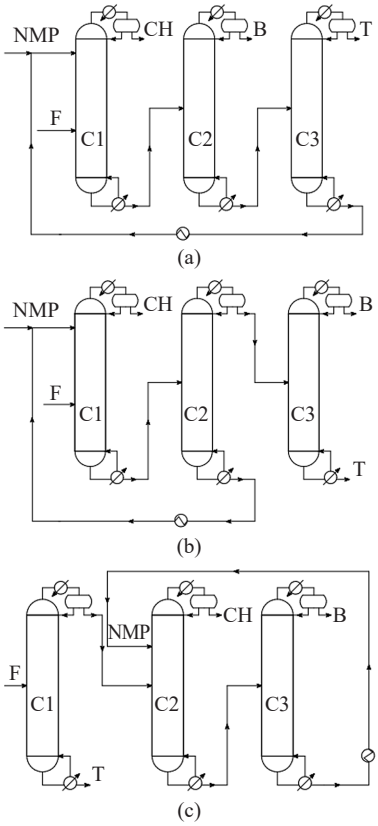

Fig. 2. Flowsheets for the ED of B–CH–T mixtures with NMP consisting of two-outlet columns:
(a) P1, (b) P2, (c) P5.
C1–C3 are distillation columns

Based on the flowsheets shown in Fig. 2, the authors of [7, 8] used an algorithm based on graph transformations that explicitly represent distillation flowsheets [20] to derive ED flowsheets for the B–CH–T mixture, including a complex column with a side section (Fig. 3). In terms of this algorithm, the flowsheets of subset P, consisting of two-outlet columns, are called pre-images, while the flowsheets of subset Θ, including a complex column with a side section, are called images.

The optimal operating parameters for the B–CH–T mixture ED systems consisting of two-outlet columns and incorporating a complex column with a side section for the two feed compositions under consideration are as published in [8] and presented in Tables 1 and 2.

In this study, an algorithm from [20] is used to synthesize flowsheets of subset I that include complex columns with a side withdrawal. A transformation of the graphs of the Θ flowsheets (in this case, they are pre-images flowsheets for the subset I) is performed using a simplification operation on the undirected edge connecting the main column to the side section (Fig. 4).

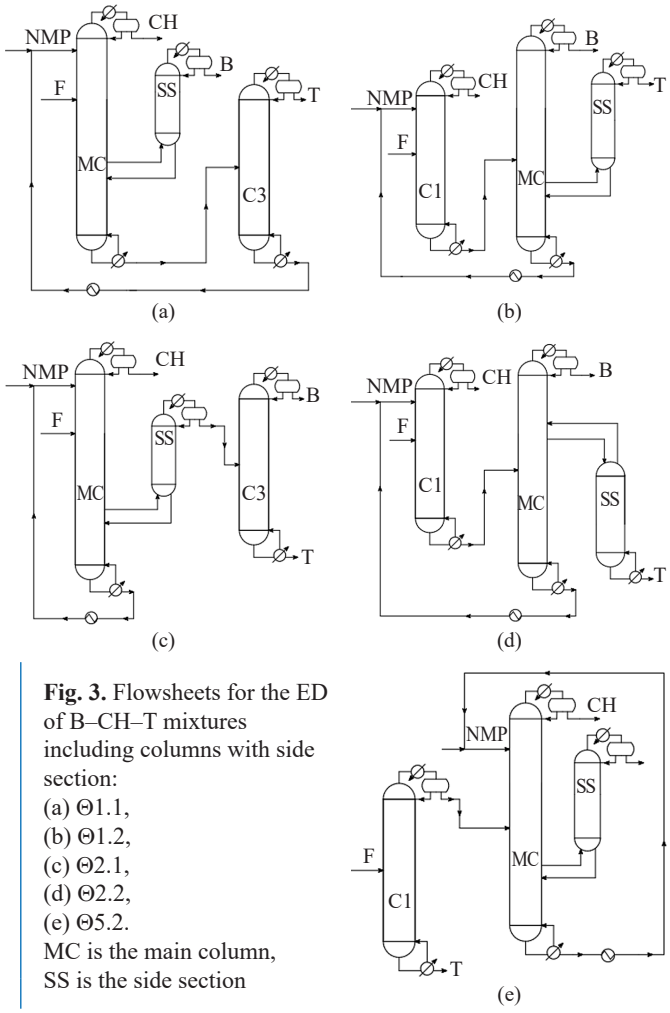

Fig. 3. Flowsheets for the ED of B–CH–T mixtures including columns with side section:
(a) Θ1.1,
(b) Θ1.2,
(c) Θ2.1,
(d) Θ2.2,
(e) Θ5.2.
MC is the main column,
SS is the side section

Table 1. Optimal parameters for ED flowsheets consisting of two-outlet columns for the separation of a B–CH–T mixture of Composition 1 (Composition 2) [8]

Flowsheet	Column	N_{total}	N_E/N_F	R	F_E, kg/h	Q_{reb}, kW	ΣQ_{reb}, kW
P1	C1	38	4/19 (4/18)	2.5 (12.4)	15033 (13746)	1509 (1398)	6695 (7093)
	C2	22	–/12 (–/12)	4.2 (3.7)	–	3656 (4113)	
	C3	14	–/8 (–/8)	0.85 (0.7)	–	1530 (1582)	
P2	C1	38	5/18 (4/16)	1.9 (8.4)	16611 (16407)	1397 (1199)	6534 (7158)
	C2	14	–/8 (–/8)	0.39 (0.33)	–	2485 (2773)	
	C3	22	–/12 (–/12)	3.0 (2.8)	–	2652 (3186)	
P5	C1	22	–/13 (–/13)	2.4 (3.1)	–	3250 (3683)	5804 (6166)
	C2	38	5/18 (4/15)	1.2 (5.2)	14301 (13696)	1082 (844)	
	C3	10	–/5 (–/5)	0.3 (0.23)	–	1472 (1639)	

Note: Composition 1 (concentrations of B, CH, and T are 40.0, 20.0, and 40.0 wt %, respectively) simulates the fraction formed in the processes of catalytic hydrotreating-hydrocracking of pyrolysis gasoline, and Composition 2 (concentrations of B, CH, and T are 50.0, 5.0, and 45.0 wt %, respectively) simulates the fraction formed in the catalytic dealkylation of pyrolysis gasoline with water vapor [21]. N_{total} is the total number of theoretical stages in the column; N_E is the feed stage of the entrainer; N_F is the feed stage of initial mixture; R is a reflux ratio; F_E is the flow rate of the entrainer; Q_{reb} is the reboiler heat duty.

Table 2. Optimal parameters for ED flowsheets including complex columns with a side section for the separation of a B–CH–T mixture of Composition 1 (Composition 2) [8]

Flowsheet	Column	N_{total}	$N_E/N_F/N_{SD}$	R	F_E, kg/h	F_{SD}, kg/h	Q_{reb}, kW	ΣQ_{reb}, kW
Θ1.1	MC	48	4/19/37 (4/18/37)	3.17 (14.14)	15033 (13746)	19000 (24500)	4119 (4531)	5649 (6113)
	SS	12	–/12/– (–/12/–)	2.28 (2.36)	–	–	–	
	C3	14	–/8/– (–/8/–)	0.85 (0.7)	–	–	1530 (1582)	
Θ1.2	C1	38	4/19/– (4/18/–)	2.5 (12.4)	15033 (13746)	–	1509 (1398)	6211 (6575)
	MC	28	–/12/24 (–/12/24)	3.6 (3.18)	–	8450 (9100)	4702 (5177)	
	SS	8	–/8/– (–/8/–)	0.7 (0.61)	–	–	–	

Table 2. Continued

Flowsheet	Column	N_{total}	$N_E/N_F/N_{SD}$	R	F_E, kg/h	F_{SD}, kg/h	Q_{reb}, kW	ΣQ_{reb}, kW
Θ2.1	MC	44	5/18/38 (4/16/38)	2.06 (8.9)	16611 (16407)	13100 (15500)	3649 (3737)	6301 (6923)
	SS	8	–/8/– (–/8/–)	0.16 (0.16)	–	–	–	
	C3	22	–/12/– (–/12/–)	3.0 (2.8)	–	–	2652 (3186)	
Θ2.2	C1	38	5/18/– (4/16/–)	1.9 (8.4)	16611 (16407)	–	1397 (1199)	5242 (5585)
	MC	26	–/20/15 (–/20/15)	3.8 (3.44)	–	19273 (22722)	2426 (2699)	
	SS	10	–/1/– (–/1/–)	–	–	–	1419 (1687)	
Θ5.2	C1	22	–/13/– (–/13/–)	2.4 (3.1)	–	–	3250 (3683)	5651 (5947)
	MC	43	5/18/37 (4/15/37)	1.06 (3.39)	14301 (13696)	6270 (7880)	2401 (2264)	
	SS	5	–/5/– (–/5/–)	0.11 (0.13)	–	–	–	

Note: N_{total} is the total number of theoretical stages in the column; N_E is the feed stage of the entrainer; N_F is the main feed stage; N_{SD} is the side draw stage; R is a reflux ratio; F_E is the flow rate of the entrainer; F_{SD} is the flow rate of the side draw stream; Q_{reb} is the reboiler heat duty. MC is the main column; SS is the side section.

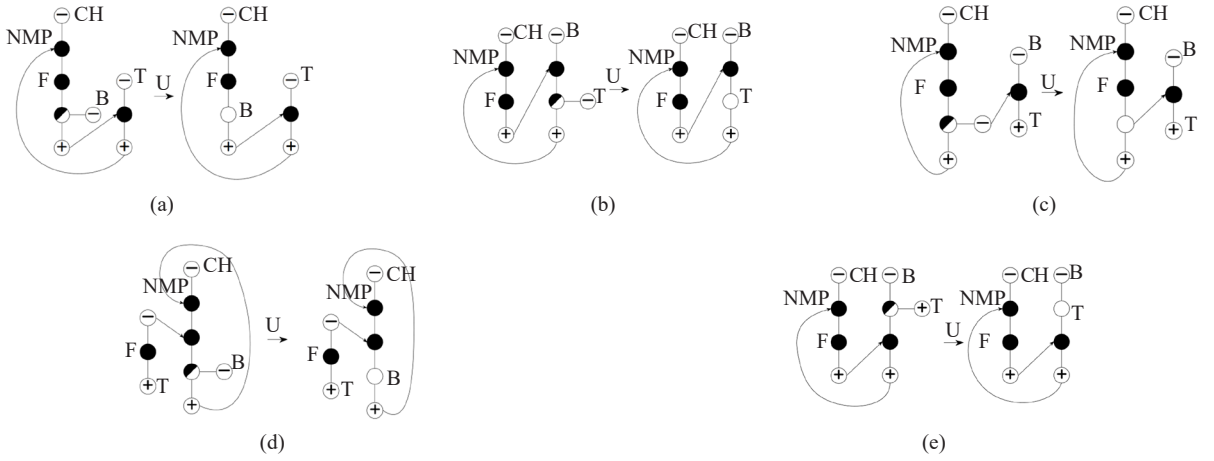

Fig. 4. Synthesis of schemes including a column with a side draw based on flowsheets:
(a) Θ1.1,
(b) Θ1.2,
(c) Θ2.1,
(d) Θ2.2,
(e) Θ5.2.
U is a simplification operation of the graph of the pre-image flowsheet on the undirected edge connecting the main column to the side section

As a result of transforming the graph of the pre-image Flowsheet Θ1.1 (Fig. 4a), a graph is obtained corresponding to Flowsheet I1.1, which includes an ED column with the entire amount of benzene contained in the initial mixture being removed in the side stream below the extractive section (Fig. 5a). The purification of benzene from T and NMP is carried out in column C2, whose bottom stream is mixed with the bottom stream of column C1 and fed for separation into column C3. In principle, another variant of this scheme is possible, where the side draw stream, consisting of B, T, and NMP, is distilled into individual components in two columns operating according to the second specified separation. However, in this case, the ED flowsheet would consist of four columns, whereas the scope of the present work is limited to a consideration of three-column ED flowsheets. Transforming the graph of the pre-image Flowsheet Θ1.2 (Fig. 4b) yields a graph corresponding to Flowsheet I1.2, which includes an NMP recovery column with the entire amount of toluene contained in the feed mixture being withdrawn as a side stream below the feed tray (Fig. 5b). The removal of NMP from toluene is carried out in column C3. Upon transformation the graph of the Flowsheet Θ2.1 (Fig. 4c), a graph corresponding to Flowsheets I2.1A and I2.1B is obtained (Figs. 5c and 5d). These flowsheets include an ED column with a side draw stream below the extractive section and differ in the sequence of separation of individual components from the side stream. In Flowsheet I2.1A, B and T are separated in the distillates of columns C2 and C3, respectively, while in Flowsheet I2.1B, NMP is separated in the bottom stream of column C2, and the mixture of B and T is distilled in column C3.

By simplifying the graph of Flowsheet Θ2.2 along the undirected edge connecting the main column and the side stripping section (Fig. 4d), we obtain the graph of Flowsheet I2.2, which includes an NMP regeneration column from which the entire amount of toluene contained in the feed mixture is withdrawn in the side stream above the feed tray (Fig. 5e). The removal of benzene from toluene is carried out in column C3. By simplifying the graph of Flowsheet Θ5.2 (Fig. 4e) along the undirected edge connecting the main column to the side rectifying section, we obtain the graph of Flowsheet I5.2, which includes an ED column with the entire amount of benzene contained in the initial mixture being withdrawn in a side stream below the feed tray (Fig. 5f). Purification of B from NMP is carried out in column C3.

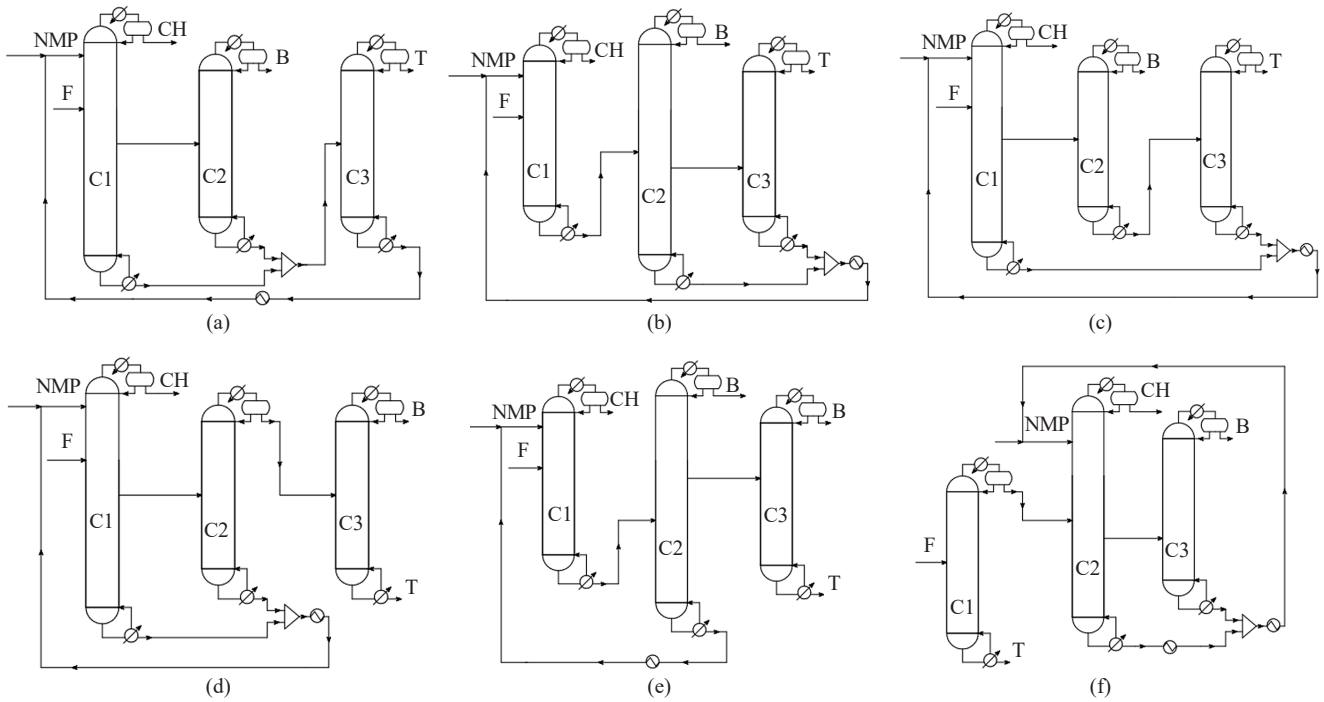

Fig. 5. Flowsheets for the ED of B–CH–T mixtures, including columns with side draw:
(a) I1.1,
(b) I1.2,
(c) I2.1A,
(d) I2.1B,
(e) I2.2,
(f) I5.2.
C1–C3 are distillation columns

Determining the optimal parameters for systems incorporating columns with a side draw

Next, we determined the optimal parameters for all the generated flowsheets, including the complex columns with a side draw, which are based on the criterion of total energy consumption in the column reboilers ($\sum Q_{reb}$). The parameters for optimization were: (1) number of trays (N_{total}); (2) position of the feed trays (N_F) in the side stream separation columns; (3) position of the side stream tray (N_{SD}); (4) side stream flow rate (F_{SD}). In this case, the columns with side draws in each flowsheet were calculated in two variants differing in the phase state of the side stream: (1) side stream is withdrawn in the vapor phase; (2) side stream is withdrawn in the liquid phase.

The initial data for modeling and optimizing flowsheets including column units with side streams are presented in Table 3.

All columns were calculated in the design and verification version, specifying the concentration of the main component in the product streams in accordance with the technical requirements for premium-grade products, namely: 99.9 wt % for cyclohexane (GOST 14198-78[4]), 99.9 wt % for benzene (GOST R 58415-2019[5]) and 99.75 wt % for toluene (GOST 14710-78[6]). The trays in the columns are theoretical.

The positions of the feed (N_F) and entrainer (N_E) trays in the ED column, as well as the entrainer flow rate (F_E) in the flowsheets of subset I, were set in accordance with the optimal values of these parameters found for the pre-image flowsheets of subset P. The number of trays in the columns with a side draw was set equal to the number of trays in the main column of the PTCDC subsystem of the corresponding pre-image flowsheets of subset Θ, which follows from the flowsheet synthesis algorithm [20]. To describe the liquid–vapor equilibrium, the Non-Random Two Liquid local composition model with the authors' parameters [8] was used. The computational experiment was performed using the Aspen Plus v.10 software package.

In the first stage, the number of plates in the side draw stream-splitting columns was selected based on an analysis of how the energy consumption in the reboilers of these columns depends on the number of plates in them, as described in [22]. In this process, the N_{SD} and the side stream flow rate were fixed in the side draw columns. Next, the optimal values of the remaining parameters were determined by scanning the range of variable changes with a specified step size (the step size for N_{SD} and N_F was equal to 1 theoretical plate; that for the side draw flow rate, 10–50 kg/h).

In Flowsheets I1.1 and I2.1B, it is not necessary to determine N_{total} and N_F for columns C3, since these columns are identical to columns C3 in the pre-image Flowsheets P1 and P2, respectively. The optimal parameters of columns C1 and C2 were determined in accordance with the procedure shown in Fig. 6. The transformation of Flowsheets P1, P2, and P5 into flowsheets of subset Θ (Θ1.1, Θ2.1, and Θ5.2, respectively) and further into the flowsheets of subset I (I1.2, I2.2, and I5.2, respectively) did not affect column C1; therefore, in Flowsheets I1.2, I2.2, and I5.2,

Table 3. Initial information for modeling and optimization of flowsheets that include complex columns with side draw [9]

Parameter	Value
Pressure in columns, kPa	101.3
Feed stream mass flow (F), kg/h	15000
NPM feed temperature to ED column, °C	70
B : CH : T concentration in feed stream, wt %	
Composition 1	40.0 : 20.0 : 40.0
Composition 2	50.0 : 5.0 : 45.0
NMP concentration in entrainer stream, wt %	99.99

Note: Composition 1 simulates the fraction formed in the processes of catalytic hydrotreating-hydrocracking of pyrolysis gasoline, and Composition 2 simulates the fraction formed in the catalytic dealkylation of pyrolysis gasoline with water vapor [21].

4 GOST 14198-78. Interstate Standard. Technical cyclohexane Specifications. Moscow: IPK Izdatelstvo standartov; 1999, 7 p. (In Russ.).

5 GOST R 58415-2019. National Standard of the Russian Federation. Petrochemical benzene. Specifications. Moscow: Standartinform; 2019, 8 p. (In Russ.).

6 GOST 14710-78. Interstate Standard. Petroleum toluene. Specifications. Moscow: IPK Izdatelstvo standartov; 2004, 4 p. (In Russ.).

it is necessary to determine the optimal parameters only for columns C2 and C3. The optimization procedure for these columns is similar to the procedure shown in Fig. 6, the only difference being that the F_{SD} value from column C2, the side draw plate in column C2, and the feed tray in column C3 are varied. Optimization criterion: $\Sigma Q_{reb2,3} = Q_{reb,C2} + Q_{reb,C3}$. The optimization procedure for Flowsheet I2.1A is shown in Fig. 7. Tables 4 and 5 present the optimal separation parameters for the B–CH–T mixture of both feed compositions under consideration in ED flowsheets including a complex column with a side draw.

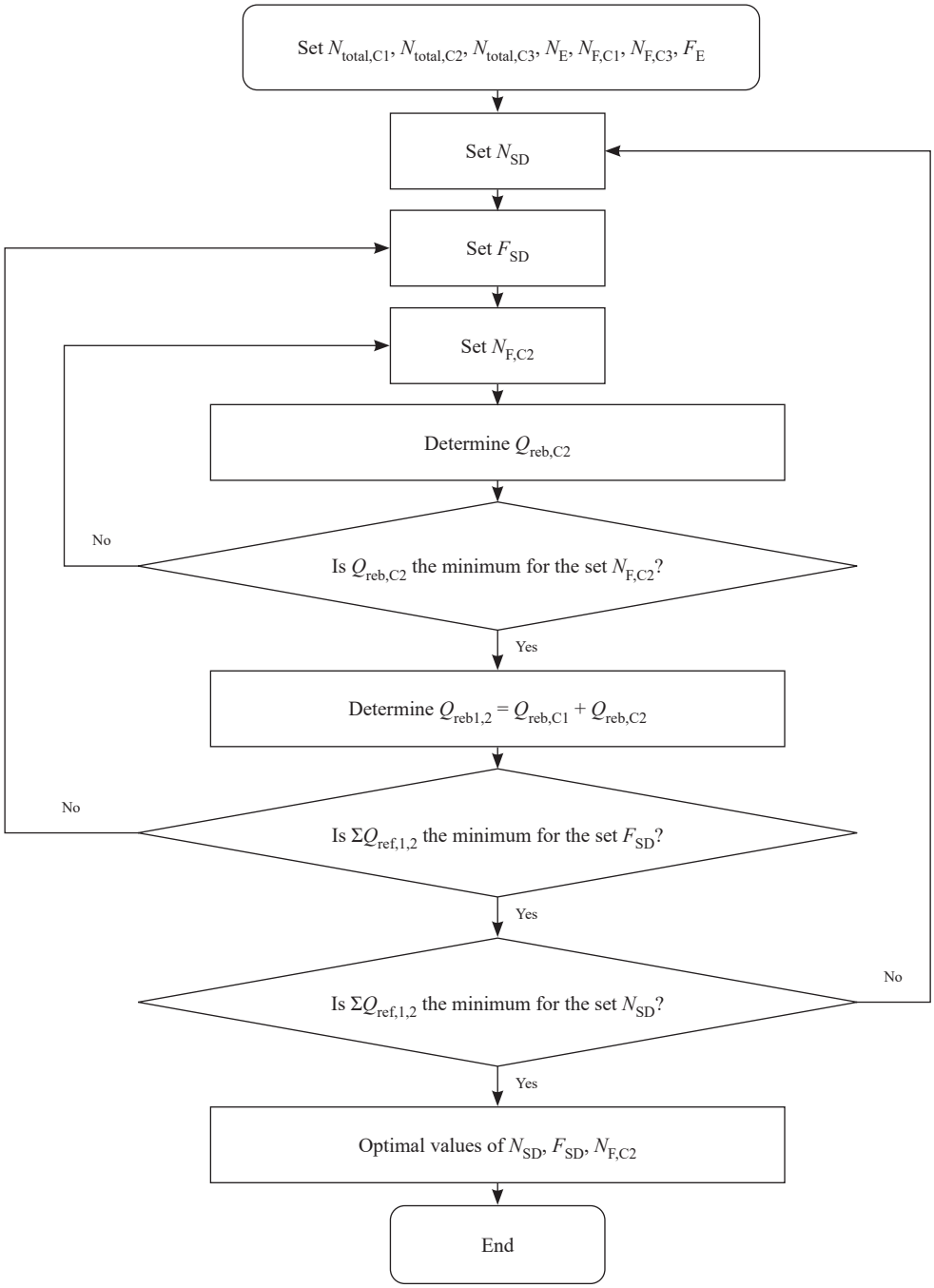

Fig. 6. Optimization procedure for Flowsheets I1.1 and I2.1B.
$N_{total,C1}$, $N_{total,C2}$, and $N_{total,C3}$ are the total number of theoretical stages in the column C1, C2, and C3, respectively;
N_E is a position of the entrainer tray in the ED column;
$N_{F,C1}$, $N_{F,C2}$, and $N_{F,C3}$ are the position of the feed tray in the column C1, C2, and C3, respectively;
F_E is entrainer flow rate;
N_{SD} is a position of the side stream tray;
F_{SD} is a side stream flow rate

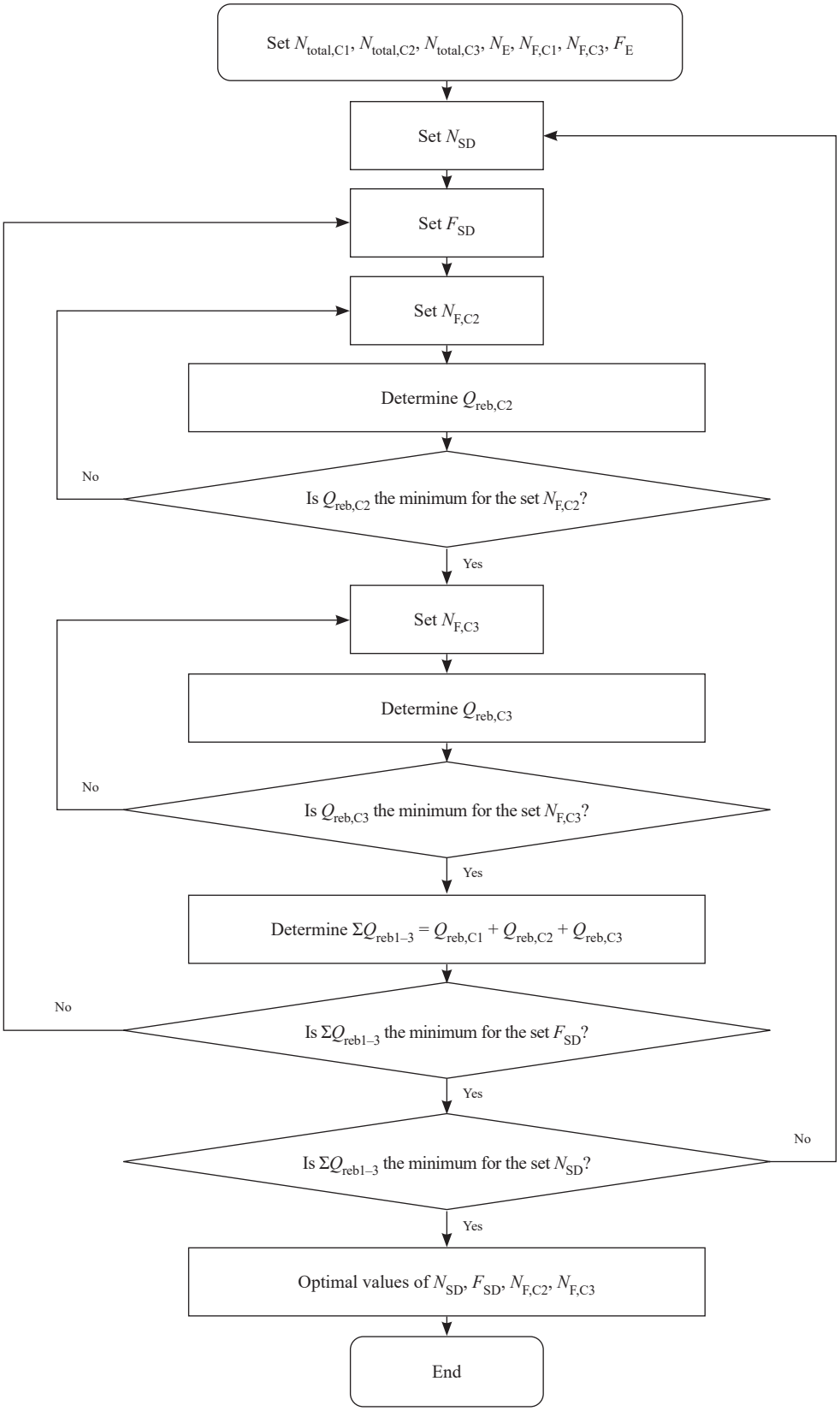

Fig. 7. Optimization procedure for Flowsheet I2.1A.
$N_{total,C1}$, $N_{total,C2}$, and $N_{total,C3}$ are the total number of theoretical stages in the column C1, C2, and C3, respectively;
N_E is a position of the entrainer tray in the ED column;
$N_{F,C1}$, $N_{F,C2}$, and $N_{F,C3}$ are the position of the feed tray in the column C1, C2, and C3, respectively;
F_E is entrainer flow rate;
N_{SD} is a position of the side stream tray;
F_{SD} is a side stream flow rate

RESULTS AND DISCUSSION

As shown in Tables 4 and 5, the phase state of the side draw flow has little effect on the total energy consumption in column boilers, although the mass flowrates of the vapor-phase and liquid-phase side draw streams differ significantly. When the side stream is carried out below the feed tray, the vapor-phase flow rate is lower than the liquid-phase flow rate; this is explained by the higher concentration of target components in the vapor phase compared to the liquid phase. For example, when separating a mixture of Composition 1, the concentration of benzene and toluene in the vapor-phase side stream from column C1 in Flowsheet I1.1 is 98.3 wt %, and in the liquid-phase side stream—61.4 wt %, this means that to recover the entire amount of benzene and toluene contained in the feed stream, 2.1 times less vapor-phase side stream is required than liquid-phase side stream.

When drawing the side stream above the feed tray (column C2 in Flowsheet I2.2), the situation is reversed: the concentration of the medium-boiling target component (toluene) in the vapor phase is 1.5 times lower than in the liquid phase, and to recover all the toluene contained in the feed mixture, 1.4 times more of the vapor-phase side draw stream must be withdrawn than of the liquid-phase side stream.

Table 4. Optimal parameters for ED flowsheets including columns with side draw for the separation of a B–CH–T mixture of Composition 1

Flowsheet	Column	N_{total}	$N_E/N_F/N_{SD}$	R	F_E, kg/h	F_{SD}, kg/h	Q_{reb}, kW	ΣQ_{reb}, kW
I1.1-V*	C1	48	4/19/36	2.83	15033	8090	2837	4932
	C2	40	–/26/–	1.32	–	–	603	
	C3	14	–/8/–	0.88	–	–	1492	
I1.1-L*	C1	48	4/19/37	2.57	15033	16860	1689	4991
	C2	32	–/18/–	1.53	–	–	1795	
	C3	14	–/8/–	0.87	–	–	1507	
I1.2-V	C1	38	4/19/–	2.5	15033	–	1509	6171
	C2	28	–/12/24	3.6	–	7570	4532	
	C3	16	–/10/–	0.7	–	–	130	
I1.2-L	C1	38	4/19/–	2.5	15033	–	1509	6010
	C2	28	–/12/24	3.3	–	16420	3199	
	C3	12	–/6/–	0.6	–	–	1302	
I2.1A-V	C1	44	5/18/38	2.0	16611	12410	3522	5250
	C2	34	–/18/–	2.7	–	–	1010	
	C3	16	–/10/–	0.16	–	–	718	
I2.1A-L	C1	44	5/18/38	1.9	16611	21160	1668	4846
	C2	32	–/17/–	1.8	–	–	2010	
	C3	16	–/9/–	0.45	–	–	1168	
I2.1B-V	C1	44	5/18/38	2.3	16611	12390	3621	6200
	C2	20	–/14/–	0.15	–	–	82	
	C3	22	–/12/–	2.8	–	–	2497	
I2.1B-L	C1	44	5/18/39	2.0	16611	22430	1660	6171
	C2	16	–/10/–	0.2	–	–	2032	
	C3	22	–/12/–	2.7	–	–	2497	

Table 4. Continued

Flowsheet	Column	N_{total}	$N_E/N_F/N_{SD}$	R	F_E, kg/h	F_{SD}, kg/h	Q_{reb}, kW	ΣQ_{reb}, kW
I2.2-V	C1	38	5/18/–	1.9	16611	–	1397	4692
	C2	26	–/20/14	4.0	–	11200	2333	
	C3	34	–/18/–	2.8	–	–	962	
I2.2-L	C1	38	5/18/–	1.9	16611	–	1397	4777
	C2	26	–/20/15	3.1	–	8330	2366	
	C3	32	–/16/–	2.9	–	–	1014	
I5.2-V	C1	22	–/13/–	2.4	–	–	3250	5654
	C2	43	5/18/36	1.09	14301	6110	2383	
	C3	12	–/7/–	0.11	–	–	21	
I5.2-L	C1	22	–/13/–	2.4	–	–	3250	5665
	C2	43	5/18/37	1.05	14301	12300	1345	
	C3	10	–/5/–	0.14	–	–	1070	

Note: N_{total} is the total number of theoretical stages in the column; N_E is the feed stage of the entrainer; N_F is the main feed stage; N_{SD} is the side draw stage; R is the reflux ratio; F_E is the flow rate of the entrainer; F_{SD} is the flow rate of the side draw stream; Q_{reb} is the reboiler heat duty.

*V—vapor; L—liquid.

Table 5. Optimal parameters for ED flowsheets including columns with side draw for the separation of a B–CH–T mixture of Composition 2

Flowsheet	Column	N_{total}	$N_E/N_F/N_{SD}$	R	F_E, kg/h	F_{SD}, kg/h	Q_{reb}, kW	ΣQ_{reb}, kW
I1.1-V	C1	48	4/18/36	12.9	13746	10040	2861	5212
	C2	36	–/24/–	1.37	–	–	808	
	C3	14	–/8/–	0.76	–	–	1543	
I1.1-L	C1	48	4/18/37	12.0	13746	19670	1490	5188
	C2	34	–/20/–	1.42	–	–	2135	
	C3	14	–/8/–	0.75	–	–	1563	
I1.2-V	C1	38	4/18/–	12.4	13746	–	1398	6543
	C2	28	–/12/24	3.2	–	8160	5021	
	C3	16	–/9/–	0.60	–	–	124	
I1.2-L	C1	38	4/18/–	12.4	13746	–	1398	6260
	C2	28	–/12/24	3.0	–	16550	3585	
	C3	14	–/7/–	0.42	–	–	1277	
I2.1A-V	C1	44	4/16/38	8.3	16407	14700	3583	5543
	C2	36	–/19/–	2.4	–	–	1153	
	C3	16	–/10/–	0.16	–	–	807	
I2.1A-L	C1	44	4/16/38	8.4	16407	24520	1429	5150
	C2	32	–/17/–	1.7	–	–	2409	
	C3	16	–/9/–	0.45	–	–	1312	

Table 5. Continued

Flowsheet	Column	N_{total}	$N_E/N_F/N_{SD}$	R	F_E, kg/h	F_{SD}, kg/h	Q_{reb}, kW	ΣQ_{reb}, kW
I2.1B-V	C1	44	4/16/38	10.3	16407	14670	3729	6811
	C2	20	–/14/–	0.14	–	–	92	
	C3	22	–/12/–	2.6	–	–	2990	
I2.1B-L	C1	44	4/16/39	9.3	16407	25500	1464	6807
	C2	16	–/10/–	0.19	–	–	2352	
	C3	22	–/12/–	2.6	–	–	2991	
I2.2-V	C1	38	4/16/–	8.4	16407	–	1199	4946
	C2	26	–/20/14	3.7	–	13400	2600	
	C3	34	–/18/–	2.5	–	–	1147	
I2.2-L	C1	38	4/16/–	8.4	16407	–	1199	5051
	C2	26	–/20/15	2.9	–	9760	2643	
	C3	32	–/16/–	2.6	–	–	1209	
I5.2-V	C1	22	–/13/–	3.1	–	–	3683	5939
	C2	43	4/15/37	3.4	13695	7650	2230	
	C3	14	–/9/–	0.12	–	–	26	
I5.2-L	C1	22	–/13/–	3.1	–	–	3683	5968
	C2	43	4/15/38	3.3	13695	16030	905	
	C3	10	–/5/–	0.16	–	–	1380	

Note: N_{total} is the total number of theoretical stages in the column; N_E is the feed stage of the entrainer; N_F is the main feed stage; N_{SD} is the side draw stage; R is the reflux ratio; F_E is the flow rate of the entrainer; F_{SD} is the flow rate of the side draw stream; Q_{reb} is the reboiler heat duty.

The optimal position of the side draw plate is practically independent of the phase state of the side stream, while the optimal values of N_{SD} in the image flowsheets of subset I and their pre-images from subset Θ practically coincide (see Tables 2, 4, 5). This is due to the fact that the number of plates in the complex column with a side draw is equal to the number of plates in the main column of the PTCDC subsystem corresponding the pre-image scheme of subset Θ, and the concentration of target components reaches its maximum value in both the vapor and liquid phases in the same zone of these units.

The energy consumption of the image flowsheets of subset I and their pre-images from subset Θ in the case of Flowsheets I1.2 and Θ1.2, I2.1B and Θ2.1, I5.2 and Θ5.2 differs only slightly, while the total number of plates in the columns of the image flowsheets is 5.0–16.2% greater than in the columns of the pre-image flowsheets. The power consumption of Flowsheets I1.1, I2.1A, and I2.2 is 8.9–25.6% lower than that of the corresponding pre-image Flowsheets Θ1.1, Θ2.1, and Θ2.2; however, the total number of plates in the columns of these image flowsheets is significantly (by 24.3–37.8%) greater than in the columns of the pre-image flowsheets. In this situation, to correctly compare flowsheets with different structures and select a technological solution for practical implementation, it is advisable to use the total annual cost (TAC) criterion, which is calculated using the formula [14]:

$$\mathrm{TAC} = \mathrm{OC} + \frac{\mathrm{CC}}{\mathrm{ET}}, \quad (1)$$

where OC represents operating costs, USD/year; CC represents capital costs, USD; ET represents the plant's exploitation time in years [14], which was assumed to be 5.

Capital and operating costs were calculated using the Aspen Process Economic Analyzer. When determining operating costs, only the costs of electricity and energy carriers (heating steam and cooling water) were taken into account. These costs were based on energy carrier prices available in the Aspen Plus v.10 software database,

namely, the cost of steam at a pressure of 689.5 kPa was 0.018 USD/kg; the cost of steam at a pressure of 2757.9 kPa was 0.026 USD/kg; the cost of cooling water was 0.032 USD/m^3. When calculating capital costs, only the cost of equipment was taken into account. For each distillation column, based on the number of theoretical plates in it, the number of NUTTER-BDP valve plates was determined, with an efficiency coefficient assumed to be 0.65.

Tables 6–8 present the values of OC, CC, and TAC for all ED flowsheets of the B–CH–T mixture shown in Figs. 2, 3, and 5. Tables 7 and 8 also present data on the energy (ΔQ_{reb}) and economic (ΔTAC) efficiency of flowsheets including a complex column with a side section and side draw. These indicators were calculated using formulas (2) and (3):

$$\Delta Q_{reb} = \frac{\sum Q_{reb}^{pr} - \sum Q_{reb}^{ref}}{\sum Q_{reb}^{pr}} \times 100\%, \quad (2)$$

where $\sum Q_{reb}^{pr}$ is the total energy consumption in the reboilers of the pre-image flowsheet based on two-outlet columns; $\sum Q_{reb}^{ref}$ is the total energy consumption in the reboilers of the image flowsheet that includes a complex column with a side section (or a complex column with a side draw).

$$\Delta TAC = \frac{TAC^{pr} - TAC^{ref}}{TAC^{pr}} \times 100\%, \quad (3)$$

where TAC^{pr} is the total annual cost of the pre-image flowsheet consisting of two-outlet columns; TAC^{ref} is the total annual cost of the image flowsheet, which includes a complex column with a side section (or a complex column with a side draw).

Table 6. Energy and economic indicators of flowsheets consisting of two-outlet columns for the separation of a B–CH–T mixture of Composition 1 (Composition 2)

Flowsheet	ΣQ_{reb}, kW	OC, USD/year	CC, USD	TAC, USD/year
P1	6696 (7093)	2269030 (2397010)	893000 (890900)	2447630 (2575190)
P2	6534 (7158)	2384770 (2620880)	878700 (899200)	2560510 (2800720)
P5	5804 (6166)	1996510 (2133090)	780000 (778600)	2152510 (2288810)

Note: ΣQ_{reb} is the total energy consumption in columns reboilers; OC are operating costs; CC are capital costs, TAC is the total annual cost.

Table 7. Energy and economic indicators of flowsheets, including complex columns with side section and side draw for the separation of a B–CH–T mixture of Composition 1

Flowsheet	ΣQ_{reb}, kW	OC, USD/year	CC, USD	TAC, USD/year	ΔQ_{reb}, %	ΔTAC, %
Θ1.1	5649	1959920	924300	2144780	15.6	12.4
Θ1.2	6211	2682210	904500	2863110	7.2	−17.0
Θ2.1	6301	2509570	910100	2691590	3.6	−5.1
Θ2.2	5242	2059080	818100	2222700	19.8	13.2
Θ5.2	5651	2112700	781400	2268980	2.6	−5.4
I1.1-V	4932	1737770	999600	1937690	26.3	20.8
I1.1-L	4991	1757850	970000	1951850	25.5	20.3
I1.2-V	6171	2661750	948900	2851530	7.8	−16.5
I1.2-L	6010	2586380	944100	2775200	10.2	−13.4
I2.1A-V	5250	2310070	944200	2498910	19.7	2.4
I2.1A-L	4846	1945130	902300	2125590	25.8	17.0
I2.1B-V	6200	2499110	1008000	2700710	5.1	−5.5
I2.1B-L	6171	2488890	910500	2670990	5.6	−4.3
I2.2-V	4692	1811300	953500	2002000	28.2	21.8
I2.2-L	4777	1842640	898600	2022360	26.9	21.0
I5.2-V	5654	2114390	824800	2279350	2.6	−5.9
I5.2-L	5665	2119350	804000	2280150	2.4	−5.9

Note: ΣQ_{reb} is the total energy consumption in columns reboilers; OC are operation costs; CC are capital costs, TAC is total annual cost.

Table 8. Energy and economic indicators of flowsheets, including complex columns with side section and side draw for the separation of a B–CH–T mixture of Composition 2

Flowsheet	ΣQ_{reb}, kW	OC, USD/year	CC, USD	TAC, USD/year	ΔQ_{reb}, %	ΔTAC, %
Θ1.1	6113	2108060	904500	2288960	13.8	11.1
Θ1.2	6575	2873790	869800	3047750	7.3	−18.4
Θ2.1	6923	2712600	895300	2891660	3.3	−3.2
Θ2.2	5585	2203860	828200	2369500	22.0	15.4
Θ5.2	5947	2177480	792500	2335980	3.6	−2.1
I1.1-V	5212	1831240	989700	2029180	26.5	21.2
I1.1-L	5188	1827570	977900	2023150	26.9	21.4
I1.2-V	6543	2858530	943000	3047130	7.8	−18.3
I1.2-L	6260	2725090	971900	2919470	11.7	−13.4
I2.1A-V	5543	2425560	997500	2625060	22.6	6.3
I2.1A-L	5150	2018720	919600	2202640	28.0	21.4
I2.1B-V	6811	2702880	992100	2901300	4.8	−3.6
I2.1B-L	6807	2701110	933800	2887870	4.9	−3.1
I2.2-V	4946	1932170	940800	2120330	30.9	24.3
I2.2-L	5051	1970680	940600	2158800	29.4	22.9
I5.2-V	5939	2173500	840200	2341540	3.7	−2.3
I5.2-L	5968	2187210	801100	2347430	3.2	−2.6

Note: ΣQ_{reb} is the total energy consumption in columns reboilers; OC are operation costs; CC are capital costs, TAC is total annual cost.

As shown in Table 6, among the two-outlet column flowsheets, Flowsheet P5 has the lowest energy, operating, capital, and total annual costs; in this flowsheet, toluene is separated from the B–CH azeotropic mixture in the bottom of the first column. Apparently, this is due to the high concentration of toluene (40 and 45 wt % for compositions 1 and 2, respectively) in the feed mixture, as well as lower NMP consumption compared to Flowsheets P1 and P2.

Among the flowsheets involving a complex column with a side section, Flowsheet Θ2.2, consisting of an ED column and an NMP regeneration column with a side stripping section (Fig. 3d), is characterized by the lowest energy consumption and the highest energy and economic efficiency in terms of separating the mixtures of both compositions. However, the lowest operating costs and TAC correspond to Flowsheet Θ1.1, consisting of an extractive column with a side rectifying section and an NMP regeneration column (Fig. 3a). This is evidently due to the fact that the NMP flow rate in Flowsheet Θ1.1 is lower than in Flowsheet Θ2.2 by 1578 kg/h (9.5%) and by 2661 kg/h (16.2%) when separating mixtures of Compositions 1 and 2, respectively. In terms of energy consumption, Flowsheet Θ1.1 ranks second and third after Flowsheet Θ2.2 when separating mixtures of compositions 1 and 2, respectively; however, the difference in energy consumption between flowsheets Θ1.1 and Θ2.2 does not exceed 10%.

Among the flowsheets incorporating a complex column with a side draw, Flowsheet I2.2-V, which includes an NMP regeneration column with a side draw in the vapor-phase above the feed tray (Fig. 5e), exhibits the lowest energy consumption and the highest energy and economic efficiency when separating the B–CH–T mixture of both compositions. This flowsheet was obtained by transforming Flowsheet Θ2.2, which is the best in terms of the specified indicators among the flowsheets incorporating columns with a side section. The lowest operating costs and TAC correspond to Flowsheet I1.1 (Fig. 5a), which includes an extractive column with a side draw stream below the feed tray in the vapor phase (for Composition 1) or in the liquid phase (for Composition 2). This flowsheet is characterized by lower NMP consumption and a smaller side draw flow rate than Flowsheet I2.2-V. It should be noted that Flowsheet I1.1 was obtained by transforming Flowsheet Θ1.1, which is optimal in terms of OC and TAC among flowsheets including columns with a side section.

At the same time, the energy consumption of the I1.1-V (for Composition 1) and I1.1-L (for Composition 2) flowsheets is approximately 5% higher than that of Flowsheet I2.2-V. The energy and economic efficiency of Flowsheets I1.1-V and I2.2-V also differ only slightly.

Certain flowsheets incorporating a complex column with a side section and a complex column with a side draw are characterized by higher TAC values than the pre-image flowsheets consisting of two-outlet columns from which they were derived. This is due to the fact that in the image flowsheets, the entrainer is eluted in the bottom flow of column (in the bottom flow of the main column of the PTCDC subsystem in the case of Flowsheets Θ1.2, Θ2.1, and Θ5.2, or in the bottom flow of the column with a side draw in the case of Flowsheets I1.2, I2.1B, and I5.2), which have a greater height than the NMP regeneration column in the pre-image flowsheet. For this reason, the temperature in the reboilers of these units differs significantly due to requiring steam of a higher temperature (and higher cost) to heat the boilers of the main column of the subsystem with the PTCDC and the complex column with a side draw than for heating the boiler of the entrainer regeneration column in the pre-image flowsheet. As a result, the operating costs and TAC of the image Flowsheets Θ1.2, Θ2.1, Θ5.2, I1.2, I2.1B, and I5.2 are higher than those of the corresponding pre-image flowsheets with two-outlet columns.

Virtually all image flowsheets in subset I are characterized by a lower TAC value than the corresponding pre-image flowsheets in subset Θ; this is mainly due to the lower energy costs associated with heating the column reboilers in the flowsheets of subset I. At the same time, the capital costs for the flowsheets in subset I are higher than those for the flowsheets in subset Θ, since the number of trays in the columns of the flowsheets in subset I is 5.0–37.8% greater than in the flowsheets of subset Θ. The TAC values for Flowsheet I5.2 are slightly higher than those for the pre-image Flowsheet Θ5.2, which is due to the 7.0–12.9% greater number of trays in the columns of these flowsheets and consequently higher capital costs, while energy and operating costs are practically equal to those of Flowsheet Θ5.2.

The minimum TAC value among all the considered flowsheets for subsets P, Θ, and I corresponds to Flowsheet I1.1 (Fig. 5a), which includes an extractive column with a side draw stream below the feed tray in the vapor phase (for Composition 1) or in the liquid phase (for Composition 2). However, when separating mixture Composition 1, the TAC value for Flowsheet I1.1 with a liquid-phase side stream is only 0.7% higher than that of the same scheme with a vapor-phase side draw. Since it is easier to take a side stream in the liquid phase than in the vapor phase, Flowsheet I1.1, which includes a complex column with a side draw in the liquid phase, can be recommended for the separation of the B–CH–T mixture of both compositions considered. Compared to Flowsheet P5, which is characterized by the lowest energy and total annual costs among flowsheets consisting of two-outlet columns, Flowsheet I1.1-L provides savings in energy consumption and TAC of 14.0% and 9.3%, respectively, when separating mixture Composition 1, and of 15.9% and 11.6%, respectively, when separating mixture Composition 2.

CONCLUSIONS

As a result of the study, based on five ED flowsheets for the B–CH–T mixture that include columns with side sections (flowsheets of subset Θ), six ED flowsheets that include columns with a side draw (flowsheets of subset I) were generated using the graph method.

The optimal parameters of the synthesized flowsheets according to the criterion of total energy consumption were determined for the separation of the B–CH–T mixture of two initial compositions. These are simplified analogs of the fractions formed during the catalytic hydrotreating-hydrocracking of pyrolysis gasolines (Composition 1) and during the catalytic dealkylation of pyrolysis gasoline with steam (Composition 2). The complex column with a side draw in each flowsheet of subset I is calculated with both vapor-phase and liquid-phase side streams.

It is established that the energy and economic efficiency of ED flowsheets involving a complex column with a side draw depends little on the phase state of the side stream. When the side stream is taken below the feed tray, the vapor-phase flow rate is lower than the liquid-phase flow rate, whereas when the side stream is taken above the feed tray, the opposite situation is observed.

A comparison was conducted of ED flowsheets with different structures based on the criteria of total energy consumption in column boilers ($\sum Q_{reb}$) and total annual costs (TAC). It was found that the minimum value of $\sum Q_{reb}$ for the separation of the B–CH–T mixture of both considered compositions corresponds to Flowsheet I2.2-V. This flowsheet consists of an extractive column, an NMP regeneration column with a vapor-phase side stream above the feed tray, and a B–T mixture distillation column. Flowsheet I1.1, which is characterized by the minimum TAC value, includes an extractive column with a side draw below the feed tray in the vapor phase (for Composition 1) or in the liquid phase (for Composition 2), as well as two side

draw distillation columns (for the B–T–NMP mixture separation). In this case, Flowsheets I1.1-V, I1.1-L, and I2.2-V have practically identical energy and economic efficiency. For the separation of the B–CH–T mixture of both considered compositions, it is recommended to use Flowsheet I1.1, which includes a complex column with a side draw in the liquid phase. This makes it easier to implement the side draw, as well as to effectively regulate its flow rate and composition.

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Authors' contributions

D.A. Ramochnikov—conducting the computational experiment to determine optimal parameters and calculate economic indicators of the flowsheets, analysis of research materials, preparation of graphical material.

E.A. Anokhina—research planning, supervision and scientific consulting, analysis of research materials, writing the article text.

P.V. Gurbanov—conducting the computational experiment to determine optimal parameters and calculate economic indicators of the flowsheets.

P.S. Klauzner—consulting on the calculation of economic indicators for the flowsheets, preparation of the article materials.

A.V. Timoshenko—formulation of the scientific concept for the work, overall supervision.

The authors declare no conflict of interest.

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