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RESEARCH ARTICLE

Flowsheets for hydroxyacetone–phenol binary mixture separation: The use of special distillation methods

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Abstract

Objectives. *To study the possibility of hydroxyacetone–phenol binary mixture (a constituent of a mixture of phenol production by the cumene method) separation in flowsheets based on the use of distillation special methods. This is the addition of separating agents to increase the relative volatility of the components of the original mixture, and the variation of pressure in the columns.*
Methods. *A computational simulation in Aspen Plus® was used as the research method. Mathematical modeling of the vapor–liquid equilibrium was carried out using a local compositions model Non-Random Two Liquid. The viability of the latter was confirmed by comparing experimental and calculated on phase equilibrium data, and azeotropic data. The average relative error does not exceed 3%.*
Results. *The dependence of the composition and boiling point of the hydroxyacetone–phenol azeotrope on pressure was determined in a computational experiment (as the pressure increases, the azeotrope is enriched with phenol). The possibility of using a complex of columns operating under different pressures to separate the mixture was shown (the shift of the azeotrope*

is about 9%). The change in the relative volatility of components of the original mixture in the presence of a high- (diethylene glycol) and a low-boiling (acetone) separating agent was investigated. Both solvents are selective agents used in extractive and re-extractive distillation processes. Three technological separation flowsheets containing two distillation columns were proposed.

***Conclusions.** The study established the operation parameters of the columns (number of theoretical stages, feed stages of the original mixture and separating agent, and reflux ratio) and energy consumption (total heat supplied to the columns boiler) of three separation flowsheets ensuring the production of products of a given quality (not less than 0.99 mol fractions). The flowsheet with diethylene glycol is characterized by the lowest energy consumption. It is recommended that complexes of extractive and re-extractive distillation be further optimized. This enables the second product of cumulus production—acetone—to be involved in the technological cycle.*

***Keywords:** phenol, hydroxyacetone, vapor–liquid equilibrium, extractive distillation, re-extractive distillation, pressure-swing distillation complexes*

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НАУЧНАЯ СТАТЬЯ

Схемы разделения бинарной смеси гидроксиацетон–фенол с использованием специальных методов ректификации

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Аннотация

***Цели.** Исследовать возможность разделения смеси гидроксиацетон-фенол (составляющей смеси производства фенола кумольным методом) в схемах, базирующихся на использовании специальных приемов ректификации: добавлении разделяющих агентов, повышающих относительную летучесть компонентов исходной смеси, и варьировании давления в колоннах.*

***Методы.** В качестве метода исследования применялся вычислительный эксперимент в среде программного комплекса Aspen Plus®. Математическое моделирование равновесия жидкость-пар проводилось с использованием модели локальных составов Non-Random Two Liquid. Адекватность последнего подтверждена сравнением экспериментальных и расчетных данных о фазовом равновесии, данных об азеотропии; средняя относительная ошибка не превышала 3%.*

***Результаты.** В вычислительном эксперименте определена зависимость состава и температуры кипения азеотропа гидроксиацетон-фенол от давления (при увеличении давления азеотроп обогащается фенолом), показана возможность использования комплекса колонн, работающих под разным давлением, для разделения смеси (сдвиг азеотропа составляет порядка 9%). Исследовано изменение относительной летучести пары компонентов исходной смеси в присутствии тяжело- (диэтиленгликоль)* *и легкокипящего (ацетон) разделяющего агента. Оба растворителя являются селективными агентами для процессов экстрактивной и реэкстрактивной ректификации. Предложены три принципиальные технологические схемы разделения, содержащие две ректификационные колонны.*

Выводы. *Определены статические параметры работы колонн (число теоретических тарелок, номера тарелок подачи исходной смеси и разделяющего агента, флегмовое число) и энергозатраты (суммарные нагрузки на кипятильники колонн) трех схем разделения, обеспечивающие получение продуктов заданного качества (не ниже 0.99 мол. долей). Наименьшими энергозатратами характеризуется схема с диэтиленгликолем. Для дальнейшей оптимизации рекомендованы комплексы экстрактивной и реэкстрактивной ректификации. Последняя позволяет вовлечь в технологический цикл второй продукт кумольного производства – ацетон.*

Ключевые слова: *фенол, гидроксиацетон, парожидкостное равновесие, экстрактивная, реэкстрактивная ректификация, комплексы с варьированием давления в колоннах*

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INTRODUCTION

Phenol is a large-scale product of industrial organic synthesis, the main amount of which is obtained by the cumene method [1–4]. The combination of an aromatic ring in the phenol molecule, which ensures a fairly high thermal stability of the compound, and a hydroxy group, which has increased polarity compared to the alcohol hydroxyl and is one of the strongest *ortho-para*-orienting substituents, creates favorable conditions for the versatile use of phenolic products [5].

Wide application of phenol in various industries[1,2] constantly tightens the requirements for the purity of the target product[3]. By-products formed at the stage of chemical transformations are dimethylbenzyl alcohol and acetophenone. In addition to these high-boiling substances, other components, such as hydroxyacetone (HA), 2-methylbenzofuran (2-MBF) and mesityl oxide, are also formed in small quantities [6–11]. The negative effect of HA on the quality of phenol is manifested in the fact that in distillation columns, as well as at the stage of catalytic purification of raw phenol from impurities using heterogeneous catalysts at high temperatures, a condensation reaction of HA with phenol occurs to form 2-MBF. This heterocyclic compound is colorless, but during storage it easily forms colored resinous products, which deteriorates the color of the phenol. Eliminating the formation of HA and completely removing it from products using

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[1] Chemie Mania: World consumption of phenol. URL: http://www.chemiemania.ru/chemies-8878-1.html. Accessed April 13, 2023.

[2] Analytical portal of the chemical industry: Global phenol market: installed capacity and demand forecast. URL: https://www.newchemistry.ru/printletter.php?n_id=4044. Accessed April 13, 2023.

[3] GOST 23519-93. Interstate Standard. Technical synthetic phenol. Specifications. Moscow: IPK Izdatelstvo standartov; 1996.

conventional distillation is a technically intractable task due to the presence of limitations imposed by vapor–liquid equilibrium (VLE) [6]. Previously, a method was proposed for producing high-quality phenol by reducing the content of 2-MBP at the stage of catalytic purification of phenol and changing the technology of distillation of the separated products. To achieve conditions that meet the requirements for phenol of the highest quality category, it was necessary to significantly complicate the traditional distillation flowsheet by introducing additional azeotropic-extractive distillation columns and installing more efficient trays in a number of columns. These measures, although not radically, solved the problem of purification from HA and 2-MBP: phenol of the required quality is produced at most plants, but it is too expensive, and any failures in the composition of the initial mixture entering the separation result in a decrease in quality [7].

Despite the proposed chemical and technological solutions, the task of improving the quality of phenol remains relevant and requires an assessment of the prospects and conditions for the use of special separation techniques in order to achieve the required purity of the target product (phenol). In this regard, the aim of this work is to find alternative options for separating a HA–phenol mixture, allowing reducing the HA content in the products of phenol synthesis using the cumene method.

OBJECTS AND METHODS OF RESEARCH

The binary component of the industrial mixture: HA–phenol was chosen as the object of study. Some physicochemical characteristics of the components at atmospheric pressure are presented in Table 1.

In order to evaluate options for the separation of a mixture of a specific composition, information is needed on the VLE under various conditions, in particular, when varying pressure and when additional substances are added to the system. To obtain the required data and further calculate the distillation process, the method of mathematical modeling of VLE in the Aspen Plus® V. 10.0 software package[4] (*AspenTech*, USA) using the Non-Random Two Liquid (NRTL) equation was used. The binary interaction parameters of the NRTL equation (Table 2) were taken from [7] and used to calculate the VLE at a pressure of 0.2 atm (Table 3).

The choice of reduced pressure is due to the fact that at atmospheric pressure there is a high probability of HA decomposition at temperatures above 145°C. At a pressure of 0.2 atm the temperature of the mixture does not exceed 135°C.

As follows from the data presented, the description of the VLE of the HA–phenol binary system at a pressure of 0.2 atm is generally satisfactory.

Table 1. Physicochemical characteristics of phenol and HA at a pressure of 1 atm [7]

Name	Gross formula	*M*, g/mol	$T_{b.p.}$, °C	n_D^{20}	d_4^{20}, g/cm^3
Phenol	C_6H_6O	94.11	181.8	1.5426	1.063
HA	$C_3H_6O_2$	74.08	145.5	1.4295	1.082

Note: M is the molar mass, g/mol; $T_{b.p.}$ is the boiling point, °C; n_D^{20} is the refractive index; d_4^{20} is density, g/cm^3.

Table 2. Binary interaction parameters for the NRTL equation [7]

Component *i*	Component *j*	a_{ij}	a_{ji}	b_{ij}	b_{ji}	c_{ij}
HA	Phenol	−0.798	−0.291	1.341	1.113	0.3

Note: a_{ij}, a_{ji}, b_{ij}, b_{ji} are parameters taking into account the binary interaction of components *i-j*, *j-i*; c_{ij} is the parameter taking into account the non-ideality of the mixture.

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[4] Aspen Plus® is a powerful software designed for modeling processes in the chemical, petroleum, energy, and many other industries. The model obtained in a computational environment allows engineers and researchers to design and optimize various chemical processes and systems.

Table 3. Comparison of experimental [7] and calculated data on the VLE of the HA (1)–phenol (2) system at a pressure of 0.2 atm

x_{HA}, mol fract.	y_{HA}, mol fact.		Uncertainty errors y_{HA}		T, °C		Uncertainty errors T	
	exp.	calc.	abs., mol fract.	rel., %	exp.	calc.	abs., °C	rel., %
0.000	0.000	0.000	0.000	0.00	131.84	131.65	0.19	0.14
0.044	0.044	0.041	0.003	6.82	133.00	131.71	1.29	0.97
0.100	0.119	0.117	0.002	1.59	132.80	131.53	1.27	0.96
0.200	0.290	0.285	0.005	1.69	131.20	130.18	1.02	0.78
0.400	0.700	0.649	0.051	7.26	125.00	123.17	1.83	1.47
0.500	0.818	0.784	0.034	4.18	120.00	118.32	1.68	1.40
0.600	0.890	0.876	0.014	1.61	115.00	113.38	1.62	1.41
0.700	0.937	0.934	0.003	0.33	110.50	108.79	1.71	1.55
0.800	0.970	0.968	0.002	0.19	105.05	104.78	0.27	0.25
0.900	0.989	0.990	−0.001	0.08	101.13	101.44	−0.31	0.31
1.000	1.000	1.000	0.000	0.000	98.45	98.78	−0.33	0.34
			Average	2.637			Average	0.87

Note: x_{HA}, y_{HA} are the HA concentrations in liquid and vapor phases, respectively, mol fract.; T is the boiling point of the mixture. (1) A component of the mixture with a lower boiling point (in this case, HA), (2) A component of the mixture with a higher boiling point (phenol).

Therefore, the parameters of the binary interaction of the NRTL equation (Table 2) can be used in the future to calculate the distillation process.

RESULTS OF COMPUTATIONAL EXPERIMENT

The HA–phenol system is characterized by the presence of an azeotrope with a maximum boiling point (at constant pressure), which indicates significant negative deviations of the system from ideal behavior and, accordingly, the predominance of strong interactions of opposite molecules. The latter imposes thermodynamic restrictions on the process of conventional distillation and requires the use of special distillation techniques based on the principle of redistribution of concentration fields [12] between separation areas with different sets of final products. The method of extractive distillation (ED) [13, 14], which has proven itself to be an energy-efficient separation process, including mixtures containing phenol, has been widely used for the separation of mixtures of various natures [15–17].

To assess the possibility of using and operating conditions for separation complexes for a HA–phenol mixture, additional information was obtained on the effect of pressure on the composition of the binary azeotrope and potential separating agents (SA) (high-boiling diethylene glycol (DEG) and low-boiling acetone) on the relative volatility of the starting components. Table 4 shows the characteristics of a binary azeotrope at different pressures, which indicate the presence of a noticeable azeotropic shift in the considered pressure range.

Table 4. Calculated characteristics of azeotropes at different pressures

Pressure, atm	x_{HA}, mol fract.	T, °C
0.1	0.990	114.07
0.2	0.959	131.71
1.0	0.902	182.45

Note: x_{HA} is the concentration of HA in azeotropic mixture; T is the azeotropic mixture boiling point.

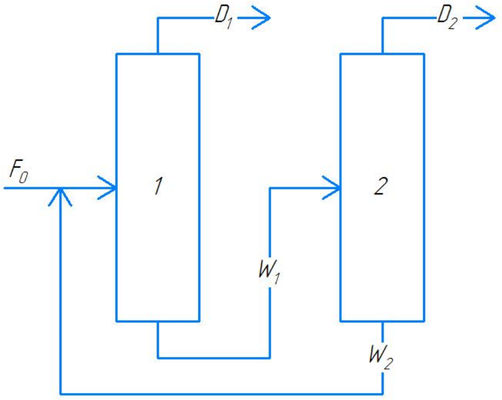

Fig. 1. Flowsheet I of separation of a mixture of HA (1)–phenol (2) at a pressure of 0.1 atm and 1.0 atm in columns *1* and *2*, respectively. F_0 is the amount of initial mixture, kmol/h; D is the distillate flow, kmol/h; W is the bottom flow, kmol/h.

Figure 1 shows a schematic diagram of separation (I), representing a complex of two columns operating at different pressures.

The calculation of the distillation process was carried out at 100 kmol/h of the initial mixture (feed to column *1*). The HA content (x_{HA}) in the initial mixture was 0.7 mol fract. (model composition). The initial mixture was fed into the column at a temperature T close to the boiling point of the mixture. Requirements for the quality of the resulting products: HA content x_{HA} = 0.995 mol fract., phenol content x_F = 0.999 mol fract. When calculating the distillation process, optimization of parameters: overall efficiency of the column N (number of theoretical stages, NTS), numbers of feed stages for the feed mixture streams (N_F) and SA (N_{SA}), as well as the reflux ratio R was carried out using the Sensitivity Analysis module. The model composition of the initial mixture was chosen to establish the general principles of separation of the HA–phenol mixture of the final composition (to exclude the situation of dilution of the mixture with the target product).

Table 5 shows the material balance and operating parameters of the columns of Flowsheet I, which represents a complex of two columns operating under a pressure of 0.1 and 1.0 atm, respectively.

The course of the lines of constant relative volatility of the HA–phenol pair in the presence of DEG (Fig. 2) and acetone (Fig. 3) shows that DEG (high-boiling SA, $T_{b.p.}$ = 244.8°C) and acetone (low-boiling SA, $T_{b.p.}$ = 56.0°C) increase the volatility of HA relative to phenol in mixtures with a high phenol content. For a model composition containing 0.7 mol fract. HA, in the presence of DEG, the relative volatility of HA decreases slightly, but remains high enough to realize the extractive effect.

Thus, in the first case, it is possible to organize the ED process [13–14], and in the second case, the process of re-extractive distillation (RED) [15].

Figure 4 shows the structures of the ED (Flowsheet II) and RED (Flowsheet III) complexes.

Flowsheets II and III are antipodean flowsheets and differ in the recovery of final products: in the first case (Fig. 4a) HA and phenol are recovered as the distillate flows; in the second (Fig. 4b)—as the bottom flows. An essential requirement for the functioning of the first column of both flowsheets is the organization of a counterflow of the initial mixture (F_0) and SA.

The calculation of the ED and RED process was carried out using the binary interaction parameters of the NRTL equation taken from [7], the NIST database[5], or modeled using the UNIFAC equation. The quantity and composition of the initial mixture, as well as the quality requirements for HA and phenol, correspond to Flowsheet I; purity of SA x_{SA} = 0.999 mol fract.

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[5] Aspen Plus® V. 10.0 database. NIST Chemistry WebBook URL: https://webbook.nist.gov/. Accessed April 22, 2023.

Table 5. Material balance and operating parameters of distillation columns at different pressures

Col. No.	*P*, atm	*N*, NTS	N_F	*R*	Distillate (*D*)	Bottom flow (*W*)	Q_{boil}, kW
					Flow rate / x_{HA} (T, °C)	Flow rate / x_{HA} (T, °C)	
1	0.1	60	3	3	70 / 0.995 (82.11)	33.41 / 0.021 (97.77)	3575.6
2	1.0	70	17	2	30 / 0.001 (165.15)	3.41 / 0.098 (182.45)	1287.8
						Total energy consumption	4863.3

Note: Flow rate is the number of flows, kmol/h; x_{HA} is the concentration of HA in the flow, mol fract.; *T* is the flow temperature (distillate/still), corresponds to the boiling temperature at a given composition of the distillate/still, °C. The plates are numbered from the top of the column. Q_{boil} is the energy consumption of the boiler, kW.

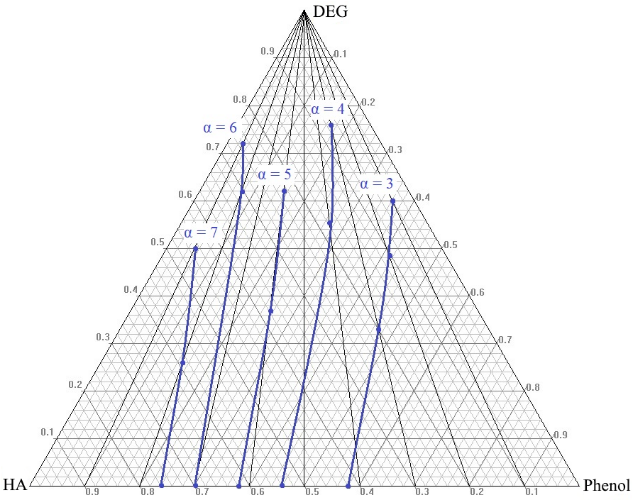


Fig. 2. Isoline diagram of the relative volatility of the HA–phenol binary system in the presence of DEG (SA) at a pressure of 0.2 atm, α is the relative volatility of the components.

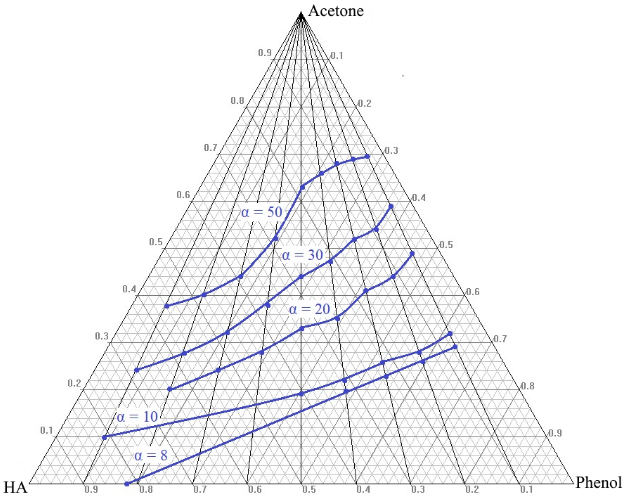
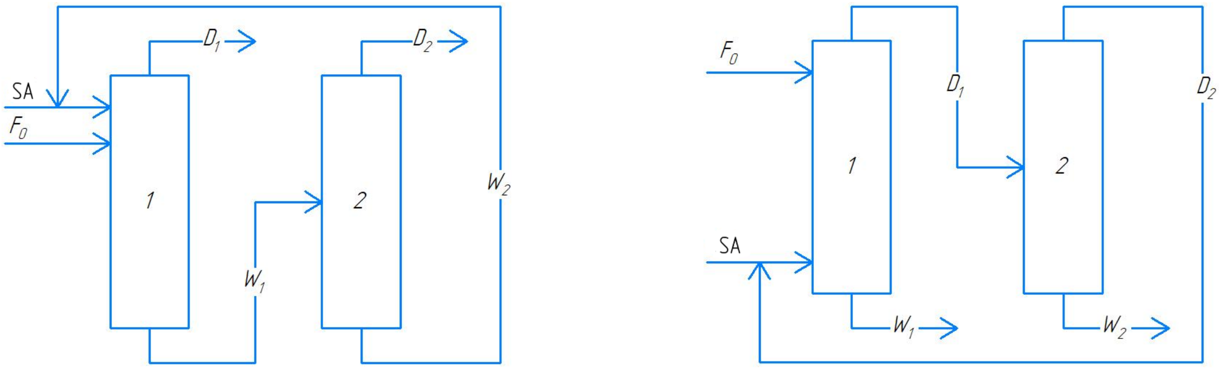


Fig. 3. Isoline diagram of the relative volatility of the HA–phenol binary system in the presence of acetone (SA) at a pressure of 0.2 atm, α is the relative volatility of the components.



(a) (b)

Fig. 4. Structures of the ED (Flowsheet II, a) and RED (Flowsheet III, b) complexes. F_0 is the flow of the initial mixture, kmol/h; *D* is the distillate flow, kmol/h; *W* is the bottom flow, kmol/h.

An important indicator of the ED and RED processes is the SA consumption, which ensures its selective action. Therefore, at the first stage of optimization of the parameters of the corresponding columns of Flowsheet II and III, a "manual" selection of the SA flow rates and pressure in the column necessary to achieve the specified purity of the product streams was carried out, and in most cases the quality of the products exceeded the specified one. Next, the Design Specs and Sensitivity Analysis modules were used.

The calculation results for the ED and RED processes are presented in Table 6.

DISCUSSION OF RESULTS

The data from the computational experiment showed that in all three options the required quality of product flows was achieved. The most efficient option for separating an HA–phenol mixture is the ED process with high-boiling SA (DEG). As one would expect, the RED mode with low-boiling SA (acetone) requires the highest (almost twice as much as in ED) energy consumption, which is due, among other things, to the higher ratio of SA (2.0 compared to 1.2 in ED), which it is necessary to evaporate twice to isolate acetone in the distillates of both columns of the RED complex. Flowsheets I and III differ slightly in energy consumption (8.6%).

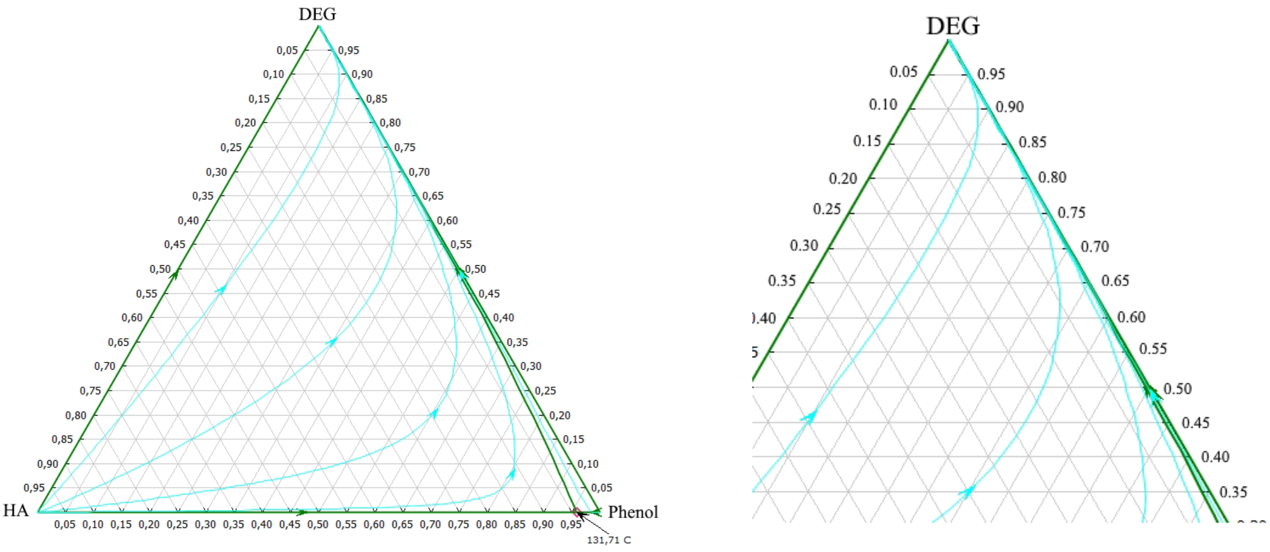
A comparison of the ED and RED modes shows a significant reduction in the total energy consumption in the first column of the ED complex, which is associated with the additional ease of isolating HA as a product with a minimum boiling point in the distillation region, which belongs to the mixture of F_0 + SA gross composition. In this case, at close levels of supply of the initial mixture and SA, we can talk about the process of conventional distillation of a ternary mixture of HA–phenol–DEG. A feature of this mode is the production in the cube of a column of a composition belonging to a separatrix [14], which, due to curvature, touches the side of the DEG–phenol triangle in the DEG concentration range of 0.65–1.0 mol fract. (Fig. 5). The latter leads to a decrease in the content of HA impurities in the bottom product of the ED column, which otherwise would be about 1.0–1.5%.

Despite the high energy consumption of the RED complex, its main advantage is the involvement of acetone in the technological process—the second target product of the cumene method

Table 6. Material balance and operating parameters of distillation columns of the ED and RED complexes

Col. No.	*P*, atm	*N*, NTS	N_F / N_{SA}	*R*	Distillate (*D*)	Bottom flow (*W*)	Q_{boil}, kW
					Flow rate / x_{HA} / x_F (*T*, °C)	Flow rate / x_{HA} / x_F (*T*, °C)	
ED complex (SA/mixture ratio = 120 : 100)							
1	0.2	16	9 / 6	0.67	70 / 0.996 / 0.004 (98.88)	150 / 0.002 / 0.198 (172.69)	1602.0
2	0.2	20	6 / –	1.45	30 / 0.001 / 0.999 (131.69)	120 / 0.000 / 0.008 (190.91)	1111.0
						Total energy consumption	2713.0
RED complex (PA/mixture ratio = 200 : 100)							
1	0.35	60	7 / 53	0.15	270 / 0.259 / 0.000 (34.24)	30 / 0.001 / 0.999 (147.44)	3050.0
2	1.0	11	7 / –	0.08	200 / 0.002 / 0.000 (56.18)	70 / 0.999 / 0.000 (143.61)	2230.0
						Total energy consumption	5280.0

Note: Flow rate is the number of flows, kmol/h; x_{HA} and x_F are concentrations of HA and phenol in the flow, respectively, mol fract.; *T* is the flow temperature (distillate/still), corresponds to the boiling temperature at a given composition of the distillate/still, °C. The plates are numbered from the top of the column. Q_{boil} is the energy consumption of the boiler, kW.



(a) (b)

Fig. 5. Distillation lines in the concentration triangle of the HA–phenol–DEG system (a) and a fragment of the diagram (b), reflecting the features of the location of the separatrix in the vicinity of the DEG–phenol side at a pressure of 0.2 atm.

for the production of phenol, which is not in full demand today. This circumstance undoubtedly increases the prospects for further optimization of the RED process and its use in industry.

CONCLUSIONS

New physicochemical information was obtained on the phase behavior of binary and ternary systems by using mathematical modeling of the VLE of the HA–phenol system at three pressures and in the presence of potential SAs (DEG, acetone). This formed the basis for the development of variant flowsheets based on the use of special techniques, and explanation of the separation results from the perspective of thermodynamic-geometric analysis of the phase diagram.

The conditions for the distillation process and the static parameters of the operation of columns of three flowsheets, based on varying the pressure in the columns and the use of ED and RED, were determined in a computational experiment using the Aspen Plus$^{®}$ software package. RED was proposed as an alternative separation option, taking into account the possibility of involving the second product of cumene production—acetone—into technological circulation.

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Authors' contribution

All authors equally contributed to the research work.

The authors declare no conflicts of interest.

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