ISSN 2070-0482, Mathematical Models and Computer Simulations, 2021, Vol. 13, No. 3, pp. 483–491. © Pleiades Publishing, Ltd., 2021.
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Mathematical Model of Rectification Process and Selection of the Separation Sequence for Multicomponent Mixtures

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Received November 18, 2019; revised January 13, 2020; accepted January 27, 2020

Abstract—Based on the equations of thermodynamic balances, a model of a stationary non-equilibrium distillation process is proposed. It is shown that the heat consumption for any given efficiency of a distillation column depends monotonically on the parameters of the reversible distillation. Using this result, the authors propose an algorithm for choosing the optimal separation sequence for a system of several columns used for multicomponent distillation process; this algorithm is based on the criterion of the minimum of the total energy consumption with the use of the coefficient of thermal efficiency which depends on the still and dephlegmator temperatures. The algorithm for calculating the coefficient of thermal efficiency in the mixture fractionation process is proposed.

Keywords: distillation, multicomponent mixture, thermal efficiency, separation sequence, maximum efficiency, minimum energy consumption

DOI: 10.1134/S2070048221030182

1. INTRODUCTION

The separation sequence problem for multicomponent mixtures in the devices such that each of them divides the mixture into two flows consists of selecting the sequence of separation boundaries in a way that minimizes the total energy consumption. If the separation process is reversible and for its realization one uses mechanical or electric energy, then the energy consumption depends only on the mixture's compositions before and after separation and does not depend on the separation sequence. The processes are close to reversible, if the values of the kinetic coefficients (dimensions of distillation apparatus) are arbitrarily large or the speed of the process is arbitrarily low. Otherwise, the separation sequence is determined by the irreversible energy consumption directly related to the entropy production.

If it is heat energy that is used in the separation process, its consumption even in the reversible case is influenced by the temperatures of its input and removal; i.e., the efficiency of a reversible process is similar to the Carnot-cycle efficiency. This factor should be considered when selecting the separation sequence together with irreversible losses. One of the most power-consuming processes is the process of liquid-mixtures separation in the cascade of distillation columns.

Numerous publications are devoted to the analysis of the processes of liquid-mixture separation in the distillation columns (see [1–10] and other publications). When separating multicomponent and continuous mixtures into fractions, one of the principal issues is estimation of the minimum consumption of the heat necessary for the separation process and selection of the separation sequence corresponding to this minimum heat consumption.

It is assumed that the concentration and boiling temperature of each component of the multicomponent mixture under consideration are known; thus, the composition and properties of the flow at the input of the cascade of distillation columns and the flows at its output are given. At first sight, the energy consumption related to the separation process without consideration of the irreversibility of the heat- and mass-transfer processes occurring in the columns depends only on the flows' compositions at the input and output of the cascade of distillation columns. This would have been correct for the reversible separation processes using mechanical energy. However, this is not so for the processes using thermal energy. The energy consumption related to separation in this case depends on the heat-injection and heat-removal temperatures; the latter are determined by selection of the separation boundary. Therefore, the total reversible energy consumption depends only on the separation sequence.

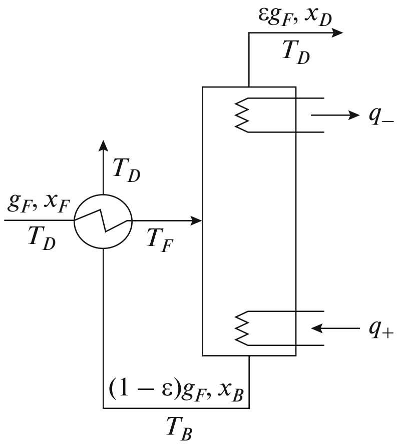

Fig. 1. Scheme of flows of a distillation column.

To select the separation sequence for multicomponent mixtures, one uses heuristic rules without any justification [3]. Below, we present an attempt to justify the selection of the separation sequence in terms of thermodynamics. It is shown that at the optimal separation sequence, the efficiency factor of a column for each cascade stage must not be lower than that at the following stage.

First, let us consider the mathematical model of a single distillation column and, simplifying our analysis under some assumptions, find a relationship between the heat consumption, efficiency, and the separation boundary. We will write down the inequality that determines the selection of the separation boundary corresponding to the heat consumption minimum at each stage in the reversible process. We will show that the column's efficiency factor with consideration of irreversibility depends monotonically on its reversible efficiency factor and, thus, the optimal separation sequence in the cascade of columns with the given efficiency must not differ from the optimal separation sequence for the reversible cascade. Moreover, for the conventional form of the heat- and mass-transfer kinetics, the efficiency factor of the column in the maximum efficiency regime does not depend on the irreversible factors and is half of the efficiency factor of the reversible column.

2. EXTREME CAPACITY OF A MULTICOMPONENT DISTILLATION COLUMN

2.1. The Main Assumptions

Let us consider a conventional construction of a distillation column with heat injection into the still and heat removal from the dephlegmator. The main assumptions used when considering the column with the given efficiency are as follows:

(1) the mass exchange is equimolar; thus, the vapor flow in the column is constant and the liquid flow changes stepwise only at the point of feed injection;

(2) in each cross section over the column height, the pressures and temperatures of the vapor and liquid flows are close to each other (they change from one cross section to another);

(3) the effects of diffusion between neighboring cross sections are negligible;

(4) the heat of output flows is transferred to the input flows entering the column; the irreversibility of this heat exchange can be neglected;

(5) the flow of the mixture subjected to separation in the form of a liquid at a boiling temperature enters the column's cross section in which the reflux temperature coincides with the temperature of this flow; the entropy of mixing that emerges because of the difference in their compositions can be neglected.

The process of separation of a multicomponent mixture into two fractions in a distillation column (Fig. 1) is characterized by the following parameters:

(1) the properties of the mixture subjected to separation: molar rates of the components in the flow subjected to separation x_{Fi} and the molar heat of evaporation of components r_i at atmospheric pressure (we assume that indices $i = 1,\dots,n$ grow as the boiling temperature of the components grows);

(2) compositions of the separation products: molar rates of the components in the dephlegmator (the light fraction, distillate) x_{Di} and in the still (the heavy fraction, bottom product) x_{Bi};

(3) mode parameters: the pressure in column P_C, temperatures in still T_B and in dephlegmator T_D, which depend on the product's composition and, thus, on the choice of the separation boundary.

Under the conditions of the given compositions of the flows at the column's input and output, these flows are proportional to each other and any of them can be chosen as the target flow, in particular, the flow g_F of the mixture subjected to separation. In this case, the column's efficiency is the number of moles of the mixture subjected to separation per unit heat q_+ injected into the column's still.

2.2. Thermodynamic Balances of Binary Distillation and the Relationship between the Heat Consumption and Column Efficiency

Let us write down the equations of thermodynamic balances of column, namely, the material, energy, and entropy balances [11, 12] on the assumption that the mixing of the heat can be neglected:

$$\begin{gathered} g_F x_{Fi} - g_F \varepsilon x_{Di} - g_F(1-\varepsilon)x_{Bi} = 0, \quad i = 1,\dots,n, \\ q_+ - q_- + g_F\sum_i h_{Fi} - g_F\varepsilon\sum_i h_{Di} - g_F(1-\varepsilon)\sum_i h_{Bi} = 0, \end{gathered} \tag{1}$$

$$g_F\varepsilon\sum_i s_{Di} + g_F(1-\varepsilon)\sum_i s_{Bi} + q_-/T_D - g_F\sum_i s_{Fi} - q_+/T_B = \sigma \ge \sigma_{\min}. \tag{2}$$

Here, $\sigma > 0$ is the entropy production in the column; h_{Fi}, h_{Di}, h_{Bi}, s_{Fi}, s_{Di}, and s_{Bi} are the molar enthalpy and entropy of the ith component in the feedstock, distillate, and bottom product, respectively, ε is the distillate takeoff per mole of the feedstock consumed (the relative takeoff).

Assuming that the column is heat-insulated and the heat losses into the environment are significantly lower than the heat flow consumed in the separation process, we can consider that $q_+ = q_- = q$. From conditions (1) and (2), we get

$$\begin{gathered} q = g_F\frac{T_B}{T_B - T_D}\left[\sum_i (s_{Fi}T_D - h_{Fi}) - \varepsilon\sum_i (s_{Di}T_D - h_{Di}) - (1-\varepsilon)\sum_i (s_{Bi}T_D - h_{Bi})\right] \\ + \sigma\frac{T_BT_D}{T_B - T_D} = q^0 + \sigma\frac{T_BT_D}{T_B - T_D}. \end{gathered} \tag{3}$$

The first term in the right-hand side of expression (3), which is denoted by q^0, is the heat consumption in the reversible process, when the heat- and mass-exchange coefficients (the column dimensions) are arbitrarily large or the efficiency is arbitrarily low. It depends only on the parameters of the input and output flows and is proportional to the column efficiency g_F; the second term corresponds to dissipative energy consumption.

Taking into account the fact that the difference $(h_i - T_Ds_i)$ for each component is equal to the molar free energy, i.e., to the chemical potential μ of the mixture at $T = T_D$, we obtain the relationship between the heat flow and efficiency in the form

$$q = g_F\frac{T_B}{T_B - T_D}\left[\varepsilon\sum_i \mu_i(T_D, x_{Di}) + (1-\varepsilon)\sum_i \mu_i(T_D, x_{Bi}) - \sum_i \mu_i(T_D, x_{Fi})\right] + \sigma\frac{T_BT_D}{T_B - T_D}. \tag{4}$$

The chemical potential of the ith component has the form [13]

$$\mu_i(T, P, x_i) = \mu_i^0(T, P) + RT\ln x_i.$$

Since in each cross section of the column, the chemical potentials correspond to the same temperature and pressure, their difference does not contain the term $\mu_i^0(T, P)$ and depends only on the flows' compositions; therefore, equality (4) can be written in the following form:

$$q = g_F\frac{T_B}{T_B - T_D}\left[A_F - \varepsilon A_D - (1-\varepsilon)A_B\right] + \sigma\frac{T_BT_D}{T_B - T_D} = \frac{p_0}{\eta_C} + \frac{\sigma T_D}{\eta_C}. \tag{5}$$

Here, $A_j = -RT_D\sum_{i=1}^n\left[x_{ji}\ln x_{ji} + (1 - x_{ji})\ln(1 - x_{ji})\right]$, $j = F, D, B$ is the reversible work of separation of one mole of the jth flow into pure components. The expression in the square brackets in equality (5) is the reversible work of the Gibbs separation of one mole of feedstock x_F into flows with compositions x_B and

x_D at temperature T_D. Let us denote it by A_G. The quantity $\eta_C = (1 - T_D/T_B)$ is the column thermal efficiency factor, which is an analog of the Carnot thermal efficiency.

Equating the entropy production in (5) to zero, we obtain the reversible estimate (the lowest boundary) $q^0 = g_F A_G/\eta_C$ of the heat consumption in the distillation process. The reversible distillation column can be compared with an ideal engine operating between reservoirs with temperatures T_B and T_D and producing the separation power $p^0 = g_F A_G$.

3. OPTIMAL SEPARATION SEQUENCE FOR A MULTICOMPONENT MIXTURE IN THE CASCADE OF REVERSIBLE COLUMNS

3.1. Two-Column Cascade

Let us consider a system of two reversible distillation columns that separate a feedstock flow with a given composition into three fractions with the given compositions. Thus, the value of the reversible separation power $p^0 = g_F A_G$ for the cascade is given. It does not depend on the separation sequence. The values of the thermal efficiency factors and the parts of reversible power γ for each column of the cascade depend on the separation sequence. There are two possible separation boundaries—let us call them the upper and lower separation boundaries—from which it is necessary to select at the first stage the boundary for which the total reversible heat consumption is less. Since the heat consumption is proportional to the feedstock consumption, we can consider that $g_F = 1$. Let us denote the thermal efficiency factor for the upper separation boundary by η_1; and for the lower separation boundary, by η_2.

Let us call the separation sequence according to which the separation is first performed with respect to the upper interface and then with respect to the lower interface the *direct* separation; the sequence when the high-boiling fraction is separated first and then the low-boiling fraction is separated from the medium fraction is called the *inverse* separation.

Let us assume that in the direct separation sequence, the first column produces the γ_1 part of the total separation work; the second column produces $(1 - \gamma_1)$. For the inverse separation sequence, these indices are γ_2 and $(1 - \gamma_2)$, respectively. Let us write down the condition of appropriateness of the direct separation sequence in the form of the following inequality:

$$\frac{\gamma_1}{\eta_{1,23}} + \frac{1-\gamma_1}{\eta_{2,3}} < \frac{\gamma_2}{\eta_{12,3}} + \frac{1-\gamma_2}{\eta_{1,2}}. \tag{6}$$

Here, the left-hand side of the inequality with the coefficient $1/A_G$ is proportional to the heat consumption per mole of mixture for the direct separation sequence; and the right-hand side, for the reverse separation sequence. The comma between indices corresponds to the position of the separation boundary. Thus, $\eta_{1,2}$ and $\eta_{2,3}$ denote the thermal efficiency factor for the separation of the first and second fractions and the second and third fractions, respectively, in the second column of the cascade.

If the inequality has the opposite sign, it is reasonable to use the inverse separation sequence. The thermal efficiency factors in inequality (6) are determined by the ratio of the boiling temperatures of the separated fractions. For the first column of cascade in the direct separation sequence, this is the ratio of the boiling temperature T_1 of the first fraction to the boiling temperature $T_{2,3}$ of the mixture of the second and third fractions; analogously, for the second column, this is the ratio of the boiling temperature of the second fraction T_2 to the boiling temperature of the third fraction T_3. The quantities in the left- and right-hand sides of inequality (6) characterize the thermodynamic difficulty of separation. Let us denote them by $C_{1,23}$ for the direct and $C_{12,3}$ for the inverse separation sequences, respectively.

Inequality (6) allows comparing the reversible heat consumptions for any two chosen separation boundaries and asserts that the optimal boundary is that for which difficulty C is lower (the reversible efficiency factor is maximum). The following necessary condition of optimality of the separation sequence for a multicomponent mixture in reversible columns is valid: *If a separation sequence corresponds to the minimum of the total heat consumption, then, for each cascade of two columns separating the incoming mixture flow into three fractions of the given composition, the separation sequence must be selected in such a way that the corresponding difficulty C is minimal.*

For a three-component mixture with component concentrations x_1, x_2, and x_3, after some simple calculations, condition (6) takes the following form:

$$[x_1 \ln x_1 + (1 - x_1)\ln(1 - x_1)]\frac{T_{23} - T_1}{T_{23}} + [x_2 \ln x_2 + x_3 \ln x_3 - (1 - x_1)\ln(1 - x_1)]\frac{T_3 - T_2}{T_3}$$

$$> [x_3 \ln x_3 + (1 - x_3)\ln(1 - x_3)]\frac{T_3 - T_{12}}{T_3} + [x_2 \ln x_2 + x_1 \ln x_1 - (1 - x_3)\ln(1 - x_3)]\frac{T_2 - T_1}{T_2}.$$

For the boiling temperatures, the following chain of inequalities is valid:

$$T_1 < T_{12} < T_2 < T_{23} < T_3.$$

In the particular case when the ratio of boiling temperatures depends only on the compositions of the fractions nearest to the separation boundary, $\eta_{1,2} \approx \eta_1$ and $\eta_{2,3} \approx \eta_2$, condition (6) takes a simpler form:

$$(\gamma_1 + \gamma_2 - 1)\left(1/\eta_1 - 1/\eta_2\right) < 0. \qquad (7)$$

In practice, a stricter assumption is often used: the hypothesis of the key components, when it is assumed that the ratio of boiling temperatures depends only on the boiling temperature of the components nearest to the separation boundary.

The sign of the first multiplier in the left-hand side of inequality (7) is positive, since the mixture flow entering the second column of the cascade is less intensive than that incoming to the first column. In this case, the following ***rule*** is valid: “the separation sequence must be selected in such a way that the thermal efficiency factor of the first stage is greater than the thermal efficiency factor of the following stage.

Since, when passing from the first to subsequent columns, the boiling temperatures of the separated fractions become closer to each other, the thermal efficiency factor decreases from the first to subsequent columns.

Therefore, for each cascade consisting of two subsequent separation stages, in the case when the temperatures in the still and in the dephlegmator are determined only by the compositions of the fractions nearest to the separation boundary, the rule of decreasing thermal efficiency factors is valid when passing from the first to subsequent stages of the cascade.

3.2. Three-Column Cascade

In a cascade that consists of three columns separating a mixture into four fractions, it is possible to select at the first column one of the separation boundaries: (1)–(234); (12)–(34); (123)–(4). For each of them, the difficulty of separation can be calculated as follows:

$$C_{1(234)} = C_{1,234} + (1 - x_1)\min[C_{2,34}; C_{23,4}],$$

$$C_{(12)(34)} = C_{12,34} + (x_1 + x_2)C_{1,2} + (x_3 + x_4)C_{3,4},$$

$$C_{(123)4} = C_{123,4} + (1 - x_4)\min[C_{1,23}; C_{12,3}].$$

The separation sequence in the cascade must correspond to the minimum of these three expressions.

4. PARAMETRIZATION OF THE DEPENDENCE OF THE COLUMN LOAD ON THE HEAT CONSUMPTION

For a column with a given load, the irreversibility of the processes passing in it plays an important role. Let us dwell upon the calculation of the entropy production depending on the column loading, which would allow us to use equality (5) and obtain a relationship between its efficiency and heat consumption.

Let us assume that the laws of heat transfer in the still and dephlegmator have the form

$$q = \beta_B(T_+ - T_B) = \beta_D(T_D - T_-),$$

where T_+ and T_- are the temperatures of the heating vapor and cooling liquid, respectively; β_B and β_D are the coefficients of heat transfer in the still and dephlegmator, respectively; and the kinetics of mass exchange between the vapor and liquid flows in each cross section of the column are characterized by the following expression:

$$g_i(y, y^0) = k\frac{[\mu_i(T, y_i^0) - \mu_i(T, y_i)]}{T}.$$

Here, y_i is the concentration of the ith component that corresponds to the operating circuit; y_i^0 is the equilibrium concentration of the ith component; k is the effective mass transfer coefficient; and T is the temperature in this cross section.

In [14], the expression for dissipation (entropy production in the column) was obtained depending on the heat flow in the following form:

$$\sigma_{\min} = q^2\left(\frac{1}{\beta_B T_B T_+} + \frac{1}{\beta_D T_D T_-} + 2\sum_i \frac{x_{Di} - x_{Bi}}{k r_i^2}\right),$$

where r_i is the heat of evaporation of the ith component.

Substituting this expression into (7), we obtain the boundary of the region of realizable regimes of the column in the form

$$g_F \le bq - aq^2, \tag{8}$$

where b and a are the characteristic coefficients that are linked with the column parameters as follows:

$$a = \left(\frac{1}{\beta_B T_B T_+} + \frac{1}{\beta_D T_D T_-} + 2\sum_i \frac{x_{Di} - x_{Bi}}{k r_i^2}\right)\frac{T_D}{A_G}, \tag{9}$$

$$b = \frac{T_B - T_D}{T_B A_G} = \frac{\eta_C}{A_G}. \tag{10}$$

Coefficient b is the reversible efficiency factor of the column; it is equal to the ratio of the thermal efficiency factor to the reversible molar work of the Gibbs separation of the incoming mixture into the desired fractions. Coefficient a characterizes the irreversibility of the processes passing in the column. The possibility of parametrization makes it possible to reveal the relationship between the efficiency factor of the reversible column and the efficiency factor taking irreversibility into consideration.

The column efficiency factor that corresponds to the boundary of the realizability region, expressed through the characteristic parameters will take the form

$$h = g_F/q = b - aq. \tag{11}$$

It follows from (11) that the efficiency factor reaches its maximum $b = \eta_{\text{rev}}$ in the reversible process when g_F and q tend to zero. The operating part of the boundary of the realizability region corresponds to those values of q at which the efficiency does not decrease with increasing heat consumption. It is bounded by the value $q^* = b/(2a)$.

Let us introduce the relative value of heat flow $q_0 = q/q^*$ and substitute it into (11) instead of q. We obtain $\eta = b(1 - 0.5q_0)$. Therefore, in the operating part $(0 < q_0 \le 1)$, the column efficiency factor, with its irreversibility taken into account, monotonically depends on the reversible efficiency factor and is half the reversible efficiency factor in the maximum-efficiency regime. This allows us to assert that the recommendations concerning the separation sequence for multicomponent mixtures for the reversible distillation columns hold also for the same cascade taking irreversible factors into considerable. If each column operates in the regime with an efficiency close to the maximum possible efficiency, then, the heat consumption will be approximately twice as much as their reversible estimate.

It should be noted that the reversible efficiency factor b depends only on the temperatures in the still and dephlegmator, as well as on the composition of the mixture subjected to separation; the irreversibility coefficient a depends also on the heat of evaporation and on the coefficients of heat- and mass-exchange kinetics.

The right-hand side of inequality (8) can serve as the approximation of the dependence of the column efficiency on the heat consumption. The characteristic coefficients can be found from the experimental data at the operating column; formulas (9) and (10) can be used to recalculate the values of these coefficients related to the possible changes in the temperatures and compositions of the flows. Let q_1, g_1, and $q_2 > q_1$, $g_2 > g_1$, be the measured heat and feedstock consumption in two modes of column operation in its operating part. Then, we get the following expressions for the characteristic coefficients:

$$a = \frac{g_1 q_2 - g_2 q_1}{q_1 q_2^2 - q_2 q_1^2}, \quad b = \frac{g_1 q_2^2 - g_2 q_1^2}{q_1 q_2^2 - q_2 q_1^2}.$$

5. THE CASE OF CLEAR-CUT SEPARATION

Let us consider the case when the separation is clear-cut, i.e., no component contained in the low-boiling fraction is contained in the high-boiling fraction and vice versa. In this case

$$\varepsilon = \sum_{i=1}^{\nu} x_{Fi}, \quad 1 - \varepsilon = \sum_{i=\nu+1}^{n} x_{Fi}.$$

Taking into account the fact that $x_{Di} = x_{Fi}/\varepsilon$ and $x_{Bi} = x_{Fi}/(1-\varepsilon)$, the expression for the molar work of mixture separation in the case of clear-cut separation will takes the form

$$A_G = -RT_D[\varepsilon \ln \varepsilon + (1-\varepsilon)\ln(1-\varepsilon)], \text{ and}$$

the value of the heat consumption per mole of the mixture subjected to separation is

$$q_m = \frac{1}{b} = -\frac{1}{\eta_C} RT_D\left[\varepsilon \ln \varepsilon + (1-\varepsilon)\ln(1-\varepsilon)\right].$$

6. CALCULATION OF THE THERMAL EFFICIENCY FACTOR IN THE PROCESS OF THE MIXTURE'S SEPARATION INTO FRACTIONS

To calculate the value of the thermal efficiency factor, it is necessary to know the values of the mixture's boiling temperature in the still and the condensation temperature in the dephlegmator, which depend on both the mixture's composition and pressure in the column. Let us present one of the possible algorithms for calculating these temperatures.

In many cases, one chooses the pressure in the column P_C in such a way that it is possible to use water or another cooling agent at an ambient temperature for vapor condensation in the dephlegmator. Then, the temperature in the dephlegmator will be close to the ambient temperature and the pressure in the column for mixtures of a different composition will change.

In the dephlegmator, the distillate extracted in the form of a vapor with a known composition x_D is in the state of thermodynamic equilibrium with the liquid that is formed due to condensation. Therefore, the pressure in the dephlegmator and, thus, in the column as a whole, can be found from the phase equilibrium condition, according to the formula

$$P_c(T) = \frac{1}{\sum_i x_{Di}/P_i(T)}. \tag{12}$$

Here, $P_i(T)$ is the saturation vapor pressure of the ith component at temperature $T = T_D$. For the mixtures close to ideal solutions, the saturation vapor pressure of components can be calculated by using the Antoine equation [1, 3]:

$$P_i(T) = \exp\left(A_i - \frac{B_i}{T + C_i}\right),$$

where A_i, B_i, and C_i are the tabulated empirical coefficients whose values for the majority of substances are presented in reference books, for example, in [15]. In the case of nonideal mixtures, it is necessary to use more complicated dependences of the saturated vapor pressure of the components on temperature that take the mixture's composition into account [7].

When the pressure in the column is found $\left(P_C(T_D) = P_C(T_B)\right)$, temperature T_B can be found from the phase equilibrium equation written down for the column still, where the bottom product of known composition x_B is in the thermodynamic equilibrium state

$$P_C(T) = \sum_i x_{Bi} P_i(T). \tag{13}$$

Here, $P_i(T)$ has the same meaning as in condition (12), $T = T_B$. Equation (13) in the majority of the cases can be solved with respect to T_B only numerically; however, since its right-hand side monotonically increases with growing T_B, it has the only real root.

If the pressure in the column is fixed for some reasons, it is possible to use equality (12), in which T_D is considered to be unknown, while P_C is given, to calculate the condensation temperature in the dephlegmator.

Table 1. Composition and coefficients of the Antoine equation of the mixture subjected to separation

i	Component	x_F	A	B	C
1	Propane	0.14	4.53678	1149.360	24.906
2	Isobutane	0.12	4.32810	1132.108	0.918
3	n-butane	0.05	4.35576	1175.581	−2.071
4	Isopentane	0.10	3.97183	1021.864	−43.231
5	n-pentane	0.26	3.98920	1070.617	−40.454
6	n-hexane	0.27	4.00266	1171.530	−48.785
7	Isohexane	0.06	3.96400	1135.410	−46.578

Table 2. Calculation results

Separation boundary	P_C, MPa	T_B, K	η_C, %
(1)–(2...7)	4.223	360	10.2
(1, 2)–(3...7)	2.479	334	3.3
(1...3)–(4...7)	2.068	352	8.3
(1...4)–(5...7)	1.274	332	2.6
(1...5)–(6, 7)	1.089	346	6.7
(1...6)–(7)	0.710	325	0.5

Knowing the values of temperatures T_D and T_B, the thermal efficiency factor of the column can be calculated by using the formula $\eta_C = 1 - T_D/T_B$.

7. EXAMPLE OF CALCULATION

Let us determine the optimal separation sequence of a hydrocarbonic mixture into components by using the rule presented above. The molar composition of the mixture taken from [7] and the coefficients of the Antoine equation of its components are presented in Table 1.

Let the temperature in the dephlegmator be $T_D = 323$ K and let us use formula (12) to calculate the pressure in the column for different separation boundaries of the mixture, assuming that the *hypothesis of the key components* is valid. The values of P_C obtained are presented in Table 2. We find the temperature in the column still by solving equation (13) for different separation boundaries of the mixture. The values of T_B are presented in Table 2. We calculate the thermal efficiency factors of the column from known temperatures T_D and T_B. Their values are also presented in Table 2.

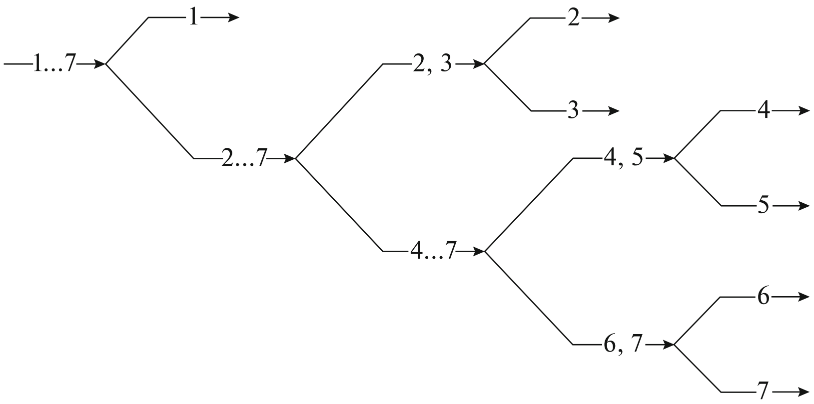

Fig. 2. Optimal mixture separation sequence.

Using the rule of the nondecreasing thermal coefficient presented above, we find the optimal separation sequence of the mixture into components, which is presented in Fig. 2.

8. CONCLUSIONS

Based on the use of the thermodynamic balances of the distillation column for ideal mixtures, it has been shown that the estimate of its efficiency in the function of heat consumption has a form of a bounded parabola, which is convex upwards, and is characterized by two parameters: the reversible efficiency factor and the irreversibility coefficient. The ultimate efficiency of the column and the efficiency factor corresponding to it are expressed through these parameters. It has been shown that the column efficiency factor is proportional to the reversible efficiency factor; the proportionality factor depends on the ratio of the heat load to its value corresponding to the maximum efficiency. In the maximum-efficiency regime, the column efficiency factor is half of the reversible efficiency factor. This makes it possible to select the separation sequence under the condition of the minimum total heat consumption by using the inequality obtained for the cascade of reversible columns.

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Translated by E. Smirnova