# **OPTIMAL SEPARATION SEQUENCE** FOR THREE-COMPONENT SYSTEMS

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#### SUMMARY

In this paper the problem of finding the optimal separation sequence for a three-component mixture in a two-stage separation system is considered. Two solutions are obtained. The first minimizes the energy used, subject to a given flow rate of the input mixture, by selecting optimal separation sequence and by distributing the contact surfaces between the first and second stages optimally. It is also shown that the input flow rate of a heat-driven two-stage separation system is bounded and that this bound (the maximal possible rate of heat-driven separation) depends on the separation sequence used. The closed-form expression for this dependence is obtained.

#### **KEY WORDS**

separation, three-component systems, zeotropic mixture

# **CLASSIFICATION**

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#### INTRODUCTION AND PROBLEM FORMULATION

Separation processes consume large amounts of energy. The lower bound on the amount of energy required is given by the reversible minimal work of separation  $A^0$  [1]. It depends on the amount of mixture, its composition and composition of the output mixtures and is equal to the increment of the mixture's free energy. For mixtures that can be considered as nearly ideal gases or nearly ideal solutions the free energy (Gibbs energy) of one mole of the i-th component in the j-th flow is equal to its chemical potential

$$\mu_{ij}(T, P_j, x_{ij}) = \mu_i^0(T, P_j) + RT \ln x_{ij}.$$
 (1)

Here *R* and *T* are the universal gas constant and mixture's absolute temperature;  $x_{ij}$  is the concentration of the i-th component in the j-th flow measured in molar fractions;  $\mu_i^0(T, P_j)$  is the chemical potential of the pure i-th component (known for most of substances) and  $P_j$  is the pressure in the j-th flow.

The reversible work of separation for  $N_0$  moles of k component mixture with concentration  $x_{i0}$  (i = 1, ...,k) (if the temperature and pressure of the mixture are equal to the temperatures and pressures of the *m* output flows of the separation system) is [2]

$$A^{0} = RN_{0}T \left[ \sum_{j=1}^{m} \gamma_{j} \sum_{i=1}^{k} x_{ji} \ln x_{ji} - \sum_{i=1}^{k} x_{i0} \ln x_{i0} \right],$$
(2)

where  $\gamma_j$  is the fraction of the input mixture that is separated into j-th flow with vector of concentrations  $x_j = (x_{j1}, ..., x_{jk})$ . In the particular case when the input mixture is separated into pure components the number of components is equal to the number of flows m = k, and the fraction of the j-th flow is equal to the concentration of the corresponding component in the input mixture:  $\gamma_j = x_{j0}, x_{jj} = 1$  and  $x_{ji} = 0$  for  $i \neq j$ .

Therefore the first term in the square brackets in (2) is equal zero and

$$A^{0} = -RN_{0}T\sum_{i=1}^{\kappa} x_{i0} \ln x_{i0} .$$
(3)

If instead of the amount the molar rate of the input mixture  $g_0$  is given together with output rates  $g_j = \gamma_j g_0$ , then the same formulas can be used to derive the power of reversible separation for an incomplete separation

$$p^{0} = -Rg_{0}T\left[\sum_{j=1}^{m} \gamma_{j} \sum_{i=1}^{k} x_{ji} \ln x_{ji} - \sum_{i=1}^{k} x_{i0} \ln x_{i0}\right].$$
(4)

and for the complete separation into pure substances

$$p^{0} = -Rg_{0}T\sum_{i=1}^{k} x_{i0} \ln x_{i0} .$$
(5)

The reversible estimates (4), (5) are realised if the rate  $g_0$  is infinitely close to zero or if the heat and mass transfer coefficients are infinitely large, that is, if the size of separation apparatus is infinitely large. These estimates are proportional to the rate  $g_0$ , depend on the compositions of the input and output flows only and do not depend on the separation sequence. Therefore these estimates do not allow us to compare different separation sequences and to choose the best sequence.

Real processes occur in finite-sized apparatus with finite rate. Irreversible losses, which increase the power required for separation, play an important role here. These losses depend on the exchange kinetics and on input/output flows' compositions and rates. These losses depend nonlinearly on the rate of the input mixture  $g_0$ . Irreversible losses are different for

separation sequences. They allow us to compare different variants with each other. Irreversible losses for separation using mechanical power are different to irreversible losses for heat-driven separation. For separation that uses mechanical energy (membrane separation, centrifuging, short-cycle absorption etc.) most of irreversibility is due to mass-transfer kinetics. For heat-driven separation that uses heat energy (distillation, boiling, drying, absorption-desorption cycles where the working solution changes temperature) irreversible losses are due to both mass transfer and heat-exchange accompanying transformation of heat energy into the work of separation.

When the number of component increases, the number of possible separation sequences increases dramatically. The problem of optimal separation sequence attracted substantial interest (see review [3]). It can only be solved if dependence of irreversible energy losses at each stage of separation for all process design as function of its rate and sizes are known.

We propose a much simpler approach in this paper. It provides coarser estimates and relies on mass and heat transfer coefficients only. Nevertheless, it allows one to find the ways to improve separation efficiency by distributing optimally contact surfaces between stages.

Estimates for the minimal power of separation in mechanical systems and for minimal amount of heat required in heat-driven separation systems with given rate were obtained in [4 - 7] under the following assumptions:

- 1. temperatures of the input molar flow  $g_0$  and output molar flows  $g_j$  (j = 1, ...,m) are equal to the same temperatures *T*,
- 2. mass transfer flows depend linearly on the chemical potentials' difference. For the i-th substance that is transferred from the flow  $g_0$  to the flow  $g_i$ ,

$$g_{ii} = \alpha_{ii} \Delta \mu_{ii}$$
, (i = 1, ..., k and j = 1, ..., m). (6)

Here  $\alpha_{ij}$  is the effective (that takes into account the area of contact surface) mass transfer coefficient for transfer of the i-th component into j-th flow,  $\Delta \mu_{ij}$  is the difference of chemical potentials for i-th component in the input mixture and in j-th flow (the driving force of mass transfer)

$$\Delta \mu_{ii} = \mu_{i0}(T, P_0, x_{i0}) - \mu(T, P_i, x_{ii}), \qquad (7)$$

3. the laws of mass transfer in heat-driven separation systems are linear

$$q = \alpha \Delta T \,, \tag{8}$$

where  $\alpha$  is the heat-transfer coefficient for the whole heat-exchange surface,  $\Delta T$  is the temperature difference between the working body and the mixture which is being heated.

The flows structure for mechanical and heat-driven separation systems m = 2 are shown in Figure 1.



Figure 1. Flows' structures in a) mechanical and b) heat-driven separation systems.

Under these assumptions it was shown [4 - 7] that the power required for separation in mechanical system can't be lower than

$$p_{1} = p^{0} + g_{0}^{2} \sum_{j=1}^{m} \gamma_{j}^{2} \sum_{i=1}^{k} \frac{x_{ij}^{2}}{\alpha_{ij}} = p^{0} + \Delta p , \qquad (9)$$

for separation into flows with compositions  $x_j$  and

$$p_2 = p_0^0 + g_0^2 \sum_{i=1}^k \frac{x_{i0}^2}{\alpha_i} = p^0 + \Delta p.$$
(10)

for separation into pure components. In (10),  $p_0$  and  $p_0^0$  corresponds to (4) and (5), respectively. The first term is proportional to the feed rate  $g_0$  of the mixture that is separated, and the second term, due to process' irreversibility, is proportional to the  $g_0^2$ .

For heat-driven separation the heat flow  $q_+$ , removed from the hot reservoir with the temperature  $T_+$ , cannot be lower than

$$q_{\nu}^{+} = \frac{p_{\nu}}{\eta(p_{\nu},\overline{\alpha})}.$$
(11)

Here v = 1 corresponds to separation into flows with given compositions, and v = 2 corresponds to separation into pure components, while  $\eta(\cdot, \cdot)$  is the maximal efficiency of irreversible transformation of heat into work with power p [5, 6]

$$\eta(p,\overline{\alpha}) = \frac{1}{2} \left[ \frac{p}{\overline{\alpha}T_{+}} + \eta_{k} + \sqrt{\left(\frac{p}{\overline{\alpha}T_{+}} + \eta_{k}\right)^{2} - \frac{4p}{\overline{\alpha}T_{+}}} \right].$$
(12)

In heat-driven separation systems heat is supplied from the hot reservoir with the temperature  $T_+$  to the mixture that is separated. Heat is also removed from the mixture into cold reservoir with the temperature T. In absorption-desorption cycle these are the temperatures in desorber and absorber, and in distillation – the temperatures in boiler and condenser. The effective heat transfer coefficient  $\alpha$  is expressed in terms of the heat transfer coefficient from the hot reservoir  $\alpha_+$  and from the cold one  $\alpha_-$  as follows

$$\overline{\alpha} = \frac{\alpha_+ \alpha_-}{\alpha_+ + \alpha_-}, \ \eta_k = 1 - \frac{T}{T_+}.$$
(13)

The formulas (9 - 13) are derived from thermodynamic balances (mass, energy and entropy balances) for separation systems. The latter balance includes entropy production, which depends on the mass and heat transfer kinetics. In [4 - 7] the minimal possible entropy production subject to given heat and mass transfer coefficients, given flow rates and mass and energy balances was derived. This result led to finding the minimal extra energy needed. It turned out that the rate of heat-driven separation systems  $g_0$  is bounded since increase of the heat flow  $q_+$  above some threshold  $\bar{q}_+$  reduces the maximal rate of heat-driven separation system. The maximal rate is [5, 8]

$$g_0^{\max} = \frac{-B + \sqrt{B^2 + 4\overline{\alpha}D(T_+^{1/2} - T^{1/2})^2}}{2D},$$
(14)

where  $\overline{\alpha}$  is given by (13), and

$$B = \frac{p^0}{g_0}, \quad D = \frac{\Delta p}{g_0^2}.$$
 (15)

Here  $p^0$  and  $\Delta p$  are defined by expressions (4) and (9) for incomplete, and by (5) and (10) for complete separations, respectively. Further in the text we will consider the problem of choosing

separation sequence for mixture of three-component mixture. The input flow  $g_0$  is described by concentrations  $x_{10}$ ,  $x_{20}$  and  $x_{30}$ ,

$$\sum_{i=1}^{3} x_{i0} = 1.$$
 (16)

We assume that separation is carried out in two stages. During the first stage one component is separated out. The residual binary mixture is separated at the second stage. For simplicity we assume that output flows consist of pure substances (Figure 2) and the compositions of the input and output flows are fixed.

This assumption means that we consider zeotropic mixtures only.



Figure 2. Schema of two-stage separation system for three-component mixture.

We would like to find out

- 1. what component should be separated out first in order to minimise the power needed for separation,
- 2. what component should be separated first in order to maximise the rate of separation,
- 3. how to distribute optimally heat and mass exchange surfaces between separation stages in order to minimize power or maximize the rate of separation.

#### **MECHANICAL SEPARATION SYSTEM**

In mechanical separation systems the minimum of the power required corresponds to the minimum of the irreversible losses. Separation is based on the differences between the properties of mixture's components (sizes of molecules, density boiling temperature, etc.).

These differences lead to different interactions between different components of the mixture and membrane or absorber, different rate at which components are transferred from liquid into gaseous phase, etc. We assume that the property used for separation can be measured quantitatively. It is also assumed here that the difference between components' properties used for separation does not depend on the composition of the mixture, which excludes separation of azeotropic mixtures.

We order components in such a way that the difference (in term of this property) between the third and the first component was maximal. Now we can compare two separation sequences only. The first sequence is when the first component is separated first. The second sequence is when the third component is separated first. For the first sequence with the unit rate ( $g_0 = 1$ ) when the first component with concentration  $x_{10}$  is separated during first stage, the irreversible losses in accordance with (10) are

$$\Delta p_1 = \frac{x_{10}^2}{\alpha_{11}} + (1 - x_{10})^2 \left[ \frac{1}{\alpha_{11}} + \frac{x_{20}^2 + x_{30}^2}{\alpha_{23}} \right],\tag{17}$$

Here  $\alpha_{11}$  and  $\alpha_{23}$  are the effective mass transfer coefficients for the first and second stages of separation where the first component is separated out first.

Similarly, when the third component is separated out first we get

$$\Delta p_3 = \frac{x_{30}^2}{\alpha_{13}} + (1 - x_{30})^2 \left[ \frac{1}{\alpha_{13}} + \frac{x_{20}^2 + x_{10}^2}{\alpha_{21}} \right],$$
(18)

where  $\alpha_{13}$  and  $\alpha_{21}$  are the effective mass transfer coefficients for the first stage when third component is separated.

Mass transfer coefficients are proportional to the contact area  $S_v$  (v = 1, 2), for apparatus used at the *v*-th stage of separation, and the specific (per unit contact area) mass transfer coefficient  $\delta$ . This coefficient depends on the properties of the second and first ( $\delta_1$ ) and second and third ( $\delta_3$ ) components. Thus

$$\alpha_{11} = S_1 \delta_1, \ \alpha_{13} = S_1 \delta_3, \ \alpha_{23} = S_2 \delta_3, \ \alpha_{21} = S_2 \delta_1.$$
<sup>(19)</sup>

Let us rewrite  $\Delta p_2$  and  $\Delta p_2$  as follows

$$\Delta p_1 = \frac{K_{11}}{S_1} + \frac{K_{23}}{S_2},\tag{20}$$

$$\Delta p_2 = \frac{K_{13}}{S_1} + \frac{K_{21}}{S_2}.$$
(21)

Here

$$K_{1i}(x_{i0},\delta_i) = \frac{x_{i0}^2 + (1 - x_{i0})^2}{\delta_i}, \quad i = 1, 3,$$
(22)

$$K_{23}(x_{10}, x_{30}, \delta_3) = \frac{(1 - x_{10})^2 [x_{30}^2 + (1 - x_{10} - x_{30})^2]}{\delta_3},$$
(23)

$$K_{21}(x_{10}, x_{30}, \delta_1) = \frac{(1 - x_{30})^2 [x_{10}^2 + (1 - x_{10} - x_{30})^2]}{\delta_1}.$$
 (24)

These expressions represent irreversible power losses for one unit contact area and one-unit feed rate of the input mixture.

Suppose that the total contact area is given as  $S = S_1 + S_2$  and it is required to distribute it between stages to minimise power needed for separation. The problem of finding the optimal  $S_1$  and  $S_2$  takes the form

$$\left[\Delta p_1(S_1, S_2) + \Delta p_2(S_1, S_2)\right] \Longrightarrow \min p_1$$

subject to  $S_1 + S_2 = S$ . Since  $\Delta p_i$  is convex on  $S_1$ ,  $S_2$  the solution of this problem is unique and is determined by the conditions

$$\frac{K_{11}}{S_1^2} = \frac{K_{23}}{S_2^2},$$

for the first sequence and

$$\frac{K_{13}}{S_1^2} = \frac{K_{21}}{S_2^2},$$

for the second one. The optimal distribution of contact area is given by the equalities

$$S_1^* = S \frac{\sqrt{K_{11}}}{\sqrt{K_{11}} + \sqrt{K_{23}}}, \ S_2^* = S \frac{\sqrt{K_{23}}}{\sqrt{K_{11}} + \sqrt{K_{23}}},$$
(25)

for the first and

$$S_1^* = S \frac{\sqrt{K_{13}}}{\sqrt{K_{13}} + \sqrt{K_{21}}}, \ S_2^* = S \frac{\sqrt{K_{21}}}{\sqrt{K_{13}} + \sqrt{K_{21}}},$$
(26)

for the second separation sequence.

Substitution of this optimal area distribution into (20) and (21) yields the following expressions for the irreversible power of separation

$$\Delta p_1 = \frac{g_0^2}{S} \left( \sqrt{K_{11}} + \sqrt{K_{23}} \right)^2, \tag{27}$$

$$\Delta p_2 = \frac{g_0^2}{S} \left( \sqrt{K_{13}} + \sqrt{K_{21}} \right)^2, \tag{28}$$

The condition when this power is lower for the first sequence takes the form

$$\left(\frac{\Delta p_1}{\Delta p_2}\right)^{1/2} = \frac{\sqrt{K_{11}(x_{10},\delta_1) + \sqrt{K_{23}(x_{10},x_{30},\delta_3)}}}{\sqrt{K_{13}(x_{30},\delta_3) + \sqrt{K_{21}(x_{10},x_{30},\delta_1)}} < 1.$$
(29)

If left-hand side of this inequality is higher than 1 then it is energetically more efficient to separate the third component first.

After substitution of (22 - 24) into (29) we get

$$\frac{\sqrt{x_{10}^2 + (1 - x_{10}^2)} - (1 - x_{30})\sqrt{x_{10}^2 + x_{20}^2}}{\sqrt{x_{30}^2 + (1 - x_{30}^2)} - (1 - x_{10})\sqrt{x_{30}^2 + x_{20}^2}} < \frac{\delta_1}{\delta_3} = K,$$
(30)

where  $x_{20} = x_{10} - x_{30}$ . The dashed areas in Figure 3 show where first separation sequence is most energy efficient for K = 0.5, K = 1 and K = 2.



**Figure 3.** Boundaries between two areas where first and second separation sequences are optimal for different *K*. Dashed area corresponds to optimal sequence with separation of first component first.

From the symmetry of the left-hand side of (30) it is clear that the boundary that corresponds to K = 1 is a straight line. Calculations show that for different values of K these boundaries are very close (with about 3 % error) to straight lines  $x_{10} = x_{30}/K$ . It allows us to write down the approximate condition which determines when separation of first component at first stage is optimal as

$$x_{10}\sqrt{\delta_1} \ge x_{30}\sqrt{\delta_3} . \tag{31}$$

In particular, if concentrations of components one and two are the same  $x_{10} = x_{20} = x_0 < 0.5$  then separation of the first component at the first stage is optimal if  $\delta_1 > \delta_3$ ; if  $\delta_1$  and  $\delta_3$  are close to each other then it is optimal to separate the first component first if  $x_{10} > x_{30}$ .

In many cases, separation of a multi-component mixture is carried out in stages, when at each stage one component with the highest or lowest value of some property is separated. Since components are numbered in an arbitrary order, we denote the component with the highest value of  $R_i = x_{i0} \cdot \delta_i^{1/2}$  as the first one. Distribution of contact surfaces here are found from (25).

For the problem where it is required to separate the middle component, the values of this property for the first and the third components are lower and higher than its value for the middle component.

#### **HEAT-DRIVEN SEPARATION**

When separation sequence is chosen for a heat-driven separation system one needs to take into account that the heat consumed at each stage of separation depend not only on the total power used at the i-th stage  $p_i = p_i^0 + \Delta p_i$ , (i = 1, 2) but also on the efficiency of the heat into work transformer  $\eta_i(p_i, \overline{\alpha}_i)$ . When  $p_i$  increases then  $\eta_i(p_i, \overline{\alpha}_i)$  decrease monotonically from  $\eta_K$  at  $p_i = 0$  to

$$\eta_i(p_i^{\max}) = 1 - \sqrt{\frac{T}{T_+}},$$
(32)

for the maximal possible power for given heat transfer coefficients. In turn, the transformer, which transforms heat into work of separation, cannot generate power that exceeds the maximal power

$$p_i^{\max} = \overline{\alpha}_i (T_{i+}^{1/2} - T_{1/2})^2.$$
(33)

When  $\overline{\alpha}_i$  increases,  $p_i$  as well as  $\eta_i$  increase (see Figure 4). Note that the expressions (32) and (33) were derived in [9] much earlier than the expression (12), which easily follows from them.



**Figure 4.** Characteristic change of the transformer's efficiency as a function of separation power and the effective heat transfer coefficient.

The maximal rate for a two-staged sequential separation system is determined by the maximal rate of the stage with the lower rate. Since the maximal rate for the i -th stage depends on the heat transfer coefficient  $\overline{\alpha}_i$ , (i = 1, 2) the maximal rate of two-stage system for the given total area of heat-transfer surfaces

$$\overline{\alpha}_1 + \overline{\alpha}_2 = \overline{\alpha} , \qquad (34)$$

is achieved when the following equality holds  $g_{01}^{\max}(\overline{\alpha}_1) = g_{02}^{\max}(\overline{\alpha}_2)$ , i.e.

$$\frac{\sqrt{B_1^2 + 4\overline{\alpha}_1 D_1 (T_{1+}^{1/2} - T^{1/2})^2} - B_1}{D_1} = \frac{\sqrt{B_2^2 + 4\overline{\alpha}_2 D_2 (T_{2+}^{1/2} - T^{1/2})^2} - B_2}{D_2},$$
 (35)

where  $B_i$  and  $D_i$ , (i = 1, 2) are defined by (15). Quantities  $g_0 B_{ij}$  and  $g_0^2 D_{ij}$  (i, j = 1, 2) represent reversible and irreversible losses of energy during the i–th stage of separation, respectively.

The conditions (34) and (35) determine the optimal distribution of heat-transfer surface  $\overline{\alpha}_1$  and  $\overline{\alpha}_2$  between two stages of heat-driven separation system. In turn, at each stage of separation for given  $\overline{\alpha}_i$  the distribution of heat-transfer surface between heating and cooling is determined by the condition of minimum of the total cost of heat-exchangers subject to (13). If these cost costs are equal, then  $\overline{\alpha}_{i+} = \overline{\alpha}_{i-} = 2\overline{\alpha}_i$ .

Since  $\eta(p, \overline{\alpha})$  decreases monotonically when *p* increases, reduction of power (for example, as a result of optimal redistribution of mass exchange surface *S*), reduces the amount of heat *q*<sub>+</sub>. That is why we assume that this surface *S* is distributed between the stages in such a way that combined irreversible power losses at these stages is minimal. This condition leads to expressions (25) or (26) for *S*<sub>i</sub><sup>\*</sup>.

Suppose that during first stage of separation the first component is separated. The concentration of the first component in the input flow with rate  $g_0$  is  $x_{10}$ . The residual binary mixture is then separated into pure components at the second stage of separation. Then for the first stage the power is  $p_1 = p_1^0 + \Delta p_{11}$ , where

$$p_1^0 = RTg_0 \left[ (1 - x_{10})(x_{20} \ln x_{20} + x_{30} \ln x_{30}) - \sum_{i=1}^3 x_{i0} \ln x_{i0} \right] = g_0 B_{11},$$
(36)

$$\Delta p_{11} = \frac{g_0^2}{S_1^*} K_{11} = \frac{g_0^2}{S_1^*} \frac{x_{10}^2 + (1 - x_{10})^2}{\delta_1} = D_{11} g_0^2.$$
(37)

Here  $S_1^*$  corresponds to the expression (25). The subscripts of  $B_{ij}$  and  $D_{ij}$  in (36) and (37) denote the separation sequence and separation stage number, respectively.

Similarly, for the second stage we have

$$p_2^0 = -RTg_0(1 - x_{10})(x_{20}\ln x_{20} + x_{30}\ln x_{30}) = g_0B_{12},$$
(38)

$$\Delta p_{12} = \frac{g_0^2 K_{23}}{S_2^*} = \frac{g_0^2 (1 - x_{10})^2}{S_2^*} \frac{x_{20}^2 + x_{10}^2}{\delta_3} = g_0^2 D_{12}.$$
(39)

We now introduce auxiliary notations for limiting power of heat into work of separation for the single-unit effective heat transfer coefficient  $r_1 = (T_{+1}^{1/2} - T^{1/2})^2$ ,  $r_2 = (T_{+3}^{1/2} - T^{1/2})^2$ . Then for the first separation sequence from power balance it follows that

$$g_{01}B_{11} + D_{11}g_{01}^2 = \alpha_1 r_1, \tag{40}$$

for the first stage of separation. Similarly for the second stage of separation we get

$$g_{01}B_{12} + D_{12}g_{01}^2 = \alpha_2 r_2.$$
(41)

Since the maximal rate of the two-stage sequence of separations is determined by the minimal rate of its stages, we assume that the heat transfer surface is distributed in such a way that the maximal rates for both stages are equal. We denote this rate for the first separation sequence as  $g_{01}$ . Let us express  $\alpha_1$  and  $\alpha_2$  from (40) and (41). After adding them together we obtain the following expression for  $g_{01}$ ,

$$\overline{\alpha} = \frac{g_{01}B_{11} + D_{11}g_{01}^2}{r_1} + \frac{g_{01}B_{12} + D_{12}g_{01}^2}{r_2} = F_1(g_{01}).$$
(42)

Similarly we get for the second separation sequence

$$\overline{\alpha} = \frac{g_{02}B_{21} + D_{21}g_{02}^2}{r_1} + \frac{g_{02}B_{22} + D_{22}g_{02}^2}{r_2} = F_2(g_{02}).$$
(43)

Solution of these equations with respect to  $g_{0i}$  gives the maximum rate for the i-th separation sequence

$$g_{0i}^{\max} = \frac{-(B_{i1}r_2 + B_{i2}r_1) + \sqrt{(B_{i1}r_2 + B_{i2}r_1)^2 + 4(D_{i1}r_2 + D_{i2}r_1)\overline{\alpha}r_1r_2}}{2(D_{i1}r_2 + D_{i2}r_1)}, i = 1, 2.$$
(44)

The closed-form expressions for  $B_{ij}$  and  $D_{ij}$  are the following:

$$\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = RT \begin{pmatrix} (1 - x_{10}) \sum_{i=2,3} x_{i0} \ln x_{i0} - \sum_{i=1}^{3} x_{i0} \ln x_{i0} & (x_{10} - 1) \sum_{i=2,3} x_{i0} \ln x_{i0} \\ (1 - x_{30}) \sum_{i=1,2} x_{i0} \ln x_{i0} - \sum_{i=1}^{3} x_{i0} \ln x_{i0} & (x_{30} - 1) \sum_{i=1,2} x_{i0} \ln x_{i0} \end{pmatrix},$$
(45)

$$\begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} = \begin{pmatrix} \frac{K_{11}}{S_1^*} & \frac{K_{23}}{S_2^*} \\ \frac{K_{13}}{S_{12}^*} & \frac{K_{21}}{S_{22}^*} \end{pmatrix} = \frac{1}{S} \begin{pmatrix} K_{11} + \sqrt{K_{11}K_{23}} & K_{23} + \sqrt{K_{11}K_{23}} \\ K_{13} + \sqrt{K_{13}K_{21}} & K_{21} + \sqrt{K_{13}K_{21}} \end{pmatrix}.$$
(46)

# SEPARATION SEQUENCE FOR THREE-COMPONENT MIXTURE IN HEAT-DRIVEN SEPARATION SYSTEMS

The choice of separation sequence with maximal rate depends on the value of  $\overline{\alpha}$  for which the maximal rates of two separation stages are equal and the curves  $F_1(g_{01})$  and  $F_2(g_{02})$  intersect. The point of intersection  $g_0$  is determined by the condition

$$g_{0} = \frac{\frac{B_{11} - B_{22}}{r_{1}} + \frac{B_{12} - B_{21}}{r_{2}}}{\frac{D_{11} - D_{22}}{r_{1}} + \frac{D_{12} - D_{21}}{r_{2}}},$$
(47)

Positive  $g_0$  exists if numerator and denominator in (47) have the same signs. Otherwise, the optimal sequence is determined by the sign of numerator in (47): it is positive then the second sequence is better, while if it is negative the first sequence has higher maximal rate. If curves intersect then this rule holds for  $g_{0i} < g_0$ . In case of  $g_{0i} > g_0$  the opposite rule holds.

It is clear that for  $r_1 = r_2$  maximal rate always corresponds to the minimal irreversible power loss for separation.

#### EXAMPLE

We consider separation of three-component mixture with initial concentrations  $x_{10} = 0,1$ ;  $x_{20} = 0,6$  and  $x_{30} = 0,3$ . The specific (per surface unit) mass transfer coefficients are  $\delta_1 = 0,2$  and  $\delta_2 = 0,1$ .

From (31) it follows that if mechanical separation is used then the third component should be separated first (0,3 > 0,141).

Let us consider heat-driven separation and assume that the temperature of the input mixture is T = 300 K, the temperature of the hot reservoir  $T_+$  are  $T_{+1} = 400$  K for separation of the first component and  $T_{+3} = 350$  K for separation of the third one. The heat transfer coefficient is  $\overline{\alpha} = 20\ 000$ . The total heat-exchange area for both stages is  $S = 10 \text{ m}^2$ .

#### Step 1

We calculate the optimal distribution of heat-exchange area between stages. From (22 - 24)  $K_{11} = 4,1$ ;  $K_{13} = 5,8$ ;  $K_{23} = 3,645$  and  $K_{21} = 0,907$ . The optimal distribution of area for the first separation sequence are  $S_1 = 5,15$ ;  $S_2 = S - S_1 = 4,85$  and  $S_1 = 7,17$ ;  $S_2 = S - S_1 = 2,83$ .

#### Step 2

For the first stage of the first separation sequence from (36) and (37) we get  $B_1 = 739,6$ ;  $D_1 = 0,8$  and for the second stage we obtain  $B_2 = 1662,5$ ;  $D_2 = 0,75$  see (38) and(39). For the second separation sequence we get  $B_{21} = 1300,3$ ;  $B_{22} = 1336,5$ ;  $D_{21} = 0,81$  and  $D_{22} = 0,32$ .

#### Step 3

See (44). For the first separation sequence (separation of the first component at first stage) we get  $g_0 = 20,48$ . For the second separation sequence we obtain  $g_0 = 22,9$ . Therefore if third component is separated first then we can separate larger flow (with the same composition) than we can if we separated the first component first.

# CONCLUSIONS

In this paper we show how to select the most efficient separation sequence for threecomponent mixtures in a two-staged separation system. We also obtained the optimal distribution of contact surfaces for mass and heat transfer between separation stages. The minimal power required for mechanical separation at given production rate is derived. For heat-driven separation we obtain the maximal flow rate of the input mixture.

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# REDOSLIJED OPTIMALNOG RAZDVAJANJA U TRO-KOMPONENTNIM SUSTAVIMA

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#### SAŽETAK

U članku se određuje optimalni slijed razdvajanja za trokomponentnu smjesu u dvostupanjskom procesu. Dva su rješenja dobivena. Prvo rješenje minimizira korištenu energiju, pri stalnom toku ulazne smjese, putem izdvajanja optimalnog slijeda razdvajanja i optimalnim dijeljenjem kontaktne plohe između prvog i drugog stupnja. Pokazano je kako je ulazni tok toplinom upravljanog dvostupanjskog procesa razdvajanja omeđena iznosom (najveće moguće brzine toplinom upravljanog razdvajanja) koji ovisi o slijedu razdvajanja. Izvedeni su izrazi za navedenu ovisnost.

#### KLJUČNE RIJEČI

razdvajanje, trokomponentni sustav, zeotropska smjesa