Minimum Energy Requirements of Thermally Coupled Distillation Systems

Energy requirements of four different thermally coupled distillation systems were minimized for an assumed ideal ternary solution being separated. Minimum vapor flows and values of decision variables have been found in the form of analytical expressions. This enables making a quick and simple comparison of these systems. The solution method can be used for synthesis of separation systems or for screening calculations.

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Introduction

Thermally coupled distillation systems consist of columns connected by liquid and vapor countercurrent streams. There are four types of these systems for separation of a ternary solution, as shown in Figures 1–4; they are called here TCS, TCS-I, TCS-R, and TCS-S. Thermodynamic aspects of the distillation process carried out in thermally coupled systems were discussed by Petlyuk et al. (1965). Spadoni and Stramigioli (1983) presented a design method for the TCS. Tedder and Rudd (1978) compared the TCS-R and the TCS-S with six other systems for separation of a ternary solution, using total annual cost as the goal function. Fidkowski and Królikowski (1986) presented an optimization procedure of the TCS based on minimization of energy requirements. The aim of the present work is to deveop the optimization procedure for three other thermally coupled systems, TCS-I, TCS-R, and TCS-S, and to compare these systems.

It is assumed that a ternary, ideal solution *ABC* with constant values of relative volatilities and equimolar internal flow rates is separated into almost pure components. Components are ranked in decreasing order of relative volatilities: $\alpha_A > \alpha_B > \alpha_C$. Feed is introduced and products are obtained in the boiling liquid state. The substitutional goal function is defined as the sum of minimum vapor flow rates from reboilers of the given system required for the demanded separation. Values of the substitutional goal function are proportional to energy requirements of separation, provided that the same cooling medium is used in all condensers and the same heating medium is used in all reboilers of the system. Energy requirements are usually the dominant factor in the total cost of a distillation plant (Doukas and Luyben, 1978; Tedder and Rudd, 1978; Nishida et al., 1981). This substitutional goal function was used by Rod and Marek (1958) and tested by Tedder and Rudd. The definition is convenient because of the universality of the goal function, which does not depend on material and energy prices. Minimum reflux ratio was calculated using the classic method of Underwood (1948).

Optimization of TCS and TCS-I

Systems TCS and TCS-I are presented in Figures 1 and 2. The optimization procedure for the TCS has been described elsewhere (Fidkowski and Królikowski, 1986). Analyzing balances of the inner liquid and vapor streams in the TCS-I one can obtain the following set of linearly independent equations:

$$V_I = L_I + A + \beta B \tag{1a}$$

$$\bar{L}_I = L_I + F \tag{1b}$$

$$\bar{V}_I = L_I + A + \beta B \tag{1c}$$

$$V_{II} = L_{II} + A \tag{1d}$$

$$\bar{L}_{II} = L_{II} - L_I \tag{1e}$$

$$\bar{V}_{II} = L_{II} - L_I - \beta B \tag{1f}$$

$$L_{III} = L_{II} - L_I - \beta \tag{1g}$$

$$V_{III} = L_{II} - L_I - \beta B \tag{1h}$$

$$\bar{L}_{III} = L_{II} + A + C \tag{1i}$$

$$\bar{V}_{III} = L_{II} + A \tag{1j}$$

where β is defined as the fraction of component *B* in the top product of the first (inner) column:

$$\beta = \frac{V_I y_B^I - L_I x_B^I}{B} \tag{2}$$

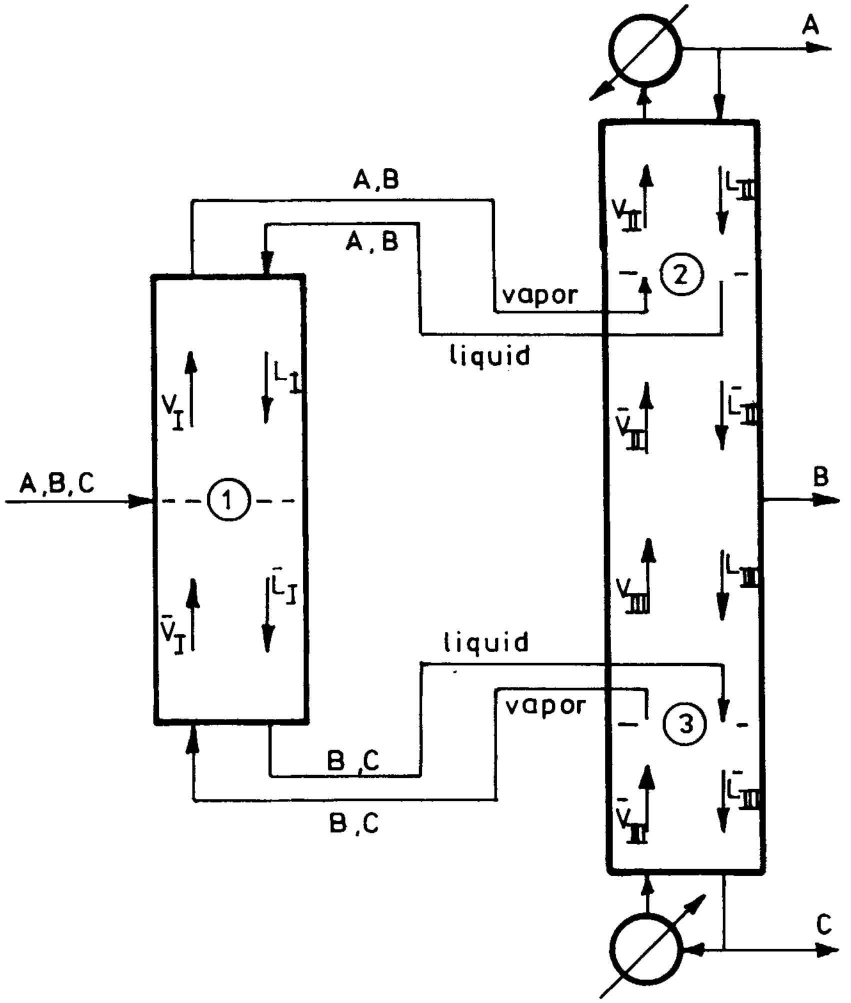

Figure 1. Thermally coupled system (TCS).

The optimization task for the TCS-I is formulated as follows: Minimize $\bar V_{III}$ subject to the inequality constraints

$$V_I \geq V_I^M$$
$$V_{II} \geq V_{II}^M$$
$$V_{III} \geq V_{III}^M \tag{3}$$

and to the equality constraints, Eqs. 1a–1j.

Balance equations and formulation of the optimization task are identical with those for the TCS, so the same solution procedure may be repeated. The solution is as follows:

$$\bar V_{III}^{opt} = \max\left\{\frac{\alpha_A A}{\alpha_A - \phi_1}, \frac{\alpha_A A}{\alpha_A - \phi_2}, \frac{\alpha_B B}{\alpha_B - \phi_2}\right\} \tag{4}$$

where ϕ_1 and ϕ_2 are roots of Underwood's equation:

$$\frac{\alpha_A A}{\alpha_A - \phi} + \frac{\alpha_B B}{\alpha_B - \phi} + \frac{\alpha_C C}{\alpha_C - \phi} = 0 \tag{5}$$

satisfying the relations:

$$\alpha_C < \phi_2 < \alpha_B < \phi_1 < \alpha_A \tag{6}$$

The optimum values of decision variables β and L_I are contained in the closed section PR on the plane (β, L_I), where coordinates of the segment ends are:

$$\beta_P = \frac{\alpha_B - \alpha_C}{\alpha_A - \alpha_C} \tag{7}$$

$$L_{I_P} = \frac{(A + B + C)\alpha_C}{\alpha_A - \alpha_C} \tag{8}$$

$$\beta_R = \frac{L_{II}^{opt}(\alpha_A - \alpha_B) - A\alpha_B}{L_{II}^{opt}\alpha_A - (L_{II}^{opt} + A + C)\alpha_C} \tag{9}$$

$$L_{I_R} = L_{II}^{opt}\left[1 - \frac{B\alpha_A}{L_{II}^{opt}\alpha_A - (L_{II}^{opt} + A + C)\alpha_C}\right] \tag{10}$$

and

$$L_{II}^{opt} = \bar V_{III}^{opt} - A \tag{11}$$

Values of the remaining operational parameters in optimal conditions may be calculated from Eqs. 1a–1j.

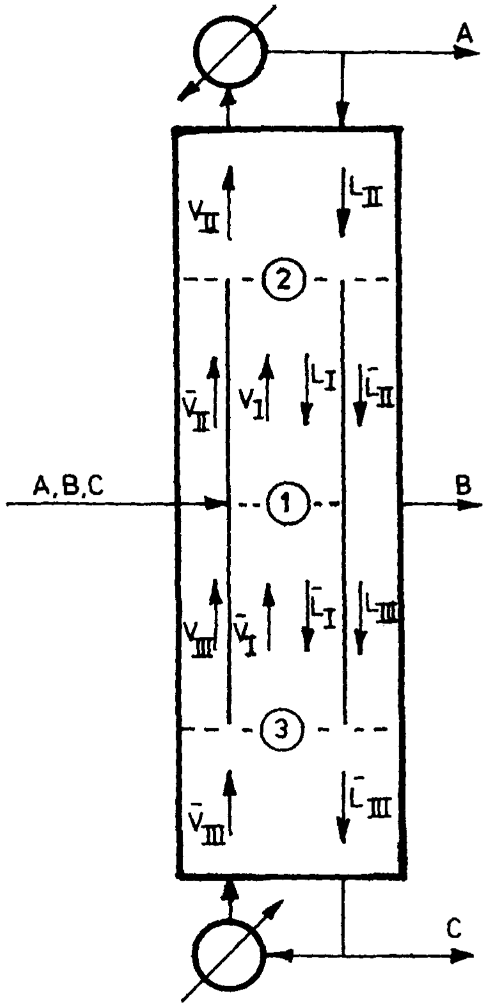

Figure 2. Thermally coupled system with inner column (TCS-I).

Optimization of TCS-R

In order to select decision variables of the TCS-R, inner streams of phases in particular sections of distillation columns were balanced, Figure 3. Linearly dependent equations were removed using the Gaussian elimination method. The final set contains six linearly independent equations with eight unknown variables.

$$V_I - L_I = A \tag{12a}$$

$$V_{III} = V_{II} - \bar{V}_I \tag{12b}$$

$$L_{II} = \bar{L}_I + L_{III} \tag{12c}$$

$$V_{II} = L_{II} - C \tag{12d}$$

$$V_{III} - L_{III} = B \tag{12e}$$

$$\bar{V}_I = V_I \tag{12f}$$

Two variables must be selected as decision variables in order to solve this series. Let them be L_{II}, the liquid flow rate in the first column below the side stream, and V_{III}, the vapor flow rate in the rectifying column. Assuming values of these variables, one can calculate all the other variables:

$$V_{II} = L_{II} - C \tag{13a}$$

$$L_{III} = V_{III} - B \tag{13b}$$

$$V_I = L_{II} - V_{III} - C \tag{13c}$$

$$L_I = L_{II} - V_{III} - A - C \tag{13d}$$

$$\bar{L}_I = L_{II} - V_{III} + C \tag{13e}$$

$$\bar{V}_I = L_{II} - V_{III} - C \tag{13f}$$

The goal function of the TCS-R is vapor flow rate V_{II} and the optimization task is formulated as follows:

Minimize V_{II} subject to

$$\begin{aligned} V_I &\geq V_I^M \\ V_{II} &\geq V_{II}^M \end{aligned} \tag{14}$$

and to the constraints given by Eqs. 13a–13f.

The problem will be expressed in terms of decision variables using these equality constraints.

Constraint $V_I \geq V_I^M$

The minimum vapor flow rate V_I^M is calculated from Underwood's equation:

$$V_I^M = \max_{i=1,2} \frac{A\alpha_A}{\alpha_A - \phi_i} \tag{15}$$

where ϕ_i are roots of Eq. 5. Because of inequalities in Eq. 6, the maximum value of V_I^M is obtained for $i = 1$:

$$V_I^M = \frac{A\alpha_A}{\alpha_A - \phi_1} \tag{16}$$

Using Eq. 13c, the first constraint in the optimization task can be rewritten as follows:

$$L_{II} \geq \frac{A\alpha_A}{\alpha_A - \phi_1} + C + V_{III} \tag{17}$$

The righthand side of the upper inequality will be denoted by $L_{II}^{(1)}$:

$$L_{II}^{(1)} = \frac{A\alpha_A}{\alpha_A - \phi_1} + C + V_{III} \tag{18}$$

Constraint $V_{II} \geq V_{II}^M$

The minimum reflux conditions for section 2 (Figure 3) are determined by the following balance and equilibrium equations:

$$L_{II}^M x_B - V_{II}^M y_B = 0 \tag{19}$$

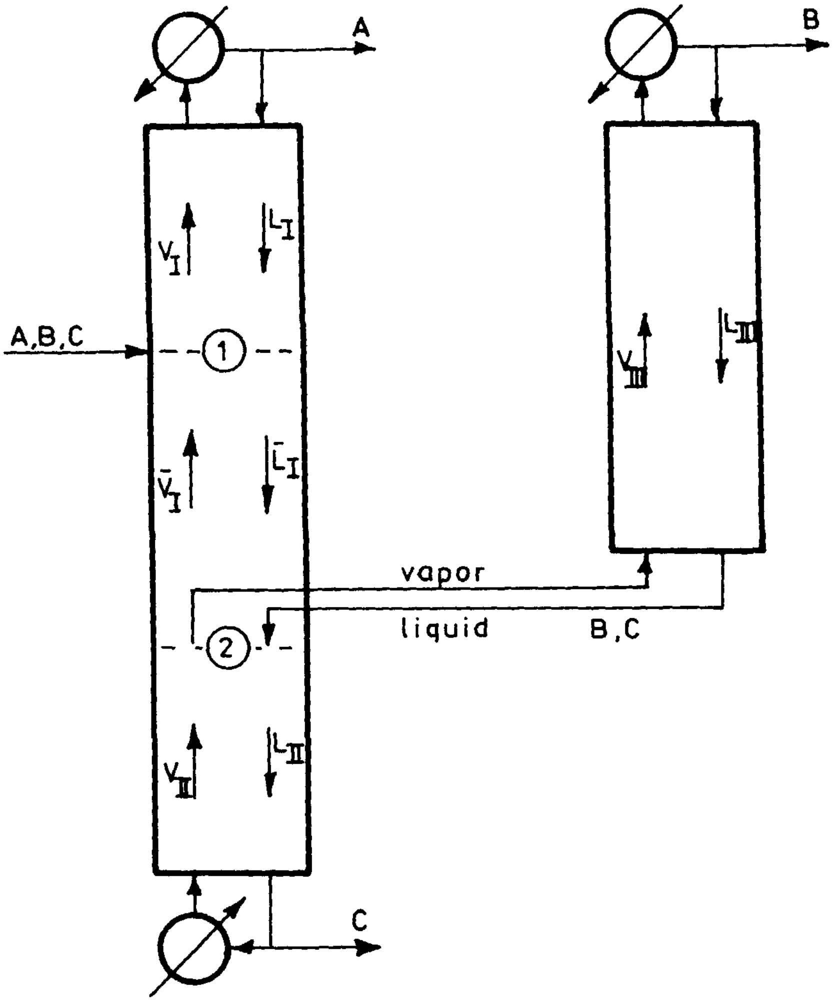

Figure 3. Thermally coupled system with rectifying column (TCS-R).

$$V_{II}^M = L_{II}^M - C \tag{20}$$

$$y_B = \frac{\alpha_B x_B}{\alpha_B x_B + \alpha_C(1 - x_B)} \tag{21}$$

where symbols x_B and y_B denote mole fraction of component B in the liquid and vapor phase, respectively, at level 2 (Figure 3). From this set of equations one can calculate V_{II}^M or L_{II}^M. The considered constraint $V_{II} \geq V_{II}^M$ is equivalent to $L_{II} \geq L_{II}^M$, so for convenience we will find L_{II}^M, which will be denoted by $L_{II}^{(2)}$:

$$L_{II}^M = L_{II}^{(2)} = \frac{C\alpha_B}{(\alpha_B - \alpha_C)(1 - x_B)} \tag{22}$$

provided that $x_B \neq 1$, and the constraint takes the form:

$$L_{II} \geq \frac{C\alpha_B}{(\alpha_B - \alpha_C)(1 - x_B)} \tag{23}$$

Finally the unknown x_B must be expressed as a function of decision variables. We obtain (see Appendix A):

$$x_B = \frac{B\alpha_C}{(V_{III} - B)(\alpha_B - \alpha_C)} \tag{24}$$

for

$$V_{III} > \frac{B\alpha_B}{\alpha_B - \alpha_C} \tag{25}$$

Solution of the optimization task

Analyzing Eq. 18 one can notice that $L_{II}^{(1)}$ is a rising function of V_{III}, whereas from Eqs. 22 and 24 we get that $L_{II}^{(2)}$ is a descending function of V_{III}:

$$V_{III} \nearrow \Longrightarrow L_{II}^{(1)} \nearrow$$

$$V_{III} \nearrow \Longrightarrow x_B \searrow \Longrightarrow L_{II}^{(2)} \searrow$$

The objective function given by Eq. 13a reaches its minimum when decision variable L_{II} is minimal and simultaneously satisfies the constraints $L_{II} \geq L_{II}^{(1)}$ and $L_{II} \geq L_{II}^{(2)}$. Because of the shape of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$, this takes place only in the case when $L_{II}^{(1)} = L_{II}^{(2)}$, and the value of decision variable V_{III} is expressed by the formula (see Appendix B):

$$V_{III}^{opt} = \frac{1}{2}\left[-\frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} + \sqrt{\left(\frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C}\right)^2 - 4\frac{A\alpha_A}{\alpha_A - \phi_1}\frac{C\alpha_C}{\alpha_B - \alpha_C}}\right] \tag{26}$$

As is proved in Appendix C, this value satisfies the inequality in Eq. 25. Finally from Eqs. 18, 26, and 13a one can calculate the optimum value of decision variable L_{II} and the minimum value of the objective function:

$$L_{II}^{opt} = \frac{A\alpha_A}{\alpha_A - \phi_1} + V_{III}^{opt} + C \tag{27}$$

$$V_{II}^{opt} = L_{II}^{opt} - C = \frac{1}{2}\left[\frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} + \sqrt{\left(\frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C}\right)^2 - 4\frac{A\alpha_A}{\alpha_A - \phi_1}\frac{C\alpha_C}{\alpha_B - \alpha_C}}\right] \tag{28}$$

Optimization of TCS-S

The optimization procedure for the TCS-S is analogous to that for the TCS-R; therefore it will be presented more briefly. The system is shown in Figure 4.

The linearly independent system of stream balance equations contains six equations with eight unknowns. Flow rates L_I and V_{III} have been selected as decision variables. The rest of variables can be expressed as follows:

$$V_I = L_I + A \tag{29a}$$

$$V_{II} = L_I - V_{III} + A \tag{29b}$$

$$L_{II} = L_I - V_{III} + A + C \tag{29c}$$

$$\bar{L}_I = L_I - V_{III} - B \tag{29d}$$

$$L_{III} = V_{III} + B \tag{29e}$$

$$\bar{V}_I = L_I - V_{III} + A \tag{29f}$$

The objective function for the TCS-R is equal to the sum of vapor flow rates V_{II} and V_{III}, and one can notice—Eqs. 29a, b—that it is equal to V_I. The optimization problem is formulated as follows:

Minimize $V_I = V_{II} + V_{III}$ subject to

$$V_I \geq V_I^M$$
$$\bar{V}_I \geq \bar{V}_I^M \tag{30}$$

and to the constraints in Eqs. 29a–29f.

Let us express this problem in terms of decision variables.

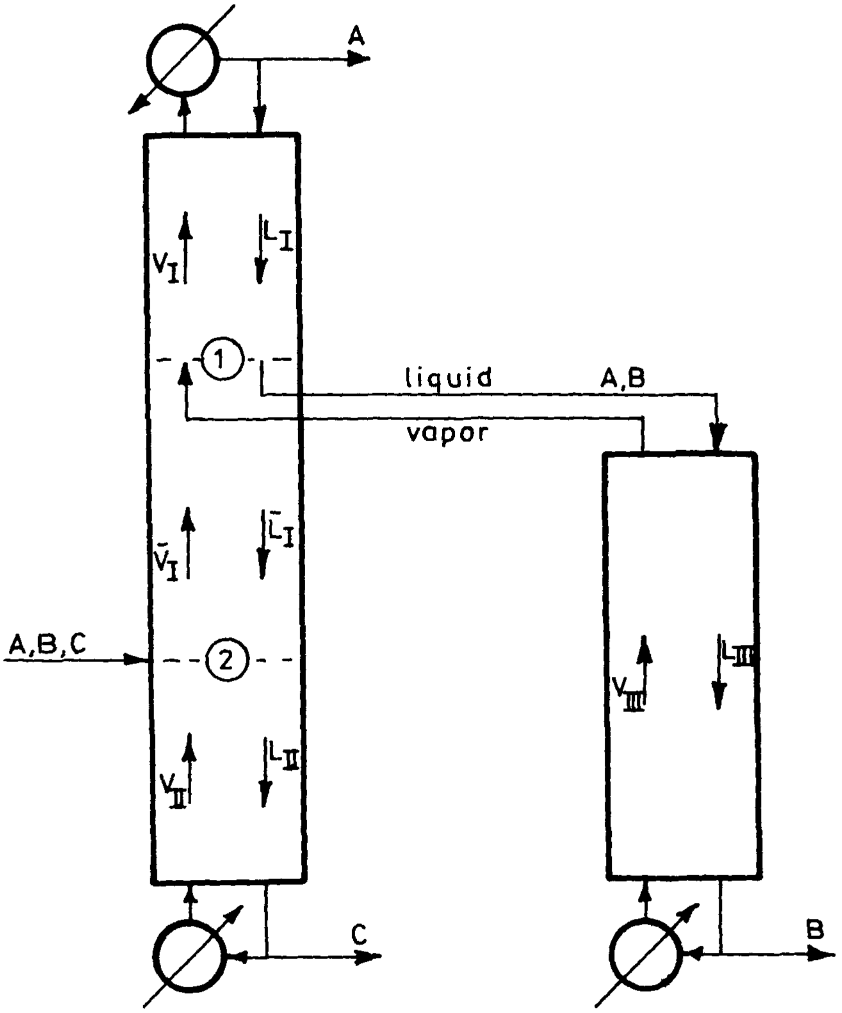

Figure 4. Thermally coupled system with stripping column (TCS-S).

Constraint $V_I \geq V_I^M$

The minimum reflux conditions in section 1 are determined by the following balance and equilibrium equations:

$$V_I^M y_A - L_I^M x_A = A \tag{31}$$

$$V_I^M = L_I^M + A \tag{32}$$

$$V_{III} y_A - L_{III} x_A = 0 \tag{33}$$

$$y_A = \frac{\alpha_A x_A}{\alpha_A x_A + \alpha_B(1 - x_A)} \tag{34}$$

where x_A and y_A denote the mole fraction of component A in the liquid and vapor stream, respectively, at level 1.

The considered constraint can be replaced by

$$L_I \geq L_I^M \tag{35}$$

where

$$L_I^M = L_I^{(1)} = \frac{A\alpha_B}{(\alpha_A - \alpha_B)x_A} \tag{36}$$

and

$$x_A = \frac{1}{\alpha_A - \alpha_B}\left(\frac{\alpha_A}{1 + \dfrac{B}{V_{III}}} - \alpha_B\right) \tag{37}$$

for $x_A \neq 0$ and $x_A \neq 1$.

The constraint, after substituting for the variable $\bar{V}_I$ the expression in Eq. 29f, takes the form:

$$L_I \geq \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} + V_{III} - A \tag{41}$$

Let us denote the righthand side of this inequality by $L_I^{(2)}$:

$$L_I^{(2)} = \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} + V_{III} - A \tag{42}$$

Solution of the optimization task

On the basis of Eqs. 36 and 37 one can deduce that $L_I^{(1)}$ is the descending function of decision variable V_{III}:

$$V_{III} \nearrow \Rightarrow x_A \nearrow \Rightarrow L_I^{(1)} \searrow$$

where $L_I^{(2)}$ is the rising function of V_{III} (Eq. 42):

$$V_{III} \nearrow \Rightarrow L_I^{(2)} \nearrow$$

The objective function depends linearly on decision variable L_I—Eq. 29a—and reaches its minimum for the least value of L_I satisfying the two constraints $L_I \geq L_I^{(1)}$ and $L_I \geq L_I^{(2)}$. Because of the shape of function $L_I^{(1)}$ and $L_I^{(2)}$, this takes place only for $L_I^{(1)} = L_I^{(2)}$. The optimum value of decision variable V_{III} can be calculated from Eqs. 36, 37, and 42 in an analogous way to the procedure for the TCS-R.

$$V_{III}^{opt} = \frac{1}{2}\left[-\left(\frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2}\right) + \frac{A\alpha_A + B\alpha_B}{\alpha_A - \alpha_B} + \sqrt{\left(\frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{A\alpha_A + B\alpha_B}{\alpha_A - \alpha_B}\right)^2 - 4\left(\frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2}\right)\frac{A\alpha_A}{\alpha_A - \alpha_B}}\right] \tag{43}$$

Let us notice that because of the condition $x_A > 0$, the following inequality must be satisfied:

$$V_{III} > \frac{B\alpha_B}{\alpha_A - \alpha_B} \tag{38}$$

Constraint $\bar{V}_I \geq \bar{V}_I^M$

The minimum vapor flow rate $\bar{V}_I^M$ is calculated from Underwood's equation:

$$\bar{V}_I^M = \max_i \left(\frac{A\alpha_A}{\alpha_A - \phi_i} + \frac{B\alpha_B}{\alpha_B - \phi_i}\right), \quad i = 1, 2. \tag{39}$$

where $\phi_i (i = 1, 2)$ are roots of Eq. 5, satisfying relations in Eq. 6, so it is easy to prove that (Fidkowski and Królikowski, 1985):

$$\bar{V}_I^M = \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} \tag{40}$$

In a similar way, as shown in Appendix B, it can be proved that V_{III}^{opt} satisfies the inequality in Eq. 25.

Finally, from Eqs. 42 and 29a we obtain the optimum value of decision variable L_I and the minimum value of the objective function:

$$L_I^{opt} = \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} + V_{III}^{opt} - A \tag{44}$$

$$V_I^{opt} = L_I^{opt} + A \tag{45}$$

Comparison of Thermally Coupled Systems

Let us define the following relations:

1. System 1 < System 2 if optimum values of objective functions for these systems satisfy the relation: V^{opt} (system 1) < V^{opt} (system 2), for all positive values of relative volatilities α_A, α_B, α_C and flow rates of components A, B, C.
2. System 1 = System 2 if optimum values of objective func-

tions for these systems are equal, for all positive values of relative volatilities and flow rates of components.

Some necessary formulas

Before the comparison, some formulas necessary for further considerations will be presented.

Underwood's equation, Eq. 5, can be transformed into a quadratic equation:

$$a\phi^2 + b\phi + c = 0 \tag{46}$$

The roots of this equation are given by:

$$\phi_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}, \quad \phi_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a} \tag{47}$$

where

$$\begin{aligned} a &= A\alpha_A + B\alpha_B + C\alpha_C \\ b &= -[A\alpha_A(\alpha_B + \alpha_C) + B\alpha_B(\alpha_A \\ &\quad + \alpha_C) + C\alpha_C(\alpha_A + \alpha_B)] \\ c &= (A + B + C)\alpha_A\alpha_B\alpha_C \end{aligned} \tag{48}$$

Using Eqs. 47 and 48 together with Vieta's formulas one can prove the following equalities:

$$(\alpha_A - \phi_1)(\alpha_A - \phi_2) = \frac{A\alpha_A(\alpha_A - \alpha_B)(\alpha_A - \alpha_C)}{A\alpha_A + B\alpha_B + C\alpha_C} \tag{49}$$

$$(\alpha_B - \phi_1)(\alpha_B - \phi_2) = -\frac{B\alpha_B(\alpha_B - \alpha_C)(\alpha_A - \alpha_B)}{A\alpha_A + B\alpha_B + C\alpha_C} \tag{50}$$

$$(\alpha_C - \phi_1)(\alpha_C - \phi_2) = \frac{C\alpha_C(\alpha_A - \alpha_C)(\alpha_B - \alpha_C)}{A\alpha_A + B\alpha_B + C\alpha_C} \tag{51}$$

$$\frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{A\alpha_A}{\alpha_A - \phi_2} = \frac{A\alpha_A + C\alpha_C}{\alpha_A - \alpha_C} + \frac{A\alpha_A + B\alpha_B}{\alpha_A - \alpha_B} \tag{52}$$

$$\frac{B\alpha_B}{\alpha_B - \phi_1} + \frac{B\alpha_B}{\alpha_B - \phi_2} = \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} - \frac{A\alpha_A + B\alpha_B}{\alpha_A - \alpha_B} \tag{53}$$

$$\frac{C\alpha_C}{\alpha_C - \phi_1} + \frac{C\alpha_C}{\alpha_C - \phi_2} = -\frac{A\alpha_A + C\alpha_C}{\alpha_A - \alpha_C} - \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} \tag{54}$$

Equivalence of TCS-R and TCS-S

We will show now that TCS-R = TCS-S. Multiplying Eq. 5 by the factor $1 + (\alpha_C - \phi_1)/(\alpha_B - \alpha_C)$, after simple rearrangements we have:

$$\frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} = -\frac{A\alpha_A}{\alpha_A - \phi_1}\frac{\alpha_C - \phi_1}{\alpha_B - \alpha_C} - \frac{C\alpha_C}{\alpha_C - \phi_1} \tag{55}$$

This expression is now introduced to Eq. 28, and after performing all the operations under the square root symbol we get the following equation:

$$V^{opt}(\text{TCS-R}) = \frac{1}{2}\left[-\frac{A\alpha_A}{\alpha_A - \phi_1}\frac{\alpha_C - \phi_1}{\alpha_B - \alpha_C} - \frac{C\alpha_C}{\alpha_C - \phi_1} + \sqrt{\left(-\frac{A\alpha_A}{\alpha_A - \phi_1}\frac{\alpha_C - \phi_1}{\alpha_B - \alpha_C} + \frac{C\alpha_C}{\alpha_C - \phi_1}\right)^2}\right] \tag{56}$$

The expression in brackets under the square root symbol is positive on the basis of Eq. 6, so the following formula is obtained:

$$V^{opt}(\text{TCS-R}) = -\frac{A\alpha_A}{\alpha_A - \phi_1} \cdot \frac{\alpha_C - \phi_1}{\alpha_B - \alpha_C} \tag{57}$$

Finally, using Eq. 51 it is transformed into the form:

$$V^{opt}(\text{TCS-R}) = \frac{A\alpha_A}{\alpha_A - \phi_1}\left(\frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2}\right)\frac{\alpha_A - \alpha_C}{A\alpha_A + B\alpha_B + C\alpha_C} \tag{58}$$

The second part of considerations referring to the TCS-S is analogous. Multiplying Underwood's equation, Eq. 5, by the factor $1 + (\alpha_A - \phi_2)/(\alpha_A - \alpha_B)$, one can obtain:

$$\frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{A\alpha_A + B\alpha_B}{\alpha_A - \alpha_B} = -\frac{C\alpha_C}{\alpha_C - \phi_2}\frac{\alpha_A - \phi_2}{\alpha_A - \alpha_B} \tag{59}$$

Introducing this expression into Eqs. 43–45, a new formula for the objective function of the TCS-S at the optimal point is obtained:

$$V^{opt}(\text{TCS-S}) = \left(\frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2}\right)\frac{\alpha_A - \phi_2}{\alpha_A - \alpha_B} \tag{60}$$

Finally after computing $(\alpha_A - \phi_2)/(\alpha_A - \alpha_B)$ from Eq. 49 and introducing that into the last equation we have:

$$V^{opt}(\text{TCS-S}) = \frac{A\alpha_A}{\alpha_A - \phi_1} \cdot \left(\frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2}\right)\frac{\alpha_A - \alpha_C}{A\alpha_A + B\alpha_B + C\alpha_C} \tag{61}$$

so

$$V^{opt}(\text{TCS-R}) = V^{opt}(\text{TCS-S}) \tag{62}$$

for all positive values of A, B, C and α_A, α_B, α_C. Thus

$$\text{TCS-R} = \text{TCS-S} \tag{63}$$

Let us notice that it is possible to find other forms of expression in Eq. 61.

From Eqs. 55, 59, and 61:

$$V^{opt}(\text{TCS-R}) = V^{opt}(\text{TCS-S}) = \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} - \frac{B\alpha_B}{\alpha_B - \phi_1} \tag{64}$$

From Eqs. 5 and 64:

$$V^{opt}(\text{TCS-R}) = V^{opt}(\text{TCS-S}) = \frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{C\alpha_C}{\alpha_C - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} \tag{65}$$

From Eqs. 53 and 64:

$$V^{opt}(\text{TCS-R}) = V^{opt}(\text{TCS-S}) = \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{A\alpha_A + B\alpha_B}{\alpha_A - \alpha_B} \tag{66}$$

The conclusion is that these both systems are equivalent. This conclusion is apparently inconsistent with results obtained by Tedder and Rudd (1978), who showed that there are some regions of optimality of TCS-R and TCS-S separately, depending on values of relative volatilities and concentration of components in the feed.

It is of course true that one of these systems might really be "better" than the other. The results of the present work show that it is only caused by differences in investment costs of these systems, differences in numbers of plates required for the given separation of components. Objective functions—minimum vapor flows and minimum energies of separation—are in both cases the same. Energies of separation in both systems may differ only in the case when heats of vaporization of components B and C are significantly different. But in this case the assumption about equimolar flow rates in columns is not satisfied.

Comparison of TCS and TCS-I with TCS-R and TCS-S

The optimum value of the goal function for the TCS is given by Eq. 4.

$$\text{If} \quad \frac{A\alpha_A}{\alpha_A - \phi_1} \geq \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} \tag{67}$$

$$\text{then} \quad V^{opt}(\text{TCS}) = \frac{A\alpha_A}{\alpha_A - \phi_1} \tag{68}$$

and, on the basis of relations in Eq. 6, the following estimation can be made:

$$\begin{aligned} V^{opt}(\text{TCS-R}) &= \frac{A\alpha_A}{\alpha_B - \phi_1} + \frac{C\alpha_C}{\alpha_C - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} \\ &> \frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B}{\alpha_B - \alpha_C} > \frac{A\alpha_A}{\alpha_A - \phi_1} = V^{opt}(\text{TCS}) \end{aligned} \tag{69}$$

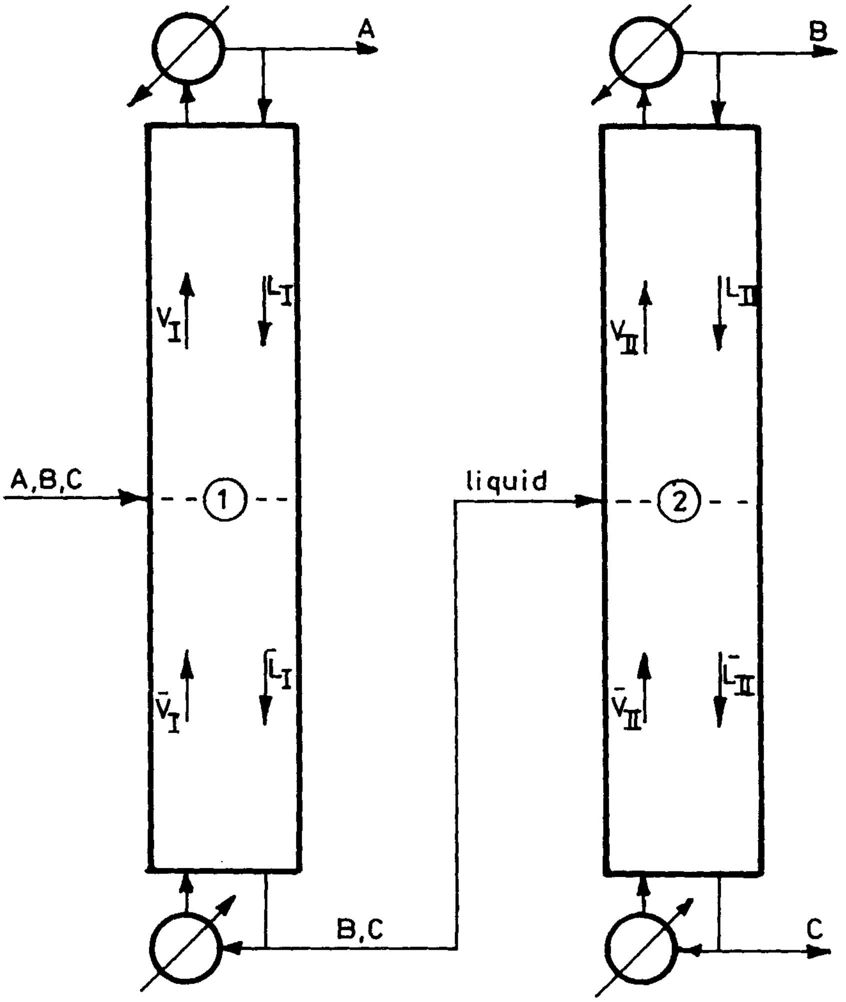

Figure 5. Direct sequence (DS_L).

In the opposite case,

$$\text{when} \quad \frac{A\alpha_A}{\alpha_A - \phi_1} < \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} \tag{70}$$

$$\text{then} \quad V^{opt}(\text{TCS}) = \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} \tag{71}$$

and in a similar way

$$V^{opt}(\text{TCS-R}) = \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{A\alpha_A + B\alpha_B}{\alpha_A - \alpha_B} > \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{A\alpha_A}{\alpha_A - \alpha_B} > \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{A\alpha_A}{\alpha_A - \phi_2} = V^{opt}(\text{TCS}) \tag{72}$$

Remembering equivalences that were proved, thermally coupled systems are ordered as follows:

$$\text{TCS} = \text{TCS-I} < \text{TCS-R} = \text{TCS-S} \tag{73}$$

Comparison of thermally coupled systems with direct and indirect sequence

Direct sequence (DS) and indirect sequence (IS) of distillation columns are the basic schemes for separation of a ternary solution, as shown in Figures 5 and 6, respectively. The DS consists of two columns connected by the stream of bottom product from the first column, whereas in the IS columns are connected by the top product. These systems can easily be decomposed into single columns, because there are no recycling streams. When columns operate at minimum reflux conditions there are no decision variables apart from the thermodynamical state of the stream connecting both columns (Fidkowski and Królikowski, 1985). Columns in the optimum DS are connected by a boiling liquid stream, whereas the stream connecting columns in the optimum IS is in a state of saturated vapor. In the optimum sequence the objective function, defined as the sum of minimum vapor flow rates in both columns, reaches its minimum value, due to the optimization task:

Minimize $V = V_I + V_{II}$ where

$$V_I \geq V_I^M$$
$$V_{II} \geq V_{II}^M \tag{74}$$

After computing minimum vapor flow rates in both columns of DS_L and IS^V, where L, V respectively denote the liquid and

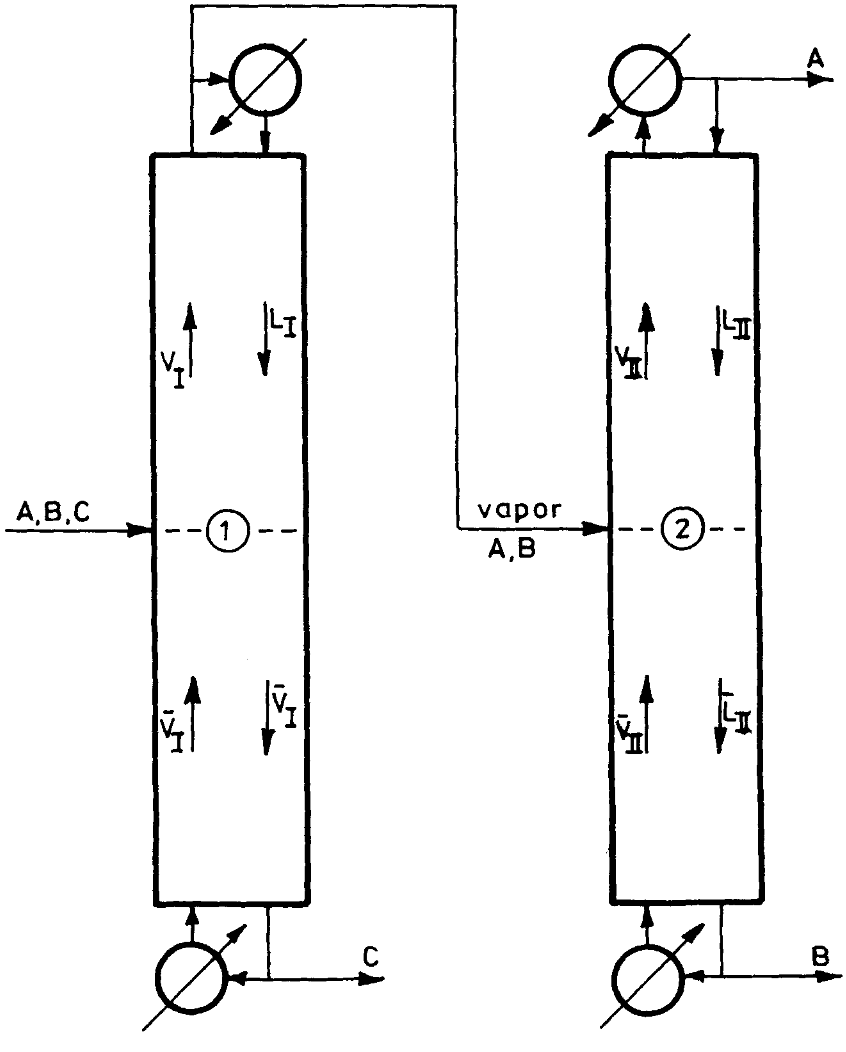

Figure 6. Indirect sequence (IS^V).

vapor states of the connecting stream, using Underwood's method we obtain the formulae:

$$V^{opt}(\mathrm{DS})_L = \frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} \tag{75}$$

$$V^{opt}(\mathrm{IS})^V = \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{(A+B)\alpha_B}{\alpha_A - \alpha_B} \tag{76}$$

These formulas together with Eqs. 6, 65, and 66 enable the following comparison of TCS-R with DS_L and IS^V:

$$\begin{aligned} V^{opt}(\text{TCS-R}) &= \frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{C\alpha_C}{\alpha_C - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} \\ &< \frac{A\alpha_A}{\alpha_A - \phi_1} + \frac{B\alpha_B + C\alpha_C}{\alpha_B - \alpha_C} = V^{opt}(\mathrm{DS}_L) \end{aligned}$$

$$\begin{aligned} V^{opt}(\text{TCS-R}) &= A + \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{(A+B)\alpha_B}{\alpha_A - \alpha_B} \\ &< \frac{A\alpha_A}{\alpha_A - \phi_2} + \frac{B\alpha_B}{\alpha_B - \phi_2} + \frac{(A+B)\alpha_B}{\alpha_A - \alpha_B} = V^{opt}(\mathrm{IS}^V) \end{aligned}$$

Finally we obtain the relations:

$$\text{TCS-R} < \mathrm{DS}_L \tag{79}$$

$$\text{TCS-R} < \mathrm{IS}^V \tag{80}$$

Summary

Minimum energy requirements of the four thermally coupled systems, TCS, TCS-I, TCS-R, TCS-S, and also of DS_L and IS^V, separating a ternary ideal solution, were calculated and compared. The result was the following sequence of systems:

$$\text{TCS} = \text{TCS-I} < \text{TCS-R} = \text{TCS-S} < \begin{cases} \mathrm{DS}_L \\ \mathrm{IS}^V \end{cases} \tag{81}$$

Energy costs are usually the dominant factor in the total annual costs of a distillation plant and may be used as a substitute objective function. Investment costs may play a more considerable role in the case of difficult separable solutions. For these cases an additional assessment of the real costs of systems should be made. Results of this work may also be used for this purpose in the calculation of energy costs.

Notation

A, B, C = flow rate of component A, B, C in the feed, kmol/s
F = feed flow rate, kmol/s
L = liquid flow rate, kmol/s
V = vapor flow rate, kmol/s
x = mole fraction in liquid phase
y = mole fraction in vapor phase
α = relative volatility
β = defined by Eq. 2
ϕ_1, ϕ_2 = roots of Underwood's equation, Eq. 5

Subscripts

A, B, C = component A, B, C
P, R = point P, R
I, II, III = section of a given system, Figures 1-6

Superscripts

M = minimum reflux conditions
opt = optimum
$-$ = section of column below feed

Appendix A

The aim of this appendix is to show how to express variable x_B (concentration of component B in section 2 of TCS-R) as the function of decision variables. In order to do that we introduce expressions given by Eqs. 21 and 13b instead of variables y_B and L_{III} to the following balance equation:

$$V_{III}y_B - L_{III}x_B = B \tag{A1}$$

After rearrangements we have the quadratic equation

$$ax_B^2 + bx_B + c = 0 \tag{A2}$$

where

$$\begin{aligned} a &= (V_{III} - B)(\alpha_B - \alpha_C) \\ b &= [(V_{III} - B)(\alpha_B - \alpha_C) - B\alpha_C] \\ c &= B\alpha_C \end{aligned} \tag{A3}$$

The discriminant of this equation is:

$$\Delta = [(V_{III} - B)(\alpha_B - \alpha_C) - B\alpha_C]^2 \tag{A4}$$

so $\Delta \geq 0$.

Two possibilities must be analyzed:

1. If $\Delta = 0$ then

$$V_{III} = B\frac{\alpha_B}{\alpha_B - \alpha_C} \tag{A5}$$

and $x_B = 1$.

2. If $\Delta > 0$ then

$$V_{III} > B\frac{\alpha_B}{\alpha_B - \alpha_C} \tag{A6}$$

and the only root of Eq. A2 satisfying inequality $0 < x_B < 1$ is

$$x_B = \frac{-b - \sqrt{\Delta}}{2a} \tag{A7}$$

which after rearrangements gives Eq. 24.

Solution 1 must be rejected as unfeasible.

Appendix B

Let us compare Eqs. 18 and 22, taking into account Eq. 24. The following quadratic equation is obtained:

$$aV_{III}^2 + bV_{III} + c = 0 \tag{B1}$$

where

$$a = \alpha_B - \alpha_C$$

$$b = \frac{A\alpha_A}{\alpha_A - \phi_1}(\alpha_B - \alpha_C) - B\alpha_B - C\alpha_C$$

$$c = -\frac{A\alpha_A}{\alpha_A - \phi_1}B\alpha_B \tag{B2}$$

It is easy to prove that the discriminant of Eq. B1 is positive:

$$\Delta = \left[\frac{A\alpha_A}{\alpha_A - \phi_1}(\alpha_B - \alpha_C) - B\alpha_B - C\alpha_C\right]^2 + 4\frac{A\alpha_A}{\alpha_A - \phi_1}(\alpha_B - \alpha_C)B\alpha_B > 0 \tag{B3}$$

and this equation has two roots:

$$V_{III,1} = \frac{-b + \sqrt{\Delta}}{2a} \tag{B4}$$

$$V_{III,2} = \frac{-b - \sqrt{\Delta}}{2a} \tag{B5}$$

Because $|b| < \sqrt{\Delta}$ then $V_{III,1} > 0$ and $V_{III,2} < 0$, so the result $V_{III,2}$ is physically infeasible. Replacing a, b, and Δ in Eq. B4 by expressions from Eqs. B2 and B3, we obtain Eq. 26.

Appendix C

We will now prove that if $L_{II}^{(1)} = L_{II}^{(2)}$, then V_{III}^{opt} given by Eq. 26 satisfies the inequality in Eq. 25.

Proof. Let us suppose that V_{III} does not satisfy the relation in Eq. 25:

$$V_{III} \leq \frac{B\alpha_B}{\alpha_B - \alpha_C} \tag{94}$$

Let us replace V_{III} by the expression given in Eq. 26, multiplying the inequality obtained by $2(\alpha_B - \alpha_C)$, and adding to both sides the following expression:

$$\frac{A\alpha_A}{\alpha_A - \phi_1}(\alpha_B - \alpha_C) - B\alpha_B - C\alpha_C$$

Because the smaller side of the inequality is positive, the inequality will still be satisfied when both sides are raised by squaring. After reduction and rearrangements one can obtain:

$$(B\alpha_B + C\alpha_C)^2 \leq (B\alpha_B - C\alpha_C)^2 \tag{95}$$

which leads to inconsistency, and the relation in Eq. 25 is satisfied.

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