Thermally Coupled System of Distillation Columns: Optimization Procedure

An analytical solution of thermally coupled system (TCS) optimization was found. Energy requirements of the TCS were minimized provided that the ternary solution being separated is ideal. The TCS is energetically profitable in comparison with other sequences of distillation columns. The solution method can be used for the synthesis of separation systems and for screening calculations, due to the great simplicity of the result.

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SCOPE

Synthesis of separation sequences is a problem repeatedly discussed in chemical engineering literature. Various synthesis techniques, algorithms, and procedures have been developed, including those by Hendry et al. (1973), Hlavacek (1978), and Nishida et al. (1981).

Before designing a synthesis, one must have algorithms with which to calculate optimal objective function values for typical subsystems of separation sequences. One of these subsystems is the thermally coupled system (TCS) of distillation columns. In the present paper, the optimization task is formulated as a nonlinear mathematical programming problem. After analysis and rearrangement of the equation system, optimum values of decision variables and the optimum value of the objective function were found in the form of analytical expressions.

CONCLUSIONS AND SIGNIFICANCE

Analytical expressions obtained as the result of the optimization task are convenient tools for quick calculation of the minimum energy requirements and optimum values of decision variables for the TCS. These may serve for quick comparison of different structures of distillation columns in the system synthesis problem. It is interesting that the optimum values of decision variables are contained in a closed section, so there is usually an infinite number of solutions.

One must remember that a minimum vapor flow rate is only a substitutional goal function of value proportional to energy costs. Sometimes, especially in the case of difficult separations, investment costs may play a considerable role. In these cases, additional assessment of investment costs might be necessary. As shown in Table 1, the TCS requires the least energy of the four systems presented in Figures 1 and 10.

Practical application of this system might be profitable, although designers might encounter here some difficulties dealt with in process automatization and control.

Introduction

The thermally coupled system of distillation columns (TCS) serves for separation of one feed stream into three product streams. It consists of two apparatuses connected by liquid and vapor streams and contains only one reboiler and one condenser, as shown in Figure 1. In the first column, the prefractionator or section I, a ternary solution ABC is split into two product streams. The top product contains only components A and B, the bottom product contains components B and C. Binary solution AB is then separated in section II, and solution BC is separated in section III.

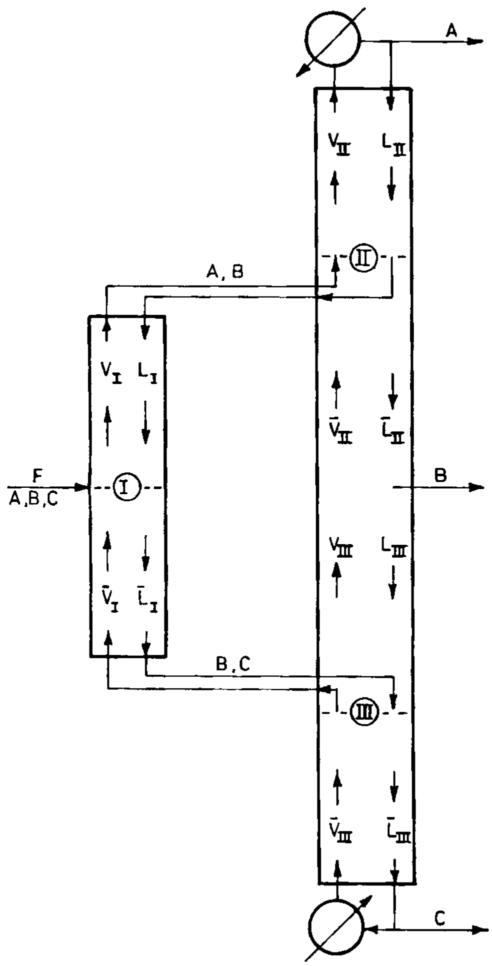

Figure 1. Thermally coupled system of distillation columns.

Thermodynamic irreversibilities and some economic aspects of the distillation process carried out in a TCS were discussed by Petlyuk et al. (1965) and Spadoni and Stramigioli (1983). Tedder and Rudd (1978) analyzed total annual costs of separation and also several substitutional objective functions for eight distinct systems for separating ternary solutions (but without the TCS considered here). Minimum energy requirements of several distillation sequences were calculated and analyzed by Kaczmarek et al. (1983), and Fidkowski (1983). The aim of the present work is to present an optimization procedure for the TCS and to compare the TCS with some other distillation sequences.

It is assumed that a ternary, ideal solution (constant values of relative volatilities and equimolar internal flow rates in columns) is separated into "almost pure" components. Although this is a great simplification, only in this case is it possible to obtain analytical results of the optimization task. Separation of nonideal solutions must be calculated using numerical procedures, and the result of a single case usually provides no wider view of the problem.

In order to avoid difficulties connected with different prices of materials and energy (depending on geographical location, inflation, etc.) a substitutional goal function was introduced. It was defined as the minimum vapor flow rate from the system's reboiler required for the demanded separation. Values of substitutional goal function are proportional to energy requirements of separation, which is usually the dominant factor in the total cost of a distillation plant.

Formulation of the Optimization Task

A steady state process of separating a ternary solution ABC into almost pure components in the TCS is considered. Constant values of component-relative volatilities are assumed. Components are ranked in decreasing order of relative volatilities: $\alpha_A > \alpha_B > \alpha_C$. Internal flow rates of phases in columns are equimolar. Feed is introduced and products are obtained in the boiling liquid state. Flow rate and composition of feed are known:

$$F = A + B + C \tag{1}$$

It is convenient to introduce the notation β, defined as the fraction of component B in the top product of the first column:

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

Linear balance equations of the inner liquid and vapor streams for particular sections of the TCS are:

$$-\bar{V}_{III} + \bar{L}_{III} = C \tag{3a}$$

$$\bar{V}_{III} - V_{III} - \bar{V}_I = 0 \tag{3b}$$

$$-\bar{L}_{III} + L_{III} + \bar{L}_I = 0 \tag{3c}$$

$$-V_{III} + \bar{V}_{II} = 0 \tag{3d}$$

$$-L_{III} + \bar{L}_{II} = B \tag{3e}$$

$$\bar{V}_{II} - V_{II} + V_I = 0 \tag{3f}$$

$$-\bar{L}_{II} + L_{II} - L_I = 0 \tag{3g}$$

$$V_{II} - L_{II} = A \tag{3h}$$

$$-\bar{V}_I + \bar{L}_I + \beta B = B + C \tag{3i}$$

$$-\bar{L}_I + L_I = -F \tag{3j}$$

$$-\bar{V}_I + V_I = 0 \tag{3k}$$

$$V_I - L_I - \beta B = A \tag{3l}$$

This system contains ten linearly independent equations:

$$V_I = L_I + A + \beta B \tag{4a}$$

$$\bar{L}_I = L_I + F \tag{4b}$$

$$\bar{V}_I = L_I + A + \beta B \tag{4c}$$

$$V_{II} = L_{II} + A \tag{4d}$$

$$\bar{L}_{II} = L_{II} - L_I \tag{4e}$$

$$\bar{V}_{II} = L_{II} - L_I - \beta B \tag{4f}$$

$$L_{III} = L_{II} - L_I - B \tag{4g}$$

$$V_{III} = L_{II} - L_I - \beta B \tag{4h}$$

$$\bar{L}_{III} = L_{II} + A + C \tag{4i}$$

$$\bar{V}_{III} = L_{II} + A \tag{4j}$$

As there are 13 variables, three of them have to be selected as decision variables; thus there are three degrees of freedom in the system. Values of these variables have to be proposed by a designer in order to minimize or maximize a given objective function. As a matter of fact, the selection of decision variables is to some extent optional. Here reflux flow rates in both columns L_I and L_{II} and the variable β have been selected as decision variables.

The substitutional goal function was defined as the minimum vapor flow rate from the system's reboiler. It is proportional to the minimum energy required for the given separation, provided the previous assumptions are satisfied. The approach is confirmed by the fact that energy costs usually far exceed the investment costs of a distillation column (Nishida, 1981; Doukas and Luyben, 1978).

Minimum reflux conditions might appear in section I, II, or III of the TCS. In the case of a single multifeed column, minimum reflux ratios are calculated for all sections and the biggest value of minimum vapor flow is selected (Yaws et al., 1981). Any smaller value of vapor flow will not ensure the required separation of components. The assumption that minimum reflux conditions occur in all of the sections of the TCS simultaneously might probably lead to inconsistency. Therefore the optimization task might be written as follows:

Minimize $\bar{V}_{III}$

subject to the inequality constraints:

C1: $V_I \geq V_I^M$

C2: $V_{II} \geq V_{II}^M$

C3: $V_{III} \geq V_{III}^M$

and to the equality constraints, Eqs. 4a–j (5)

where the objective function and constraints depend only on the previously selected decision variables L_I, L_{II}, and β.

Analysis of the Optimization Task

Let us express the objective function and the constraints as functions of decision variables.

Objective function

From Eq. 4j it results at once that the objective function depends only on one of the decision variables, L_{II}.

Constraint C1

Minimum vapor flow in the first column was calculated using Underwood's classic method (Underwood, 1948; Nandakumar and Andres, 1981). At the first step one has to find the roots ϕ of the equation:

$$\frac{\alpha_A A}{\alpha_A - \phi} + \frac{\alpha_B B}{\alpha_B - \phi} + \frac{\alpha_C C}{\alpha_C - \phi} = 0 \tag{6}$$

which after transformation has the form of the quadratic equation:

$$a\,\phi^2 + b\phi + c = 0 \tag{7}$$

where

$$\begin{aligned} a &= A\alpha_A + B\alpha_B + C\alpha_C \\ b &= -\,[A\alpha_A(\alpha_B + \alpha_C) + B\alpha_B(\alpha_A + \alpha_C) \\ &\quad + C\alpha_C(\alpha_A + \alpha_B)] \\ c &= (A + B + C)\,\alpha_A\alpha_B\alpha_C \end{aligned} \tag{8}$$

Equation 7 is satisfied by the two roots:

$$\phi_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}, \quad \phi_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a} \tag{9}$$

values of which can be ranked in the following order:

$$\alpha_C < \phi_2 < \alpha_B < \phi_1 < \alpha_A \tag{10}$$

Minimum vapor flow rate is then calculated from the equation:

$$V_I^M = \max_j \left[\frac{\alpha_A A}{\alpha_A - \phi_j} + \frac{\alpha_B B}{\alpha_B - \phi_j}\beta\right] \tag{11}$$

Taking into account Eqs. 4a and 11, constraint C1 might be replaced by the inequalities:

$$L_I \geq \frac{B\phi_1}{\alpha_B - \phi_1}\beta + \frac{A\phi_1}{\alpha_A - \phi_1}$$

and

$$L_I \geq \frac{B\phi_2}{\alpha_B - \phi_2}\beta + \frac{A\phi_2}{\alpha_A - \phi_2} \tag{12}$$

Let us denote the straight lines staking out the area defined by these constraints, Eq. 12, by φ_j ($j = 1, 2$), Figure 2.

$$\varphi_j : L_I = \frac{B\phi_j}{\alpha_B - \phi_j}\beta + \frac{A\phi_j}{\alpha_A - \phi_j} \qquad j = 1, 2 \tag{13}$$

From the inequalities in Eq. 10, it results that the slope of the line φ_1 is negative and the slope of φ_2 is positive:

$$\frac{B\phi_1}{\alpha_B - \phi_1} < 0 \quad \text{and} \quad \frac{B\phi_2}{\alpha_B - \phi_2} > 0 \tag{14}$$

At the intersection point P of lines φ_1 and φ_2, the vapor flow rate

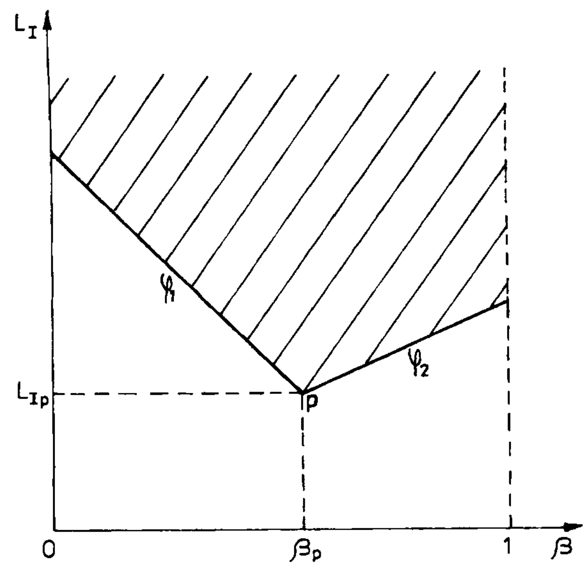

Figure 2. Area of feasible solutions.

in section I reaches its minimum value. The coordinates of P can be calculated from Eqs. 8, 9 and 13:

$$\beta_P = \frac{\alpha_B - \alpha_C}{\alpha_A - \alpha_C} \tag{15}$$

$$L_{Ip} = \frac{F\alpha_C}{\alpha_A - \alpha_C} \tag{16}$$

One can notice that the values of β_P and L_{Ip} do not depend on feed composition.

Constraint C1 can finally be rewritten in the following manner:

$$L_I \geq \begin{cases} \dfrac{B\phi_1}{\alpha_B - \phi_1}\beta + \dfrac{A\phi_1}{\alpha_A - \phi_1} & \text{for } 0 \leq \beta \leq \beta_P \\ \dfrac{B\phi_2}{\alpha_B - \phi_2}\beta + \dfrac{A\phi_2}{\alpha_A - \phi_2} & \text{for } \beta_P \leq \beta \leq 1 \end{cases} \tag{17}$$

Constraint C2

Taking into account Eq. 4d and the analogous balance equation written for minimum reflux conditions in section II:

$$V_{II}^M = L_{II}^M + A \tag{18}$$

constraint C2 can be written in a new form:

$$L_{II} \geq L_{II}^M \tag{19}$$

The reflux in section II is minimal when liquid and vapor in the feed level are in equilibrium. In this section binary solution AB is separated.

$$y_A^I = \frac{\alpha_A x_A^I}{\alpha_A x_A^I + \alpha_B(1 - x_A^I)} \tag{20}$$

The component A balance equation for the upper part of section II in minimum reflex conditions is as follows:

$$V_{II}^M y_A^I - L_{II}^M x_A^I = A \tag{21}$$

Eliminating variables V_{II}^M and y_A^I from Eqs. 18, 20, and 21, one can obtain the equation:

$$L_{II}^M(\alpha_A - \alpha_B)(1 - x_A^I)x_A^I = A\alpha_B(1 - x_A^I) \tag{22}$$

The factor $1 - x_A^I$ is usually positive and only in the boundary case does $x_A^I = 1$. Excluding this case from further consideration, one can calculate minimum reflux in section II as follows:

$$L_{II}^M = \frac{A\alpha_B}{(\alpha_A - \alpha_B)x_A^I} \tag{23}$$

At the end the unknown x_A^I must be expressed as a function of the decision variables. To do that component A must be balanced in section II:

$$V_I y_A^I - L_I x_A^I = A \tag{24}$$

Then it is possible to eliminate unknowns V_I and y_A^I from Eqs. 4a, 20, and 24, obtaining finally the following quadratic equation:

$$a(x_A^I)^2 + bx_A^I + c = 0 \tag{25}$$

where

$$a = L_I(\alpha_A - \alpha_B)$$
$$b = -[\beta B\alpha_A + L_I(\alpha_A - \alpha_B) + A\alpha_B]$$
$$c = A\alpha_B \tag{26}$$

This equation has two roots, but it can be proved (Fidkowski and Królikowski, 1983) that only one of them,

$$x_A^I = \frac{-b - \sqrt{b^2 - 4ac}}{2a} \tag{27}$$

satisfies the relation

$$0 < x_A^I < 1. \tag{28}$$

Finally the constraint C2 has the form:

$$L_{II} \geq \frac{A\alpha_B}{(\alpha_A - \alpha_B)x_A^I} \tag{29}$$

Constraint C3

Minimum reflux conditions for section III can be formulated in a way analogous to that used for section II.

$$\bar{y}_B^I = \frac{\alpha_B \bar{x}_B^I}{\alpha_B \bar{x}_B^I + \alpha_C(1 - \bar{x}_B^I)} \tag{30}$$

$$V_{III}^{M}\,\bar{y}_B^{I} - L_{III}^{M}\,\bar{x}_B^{I} = (1-\beta)\,B \quad (31)$$

$$V_{III}^{M} - L_{III}^{M} = (1-\beta)\,B \quad (32)$$

From the above set of equations one can calculate L_{III}^{M} in dependence on $\bar{x}_B^{I}$, excluding the boundary case when $\bar{x}_B^{I} = 0$.

$$L_{III}^{M} = \frac{(1-\beta)\,B\alpha_C}{(\alpha_B-\alpha_C)\,\bar{x}_B^{I}} \quad (33)$$

The mole fraction of component B in the stream $\bar{L}_I$ can be calculated from Eqs. 4b, 4c, and 30 with the following balance:

$$-\bar{V}_I\bar{y}_B^{I} + \bar{L}_I\bar{x}_B^{I} = (1-\beta)\,B \quad (34)$$

The result is the quadratic equation with unknown $\bar{x}_B^{I}$, the solution of which for values in the range (0, 1) is written (Fidkowski and Królikowski, 1983):

$$\bar{x}_B^{I} = \frac{-b+\sqrt{b^2-4ac}}{2a} \quad (35)$$

where

$$\begin{aligned} a &= (L_I+F)(\alpha_B-\alpha_C)\\ b &= (1-\beta)\,B\alpha_C + C\alpha_B - (L_I+F)(\alpha_B-\alpha_C)\\ c &= -(1-\beta)\,B\,\alpha_C \end{aligned} \quad (36)$$

Taking into account Eqs. 4h and 32, one can finally write constraint C3 in the following form:

$$L_{II} \geq \frac{(1-\beta)\,B\alpha_C}{(\alpha_B-\alpha_C)\,\bar{x}_B^{I}} + L_I + B \quad (37)$$

Simplification of the original task

Let us denote:

$$L_{II}^{(1)} = \frac{\alpha_B}{\alpha_A - \alpha_B\,x_A^{I}}\,A \quad (38)$$

$$L_{II}^{(2)} = \frac{\alpha_C}{\alpha_B-\alpha_C}\,\frac{(1-\beta)\,B}{\bar{x}_B^{I}} + L_I + B \quad (39)$$

where x_A^{I} and $\bar{x}_B^{I}$, Eqs. 27 and 35, depend only on two decision variables – L_I and β.

Analyzing Eq. 4j, the definition of the goal function, one can notice that instead of minimizing the value of $\bar{V}_{III}$, the least feasible value of variable L_{II} may be taken as the solution. The original optimization task, Eq. 5, may now be rewritten in the following way:

$$\text{Minimize } L_{II} = \begin{cases} L_{II}^{(1)} & \text{when } L_{II}^{(1)} > L_{II}^{(2)} \\ L_{II}^{(2)} & \text{in the opposite case} \end{cases} \quad (40)$$

subject to constraint C1, Eq. 17.

Let us notice that the problem can be analyzed in terms of two decision variables, L_I and β, due to the fact that L_{II} appears linearly in the objective function.

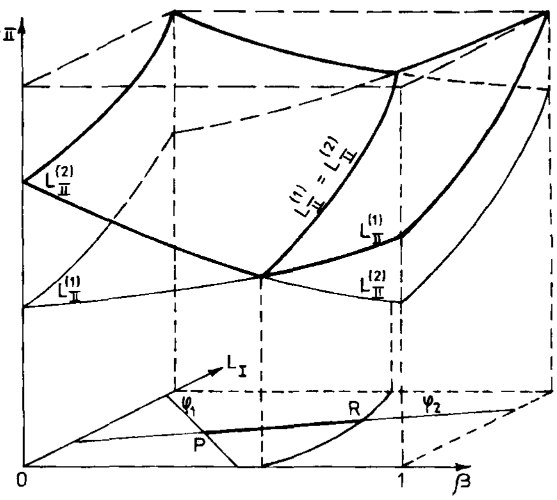

Figure 3. Diagram of the objective function L_{II}.

As shown in Appendix 1, the solution lies on the edge of the feasible area (Figure 2) that has a mean on line φ_1 or φ_2. Therefore the inequality constraint, Eq. 17, may be replaced by the equality constraint:

$$L_I = \begin{cases} \dfrac{B\phi_1}{\alpha_B-\phi_1}\beta + \dfrac{A\phi_1}{\alpha_A-\phi_1} & \text{for } 0 \leq \beta \leq \beta_P \\[2ex] \dfrac{B\phi_2}{\alpha_B-\phi_2}\beta + \dfrac{A\phi_2}{\alpha_A-\phi_2} & \text{for } \beta_P \leq \beta \leq 1 \end{cases} \quad (41)$$

A diagram of the objective function and constraints is presented in Figure 3.

The task can be interpreted in the following way: The value of β should be found for which minimum reflux in the second column reaches the lowest value; both columns operate at minimum reflux conditions. Minimum reflux in the second column is understood as the maximum value from minimum refluxes (L_{II}) calculated for sections II and III.

Solution of the Optimization Task

Let us imagine the shape of the goal function $L_{II} = L_{II}(\beta, L_I)$ given by Eq. 40. Remembering the shape of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$, Appendix 1, one can conclude that it looks like a ravine descending toward the axis β (Figure 3). The rectangular projection of the ravine bottom on the plane (β, L_I) intersects with the line φ_1 or φ_2 at point R. In order to solve the optimization task we need some more detailed information.

Level lines of the goal function

One can find, on the plane of decision variables (β, L_I), the lines on which the function $L_{II}^{(1)}$ is of constant value. These lines are also level lines of the goal function L_{II} in the area where $L_{II}^{(1)} > L_{II}^{(2)}$. Introducing into Eq. 38 expressions 26 and 27, after rearrangements one can obtain:

$$L_I = L_{II}^{(1)} - \frac{\beta B\alpha_A}{\alpha_A - \alpha_B - \dfrac{A\alpha_B}{L_{II}^{(1)}}} \quad (42)$$

For a constant value of $L_{II}^{(1)}$, Eq. 42 describes the level line of function $L_{II}^{(1)}$. It is a straight line on the plane (β, L_I). In the next step we can consider level lines of the function $L_{II}^{(2)}$, which are also level lines of the goal function in the area where $L_{II}^{(2)} \geq L_{II}^{(1)}$. From Eqs. 35, 36, and 39 we get:

$$L_I = L_{II}^{(2)} - B - \frac{(1-\beta)B\alpha_C}{\alpha_B - \alpha_C - \dfrac{C\alpha_B}{L_{II}^{(2)} + A + C}} \tag{43}$$

The level line of function $L_{II}^{(2)}$ is also a straight line on the plane of decision variables.

As shown in Appendix 2, lines φ_1 and φ_2 are level lines on which functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$, respectively, reach their minimum feasible values:

$$L_{II\varphi_1}^{(1)} = \frac{A\phi_1}{\alpha_A - \phi_1} \tag{44}$$

$$L_{II\varphi_2}^{(2)} = \frac{A\phi_2}{\alpha_A - \phi_2} + \frac{\alpha_B B}{\alpha_B - \phi_2} \tag{45}$$

Equality line of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$

Let us name the rectangular projection of the ravine bottom on the plane of decision variables by the equality line of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$, that is the line where $L_{II}^{(1)} = L_{II}^{(2)}$, Figure 4. Now we will find parametric equations of this line. Denoting $L_{II}^{(1)}$ and $L_{II}^{(2)}$ by the common symbol L_{II}, from Eqs. 42 and 43 we obtain the following formulae:

$$\beta = \frac{L_{II}(\alpha_A - \alpha_B) - A\alpha_B}{L_{II}\alpha_A - (L_{II} + A + C)\alpha_C} \tag{46}$$

$$L_I = L_{II}\left[1 - \frac{B\alpha_A}{L_{II}\alpha_A - (L_{II} + A + C)\alpha_C}\right] \tag{47}$$

where L_{II} plays the role of parameter.

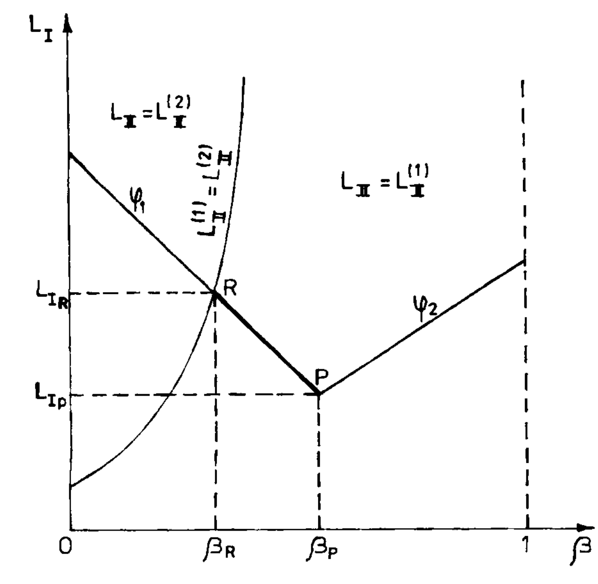

Figure 4. The set of optimal solutions when $L_{II\varphi_1}^{(1)} > L_{II\varphi_2}^{(2)}$.

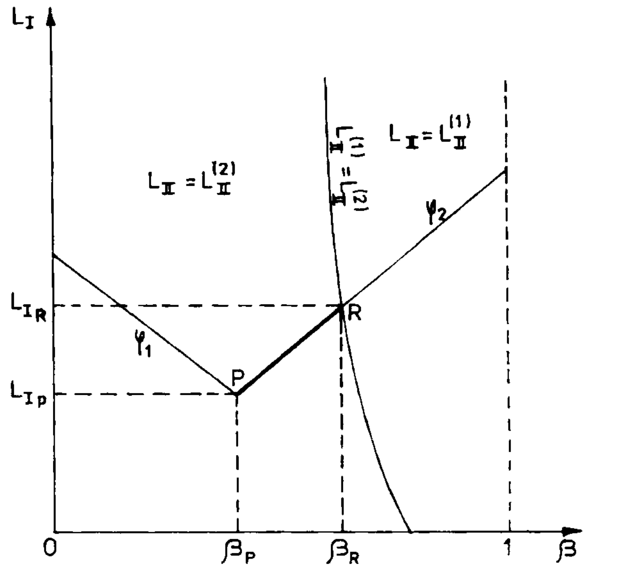

Figure 5. The set of optimal solutions when $L_{II\varphi_1}^{(1)} < L_{II\varphi_2}^{(2)}$.

A nonparametric equation describing the equality line is given in the work of Fidkowski and Królikowski (1983).

Optimal solution

Depending on values of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$ on lines φ_1 and φ_2, respectively, there are three possibilities:

1. If $L_{II\varphi_1}^{(1)} > L_{II\varphi_2}^{(2)}$, then $0 < \beta_R < \beta_P < 1$, and the set of optimal solutions lies in the closed segment $\overline{RP}$ on the line φ_1; see Figure 4. The value of the goal function on this segment is $L_{II\varphi_1}^{(1)}$, Appendix 3.
2. If $L_{II\varphi_1}^{(1)} < L_{II\varphi_2}^{(2)}$, then $0 < \beta_P < \beta_R \leq 1$, and the set of optimal solutions lies in the closed segment $\overline{PR}$: (β_P, L_{I_P}), (β_R, L_{I_R}) on the line φ_2; see Figure 5. The goal function value is $L_{II\varphi_2}^{(2)}$. The proof is analogous to the previous case (Fidkowski and Królikowski (1983).
3. If $L_{II\varphi_1}^{(1)} = L_{II\varphi_2}^{(2)}$, then $\beta_P = \beta_R$ and solution of the optimization task is at point P: (β_P, L_{I_P}). The goal function value is equal to $L_{II\varphi_1}^{(1)}$ or $L_{II\varphi_2}^{(2)}$. Let us notice that in this case $L_{II_P}^{(1)} = L_{II_P}^{(2)}$. This means that the equality line of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$ passes through the intersection point of lines φ_1 and φ_2. At this point the goal function reaches the minimum. This can be proved by analysis of values of function $L_{II}^{(1)}$ on the line φ_2 and $L_{II}^{(2)}$ on the line φ_1. The set of optimal solutions is in this case reduced to one point.

Recapitulation

The minimum of the goal function, according to Eq. 40, is expressed by the formula:

$$L_{II}^{opt} = \max\{L_{II\varphi_1}^{(1)}, L_{II\varphi_2}^{(2)}\} \tag{48}$$

From Eqs. 44 and 45 we get:

$$L_{II}^{opt} = \max\left\{\frac{A\phi_1}{\alpha_A - \phi_1}, \frac{A\phi_2}{\alpha_A - \phi_2} + \frac{\alpha_B B}{\alpha_B - \phi_2}\right\} \tag{49}$$

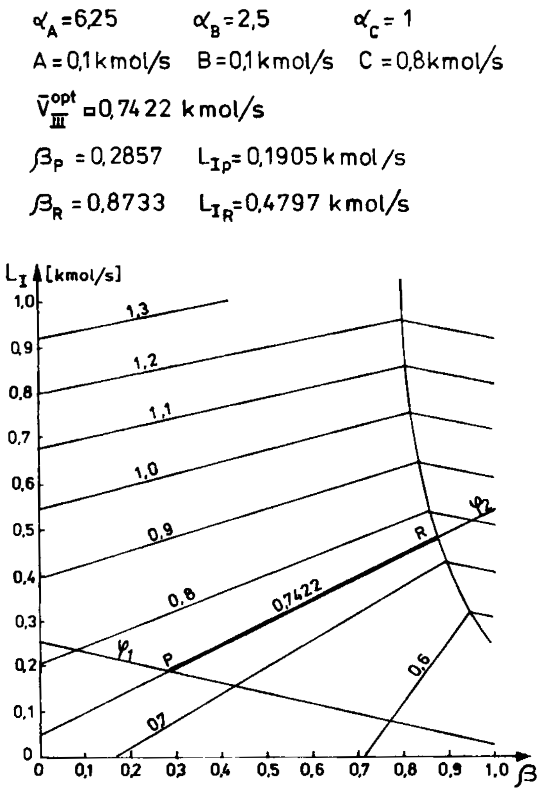

Figure 6. Results of calculations.

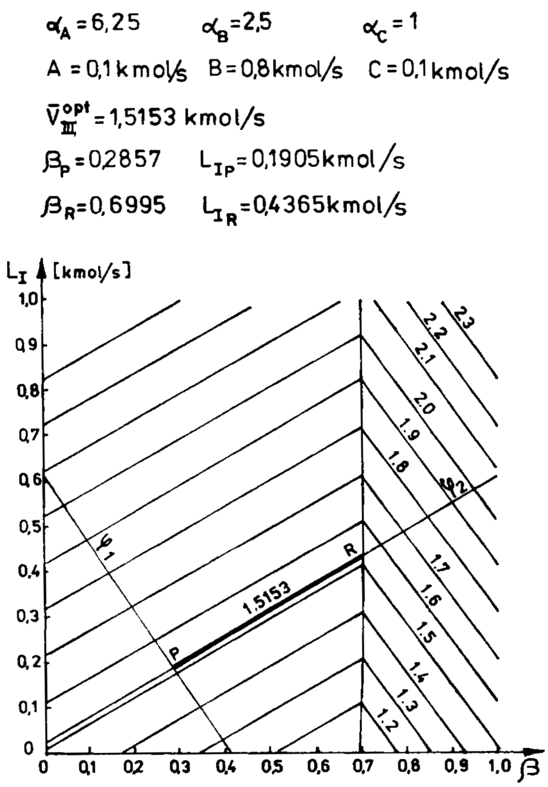

Figure 7. Results of calculations.

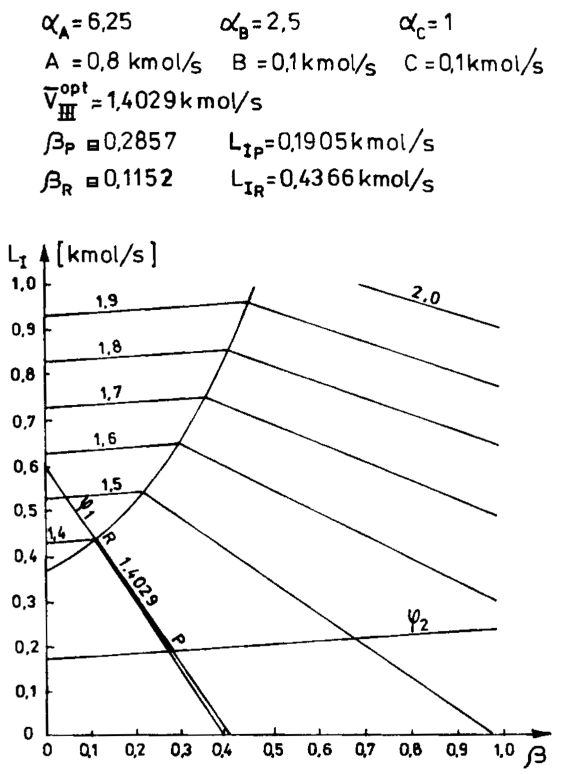

Figure 8. Results of calculations.

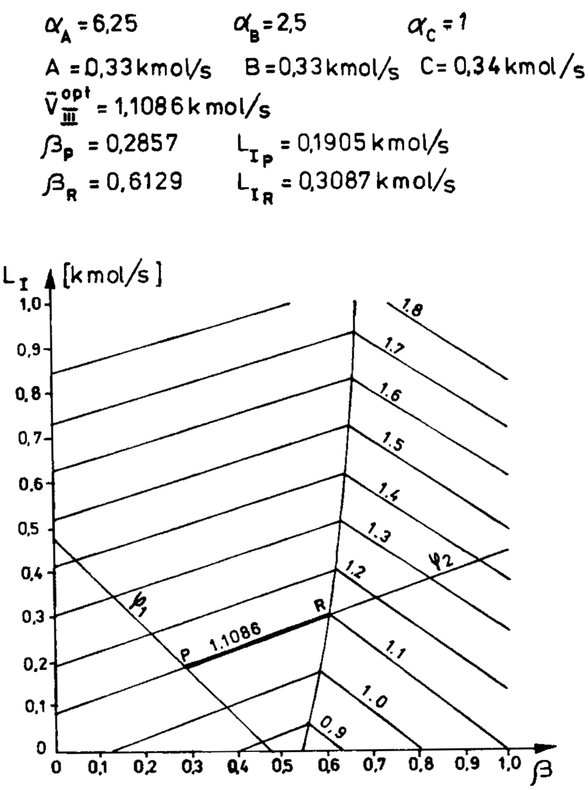

Figure 9. Results of calculations.

whereas the minimum goal function value of the original task is:

$$\bar{V}_{III}^{opt} = L_{II}^{opt} + A = \max\left\{\frac{\alpha_A A}{\alpha_A - \phi_1}, \frac{\alpha_A A}{\alpha_A - \phi_2} + \frac{\alpha_B B}{\alpha_B - \phi_2}\right\} \quad (50)$$

where ϕ_1 and ϕ_2 are roots of Underwood's equation given by Eq. 9.

The set of optimal solutions may be graphically presented on the plane of decision variables (β, L_I) as the closed segment having the ends (β_p, L_{I_p}) and (β_R, L_{I_R}). The coordinates of the segment ends are given by the following formulae:

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

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

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

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

where L_{II}^{opt} is given by Eq. 49.

Results

Some calculated examples of thermally coupled system optimization are presented in Figures 6–9. In these figures one can find level lines of the original goal function $\bar{V}_{III}$, lines φ_1 and φ_2, the rectangular projection of the ravine bottom—the equality line where $L_{II}^{(I)} = L_{II}^{(2)}$—and the set of optimal solutions, indicated by the heavy line segments *R-P* or *P-R*. The data to be calculated—relative volatilities, feed composition, and molar flow rate—are also given.

In Table 1 results of the optimization of the four sequences of distillation columns for four different feed compositions and four types of solutions are presented. The sequences are: *SC*, separation complex; *DS*, direct sequence; *IS*, indirect sequence; *TCS*, thermally coupled system (see Figures 1 and 10).

The substitutional goal function was defined as the sum of minimum vapor flow rates in distillation columns. Calculation algorithms for *SC*, *DS*, and *IS* have been presented elsewhere (Fidkowski, 1983). As one can see in Table 1, energy requirements of separation are the least in the TCS. The goal function is a nonlinear function of relative volatilities and flow rates of components in the feed. Changes in one parameter may cause an increase or decrease of the goal function value, depending on the values of the rest of parameters. Therefore not all rows and columns in Table 1 follow the same trend.

It must be stated that the result obtained is the minimum value of minimal vapor flow rate. It is accurate provided all the assumptions are satisfied. Of course a real vapor flow rate might be controlled by the purity of product *B* in the TCS when the number of plates is given. Therefore rigorous methods must be used for design purposes. Nevertheless, the formulae are also useful in the case presented here because they enable us to calculate minimum vapor flow rate at once. But in the case of synthesis of separation sequences the use of shortcut methods is necessary because of the complexity of the problem.

Our future works is directed toward the analytical comparison of energy requirements in alternative distillation sequences, using previously elaborated goal function formulae.

Table 1. Optimum Values of Goal Function—Minimum Vapor Flow Rates kmol/s

Relative Volatilities	Sequence	Flow Rates of Feed Components, kmol/s: $A = 0.1$, $B = 0.1$, $C = 0.8$	$A = 0.1$, $B = 0.8$, $C = 0.1$	$A = 0.8$, $B = 0.1$, $C = 0.1$	$A = 0.33$, $B = 0.33$, $C = 0.34$
$\alpha_A = 6.25$	SC	0.9713	1.5381	2.3715	1.2343
$\alpha_B = 2.5$	DS	1.0549	2.1176	1.6362	1.5871
$\alpha_C = 1.0$	IS	0.9754	2.2153	2.5455	1.8786
	TCS	0.7422	1.5153	1.4029	1.1086
$\alpha_A = 2.75$	SC	9.7143	10.0145	3.4144	7.7425
$\alpha_B = 1.1$	DS	9.7822	10.5563	3.5322	7.9803
$\alpha_C = 1.0$	IS	9.3418	10.6468	4.3474	8.0752
	TCS	9.1203	9.9422	2.9470	7.3151
$\alpha_A = 2.75$	SC	2.7142	9.3299	17.8595	7.6471
$\alpha_B = 2.5$	DS	3.0646	10.5668	10.0416	7.8116
$\alpha_C = 1.0$	IS	2.9244	10.6561	11.2753	8.2098
	TCS	2.3616	9.1512	9.8067	7.0315
$\alpha_A = 1.21$	SC	13.5048	10.8510	20.1238	10.5429
$\alpha_B = 1.1$	DS	14.6251	19.4032	11.9978	15.0481
$\alpha_C = 1.0$	IS	11.3520	19.4383	16.0951	15.3982
	TCS	9.2308	10.3456	9.8989	8.4346

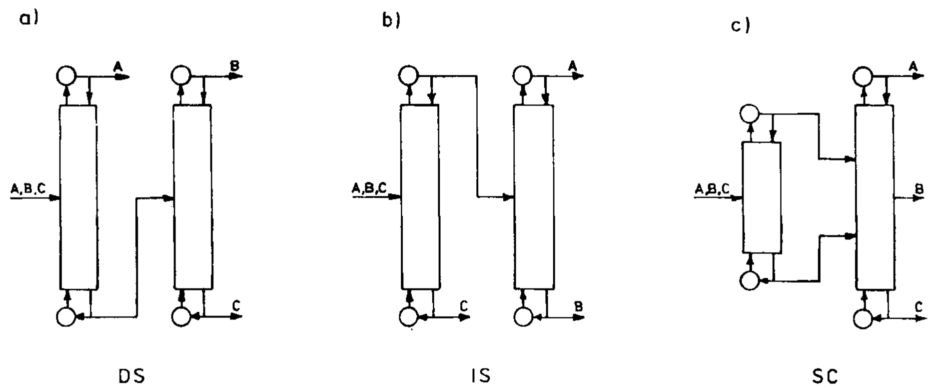

Figure 10. Sequences of distillation columns separating ternary solutions.
(a) Direct sequence *DS*. (b) Indirect sequence *IS*. (c) Separation complex *SC*.

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
$L_{II}^{(1)}, L_{II}^{(2)}$ = functions of decision variables, Eqs. 38 and 39
V = vapor flow rate, kmol/s
x_A^I = mole fraction of component A in stream L_I
$\bar{x}_B^I$ = mole fraction of component B in stream $\bar{L}_I$
y_A^I = mole fraction of component A in stream V_I
$\bar{y}_B^I$ = mole fraction of component B in stream $\bar{V}_I$
α = relative volatility
β = defined by Eq. 2
ϕ_1, ϕ_2 = roots of Underwoods equation, Eq. 9
φ_1, φ_2 = straight lines, Eq. 13

Subscripts

A, B, C = component A, B, C
P, R = point P, R
φ_1, φ_2 = line φ_1, φ_2
I, II, III = sections of the TCS, Figure 1

Superscripts

M = minimum reflux conditions
opt = optimum
$\bar{\ }$ = refers to the section of the column below the feed.

Appendix 1

Let us examine in what way the new objective function L_{II} (Eq. 40) depends on decision variables. It might be realized by differentiating Eqs. 38 and 39 in respect to L_I and β and by examining the signs of partial differentials. However, the same analysis can be made in the following, simpler way:

From Eq. 4a,

$$V_I = L_I + A + \beta B$$

with the result that the value of V_I increases when L_I or β rises:

$$V_I \nearrow \quad \text{when } L_I \nearrow \text{ and } \beta = \text{const.}$$

$$V_I \nearrow \quad \text{when } L_I = \text{const. and } \beta \nearrow$$

The equilibrium relation, Eq. 20, can be written in linearized form:

$$y_A^I = kx_A^I \tag{51}$$

where the equilibrium coefficient k is greater than 1 ($k > 1$) in the binary system AB. Introducing y_A^I from Eq. 51 into Eq. 24, one can obtain:

$$V_I k - L_I = \frac{A}{x_A^I} \tag{52}$$

As was shown, V_I is the rising function of L_I and $k > 1$, so the value of the expression $V_I k - L_I$ increases when L_I or β rises; that is:

$$(V_I k - L_I) \nearrow \quad \text{when } L_I \nearrow \text{ and } \beta = \text{const.}$$

and

$$(V_I k - L_I) \nearrow \quad \text{when } L_I = \text{const. and } \beta \nearrow .$$

Finally, from Eq. 52 and 38 it results that $L_{II}^{(1)}$ is the rising function of the decision variables:

$$L_{II}^{(1)} \nearrow \quad \text{when } L_I \nearrow \text{ and } \beta = \text{const.}$$

and

$$L_{II}^{(1)} \nearrow \quad \text{when } L_I = \text{const. and } \beta \nearrow .$$

An analogous analysis might be made for section III (for function $L_{II}^{(2)}$), considering the following equations:

$$L_I + F - V_I = (1 - \beta)B + C \tag{53}$$

$$(L_I + F)\bar{x}_B^I - V_I\bar{y}_B^I = (1 - \beta)B \tag{54}$$

$$\bar{y}_B^I = \bar{k}\bar{x}_B^I \tag{55}$$

where $\bar{k} > 1$ in the binary system BC. The variable $\bar{x}_B^I$ is calculated from this set of equations by elimination of $\bar{y}_B^I$ and V_I, and introduced into Eq. 39.

$$L_{II}^{(2)} = \frac{\alpha_B - \bar{k}\alpha_C}{\alpha_B - \alpha_C} L_I + \frac{\alpha_C}{\alpha_B - \alpha_C}[F - \bar{k}(A + \beta B)] + B \tag{56}$$

One can notice that the coefficient multiplied by L_I is positive, whereas the coefficient multiplied by β is negative. This means that $L_{II}^{(2)}$ is the rising function of L_I and the descending function of β.

$$L_{II}^{(2)} \nearrow \quad \text{when } L_I \nearrow \text{ and } \beta = \text{const.}$$

and

$$L_{II}^{(2)} \searrow \quad \text{when } L_I = \text{const. and } \beta \nearrow .$$

An approximate shape of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$, without any proportions, is shown in Figure 3.

As was shown, the objective function value rises when variable L_I increases its value. This leads to the conclusion that the optimum solution must lie on the edge of the area of feasible solutions (Figure 2), that is, on the line φ_1 or φ_2.

Appendix 2

The question arises whether lines φ_1 and φ_2 are also the level lines of the objective function. We will show that the answer is affirmative.

Let us concentrate our attention on line φ_1 and the function $L_{II}^{(1)}$. From many level lines of $L_{II}^{(1)}$ we select the one running through the same point as line φ_1, that is:

$$\left(0, \ \frac{A\phi_1}{\alpha_A - \phi_1}\right)$$

The function value on this level line, calculated from Eq. 42, is:

$$L_{II}^{(1)} = \frac{A\phi_1}{\alpha_A - \phi_1} \tag{57}$$

Substituting $\beta = 1$ and the above function value into Eq. 42, we obtain:

$$L_I = \frac{B\phi_1}{\alpha_B - \phi_1} + \frac{A\phi_1}{\alpha_A - \phi_1} \tag{58}$$

The same value of L_I, for $\beta = 1$, can be obtained from the equation defining line φ_1 (Eq. 13). This means that line φ_1 and the level line of $L_{II}^{(1)}$ pass through the same two points:

$$\left(0, \quad \frac{A\phi_1}{\alpha_A - \phi_1}\right) \left(1, \quad \frac{B\phi_1}{\alpha_B - \phi_1} + \frac{A\phi_1}{\alpha_A - \phi_1}\right)$$

so it is the same straight line.

It is easy to prove in the same way (Fidkowski and Królikowski, 1983), that line φ_2 is the level line of function $L_{II}^{(2)}$. The function value on this line is:

$$L_{II}^{(2)} = \frac{\alpha_B B}{\alpha_B - \phi_2} + \frac{A\phi_2}{\alpha_A - \phi_2} \tag{59}$$

Appendix 3

Let $\beta_P \leq \beta_R$, the equality line of functions $L_{II}^{(1)}$ and $L_{II}^{(2)}$ intersects line φ_2 (see Figure 5). The slope of line φ_2 is positive, from the inequality Eq. 14. This implies that $L_{I_P} \leq L_{I_R}$. $L_{II}^{(1)}$ is the rising function of decision variable β, so $L_{II_P}^{(1)} \leq L_{II_R}^{(1)}$. On the other hand $L_{II_R}^{(1)} = L_{II_R}^{(2)}$, which is evident, and $L_{II_R}^{(2)} = L_{II_P}^{(2)}$, because φ_2 is a level line of the function $L_{II}^{(2)}$. Therefore $L_{II_P}^{(1)} \leq L_{II_P}^{(2)}$ and consequently $L_{II\varphi_1}^{(1)} \leq L_{II\varphi_2}^{(2)}$. Now, on the basis of contraposition law, if $L_{II\varphi_1}^{(1)} > L_{II\varphi_2}^{(2)}$, then $\beta_R < \beta_P$. Because $\beta_P < 1$ (see Eq. 15), in order to finish the first part of the proof it is enough to show that $\beta_R > 0$.

The point R lies on line φ_1 because $\beta_R < \beta_P$. Let us compare Eq. 47 for the ordinate of the equality line with Eq. 13 for line φ_1, replacing L_{II} by expression 44. We obtain the following expression:

$$\beta_R = \frac{A(\phi_1 - \alpha_B)\alpha_A}{(\phi_1 - \alpha_C)(A\alpha_A + C\alpha_C)} \tag{60}$$

The conclusion is that $\beta_R > 0$, because all the factors in Eq. 60 are positive.

Let us move to the second part of the proof. Because $0 < \beta_R < \beta_P < 1$, then the segment $\overline{RP}$—whose ends are (β_R, L_{I_R}) and (β_P, L_{I_P})—lies on line φ_1 in the area where $L_{II}^{(1)} > L_{II}^{(2)}$; see Figure 4. The line φ_1 is the level line of the function $L_{II}^{(1)}$, which means that the objective function, Eq. 40, has in this segment the constant value $L_{II\varphi_1}^{(1)}$. The slope of line φ_2 is positive—Eq. 14—and L_I increases when β rises. $L_{II}^{(1)}$ is the rising function of β and L_I, so its values (and also the values of the goal function) on line φ_2, for $\beta > \beta_P$, are greater than $L_{II\varphi_1}^{(1)}$. For $\beta < \beta_R$ points on the line φ_1 are in the area where $L_{II}^{(2)} > L_{II}^{(1)}$. The slope of φ_1 is negative and L_I rises when the value of β decreases. Because $L_{II}^{(2)}$ rises when the value of L_I increases and the value of β decreases, so the values of function $L_{II}^{(2)}$ (and also the values of the goal function) on line φ_1, for $\beta < \beta_R$, are greater than $L_{II\varphi_1}^{(1)}$. The objective function has therefore its minimum value, equal to $L_{II\varphi_1}^{(1)}$, on the segment $\overline{RP}$: (β_R, L_{I_R}), (β_P, L_{I_P}).

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