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THE DESIGN OF OPTIMAL RECTIFICATION CASCADES

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F. B. Petlyuk, V. M. Platonov, and I. V. Girsanov

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The separation of mixtures by rectification [fractionation] is extensively used in the chemical, petroleum, and gas industries, and also in processes of isotope separation. As a rule, adiabatic rectification columns with constant reflux and vapor [boil-up] rates are employed here. However, the thermodynamic efficiency of an adiabatic process is often very low. Thus, in the case of energy-wasting separation processes such as, for example, low-temperature gas separation, attempts to improve their thermodynamic efficiency (by decreasing the irreversibility) have been made by means of certain design and construction modifications, having as their aim the rejection of the adiabatic principle.

In other cases, where the work of separation comprises only a small portion of the total expenditure (isotope separation), the rejection of the adiabatic principle results chiefly from a tendency to reduce the volume of equipment required, and also to decrease extraneous power consumption (for pumping of liquids and so forth).

So-called "multistage cascading" [1, 2] is employed in isotope separation; columns with intermediate reflux feed, columns with interjacent reboilers and partial condensers, sectionalized columns, condensation-evaporation units and others [3-6] have been suggested for low-temperature gas separation also. In all of these cases, energy is supplied either at certain intermediate points of the columns, or else along the whole mass-transfer surface.

However, all of these attempts to improve the rectification process have an empirical nature; in other cases, approximate optimal solutions, valid only for specific conditions [7], have been proposed. At the present time the need for methods of computing the thermodynamically optimal separation process in a real column (that is, in a column with a finite number of stages) has developed. The formulation of such a separation process would make it possible to indicate the direction of the desired thermodynamic improvement and also its upper limit.

A thermodynamically optimal separation in a column with a given number of stages would serve as a standard for industrial units, on which their efficiency

could be based. However, the practical usage of a reversible separation process (in an infinite column) [8] for these objectives would not be feasible and would not permit even an approximate estimation of the possibility of thermodynamic improvement of a process in a real column, if only because of the fact that the work of a reversible separation [9] does not depend on the physical properties of the mixture being separated (including here the volatility).

Thus, the thermodynamic improvement of processes for the separation of various mixtures must be based on an analysis of the thermodynamically optimal process in a real column, in which the physical properties of the mixture being separated must be accurately taken into consideration insofar as possible.

Together with the task of computing such a process, the problem of designing a cascade that is optimal from the economic standpoint (that is, with a consideration of capital and other expenses for the separation), is of considerable practical significance, especially in the case of isotope separation.

A thermodynamically optimal process, carried out in both finite and infinite columns, and also methods for computing optimal cascades for binary and multi-component rectification on the basis of various criteria, are presented below.

Separation in columns with an infinite number of stages (completely reversible process). Such a process has been described for both binary [9, 10] and multi-component [11, 12] rectification. However, a number of important assumptions regarding these processes were not clearly formulated. An optimal rectification process is characterized at each point of the column by minimum reflux and vapor [boil-up] rates and by zero driving forces for the process, that is, by equilibrium between the liquid and the vapor.

Thus, considering these features, a process of optimal rectification may be described by the following system of equations (material balance and phase-equilibria equations):

$$\begin{aligned} x_i(V + W) &= y_i V + x_{Wi} \cdot W \\ y_i &= K_i(T)x_i \\ (i &= 1, 2, \dots, n) \end{aligned} \quad (1)$$

(this system is written for the stripping section; an analogous system results for the rectifying [enrichment] section).

Applying system (1) to the feed point, we obtain:

$$\begin{aligned} x_{Fi}(V + W) &= y_{Fi} V + x_{Wi} \cdot W \\ (i &= 1, 2, \dots, n) \end{aligned} \quad (2)$$

System (2) contains n equations with $n + 2$ unknowns (x_{Wi} , W , and V). Specification of any two parameters, for example, the concentrations of the key components in the bottoms product, uniquely defines the solution to system (2) and, consequently, the complete process of reversible rectification. Having determined x_{Wi} and W from system (2), one may, by using system (1), compute the magnitudes of the liquid and vapor rates and the concentrations of all of the components for any given temperature level in the column.

However, system (2) guarantees a non-negative solution only for a certain specification of the parameters. The maximum vapor-to-liquid ratio in the stripping section during reversible rectification corresponds to a zero concentration of the lightest [1st] component in the bottoms product.

For this case we obtain from system (2):

$$\frac{V}{V+W} = \frac{V}{L} = \frac{x_F^{1st}}{y_F^{1st}} = \frac{1}{K_F^{1st}} \quad (3)$$

Analogously, the maximum liquid-to-vapor ratio in the rectifying [enrichment] section corresponds to a zero concentration of the heaviest [hst] component in the distillate and is equal to K_F^{hst} . For higher values of the vapor-to-liquid ratio in the stripping section and the liquid-to-vapor ratio in the rectifying [enrichment] section, the solution to system (2) loses physical meaning (the concentrations of the lightest components in the bottoms product and of the heaviest components in the distillate will be found to be negative). Thus, reversible rectification is possible only for:

$$\left(\frac{V}{L}\right)_{\text{strip}} \leq \frac{1}{K_F^{1st}}$$

and

$$\left(\frac{L}{V}\right)_{\text{rect}} \leq K_F^{hst}$$

This corresponds to the so-called first class of fractionation [13].

A sharper separation by means of reversible rectification is impossible in a single column.

For binary rectification, the limiting case corresponds to complete separation of the initial mixture into its pure components.

A thermodynamically reversible rectification process has been described, proceeding from purely physical considerations. However, it may be shown in rigorous mathematical fashion that the entropy change during such a process is equal to the entropy change that occurs during separation of the mixture into the corresponding products, computed on the basis of the concept of semipermeable membranes [14].

A short exposition of this derivation for the case of binary rectification of ideal closely boiling solutions is given below.

The entropy of separation (the entropy change in external energy sources during separation) is equal to:

$$\Delta S_{\text{sep}} = - \int_{x_W}^{x_D} \frac{dQ}{T} \quad (4)$$

If the heat content of the feed and of the separated products are selected such that:

$$\int_{x_W}^{x_D} dQ = 0$$

(that is, for example, all of the entering and exiting streams are saturated liquids), then, integrating by parts, we obtain:

$$- \int_{x_W}^{x_D} \frac{dQ}{T} = \int_{x_W}^{x_D} Q d\left(\frac{1}{T}\right) \quad (5)$$

From the Clapeyron-Clausius equation:

$$\frac{dP}{dT} = \frac{\lambda}{T(V_g - V_{liq})} \quad (6)$$

assuming that $V_{liq} = 0$ and $V_g = RT/P$, and after some simple transformations, we obtain for closely boiling ideal solutions:

$$\frac{1}{T} = \frac{R}{\lambda} \{ \ln [1 + (\alpha - 1)x] + C \}$$

$C = \frac{\lambda}{R} \cdot \frac{1}{T_H}$ for $d = \frac{P_i}{P_0^H}$ (7)

$$d\left(\frac{1}{T}\right) = \frac{R}{\lambda} \cdot \frac{\alpha - 1}{1 + (\alpha - 1)x} dx \quad (8)$$

$$Q_{strip}^x = \lambda \cdot W \frac{x - x_W}{y - x} \quad (9)$$

$$Q_{rect}^x = \lambda \cdot D \frac{x_D - x}{y - x} \quad (10)$$

Assuming the existence of phase equilibrium at each point, we finally have:

$$\begin{aligned} \Delta S_{sep} = & \int_{x_W}^{x_F} \lambda \cdot W \frac{x - x_W}{\frac{\alpha x}{1 + (\alpha - 1)x} - x} \cdot \frac{R}{\lambda} \cdot \frac{\alpha - 1}{1 + (\alpha - 1)x} dx + \\ & + \int_{x_W}^{x_D} \lambda \cdot D \frac{x_D - x}{\frac{\alpha x}{1 + (\alpha - 1)x} - x} \cdot \frac{R}{\lambda} \cdot \frac{\alpha - 1}{1 + (\alpha - 1)x} dx = \end{aligned} \quad (11)$$

? $F \cdot W$

$$= R[W(1 - x_W) \ln(1 - x_W) + W \cdot x_W \cdot \ln x_W +$$

$$+ D(1 - x_D) \ln(1 - x_D) + D x_D \cdot \ln x_D - F(1 - x_F) \ln(1 - x_F) - F x_F \ln x_F]$$

While the thermodynamically optimal separation process in infinite columns may be computed via elementary means, the calculation of such a process in the case of real rectification columns (which represent the greatest practical interest) is possible only by recourse to the apparatus of dynamic and nonlinear programming and with the application of digital computers.

In conjunction with the emergence of the need for isotope separation, a theory of ideal cascades was developed [15], which is applicable to various methods of separation, including rectification. This theory was recently extended to the separation of multi-component mixtures [16]. This theory is adaptable to processes with a finite number of separation stages.

However, it describes separation processes which are characterized by a minimum total interstage flow (the functional $\int_0^n Vdn$ is a minimum), and not by a minimum work of separation, as will be shown below.

The ideal cascade guarantees a minimum expenditure of energy on separation only for processes with an irreversible elementary act (gaseous diffusion, atomolysis, etc.), for which the energy expenditure on separation is proportional to the total interstage flow. For an ideal cascade, $n = 2n_{\min}$, and if $\alpha - 1 \ll 1$ at each stage $V \approx 2V_{\min}$. The theory of ideal cascades yields a simple analytical solution to the problem of minimizing the functional $\int_0^n Vdn$ under the condition $\alpha - 1 \ll 1$. A number of papers by Soviet and foreign authors [1, 2, 7] have been devoted to the application of the theory of ideal cascades to the design of rectification plants. However, several authors [4] have also made unsuccessful attempts to:

first, consider the ideal cascade as guaranteeing the minimum work of separation and use such concepts of the theory of ideal cascades as the separation potential to estimate the efficiency of rectification plants;

second, extend the theory of ideal cascades to widely boiling mixtures.

An ideal cascade as applied to a rectification plant is not thermodynamically optimal. The problem of minimizing the work of separation or the entropy of separation, which is proportional to the latter, as expressed by the functional

$-\int_0^n dQ/T$ is a considerably more difficult variational ("non-classical") problem than the problem of minimizing the functional $\int_0^n Vdn$.

The study carried out by the present authors showed that the method of dynamic programming [16] may be effectively used to solve this problem for the case of binary rectification.

Separation of a binary mixture in a plate column with an energy supply at each stage. The optimality criterion [function] is

$$- \sum_{j=1}^n \frac{Q_j}{T_j}$$

Using the material and heat [enthalpy] balance equations, we obtain (for the stripping section):

$$V_j = \frac{x_{j+1} - x_W}{y_j - x_{j+1}} \cdot W \quad (12)$$

$$Q_j = V_j H_j - (V_j + W)h_{j+1} - V_{j-1}H_{j-1} + (V_{j-1} + W)h_j \quad (13)$$

where y_j , H_j and h_j for the binary rectification are functions of x_j .

Analogous equations result for the rectifying [enrichment] section.

Thus, the problem reduces to a minimization of the functional:

$$- \sum_{j=1}^n Q_j(x_{j-1}, x_j, x_{j+1}) \cdot \frac{1}{T_j(x_j)}$$

Using the method of dynamic programming, we construct a system of Bellman recursion equations [17]:

$$F_{j-2}(x_j, x_{j+1}) = \min \left[F_{j-3}(x_{j-1}, x_j) - \frac{Q_j(x_{j-1}, x_j, x_{j+1})}{T(x_j)} \right]$$

$$j = 3, 4, \dots, n$$

$$F_0(x_2, x_3) = - \frac{Q_1(x_2)}{T(x_1)} - \frac{Q_2(x_2, x_3)}{T(x_2)} \quad (14)$$

This system was solved numerically on a "Ural" digital computer, using the so-called "tube" method.*

Although the method developed is applicable to any arbitrary mixture, an ideal mixture, subject to equalities (7), (9), and (10), was chosen as the object of this study; thus, there was the possibility of comparing the results with the data from the theory of ideal cascades.

The process of searching for the optimum (the results of successive iterations) is shown in Fig. 1 in $V - n$ coordinates ($n = 23$, $n_{strip} = 11$, $\alpha = 1.44$, $\lambda = 5810$, $F = 100$, $x_F = 0.5$, $x_W = 0.11865$, $x_D = 0.91452$, liquid feed, total condenser).

The parameters of the process (separation, number of plates, and relative volatility) were selected in accordance with the theory of ideal cascades. For purposes of demonstration, the stepwise variation of the vapor flow up the column is shown as continuous. An ideal cascade was selected as the initial trajectory. As the result of successive iterations, the trajectory approaches the form for a thermodynamically optimal cascade and acquires a monotonic nature for each section, corresponding to the supply of heat to all of the plates of the stripping section and to the removal of heat from all of the plates of the rectifying section.

The relationships n vs. x and n vs. V for a thermodynamically optimal cascade for various values of α are constructed in Figs. 2 and 3, respectively. For $\alpha = 1.44$ the corresponding relationships for an adiabatic column and an ideal cascade are shown, while in Fig. 3 the curve for V_{min} is also given. It is seen from these Figures that the thermodynamically optimal cascade occupies an intermediate position between an adiabatic column (where $V = \text{const}$) and an ideal cascade (where $V = 2V_{min}$ for each tray) with respect to both the distribution of the vapor flow

* The "tube" method is a technique for solving systems of functional equations of the type (14) for rectification problems - has been described in detail earlier [18].

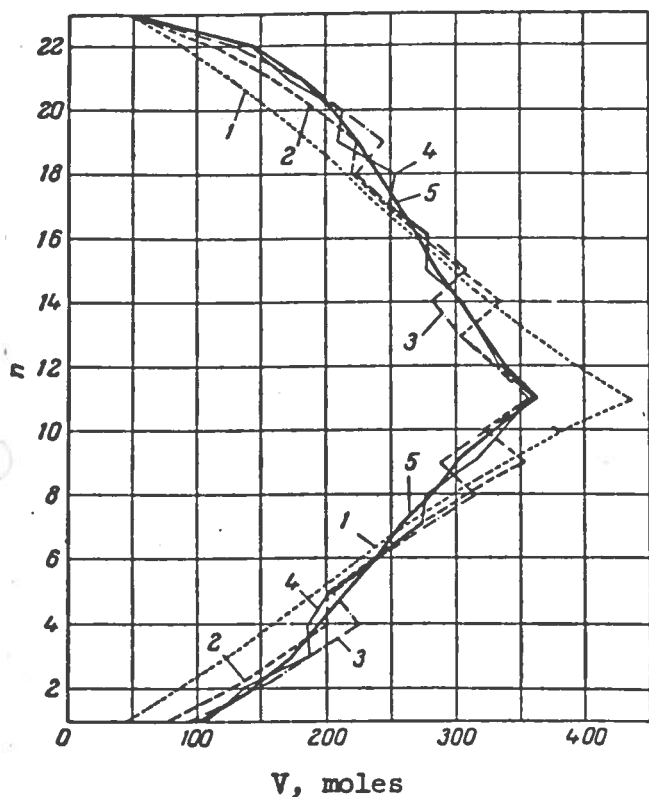


Fig. 1. Results of successive iterations in the process of approaching the thermodynamically optimal cascade: 1) initial trajectory (ideal cascade), $\Delta S = 147.0$ kcal per deg per 100 moles of initial mixture; 2) results of the 1st iteration, $\Delta S = 141.0$; 3) results of the 2nd iteration, $\Delta S = 140.2$; 4) results of the 3rd iteration, $\Delta S = 139.5$; 5) results of the 6th iteration, $\Delta S = 139.2$.

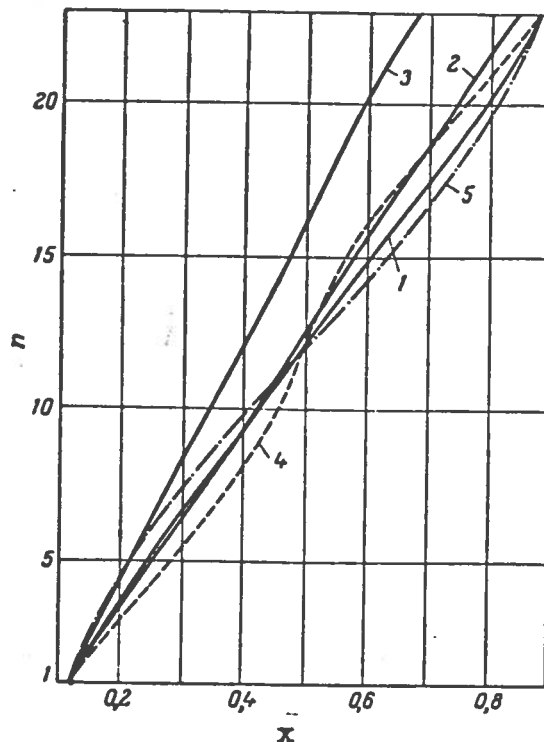


Fig. 2. Dependence of n on x for a thermodynamically optimal cascade for various values of α : 1) thermodynamically optimal cascade, $\alpha = 1.44$; 2) the same, $\alpha = 2.0$; 3) the same, $\alpha = 5.0$; 4) adiabatic column, $\alpha = 1.44$; 5) ideal cascade, $\alpha = 1.44$.

and the variation of the concentration with the height of the column.

It is of interest to note that the variation of the concentration with height during the separation of ideal solutions in thermodynamically optimal cascades has an approximately linear nature (here, the optimal distribution of the plates with respect to the sections of the column is proportional to the differences $(x_D - x_F)$ and $(x_F - x_W)$).

As is seen from Fig. 4, this corresponds to approximate equality of the driving forces at each level of the cascade. For an ideal mixture, having the properties (7) and (9), the entropy of separation (the function

$$- \sum_{j=1}^n \frac{Q_j}{T_j}$$

is obviously independent of the latent heat of vaporization.

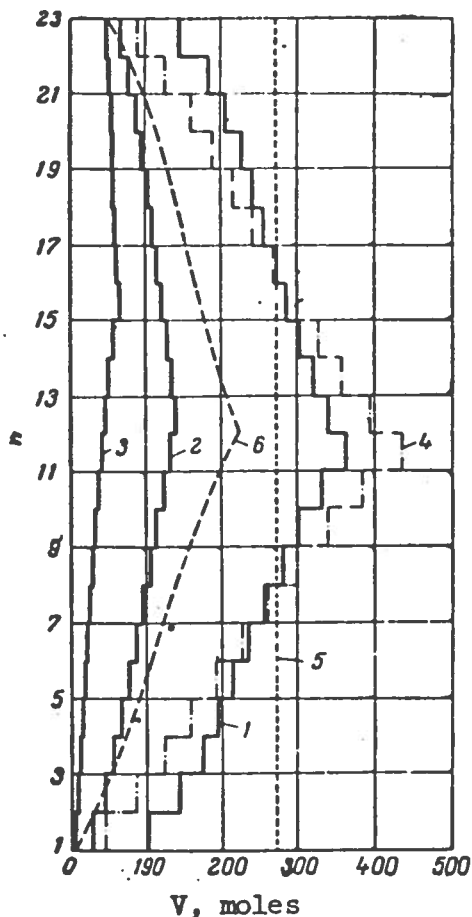


Fig. 3. Dependence of n on V for a thermodynamically optimal cascade for various values of α : 1) thermodynamically optimal cascade, $\alpha = 1.44$; 2) the same, $\alpha = 2.0$; 3) the same, $\alpha = 5.0$; 4) ideal cascade, $\alpha = 1.44$; 5) adiabatic column, $\alpha = 1.44$; 6) minimum vapor flow V_{min} , $\alpha = 1.44$.

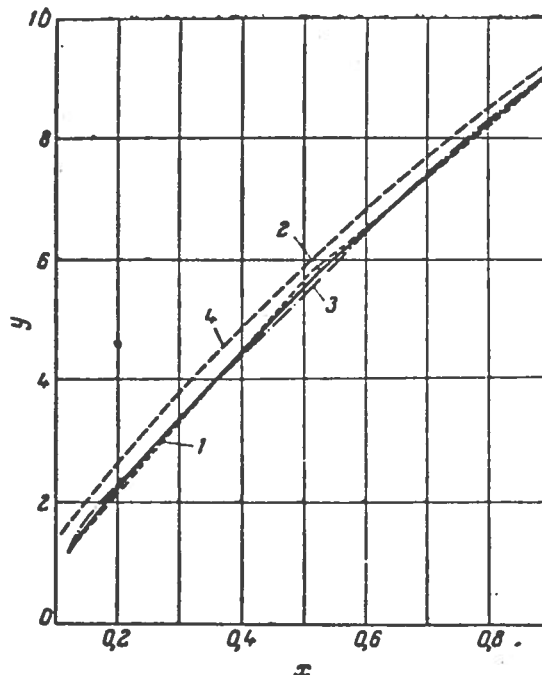


Fig. 4. Dependence of y on x for an adiabatic column, an ideal cascade, and a thermodynamically optimal cascade ($\alpha = 1.44$): 1) adiabatic column; 2) thermodynamically optimal cascade; 3) ideal cascade; 4) equilibrium curve.

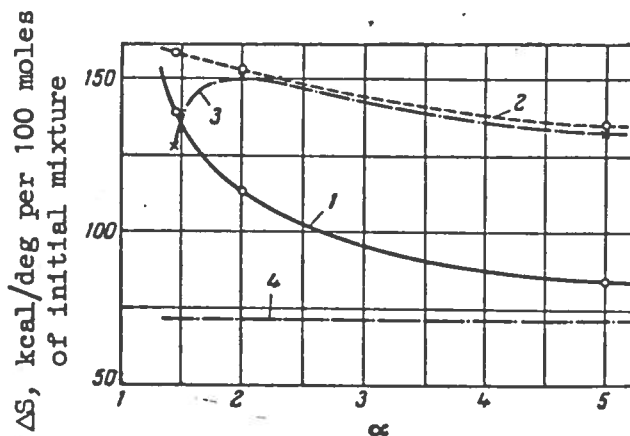


Fig. 5. Dependence of ΔS_{sep} on α : 1) thermodynamically optimal cascade ($n = 23$); 2) adiabatic column ($n = 23$); 3) infinite adiabatic column; 4) reversible rectification.

The entropy of separation for a thermodynamically optimal cascade as a function of the relative volatility α for a given number of trays ($n = 23$) is shown in Fig. 5. The corresponding relationship for adiabatic columns is also presented in this Figure for comparative purposes. It is seen that the entropy of separation for a thermodynamically optimal cascade as $\alpha \rightarrow \infty$ asymptotically approaches the entropy for reversible separation (the same thing is observed for $\alpha = \text{const}$ and $n \rightarrow \infty$).

For $\alpha = \text{const}$ and $n \rightarrow \infty$, and also for $n = \text{const}$ and $\alpha \rightarrow \infty$, the deviation from equilibrium of the liquid and vapor streams mixing on each stage is diminished and, accordingly, the work of separation converges to the reversible work.

A comparison of the thermodynamically optimal cascade with an adiabatic column and with an ideal cascade for the above-indicated values of the process parameters ($\alpha = 1.44$, $n = 23$) shows that the entropy of separation for the thermodynamically optimal cascade is 139.15, for the ideal cascade it is 146.97, and for the adiabatic column it is 158 kcal/deg per 100 moles of initial mixture (compare: the entropy of reversible separation is equal to 72.24 and the entropy of separation in an infinite adiabatic column is 127.92). This corresponds to an efficiency for the ideal cascade of 0.945 and an efficiency for the adiabatic column of 0.88. It should be appreciated that these efficiencies may vary over a wide range depending on the separation conditions; thus, the efficiency of an adiabatic column falls sharply with an increase in the degree of enrichment in the column.

The total interstage flow, $\sum_{j=1}^n V_j$, is, as one would expect the least for an ideal cascade (5268 moles per 100 moles of initial mixture); for the thermodynamically optimal cascade it is equal to 5413 and for an adiabatic column it is 6030.

If the mixture is close-boiling, the losses due to irreversibility in such a column amount to only a small portion of the total irreversible losses, which occur primarily in reboilers and condensers.

The method developed here may be easily used to find the minimum energy expenditure with an allowance for losses due to incomplete recovery in the heat exchangers. It is only necessary in system (14) to substitute $T + \Delta T$ for T in the stripping section and $T - \Delta T$ for T in the rectifying section (ΔT is the temperature difference in the heat exchangers).

Another approach should be possible for the solution of the problem of determining the minimum work of separation. The minimum work of separation in a real column must correspond to the minimum total of the entropies of mixing of the vapor and liquid streams on all of the stages of separation. In reversible rectification this sum is equal to zero, and the entropy change in external energy sources is equal to the entropy change in the separation products. In a real column the entropy change in external energy sources is greater than the entropy change in the separation products by an amount equal to the sum of the entropies of mixing on all of the separation stages:

$$\Delta S_{\text{real}} - \Delta S_{\text{revers}} = \sum_{j=2}^{n-1} \Delta S_{\text{mix}}^j$$

The minimization of the quantity, $\sum_{j=2}^{n-1} \Delta S_{\text{mix}}^j$, may be done using the "tube" method. Here, we obtain the following system of Bellman equations:

$$F_{j-2}(x_j, x_{j+1}) = \min_{x_{j-1}} [F_{j-3}(x_{j-1}, x_j) + \Delta S_{\text{mix}}^j(x_{j-1}, x_{j+1})] \quad (i = 3, 4, \dots, n)$$

$$F_0(x_3) = \Delta S_{\text{mix}}^2(x_3) \quad (15)$$

The systems of functional equations (14) and (15) are equivalent.

This method of dynamic programming may be used extensively for solving other optimality problems of binary rectification.

The optimality criterion [function] is $\sum_{j=1}^n V_j$. The problem of minimizing

the total interstage flow is solved in the same fashion as in the theory of ideal cascades. However, a mixture with any arbitrary properties, including widely boiling ones, may be studied via this method.

The system of Bellman equations in this case assumes the following form:

$$F_{j-2}(x_j) = \min_{x_{j-1}} [F_{j-3}(x_{j-1}) + V_{j-1}(x_{j-1}, x_j)] \quad (16)$$

$$(j = 3, 4, \dots, n)$$

$$F_0(x_2) = V_1(x_2)$$

Systems (14) and (16) have an identical structure, but system (14) is doubly connected while (16) is simply connected. This merely leads to a corresponding decrease in the computation time.

The computations that were carried out showed that, for an ideal mixture and $\alpha = 1.44$, the optimal parameters were close to the results from the theory of ideal cascades.

It should be pointed out that this method guarantees that a minimum interstage flow will be found for a fixed number of separation stages. A series of computations with various values of n must be carried out in order to find the overall minimum.

Economic optimality criterion. The problems treated above are primarily of a theoretical nature. Of greater practical interest, particularly as applied to the separation of isotopes, is the case wherein heat or cold is fed not to each tray, but rather only at certain intermediate points (that is, by sections), and wherein the functional to be minimized includes dissimilar expenditures for the separation (energy and capital expenditures).

If we take the expenditures [in reduced form] for the separation E (the sum of the energy and capital expenditures with pay-out time taken into account), as such a functional, we then have for each section:

$$E_j = a_1 Q_j \varphi(T_j) + a_2 V_j + a_3 V_j n_j + a_4 \frac{V_j}{\Delta T_j} + a_5 \quad (17)$$

Here the function $\varphi(T)$ may, first, have a step-like form in conformity with the discrete set of isotherms for the heating or cooling agents at hand, and, second, take into consideration incomplete recovery in the reboilers and condensers (in the separation of isotopes $T \approx \text{const}$).

The first term of expression (17) includes direct expenditures of energy for the supply of heat or cold to the given section.

The second term includes expenditures for piping, fittings, storage tanks, compressors, and pumps.

The third term includes expenditures on the rectifying section itself (shell, trays or packing), and also energy expenditures to overcome hydraulic resistance.

The fourth term includes expenditures on reboilers and condensers.

Finally, the fifth term includes expenditures for instrumentation and certain other fixed expenditures.

The problem consists in the optimal selection of the points for intermediate supply of heat and cold and of the quantities Q_j , corresponding to a minimum

value of $\sum_{j=1}^k E_j$, where k is the number of sections.

The semianalytical solution of such a problem for the particular case of isotope separation, with a number of simplifying assumptions ($x_F \ll 1$), was attempted by Dipak [7]. A method of rigorous solution of such a problem for the general case is presented below.

In solving this problem by the "tube" method, it is convenient to select as the independent variables V_j (the vapor flow in the j -th section) and x_j (the concentration of the light component at the exit from the j -th section; x_0 and x_k are fixed by the separation conditions*).

With this selection of the independent variables, we then obtain:

$$Q_j = f_1(x_{j-1}, V_{j-1}, V_j) \quad (18)$$

(in the particular case of ideal solutions with $\lambda = \text{const}$, $Q_j = f_1(V_{j-1}, V_j)$), and:

$$\varphi(T_j) = f_2(x_{j-1}) \quad (19)$$

$$n_j = f_3(x_{j-1}, x_j, V_j) \quad (20)$$

$$\Delta T_j = f_4(x_{j-1}) \quad (21)$$

Thus:

$$E_j = \psi_j(x_{j-1}, x_j, V_{j-1}, V_j) \quad (22)$$

Finally the problem is set up to find:

$$\min \sum_{j=1}^k \psi_j(x_{j-1}, x_j, V_{j-1}, V_j)$$

with the conditions $x_0 = x_W$, $x_k = y_D/K$ and the restrictions:

$$V_j > V_{j_{\min}}; \quad x_j > x_{j-1}$$

The system of Bellman equations for this problem has the following form:

$$F_{j-1}(V_j) = \min[F_{j-2}(x_{j-1}, V_{j-1}) + \psi_j(x_{j-1}, V_{j-1}, V_j)] \quad (23)$$

$$x_{j-1}, V_{j-1} \quad (j = 2, 3, \dots, k)$$

*The more general problem of optimal design with variable degrees of recovery and purity of the products is not considered here.

The process of solving this system may be considered as two-dimensional and simply connected.

The computation for each section (determination of n_j) is carried out via the "tray-to-tray" method using the equations of phase equilibrium, material balance and, if necessary, enthalpy balance.

A fractional number of theoretical trays in each section may be obtained here.

The coefficients a_1 - a_5 , the functions $\varphi(T_j)$, and the ΔT_j are derived from a consideration of the actual engineering, economic, thermodynamic, and physical parameters of the process.

It should be noted that, in expression (17), several of the component expenditures are estimated approximately. For example, the capital expenditures on the rectifying section itself have been assumed to be proportional to V_j and n_j , no precise relationship between the diameter of the column, the tray spacing and the V_j has been incorporated, no proportionality between the cost of the column and the weight of the material has been included, the tray efficiencies have been assumed to be constant, and so forth.

The problems of a more accurate consideration of these factors have been treated in the literature [19, 20]. However, the method presented here retains its merit completely even if all of these complicating factors are considered. The structure of expression (22) and of the system of equations (23) is completely preserved here.

The dynamic programming method described herein has been found to be universal and very effective in its application to various optimality problems of binary rectification.

Depending on the formulation of the problem and the selection of the optimality criterion (the functional to be minimized), simply connected or doubly connected one-dimensional or two-dimensional processes for solving the system of Bellman functional equations have been encountered.

In this connection, the problem of minimizing a function of many variables is replaced with a set of sequentially solved problems of minimization of functions of one or two variables.

The advantage of the dynamic programming method in comparison with other methods (for example, a gradient method) is demonstrated rather forcefully if there is a large number of independent variables, which may occur, for example, in the computation of optimal cascades for isotope separation.

The "tube" method is less sensitive than the gradient method with respect to local optima and is not endangered by limits; moreover, considerably more information about the system is obtained (instead of a single optimal trajectory there is an envelope of trajectories, which correspond to partial optima with respect to segments of the system).

However, the dynamic programming method is particularly effective in its application to the problem of optimizing a chain of elements (the elements may be the trays of a rectification column, the rectangular sections of a rectification cascade, rectification columns in complex separation installations, and even

different industrial units in a single industrial sequence), if the process in each element depends on no more than one or two input parameters and a small number of control parameters.

In the binary rectification problems described above, the process in each element did indeed depend on one (simply connected process) or two (doubly connected process) input parameters and on one (one-dimensional process) or two (two-dimensional process) control parameters.

Separation of a multi-component mixture. In the case of multi-component rectification the process in each element depends on many input parameters (that is, it is multiply connected); the concentrations of all of the components of the mixture entering the element or the control parameters of all of the preceding elements may be taken as such input parameters.

Thus, the dynamic programming method for the problem of multi-component rectification is not very effective. Nonlinear programming methods, in particular gradient methods, would be more efficient.

Let us consider the problem of determining the minimum work of separation of a multi-component mixture in a real column with a given number of theoretical stages of separation.

The following are given: the composition and thermodynamic state of the feed, the total number of theoretical stages of separation, and the separation with respect to the key components.

In this case it is convenient to select as the independent variables (control parameters) the amount of vapor leaving each tray V_j , and the number of trays in one of the sections of the column m . Here $V_n = D$, while V_{n-1} for fixed V_j ($j = 1, 2, \dots, n-2$) is uniquely determined by the given separation.

The process of multi-component rectification under the given conditions is completely determined by the distribution of the vapor stream up the column, V_1, V_2, \dots, V_{n-2} , and may be computed by one of the "tray-to-tray" methods.

Thus, the problem reduces to the minimization of some undefined function of the $n-1$ variable:

$$- \sum_{j=1}^n \frac{Q_j}{T_j} = F(V_1, V_2, \dots, V_j, \dots, V_{n-2}, m) \quad (25)^*$$

The functional restrictions are placed on the independent variables:

$$V_j > V_j^{\min} \\ (j = 1, 2, \dots, n-1)$$

From a physical sense of the problem, the optimal trajectory (the optimal set of the V_j) must completely lie strictly inside the restrictions [limits].

This makes it possible to use the method of steepest descent for solving this problem, without any serious complications of the algorithm associated with searching for the optimum on a boundary. The method consists in determining

* Translator's Note: paper contains no equation number 24.

particular increments of the function $-\sum_{j=1}^n \frac{Q_j}{T_j}$ with respect to each of the independent variables (that is, the direction of the gradient) and in moving in a direction opposite to the gradient.

The solution of this problem is of interest for the proper design of low-temperature gas-separation plants. The individual units of these plants are characterized by a low temperature of the refrigeration being supplied (high power cost) and a large temperature drop between the top and bottom of the columns. This results in a high percentage of the total energy expenditures going directly to the separation, the total expenditures being associated with, for example, irreversibility in the reboilers and condensers.

The method of steepest descent also makes it possible to solve the important practical problem of the optimal, in an economic sense, supply of heat and cold to the sections of a column. The problem formulation does not differ from that described above in the section on binary rectification.

However, it is more convenient in this case to consider the reduced expenditures being minimized as a function of the number of trays n_j and the vapor flows V_j in each section:

$$E = F(n_1, V_1, n_2, V_2, \dots, n_k, V_k) \tag{26}$$

One of the variables, for example, n_k , is not independent. It is uniquely defined by the selection of the remaining variables and the given separation. Thus, the problem consists in minimizing the function of the $(2k - 1)$ th variable (if the number of the feed tray m is also considered to be a variable, then there are $2k$ variables) with the restrictions, $V_j > V_j^{\min}$ ($j = 1, 2, \dots, k$).

The method of steepest descent for this problem does not differ from that described above.

SUMMARY

1. An expression for the entropy change during completely reversible separation of a binary mixture has been obtained without using any concepts of hypothetical semipermeable membranes.
2. Methods for computing thermodynamically or economically optimal rectification cascades have been developed.
3. It has been shown that a dynamic programming method is the most efficient for the computation of optimal cascades for binary rectification, while the method of steepest descent is best for multi-component rectification.
4. The results of a computer study of the thermodynamically optimal cascade for binary rectification have been presented.
5. It has been shown that an ideal cascade does not necessarily guarantee the minimum work of separation.

SYMBOLS

- V - vapor flow up the column
- L - liquid flow down the column

F - feed to the column
D - distillate product
W - bottoms product
T - temperature
P - pressure
H - heat content of the vapor
h - heat content of the liquid
S - entropy
K - phase equilibrium constant
 α - relative volatility
 λ - latent heat of vaporization
x - concentration of a component in the liquid
y - concentration of a component in the vapor
Q - amount of heat

Q_{strip}^x - amount of heat supplied to the portion of the stripping section located from the bottom of the column up to the point with the concentration x

Q_{rect}^x - amount of heat removed from the portion of the rectifying [enrichment] section located from the top [Translator's Note: text says "from the bottom"] down to the point with the concentration x

R - universal gas constant
k - number of sections
n - total number of trays
m - number of trays in a single section
C - integration constant

SUBSCRIPTS AND SUPERSSCRIPTS

j - tray number
i - component number
F - feed
W - bottoms product
D - distillate product
lst - lightest component
hst - heaviest component
g - gas
liq - liquid

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