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Degree of Separation in a Gas Thermal Diffusion Column Depending on the Parameters of the Gas Mixture, the Geometry, and the Column Productivity

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Degree of Separation in a Gas Thermal Diffusion Column Depending on the Parameters of the Gas Mixture, the Geometry, and the Column Productivity

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Abstract

Analytical dependencies have been obtained for the degree of separation in a gas thermal diffusion column separating a binary gas mixture under dynamic working conditions (with product extraction), as well as for calculating the convective gas flows in the column. The dependence of the degree of separation from thermodynamic parameters of the gas mixture and from both the geometry and the productivity of the column has been shown.

1. INTRODUCTION

The first analytical dependencies for the degree of separation in thermal diffusion columns under dynamic working conditions, i.e., product extraction column, were derived by Rozen (*1*). Moreover, he examined the influence of some parameters on the degree of separation in the column. The dependencies obtained in Ref. *1* were general for the separation of both isotope gas mixtures and mixtures consisting of gases with similar physical properties. When such mixtures separate, the coefficient of separation $q \rightarrow 1$ and the coefficient of enrichment $\epsilon \rightarrow 0$. In that case, the dependencies are simple, but they do not reflect all the processes in the thermal diffusion column (TDC). Moreover, those dependencies misrepresent the process of separation of mixtures of quite different gases.

The aim of the present work is to provide a more general examination of the processes of separation of several binary gas mixtures in TDC and to derive more general and more universal dependencies than those in Ref. *1*. This will make it possible to account for all the parameters that exert an influence on the degree of separation.

This work is a continuation of our previous work (*2*) which examined identical problems of TDC under steady-state conditions (taking no product from the column).

2. FLOWS IN THE THERMAL DIFFUSION COLUMNS AND RELATIVE EXTRACTION

2.1. Flows in TDC

A single TDC and a thermal diffusion cascade (TD-cascade) are shown schematically in Figs. 1 and 2, respectively. The gas flows in a single column or in the individual stages of a cascade are shown in the two figures.

Using the material balance of the TDC or TD-cascade, it can be shown that

$$L_0 = P + W = (L - G) + (G - L_f) \quad (1)$$

$$L_0 x_0 = P x_p + W x_w \quad (2)$$

Under dynamic working conditions, TDC (TD-cascade) is assumed to consist of two connected columns (cascades) which we will call lower and upper. If the product of the separation is only the heavier gas (with larger molecular weight), the lower column appears to be concentrating while the upper column is extracting, and if the lighter gas is extracting, the picture is just the opposite. In fact, for each case it can be accepted that the upper column is concentrating the light gas while the lower column is concentrating the heavy gas. In the present work, this convention is adopted. For convenience, the derivation of the equations concerning the upper column (cascade) will appear on the left-hand side of the printed page while those concerning the lower column will appear on the right-hand side. Expressions common to both parts of the column will be written in the middle of the page. We will use the concentrations of the light gas in the derivations for the upper column (cascade) and the concentrations of the heavy gas in the derivations for the lower column.

2.2. Equilibrium Curve and Equation of Working Line

The equilibrium curve for binary gas mixture is shown to be described by the equation (*1*):

$$y_e = \frac{x}{q - (q - 1)x} = \frac{(1 - \epsilon)x}{1 - \epsilon x} \qquad y_e = \frac{qx}{1 + (q - 1)x} = \frac{x}{1 - \epsilon(1 - x)} \quad (3)$$

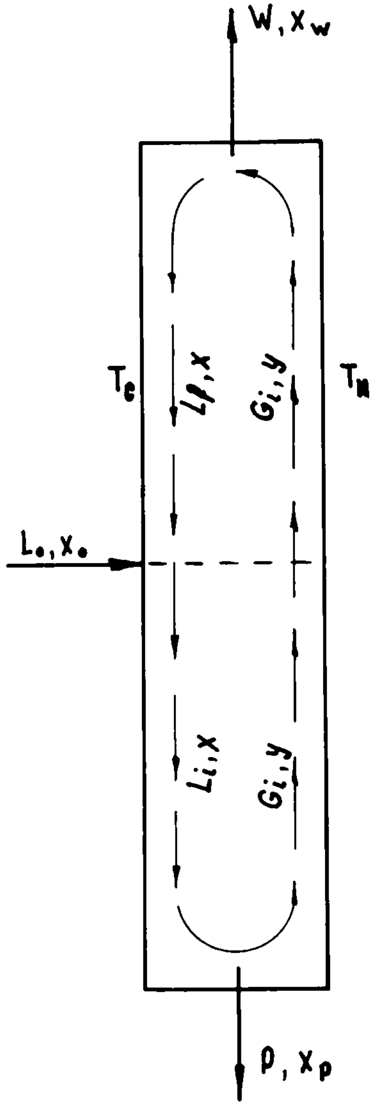

FIG. 1. Scheme of gas flows in a single TDC.

where

$$q = (T_H/T_C)^{\alpha_T} \tag{4}$$

$$\epsilon = (q - 1)/q \tag{5}$$

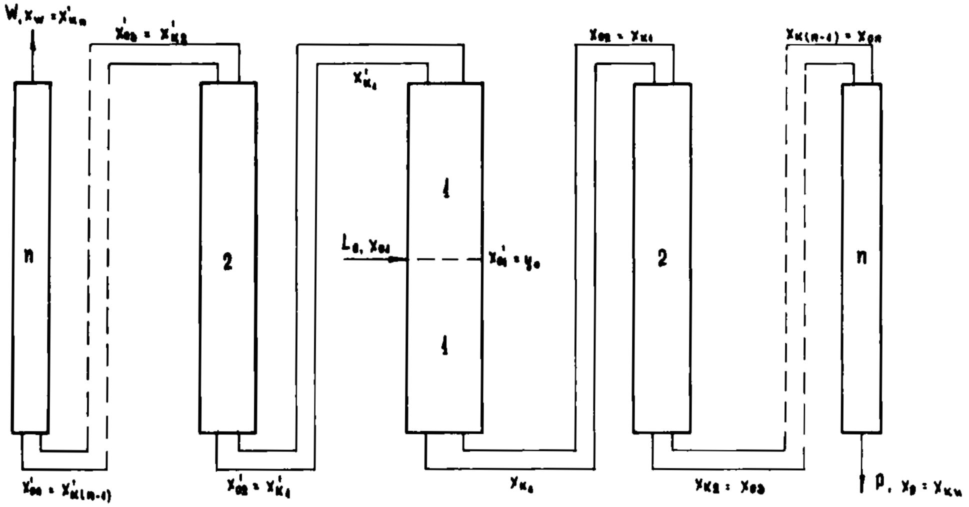

FIG. 2. Scheme of gas flows in a TD-cascade.

Under steady-state conditions, the equation of the working line was given by the expression (see Ref. *1*)

$$y = x$$

This is the diagonal in the x–y diagram of the process (see Position 2 of Figs. 3a and 3b). Under dynamic conditions the picture is different. From

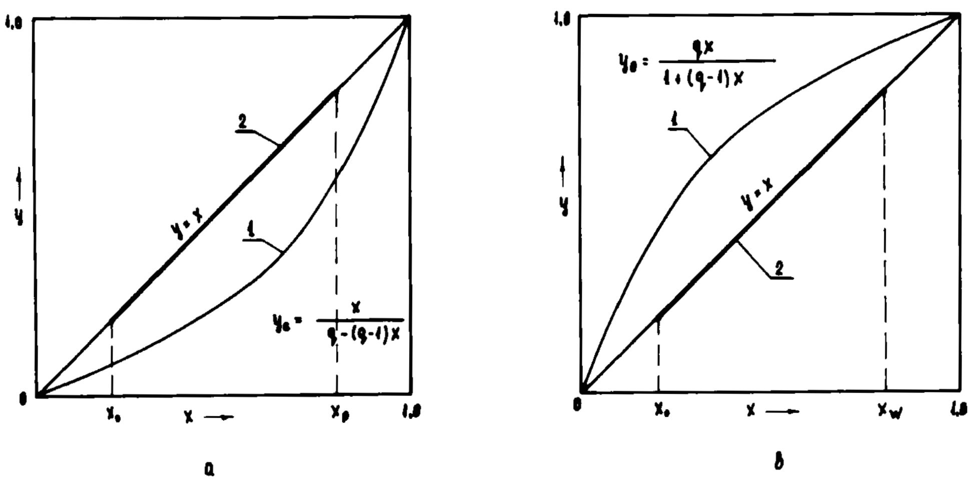

FIG. 3. Presentation of the processes of separation in TDC and TD-cascade in x–y coordinates under static conditions for: (a) lower column (cascade); (b) upper column (cascade).

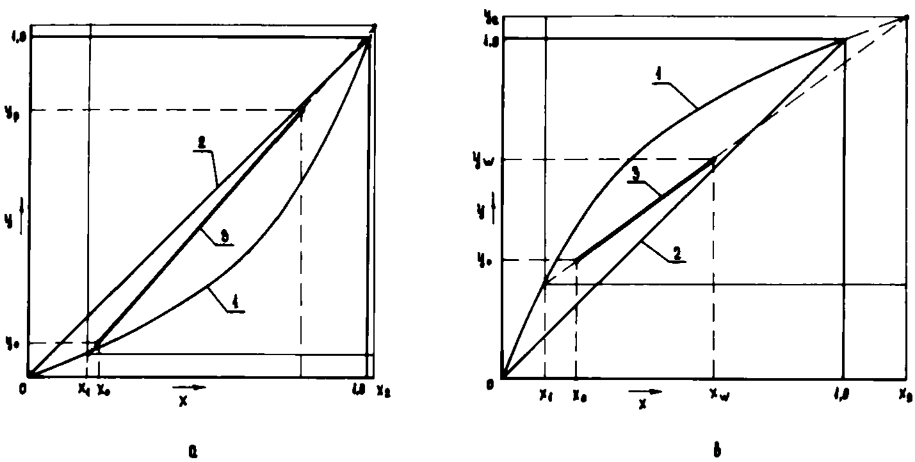

FIG. 4. Presentation of the processes of separation in TDC and TD-cascade in x–y coordinates under dynamic conditions for: (a) lower column (cascade); (b) upper column (cascade).

the material balance of either of the columns (cascades)—upper and lower—the following expressions can be obtained (*1*) (see Curve 3 of Figs. 4a and 4b).

$$Px_p = Lx - Gy \qquad Wx_w = Gy - L_f x \tag{6}$$

From Eq. (6), after elementary transformations are obtained:

$$y = \lambda x - (\lambda - 1)x_p \qquad y = \lambda_f x - (\lambda_f - 1)x_w \tag{7}$$

where

$$\lambda = L/G \qquad \lambda_f = L_f/G \tag{8}$$

$$\lambda - 1 = P/G \qquad \lambda_f - 1 = W/G \tag{9}$$

2.3. Relative Extraction

If L_0, x_p, x_w, and x_0 (for column from cascade x_{0i}) are given, the productivity of the TDC (the TD-cascade) with respect to the quantity of extracted product (Px_p or Wx_w) will depend only on the molar concentration of the extracted gas in the gas flow going up at the inlet of the respective column (y_0). The lower value of y_0 in Eq. (3) will give smaller value of Gy and higher values for both Px_p and Wx_w. Consequently, the productivity of the TDC will also be larger. As the concentration of the extraction gas in the convective flow going up cannot be lower than equilibrium concentration, the maximum productivity of the column with respect to the extraction product will correspond to $y = y_e(y_0)$ (*1*). If we denote

$$P_{\max} = P_0 \qquad W_{\max} = W_0$$

and take into consideration Eqs. (1), (2), and (3) for each column of the cascade or for the single column from Eq. (6), we obtain

$$P_{0i} = \frac{x_{0i} - y_e}{x_p - x_{0i}} = \frac{G_i \epsilon_i x_{0i}(1 - x_{0i})}{(x_p - x_{0i})(1 - \epsilon_i - x_{0i})} = \frac{L_i \epsilon_i x_{0i}(1 - x_{0i})}{x_p - x_{0i}[1 - \epsilon_i(1 - x_p)]} \tag{10}$$

$$W_{0i} = \frac{y_e - x_{0i}}{x_w - x_{0i}} = \frac{G_i \epsilon_i x_{0i}(1 - x_{0i})}{(x_w - x_{0i})[1 - \epsilon_i(1 - x_{0i})]} = \frac{L_{fi} \epsilon_i x_{0i}(1 - x_{0i})}{[1 - \epsilon_i(1 - x_{0i})]x_w - x_{0i}} \tag{10}$$

According to Ref. *1*, the relationship between the real and utmost productivity is called relative extraction, so that for the *i*th stage in TD-cascade or for a single column:

$$\theta_i = P/P_{0i} \qquad \theta_i = W/W_{0i} \tag{11}$$

It is obvious that $0 < \theta < 1$. After that, from Eqs. (10) and (11) the following expressions for the convection flows in TDC are obtained:

$$L_i = P\frac{x_p - x_{0i}[1 - \epsilon_i(1 - x_p)]}{\theta_i \epsilon_i x_{0i}(1 - x_{0i})} \tag{12}$$

$$G_i = P\frac{(x_p - x_{0i})[1 - \epsilon_i(1 - x_{0i})]}{\theta_i \epsilon_i x_{0i}(1 - x_{0i})} \tag{13}$$

$$L_{fi} = W\frac{[1 - \epsilon_i(1 - x_{0i})]x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})} \quad (12)$$

$$G_i = W\frac{(x_w - x_{0i})[1 - \epsilon_i(1 - x_{0i})]}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})} \quad (13)$$

In general, Expressions (12) and (13) are relatively complicated, but for certain regions of application they are considerably simplified. In fact, all cases of interest for the practice can be reduced to four.

1) Low concentrations of extraction gas ($x << 1$) and low degree of separation in TDC or TD-cascade when considered from the current to the final stage (this is a typical case for the final 1–3 stages of TD-cascade).

$x_{0i}/x_p > 0.1$ and $x_p < 0.5$ $\qquad$ $x_{0i}/x_w > 0.1$ and $x_w < 0.5$

For $x << 1$, it can be assumed that $1 - x \approx 1$ and Expressions (12) and (13) are simplified to

$$L_i \cong P\frac{x_p - (1 - \epsilon_i)x_{0i}}{\theta_i\epsilon_i x_{0i}} \qquad L_{fi} \cong W\frac{(1 - \epsilon_i)x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}}$$

$$G_i \cong P\frac{x_p - x_{0i}}{\theta_i\epsilon_i x_{0i}} \qquad G_i \cong W\frac{(x_w - x_{0i})(1 - \epsilon_i)}{\theta_i\epsilon_i x_{0i}}$$

If $\epsilon << 1$, then $1 - \epsilon$ is negligible and can be ignored. After that, Expressions (12) and (13) are reduced to the well-known forms (*1*)

$$L_i \cong P\frac{x_p - x_{0i}}{\theta_i\epsilon_i x_{0i}} \qquad L_{fi} \cong W\frac{x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}}$$

$$G_i \cong P\frac{x_p - x_{0i}}{\theta_i\epsilon_i x_{0i}} \qquad G_i \cong W\frac{x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}}$$

2) Moderate concentrations of final products and not a very high degree of separation (comparable to Part 1).

$x_{0i}/x_p > 0.1$ and $0.05 \leq x_p \leq 0.95$

$x_{0i}/x_w > 0.1$ and $0.05 \leq x_w \leq 0.95$

In this case, it can be assumed with sufficient accuracy that

$$L_i \cong P\frac{x_p - (1 - \epsilon_i)x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})} \qquad L_{fi} \cong W\frac{(1 - \epsilon_i)x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})}$$

$$G_i \cong P\frac{x_p - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})} \qquad G_i \cong W\frac{(x_w - x_{0i})(1 - \epsilon_i)}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})}$$

If, however, $x_{0i} > 0.5$, for higher precision the following expressions can be used:

$$L_i \cong P\frac{x_p - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})} \qquad L_{fi} \cong W\frac{x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})}$$

$$G_i \cong P\frac{(x_p - x_{0i})(1 - \epsilon_i x_{0i})}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})} \qquad G_i \cong W\frac{x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})}$$

If $\epsilon << 1$:

$$L_i \cong G_i \cong P\frac{x_p - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})} \qquad L_{fi} \cong G_i \cong W\frac{x_w - x_{0i}}{\theta_i\epsilon_i x_{0i}(1 - x_{0i})}$$

3) Arbitrary concentration of final products and high degrees of separation in TDC or in TD-cascade, comparable to Part 1.

$$x_{0i}/x_p > 0.1 \qquad x_{0i}/x_w > 0.1$$

Since under these conditions

$$x_{0i} << x_p < 1 \qquad x_{0i} << x_p < 1$$

it can be assumed that $1 - x \approx 1$, and

$$x_p - x_{0i} \approx x_p \qquad x_w - x_{0i} \approx x_w$$

Using these approximations, Expressions (12) and (13) are simplified to

$$L_i \cong G_i \cong Px_p/\theta_i\epsilon_i x_{0i} \qquad L_{fi} \cong G_i \cong Wx_w(1 - \epsilon_i)/\theta_i\epsilon_i x_{0i}$$

For $\epsilon_i << 1$, the part $1 - \epsilon_i$ in the expression for the upper column can be neglected.

4) High concentration of final products for arbitrary degrees of separation.

$$x_p > 0.95 \qquad x_w > 0.95$$

For such high concentrations of the final products it can be assumed that $x_p \approx 1$ and $x_w \approx 1$. In this case, Expressions (12) and (13) are simplified even more:

$$L_i \cong G_i \cong P/\theta_i \epsilon_i x_{0i} \qquad L_{fi} \cong G_i \cong W(1 - \epsilon_i)/\theta_i \epsilon_i x_{0i}$$

As for $\epsilon_i << 1$, the term $1 - \epsilon_i$ can be neglected.

2.4. Shortening of the Convection Flows in TD-Cascade

For a concrete problem, the values of P, W, θ, x_p, and x_w are known, and in this case from Expressions (12) and (13) it follows that L_i, L_{fi}, and G_i are functions of x_{0i}, and to a first-order approximation there are $\sim 1/x_{0i}$. The result from this is that the longitudinal section of the ideal TDC or TD-cascade must approximately look as shown in Fig. 5(a). The practical realization of this TDC or TD-cascade is very hard to fulfill, and in some cases it is impossible. The TDC or the stage in the cascade usually has a constant section along the height of the column, and the real cascade looks approximately as shown in Fig. 5(b), while the convectional flows

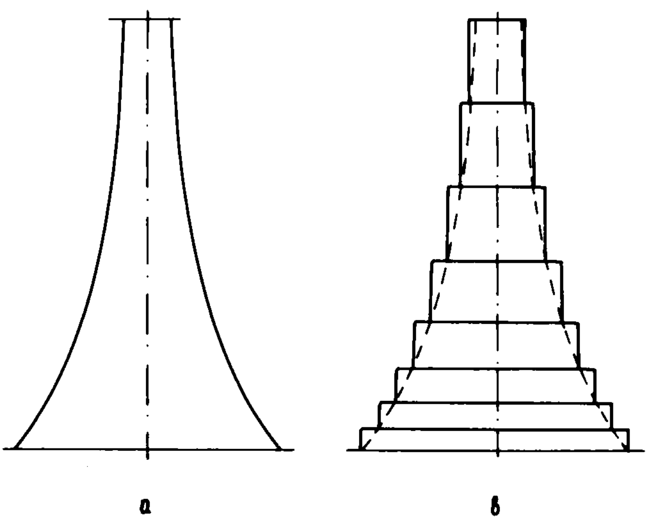

FIG. 5. Schematic setup of TD-cascade: (a) ideal cascade; (b) real orthogonal cascade.

in the separate stages decrease as one moves away from the inlet point of the initial gas mixture.

If expressions (12) and (13) are written as

$$L_i = A_{Li}P/\theta_i\epsilon_i x_{0i} \qquad L_{fi} = A_{Li}W/\theta_i\epsilon_i x_{0i} \tag{14}$$

$$G_i = A_{Gi}P/\theta_i\epsilon_i x_{0i} \qquad G_i = A_{Gi}W/\theta_i\epsilon_i x_{0i} \tag{15}$$

where

$$A_{Li} = \frac{x_p - x_{0i}[1 - \epsilon_i(1 - x_p)]}{1 - x_{0i}} \tag{16}$$

$$A_{Gi} = \frac{(x_p - x_{0i})(1 - \epsilon_i x_{0i})}{1 - x_{0i}} \tag{17}$$

$$1A_{Li} = \frac{[1 - \epsilon_i(1 - x_{0i})]x_w - x_{0i}}{1 - x_{0i}}A_{Gi}x_{0i} \quad (16)$$

$$A_{Gi} = \frac{(x_w - x_{0i})[1 - \epsilon_i(1 - x_{0i})]}{1 - x_{0i}} \quad (17)$$

the shortening of the convectional flows in the cascade, σ, under the orthogonal cascade (see Fig. 5b) will be obvious (see also Ref. *1*).

$$\sigma_{Li} = L_i/L_{i+1} = \frac{A_{Li}\theta_{i+1}\epsilon_{i+1}x_{0(i+1)}}{A_{L(i+1)}\theta_i\epsilon_i x_{0i}} \tag{18}$$

$$\sigma_{Gi} = G_i/G_{i+1} = \frac{A_{Gi}\theta_{i+1}\epsilon_{i+1}x_{0(i+1)}}{A_{G(i+1)}\theta_i\epsilon_i x_{0i}} \tag{19}$$

For $\epsilon \to 0$ ($q \to 1$), Eqs. (16) and (17) are greatly simplified:

$$A_{Li} = \frac{x_p - x_{0i}}{1 - x_{0i}} \qquad A_{Li} = \frac{x_w - x_{0i}}{1 - x_{0i}}$$

$$A_{Gi} = \frac{x_p - x_{0i}}{1 - x_{0i}} \qquad A_{Gi} = \frac{x_w - x_{0i}}{1 - x_{0i}}$$

The degree of separation Q in an apparatus for gas separation is defined as (see Refs. 1 and 2)

$$Q = Q_L Q_H = (x_{L1}/x_{L2})(x_{H2}/x_{H1}) \tag{20}$$

where

$$Q_L = x_{L1}/x_{L2} \tag{21}$$

$$Q_H = x_{H2}/x_{H1} \tag{22}$$

$$x_{L1} = 1 - x_{H1} \tag{23}$$

$$x_{L2} = 1 - x_{H2} \tag{24}$$

From Eqs. (21) and (22) it follows that for the ith stage in a TD-cascade (see Fig. 2):

$$Q_{Hi} = x_{0(i+1)}/x_{0i} \qquad Q_{Hi} = (1 - x_{0i})/(1 - x_{0(i+1)}) \tag{25}$$

$$Q_{Li} = (1 - x_{0i})/(1 - x_{0(i+1)}) \qquad Q_{Li} = x_{0(i+1)}/x_{0i} \tag{26}$$

Furthermore, even though ϵ_i depends on x_{0i}, for small differences in the absolute values of x_{0i} as is the case in adjacent stages in the TD-cascades, it can be accepted that $\epsilon_{i+1} \cong \epsilon_i$ for each couple of two adjacent stages in the TD-cascade. Taking this into account, and Expressions (25) and (26), Eqs. (18) and (19) can be simplified to

$$\sigma_{Li} = \frac{A_{Li}\theta_{i+1}}{A_{L(i+1)}\theta_i} Q_{Hi} \qquad \sigma_{Li} = \frac{A_{Li}\theta_{i+1}}{A_{L(i+1)}\theta_i} Q_{Li} \tag{27}$$

$$\sigma_{Gi} = \frac{A_{Gi}\theta_{i+1}}{A_{G(i+1)}\theta_i} Q_{Li} \qquad \sigma_{Gi} = \frac{A_{Gi}\theta_{i+1}}{A_{G(i+1)}\theta_i} Q_{Hi} \tag{28}$$

Usually $\theta = 0.7 \div 0.9$ (see Ref. 1), and since in adjoining stages of the cascade the conditions are similar, it can be assumed with sufficient accuracy that $\theta_i \cong \theta_{i+1}$. Then, from Eqs. (18) and (19) one finally obtains

$$\sigma_{Li} = \frac{A_{Li}}{A_{L(i+1)}} Q_{Hi} \qquad \sigma_{Li} = \frac{A_{Li}}{A_{L(i+1)}} Q_{Li} \tag{29}$$

$$\sigma_{Gi} = \frac{A_{Gi}}{A_{G(i+1)}} Q_{Li} \qquad \sigma_{Gi} = \frac{A_{Gi}}{A_{G(i+1)}} Q_{Hi} \tag{30}$$

For the four particular cases defined above, Eqs. (16), (17), (29), and (30) are essentially simplified.

1) $x_{0i}/x_p > 0.1$ and $x_p < 0.5$ $\quad$ $x_{0i}/x_w > 0.1$ and $x_w < 0.5$

Under $x << 1$:

$$A_{Li} \cong x_p - (1 - \epsilon_i)x_{0i} \qquad A_{Li} \cong (1 - \epsilon_i)x_w - x_{0i}$$

$$A_{Gi} \cong x_p - x_{0i} \qquad A_{Gi} \cong (1 - \epsilon_i)(x_w - x_{0i})$$

$$Q_{Li} \cong 1 \qquad Q_{Hi} \cong 1$$

$$Q_{Hi} \cong Q_i \qquad Q_{Li} \cong Q_i$$

and respectively

$$\sigma_{Li} \cong \frac{q_i x_p - x_{0i}}{q_{i+1}x_p - x_{0(i+1)}} Q_i \qquad \sigma_{Li} \cong \frac{x_w - q_i x_{0i}}{x_w - q_{i+1}x_{0(i+1)}} Q_i$$

$$\sigma_{Gi} \cong \frac{x_p - x_{0i}}{x_p - x_{0(i+1)}} Q_i \qquad \sigma_{Gi} \cong \frac{x_w - x_{0i}}{x_w - x_{0(i+1)}} Q_i$$

For $q_i \rightarrow 1$ ($\epsilon_i \rightarrow 0$):

$$\sigma_{Li} \cong \sigma_{Gi}$$

2) $x_{0i}/x_p > 0.1$ and $0.05 \leq x_p \leq 0.95$

$x_{0i}/x_w > 0.1$ and $0.05 \leq x_w \leq 0.95$

$$A_{Li} \cong \frac{x_p - x_{0i}}{1 - x_{0i}} \qquad A_{Li} \cong \frac{(1 - \epsilon_i)x_w - x_{0i}}{1 - x_{0i}}$$

$$A_{Gi} \cong \frac{x_p - x_{0i}}{1 - x_{0i}} \qquad A_{Gi} \cong \frac{(1 - \epsilon_i)(x_w - x_{0i})}{1 - x_{0i}}$$

$$\sigma_{Li} \cong \frac{x_p - x_{0i}}{x_p - x_{0(i+1)}} \frac{Q_{Hi}}{Q_{Li}} \qquad \sigma_{Li} \cong \frac{x_w - q_i x_{0i}}{x_w - q_{i+1}x_{0(i+1)}} \frac{Q_{Li}}{Q_{Hi}}$$

$$\sigma_{Gi} \cong \frac{x_p - x_{0i}}{x_p - x_{0(i+1)}} \frac{Q_{Hi}}{Q_{Li}} \qquad \sigma_{Gi} \cong \frac{x_w - x_{0i}}{x_w - x_{0(i+1)}} \frac{Q_{Li}}{Q_{Hi}}$$

For $q_i \rightarrow 1$ ($\epsilon_i \rightarrow 0$) and in the upper column, $\sigma_{Li} = \sigma_{Gi}$.

3) $x_{0i}/x_p > 0.1$ $\qquad x_{0i}/x_w > 0.1$

Under a high degree of separation

$$A_{Li} \cong A_{Gi} \cong x_p \qquad A_{Li} \cong A_{Gi} \cong (1 - \epsilon_i)x_w$$

$$\sigma_{Li} \cong \sigma_{Gi} \cong Q_{Hi} \qquad \sigma_{Li} \cong \sigma_{Gi} \cong Q_{Li}$$

For Case *4*:

$$x_p > 0.95 \qquad x_w > 0.95$$

$$A_{Li} \cong A_{Gi} \cong 1 \qquad A_{Li} \cong A_{Gi} \cong 1 - \epsilon_i$$

$$\sigma_{Li} \cong \sigma_{Gi} \cong Q_{Hi} \qquad \sigma_{Li} \cong \sigma_{Gi} \cong Q_{Li}$$

If, furthermore, $x_{0i} > 0.9$, it can be assumed that

$$Q_{Hi} \cong 1 \qquad Q_{Li} \cong 1$$

and, respectively,

$$\sigma_{Li} \cong \sigma_{Gi} \cong 1 \qquad \sigma_{Li} \cong \sigma_{Gi} \cong 1$$

As can be seen from the last equations, for high concentrations of the final products, the convection flows stay practically constant.

3. DEGREE OF SEPARATION IN TDC

The degree of separation in TDC in static conditions (no gas production) can be defined by using the formula of Fenske (*3*):

$$Q_0 = q^{N_T} \tag{31}$$

as well as by using the formula suggested by Rozen (*1*) and modified by the authors (*2*):

$$\ln Q_0 = \epsilon(N + \ln Q_L) = \bar{\epsilon}N \tag{32}$$

where

$$\bar{\epsilon} = \epsilon/[1 - \epsilon/(1 + m)] \tag{33}$$

$$m = \ln Q_H/\ln Q_L \tag{34}$$

For TDC working in dynamic conditions (with product extraction), the determination of the degree of separation, Q, cannot be done using the above formulas. According to Rozen (*1*), their application is possible if X–Y coordinates are used for the graphic description of the process in TDC instead of the conventional x–y coordinates (see Figs. 3 and 4). X and Y are defined as

$$X = (x - x_1)/(x_2 - x_1) \tag{35}$$

$$Y = (y - y_1)/(y_2 - y_1) \tag{36}$$

In Eqs. (35) and (36), (x_1,y_1) and (x_2,y_2) are denoted as the coordinates of the intersection points of the equilibrium and working lines, shown in Figs. 4(a) and 4(b). In fact, they are the roots of the equation

$$y - y_e = 0 \tag{37}$$

or taking into account Eqs. (2) and (3),

$$\lambda x - (\lambda - 1)x_p - (1 - \epsilon)x/(1 - \epsilon x)$$

$$\lambda_f x - (\lambda_f - 1)x_w - x/[1 - \epsilon\,(1 - x)] \tag{38}$$

In the new coordinates, the equation of the working line is transformed into (for more details see Ref. *1*)

$$Y = X \tag{39}$$

Obviously this equation is described by the diagonal of the X–Y diagram, as it is in the x–y diagram under static conditions. This circumstance also permits the use of Eq. (32) under dynamic conditions.

As shown in Ref. *1*, in X–Y coordinates, Eq. (3) is transformed into

$$Y_e = \frac{X}{q^* - (q^* - 1)X} \qquad Y_e = \frac{q^*X}{1 + (q^* - 1)X}$$

$$= \frac{(1 - \epsilon^*)X}{1 - \epsilon^*X} \qquad \frac{X}{1 - \epsilon^*\,(1 - X)} \tag{40}$$

It is not difficult to show that

$$q^* = \frac{q - (q - 1)x_1}{q - (q - 1)x_2} \qquad q^* = \frac{q + (q - 1)x_2}{q + (q - 1)x_1}$$

$$= \frac{1 - \epsilon x_1}{1 - \epsilon x_2} \qquad = \frac{1 - \epsilon(1 - x_2)}{1 - \epsilon(1 - x_1)} \tag{41}$$

$$\epsilon^* = \frac{q^* - 1}{q^*} \qquad \epsilon^* = \frac{q^* - 1}{q^*}$$

$$= \frac{\epsilon(x_2 - x_1)}{1 - \epsilon x_1} \qquad = \frac{\epsilon(x_2 - x_1)}{1 - \epsilon(1 - x_2)} \tag{42}$$

For the determination of x_1 and x_2, Eq. (38) has to be solved. For this, x_2 is transformed by taking into account Eqs. (7), (8), (9), (12), and (13). As a result, the following quadratic equation is obtained:

$$x^2 + Fx + R = 0 \tag{43}$$

for the ith stage in the TD-cascade, as well as for a single TDC:

$$F_i = 1 + \theta_i x_{0i}(A_i^* + 1) \tag{44}$$

$$R_i = \theta_i x_{0i}(1 + x_{0i}A_i^*) \tag{45}$$

$$A_i^* = \frac{(1 - \epsilon_i)(1 - x_p)}{x_p - x_{0i}[1 - \epsilon_i(1 - x_p)]}$$

$$A_i^* = \frac{1 - x_w}{[1 - \epsilon_i(1 - x_{0i})]x_w - x_{0i}} \tag{46}$$

The solution of the quadratic equation (43) presents no difficulty. As a result, the following expressions for x_{1i} and x_{2i} are obtained:

$$x_{1i} = \theta_i x_{0i}\{1 + a_i^*[1 + \theta_i x_{0i}[A_i^* - 1)]/2\theta_i x_{0i}\} \tag{47}$$

$$x_{2i} = 1 + \theta_i x_{0i} A_i^*\{1 - a_i^*[1 + \theta_i x_{0i}(A_i^* - 1]/2\theta_i x_{0i} \tag{48}$$

where

$$a_i^* = 1 - \{1 - 4(1 - \theta_i)\theta_i x_{0i}^2 A_i^*/[1 + \theta_i x_{0i}(A_i^* - 1)]^2\}^{1/2} \tag{49}$$

Analysis of Eq. (49) shows that

$$4(1 - \theta_i)\theta_i \leq 1$$

$$x_{0i}A_i^* < 1$$

$$0.9 < 1 + \theta_i x_{0i}(A_i^* - 1) < 2$$

from which it follows that

$$a_i^* << 1$$

$$0.5a_i^*[1 + \theta_i x_{0i}(A_i^* - 1)] << \theta_i x_{0i} < 1$$

$$0.5a_i^*[1 + \theta_i x_{0i}(A_i^* - 1)] << \theta_i x_{0i} A_i^* < 1$$

With this in mind, and an error within 5%, it can be shown that

$$x_{1i} \cong \theta_i x_{0i} \quad (50)$$

$$x_{2i} \cong 1 + \theta_i x_{0i} A_i^* \quad (51)$$

Only for low degrees of separation and low concentrations can the determination of x using Eq. (50) have an error of more than 5%. This possibility will be assumed below.

For the four particular cases described above, Eqs. (46), (50), and (51) are modified as follows.

1) $x_{0i}/x_p > 0.1$ and $x_p < 0.5$ $\qquad$ $x_{0i}/x_w > 0.1$ and $x_w < 0.5$

As shown above, if x_{1i} is calculated from Eq. (50), in some cases the error can be higher than 5%. On the other hand, Expression (47) is rather complicated and inconvenient for practial application. However, for $x <<$ 1 for the point whose coordinates are x_1 and y_1, the equation of the equilibrium line can be approximated with a straight line.

$$y_e \cong (1 - \epsilon)x \qquad y_e \cong qx \quad (52)$$

In this case, Eq. (38) can be written as

$$\lambda x - (\lambda - 1)x - (1 - \epsilon)x = 0$$

$$\lambda_f x - (\lambda_f - 1)x - qx = 0 \quad (53)$$

Taking into account Eqs. (8), (9), (12), and (13), from Eq. (53) the expression for x_{1i} is obtained:

$$x_{1i} = \theta_i x_{0i}/[1 - (1 - \theta_i)x_{0i}/q_i x_p]$$

$$x_{1i} = \theta_i x_{0i}/[1 - (1 - \theta_i)q_i x_{0i}/x_w] \quad (54)$$

From the properties of quadratic equations, it is known that

$$F_i = x_{1i} + x_{2i} \quad (55)$$

If x_{2i} is calculated from Eqs. (54) and (55), Expression (51) will be obtained again, as in this case

$$A_i^* \cong 1/(q_i x_p - x_{0i}) \qquad A_i^* \cong 1/[(1 - \epsilon_i)x_w - x_{0i}]$$

from which it follows that

$$x_{2i} \cong 1 + \theta_i x_{0i}/(q_i x_p - x_{0i}) \qquad x_{2i} \cong 1 + \theta_i x_{0i}/[(1 - \epsilon_i)x_w - x_{0i}]$$

2) $x_{0i}/x_p > 0.1$ and $0.05 \leq x_p \leq 0.95$

$x_{0i}/x_w > 0.1$ and $0.05 \leq x_w \leq 0.95$

In this case the expression for A_i^* is reduced to

$$A_i^* \cong (1 - x_p)/(q_i x_p - x_{0i}) \qquad A_i^* \cong (1 - x_w)/[(1 - \epsilon_i)x_w - x_{0i}]$$

and respectively

$$x_{1i} \cong \theta_i x_{0i}$$

$$x_{2i} \cong 1 + \theta_i x_{0i}(1 - x_p)/(q_i x_p - x_{0i})$$

$$x_{2i} \cong 1 + \theta_i x_{0i}(1 - x_w)/[(1 - \epsilon_i)x_w - x_{0i}]$$

If $q > 1.1$ and

$$x_p > 0.5 \qquad x_{0i} > 0.5$$

the determination of A_i^* and x_{2i} can be made from the more exact equations

$$A_i^* \cong (1 - x_p)/q_i(x_p - x_{0i}) \qquad A_i^* \cong (1 - x_w)/(x_w - x_{0i})$$

$$x_{2i} \cong 1 + \theta_i x_{0i}(1 - x_p)/q_i(x_p - x_{0i})$$

$$x_{2i} \cong 1 + \theta_i x_{0i}(1 - x_w)/(x_w - x_{0i})$$

3) $x_{0i}/x_p > 0.1 \qquad x_{0i}/x_w > 0.1$

For high degrees of separation:

$$A_i^* \cong (1 - x_p)/q_i x_p \qquad A_i^* \cong (1 - x_w)/(1 - \epsilon_i)x_w$$

As a result of this, it can be shown that

$$\theta_i x_{0i} A_i^* << 1$$

and then

$$x_{1i} \cong \theta_i x_{0i}$$

$$x_{2i} \cong 1$$

4) $x_p > 0.95 \qquad x_w > 0.95$

It is not difficult to see that for high concentrations

$$A_i^* \cong 0$$

and then

$$x_{1i} \cong \theta_i x_{0i}$$

$$x_{2i} \cong 1$$

As x_{1i} and x_{2i} are known, an analytical expression for the degree of separation under dynamic conditions can be deduced. From Eq. (20) it follows that the degree of separation in X–Y coordinates can be written

$$Q_i^* = X_{ki}(1 - X_{0i})/X_{0i}(1 - X_{ki}) \tag{56}$$

For the upper column and for each column from the upper cascade, the gas mixture to be separated goes in at the bottom of the TDC and the extracted gas goes out at the top. For the lower column and each column from the lower cascade, the inlet is at top and the outlet is at the bottom of the TDC.

Taking into account Eq. (35), Expression (56) has the form

$$Q_i^* = \frac{(x_{ki} - x_{1i})(x_{2i} - x_{0i})}{(x_{0i} - x_{1i})(x_{2i} - x_{ki})} \tag{57}$$

On the other hand, from Eqs. (22), (23), and (28) it follows that (see Ref. *1*)

$$\ln (Q_{Hi}^* Q_{Li}^{*(1-\epsilon_i^*)}) = \epsilon_i^* N_i = \mu_i \epsilon_i N_i = \mu_i \ln (Q_{Hi} Q_{Li}^{(1-\epsilon)}) \tag{58}$$

where

$$\mu_i = (x_{2i} - x_{1i})/(1 - \epsilon_i x_{1i})$$

$$\mu_i = (x_{2i} - x_{1i})/[1 - \epsilon_i(1 - x_{2i})] \tag{59}$$

$$Q_{0i} \cong Q_{Hi} Q_{Li} \tag{60}$$

In this situation it can be assumed that

$$\ln Q_i^* = \mu_i \ln Q_{0i} \tag{61}$$

The degree of separation in TDC, using x–y coordinates, can be written (see Eq. 20) as

$$Q = x_{ki}(1 - x_{0i})/x_{0i}(1 - x_{ki}) \tag{62}$$

and then from Eqs. (57), (58), (60), and (62), after some transformations, the following expression is obtained for the degree of separation under dynamic conditions:

$$Q_i - 1 = (Q_{0i}^{\mu_i} - 1) k_{xi} k_{ri} \tag{63}$$

where

$$k_{xi} = (1 - x_{1i}/x_{0i})/(1 - x_{1i}) \tag{64}$$

$$k_{ri} = 1 \bigg/ \left[1 - Q_{0i} \frac{(x_{2i} - 1)(x_{0i} - x_{1i})}{(x_{2i} - x_{0i})(1 - x_{1i})} \right] \tag{65}$$

Equations (59), (63), (64), and (65) for each of above described particular cases (keeping in mind the values of x_{1i} and x_{2i}) are

1) $x_{0i}/x_p > 0.1$ and $x_p < 0.5$ $\qquad$ $x_{0i}/x_w > 0.1$ and $x_w < 0.5$

$$\mu_i \cong x_{2i}$$

$$k_{xi} \cong (1 - \theta_i)(1 - \theta_i x_{0i}/q_i x_p) \qquad k_{xi} \cong (1 - \theta_i)(1 - x_{0i}/x_w)$$

$$k_{ri} \cong 1$$

$$Q_i - 1 \cong (Q_{0i}^{x_{2i}} - 1)(1 - \theta_i)(1 - \theta_i x_{0i}/q_i x_p)$$

$$Q_i - 1 \cong (Q_{0i}^{x_{2i}} - 1)(1 - \theta_i)(1 - x_{0i}/x_w)$$

2) $x_{0i}/x_p > 0.1$ and $0.05 \le x_p \le 0.95$

$x_{0i}/x_w > 0.1$ and $0.05 \le x_w \le 0.95$

$$\mu_i \cong x_{2i} - x_{1i}$$

$$k_{xi} \cong (1 - \theta_i)/(1 - \theta_i x_{0i})$$

$$k_{ri} \cong 1 \bigg/ \left[1 - Q_{0i}^{\mu_i} \frac{(1 - \theta_i)\theta_i x_{0i}^2 A_i^*}{(x_{2i} - x_{0i})(1 - \theta_i x_{0i})}\right]$$

$$Q_i - 1 \cong (Q_{0i}^{\mu_i} - 1)(1 - \theta_i)k_{ri}/(1 - \theta_i x_{0i})$$

3) $x_{0i}/x_p > 0.1$ $\qquad$ $x_{0i}/x_w > 0.1$

In this case $Q_i >> 1$ and $Q_{0i} >> 1$, so that

$$\mu_i \cong 1$$

$$k_{xi} \cong 1$$

$$k_{ri} \cong 1 - \theta_i$$

$$Q_i \cong Q_{0i}(1 - \theta_i)$$

4) $x_p > 0.95$ $x_w > 0.95$

$$\mu_i \cong 1 - \theta_i x_{0i}$$

$$k_{xi} \cong (1 - \theta_i)/(1 - \theta_i x_{0i})$$

$$k_{ri} \cong 1$$

$$Q_i - 1 \cong (Q_{0i}^{x_{2ii}} - 1)(1 - \theta_i)/(1 - \theta_i x_{0i})$$

Further, from Eqs. (63), (64), and (65), it is obvious that for concrete TDC:

$$Q_i = f(Q_{0i},\theta_i,x_{0i}) \quad (66)$$

On the other hand, having shown in Ref. *2* that

$$Q_i = f(x_{0i},\alpha_T,T_H^*,T_C^*,p,h,\delta,k_{pi}) \quad (67)$$

and using Eqs. (12) and (13), it can be written that

$$\theta_i = f(L,P,x_{0i},\alpha_T,T_H^*,T_C^*,p,x_p)$$

$$\theta_i = f(L_f,W,x_{0i},\alpha_T,T_H^*,T_C^*,p,x_w) \quad (68)$$

Analysis of Eqs. (66), (67), and (68) shows that the degree of separation Q under dynamic conditions depends on the initial concentration of the separated gas mixture, the temperatures of the hot and cold walls of TDC, the pressure, the geometry, and the perfection of the column. Since

$$Q - 1 \sim Q_0^{\mu} - 1$$

it is obvious that all conclusions made in Ref. *2* concerning the optimal thermodynamic parameters of the separating gas mixture for the work of the column under static conditions are also valid under dynamic conditions. The agreement is very good for high degrees of separation ($Q >> 1$), because then it can be assumed that

$$Q \cong Q_0(1 - \theta)$$

or

$$Q \sim Q_0$$

The influence of the productivity of TDC upon the degree of separation is taken into account by the coefficient of the relative extraction θ. From Eq. (61) it can be seen that in first approximation,

$$Q - 1 \sim 1 - \theta$$

It is obvious that for $\theta = 0$ (work under static conditions), $Q = Q_0 =$ maximum, and for $\theta = 1 - Q = 1 =$ minimum, i.e., there is no separation of the gas mixture in a column with limited height. This shows the importance of the value of the coefficient of relative extraction for the work of a TDC. Its variation leads to a change of the working volume and the productivity of a TDC. In fact, from Eqs. (12) and (13) it follows that for constant P and W:

$$L \sim 1/\theta \qquad L_f \sim 1/\theta$$

$$G \sim 1/\theta \qquad G \sim 1/\theta$$

and if L, L_f, and G are constant:

$$P \sim \theta \qquad W \sim \theta$$

From the above, it is obvious that when calculations are made for a real column, the optimal value of θ has to be found from an energetic and instrumental point of view, but not with respect to the degree of separation. The question of obtaining the optimal θ is complicated, and it requires special attention. It will be described in another paper.

The initial concentration of a gas mixture (x_0) similarly influences the degree of separation. If x_0 increases, Q also increases, although this influence of x_0 on Q is small. Furthermore, for a concrete problem, x_0 is given or it can vary within a limited region. In our opinion, the optimization of the process by this parameter is not needed and is hardly possible.

4. CONCLUSIONS

The analytical expressions obtained for the degree of separation in a TDC under dynamic conditions permit, on the basis of experimental data for the dependence of the thermal diffusion factor or the degree of separation under static conditions, and on the thermodynamic parameters of a gas mixture (temperature and pressure), the optimal conditions for the separation of a concrete gas mixture to be chosen. The common analytical dependencies derived allow the energetic and instrumental optimization of a TDC or a TD-cascade. The results of these investigations will be reported later.

SYMBOLS

A^*	coefficient introduced for convenience
A_G	coefficient introduced for convenience
A_L	coefficient introduced for convenience
a^*	coefficient introduced for convenience
G	convection flow going up (mol/s)
h	geometrical height of TDC (m)
k_p	coefficient taking into account the imperfection of TDC
k_r	coefficient introduced for convenience
k_x	coefficient introduced for convenience
L, L_f	convection flow going down in lower and upper column, respectively (mol/s)
L_0	gas mixture entering into TDC (mol/s)
m	coefficient introduced for convenience
N	number of transfer unit height in TDC
N_T	number of the theoretical plates in TDC
P	product extracted from the bottom of the lower column (mol/s)
p	pressure (N/m^2)
Q	degree of separation in TDC
Q_0	degree of separation in TDC without gas production
Q_H	degree of enrichment in TDC of the heavy gas in the mixture
Q_L	degree of enrichment in TDC of the light gas in the mixture
q	coefficient of separation
q^*	coefficient of separation in X–Y coordinates
T_C	temperature of the cold wall in TDC (K)
T_H	temperature of the hot wall in TDC (K)
T_C^*	average temperature of the convection flow going down (K)
T_H^*	average temperature of the convection flow going up (K)
W	product extracted from the top of the upper column (mol/s)
X, Y	conditional concentrations of extracting gas
x, y	molar concentration of extracting gas in the convection flows going up and down respectively
x_1, x_2, y_1, y_2	coordinates of the two intersection points of the equilibrium and working lines
x_k	molar concentration of extracting gas at the outlet of the corresponding stage of TD-cascade
x_0	molar concentration of extracted gas at the inlet of TDC
x_p	molar concentration of extracted gas in the product

x_w molar concentration of extracted gas in the waste product
x_{H1} molar concentration of the heavy gas at the top of TDC
x_{H2} molar concentration of the heavy gas at the bottom of TDC
x_{L1} molar concentration of the light gas at the top of TDC
x_{L2} molar concentration of the light gas at the bottom of TDC
Y_e equilibrium concentration of extracted gas in convection flow going up under X–Y coordinates
y_e equilibrium concentration of extracted gas in convection flow going up
y molar concentration of extracted gas in the convection flow going up at the outlet of TDC

Greek Letters

α_T thermal diffusion factor
δ distance between the hot and cold walls in TDC (m)
ϵ coefficient of enrichment
$\bar{\epsilon}$ relative coefficient of enrichment
ϵ^* coefficient of enrichment in X–Y coordinates
μ coefficient introduced for convenience
σ_G shortening of convection flow going up in TDC
σ_L shortening of convection flow going down in TDC
θ relative extraction in TDC

REFERENCES

1. A. M. Rozen, *Theory of Separation of Isotopes in a Column,* Atomizdat, Moscow, 1960 (in Russian).
2. E. I. Leyarovski, J. K. Georgiev and A. L. Zahariev, *Sep. Sci. Technol., 25,* 557 (1990).
3. M. Fenske, *Ind. Eng. Chem., 24,* 482 (1932).
4. A. Colburn and T. Chilton, *Ibid., 26,* 1883 (1934).

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