COMPUTER CALCULATION OF NONSTATIONARY PROCESSES IN MULTISTAGE CASCADES FOR THE SEPARATION OF TWO-COMPONENT ISOTOPE MIXTURES

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A " systemic" method of integrating differential equations is used for working out a process for the numerical calculation of nonstationary processes using electronic computers.

Problems relating to the use of computers for the numerical solution of equations describing a nonstationary process in separating cascades have been discussed in [1-5]. However, the mathematical methods used in these studies either require too much machine time or have a limited region of practical applicability.

We have made an attempt to construct a mathematical model which describes sufficiently completely a nonstationary process taking place in cascades of arbitrary profile and to work out methods to use it on an electronic computer for rapidly obtaining solutions over an arbitrary range of concentrations.

As a rule, all separating installations consist of sections with constant flow between stages; i. e., they are squared-off cascades. If there is a sufficiently large number of sections, the profile of the flow in a cascade is taken to be close to the profile of an ideal cascade. The use of an ideal-cascade model makes it possible to simplify considerably the calculation of nonstationary processes taking place in multistage installations. Therefore, for a solution of practically all separation problems, it is sufficient to investigate the cases of squared-off cascades and ideal cascades.

We consider a squared-off cascade used for separating a two-component isotope mixture by the single-phase method. Suppose that at some intermediate point of the cascade there is an input flow F and from the ends of the cascade we remove the flows P (product) and W (waste). The quantities P, F, and W may be functions of time but must satisfy the following balance equation:

$$F = P + W. \tag{1}$$

The transfer of the valuable component in the direction from the waste outlet to the product outlet for the enriching and stripping parts of the cascade, respectively, can be written in the form

$$j = -L\frac{\partial c}{\partial s} + \varepsilon Lc(1-c) + Pc, \tag{2}$$

$$j = -L\frac{\partial c}{\partial s} + \varepsilon Lc(1-c) - Wc. \tag{3}$$

Substituting (2) and (3) into the fundamental equation describing the nonstationary process [6]

$$\rho L\frac{\partial c}{\partial t} = -\operatorname{div} j \tag{4}$$

and writing

$$l = \varepsilon s, \qquad \tau = \frac{\varepsilon^2 t}{\rho}, \qquad G = \varepsilon L, \tag{5}$$

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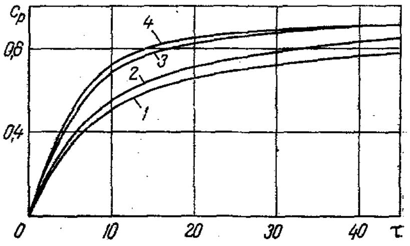

Fig. 1

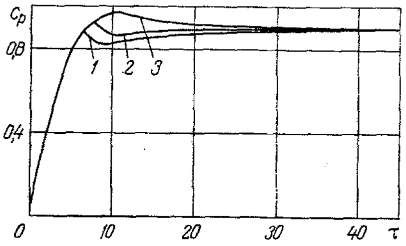

Fig. 2

Fig. 1. Kinetic curves of squared-off and ideal cascades in a regime with the product outlet constantly connected: 1) single-section cascade (η = 0.6); 2) two-section cascade (η = 0.83); 3) four-section cascade (η = 0.95); 4) ideal cascade.

Fig. 2. Kinetic curves of an ideal cascade when the product outlet is connected at different instants of time. Points 1, 2, and 3 correspond to the times at which the product outlet is connected.

we obtain

$$\frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial l^2} - \frac{\partial c}{\partial l}\left(1 + \frac{P}{G} - 2c\right), \tag{6}$$

$$\frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial l^2} - \frac{\partial c}{\partial l}\left(1 - \frac{W}{G} - 2c\right). \tag{7}$$

Equation (6) holds for all the sections of the enriching part and (7) holds for the stripping part of the cascade. The connection between the nonstationary-process equations at the "junction" point between adjacent sections can be obtained from the condition of conservation of mass transport at that point:

$$G_i \frac{\partial c^-}{\partial l} - G_{i+1} \frac{\partial c^+}{\partial l} - (G_i - G_{i+1})\, c^* (1 - c^*) = 0, \tag{8}$$

where the signs "+" and "−" denote the derivative on the left and on the right of the "junction" point, respectively.

If at the "junction" between the i-th and (i + 1)-th sections there is an input flow, then Eq. (8), taking account of (1), can be rewritten in the form

$$G_i \frac{\partial c^-}{\partial l} - G_{i+1} \frac{\partial c^+}{\partial l} - (G_i - G_{i+1})\, c_f (1 - c_f) = (c_f - c_F)(P + W). \tag{9}$$

The boundary conditions for the ends are obtained from the following equations:

$$j_1 = -Wc_W(\tau), \tag{10}$$

$$j_N = Pc_P(\tau). \tag{11}$$

Substituting (2) and (3), respectively, into (10) and (11), we rewrite the boundary conditions in the form

$$\left.\frac{\partial c}{\partial l}\right|_{l=0} = c(1 - c)|_{l=0}, \tag{12}$$

$$\left.\frac{\partial c}{\partial l}\right|_{l=l_P} = c(1 - c)|_{l=l_P}. \tag{13}$$

For a solution of the boundary-value problem we also must specify the initial condition in the form of a distribution of concentration along the cascade at time 0. In particular, if the cascade is filled with a homogeneous mixture whose concentration is c_F, the initial condition takes the form

$$c(l,\ 0) = c_F. \tag{14}$$

Equations (6) and (7), together with the "junction" conditions (8) and (9), the boundary conditions (12) and (13), and the initial condition (14), form a boundary-value problem describing the nonstationary process of separation taking place in a squared-off cascade.

The equation describing the nonstationary process in an ideal cascade has the form [6]

$$\frac{\partial c}{\partial \tau}=\frac{\partial^2 c}{\partial l^2}+\left(\frac{\partial \ln G}{\partial l}-\frac{P}{G}-1+2c\right)\frac{\partial c}{\partial l}-c(1-c)\frac{\partial \ln G}{\partial l}. \tag{15}$$

If the waste point is taken as the origin of our coordinate system, the flow distribution in the stripping and enriching parts of the cascade will have the form

$$G=2W\frac{\left[1+\mu\exp\left(\frac{l-l_W}{2}\right)\right]\left[1-\exp\left(-\frac{l_W}{2}\right)\right]}{1+\mu\exp\left(-\frac{l_W}{2}\right)}, \tag{16}$$

$$G=2P\frac{\left[1-\mu\exp\left(\frac{l-l_P}{2}\right)\right]\left[\exp\left(\frac{l_P-l}{2}\right)-1\right]}{1+\mu\exp\left(\frac{l_P-l_W}{2}\right)}, \tag{17}$$

where $\mu = c_F/(1-c_F)$.

Substituting (16) and (17) into Eq. (15), we obtain

$$\frac{\partial c}{\partial \tau}=\frac{\partial^2 c}{\partial l^2}$$

$$-\frac{\partial c}{\partial l}\left\{\frac{\mu\exp\left(\frac{l-l_W}{2}\right)+\exp\left(-\frac{l}{2}\right)+w\left[1+\mu\exp\left(-\frac{l_W}{2}\right)\right]}{2\left[\exp\left(-\frac{l}{2}\right)+\mu\exp\left(-\frac{l_W}{2}\right)\right]\left[1-\exp\left(-\frac{l}{2}\right)\right]}\right.$$

$$\left.+1-2c\right\}+\frac{\mu\exp\left(\frac{l-l_W}{2}\right)-\exp\left(-\frac{l}{2}\right)}{2\left[\exp\left(-\frac{l}{2}\right)+\mu\exp\left(-\frac{l_W}{2}\right)\right]\left[1-\exp\left(\frac{l}{2}\right)\right]}c(1-c), \tag{18}$$

$$\frac{\partial c}{\partial \tau}=\frac{\partial^2 c}{\partial l^2}-\frac{\partial c}{\partial l}$$

$$-\left\{\frac{\mu\exp\left(\frac{l-l_W}{2}\right)+\exp\left(\frac{l_P-l}{2}\right)+p\left[1+\mu\exp\left(\frac{l_P-l_W}{2}\right)\right]}{2\left[\exp\left(\frac{l_P}{2}\right)-\exp\left(\frac{l}{2}\right)\right]\left[\mu\exp\left(-\frac{l_W}{2}\right)+\exp\left(-\frac{l}{2}\right)\right]}+1-2c\right\}$$

$$+\frac{\exp\left(\frac{l_P-l}{2}\right)+\mu\exp\left(\frac{l-l_W}{2}\right)}{2\left[\exp\left(\frac{l_P}{2}\right)-\exp\left(\frac{l}{2}\right)\right]\left[\mu\exp\left(-\frac{l_W}{2}\right)+\exp\left(-\frac{l}{2}\right)\right]}c(1-c), \tag{19}$$

where the coefficients p, w are equal to unity if the cascade includes the product outlet or the waste outlet, and equal to zero, otherwise.

Since the flow values for the enriching and stripping parts at the point of input in ideal cascades are equal, the "junction" condition for Eqs. (18) and (19) takes the simple form

$$\left(\frac{\partial c^+}{\partial l}-\frac{\partial c^-}{\partial l}\right)\Big|_{l=l_W}=(c_f-c_F)\frac{P+W}{G(l_W)}. \tag{20}$$

The boundary and initial conditions (12), (13), and (14) also hold for an ideal cascade.

In calculations for cascade installations based on the use of reversible methods, such as distillation or chemical exchange, we must take account of the process of accumulation of an isotope in the phase-reversal devices. In this case the equations have a form analogous to (6) and (7), and the "junction" and boundary conditions can be written in the form

$$G_i\frac{\partial c^-}{\partial l}-G_{i+1}\frac{\partial c^+}{\partial l}-(G_i-G_{i+1})c^*(1-c^*)+E_i\frac{dc^*}{dt}=0, \tag{21}$$

$$G_1 \frac{\partial c}{\partial l}\Big|_{l=0} - G_1 c_W (1 - c_W) = E_0 \frac{dc_W}{dt}, \tag{22}$$

$$-G_N \frac{\partial c}{\partial l}\Big|_{l=l_W+l_P} + G_N c_P (1 - c_P) = E \frac{dc_P}{dt}. \tag{23}$$

We have shown that in the cases under consideration the nonstationary separation process can be described by a nonlinear boundary-value problem, where the "junction" and boundary conditions can be given in the form of ordinary differential equations. In the general case an analytic solution of such boundary-value problems is impossible. Moreover, the complex structure of the equations requires the development of special methods of solution and the construction of a form of mathematical model that is suitable for use on an electronic computer.

In the present paper we investigate a differential-difference model for the equations of the nonstationary process. This model may be regarded as the limiting case of a network model, when one of the linear dimensions of the network (in this case the dimension along the time coordinate) approaches zero. In the literature this model is known as the "method of straight lines" [7].

The essence of this method as applied to our boundary-value problem is that the interval of the variation of the coordinate l for each section of the cascade is divided into n parts with step h and a family of parallel lines is drawn through the interior points of division. On each line the partial differential equation is replaced with an ordinary differential equation for the function $c\,(l_i + kh, \tau) = c^i_k(\tau)$. Thus, the boundary-value problem is reduced to a Cauchy problem for a system of ordinary differential equations with time as the independent variable.

For the transition to the Cauchy problem we replace the first and second derivatives on the selected lines with symmetric finite-difference relations [8]

$$\frac{\partial c_k}{\partial l} = \frac{c_{k+1} - c_{k-1}}{2h}, \tag{24}$$

$$\frac{\partial^2 c_k}{\partial l^2} = \frac{c_{k+1} - 2c_k + c_{k-1}}{h^2}. \tag{25}$$

At the "junction" points between the sections and at the ends of the cascade formula (24) cannot be used, since at these points we have only one-sided derivatives. The choice of difference formulas for representing one-sided derivatives is a matter of theoretical importance and significantly affects the accuracy of the calculation, since the relations (8), (9), (12), and (13) close the system of differential equations. Good results have been obtained by using the Adams—Bashforth and Adams—Moulton [9] second-degree difference formulas for the beginning and end of the interval, respectively:

$$c_2 = c_1 + \frac{1}{2} h (3c'_1 - c'_0), \tag{26}$$

$$c_n = c_{n-1} + \frac{1}{2} h (c'_n - c'_{n-1}); \tag{27}$$

where the derivatives at the interior points c'_1 and c'_{n-1} are calculated by the formulas of (24).

Substituting (24) and (25) into Eqs. (6) and (7), we obtain a system of ordinary differential equations describing the nonstationary process:

$$\frac{dc^i_k}{d\tau} = f(c^i_{k+1}, c^i_k, c^i_{k-1}), \quad 1 \leqslant i \leqslant N, \quad 0 \leqslant k \leqslant n. \tag{28}$$

Substituting (24), (26), (27) into (8), (9), (12), and (13) and taking account of the conditions for continuity of concentration, we obtain the following functional relationships:

$$f(c^*_i, c^i_{n-1}, c^i_{n-2}, c^{i+1}_1, c^{i+1}_2) = 0, \tag{29}$$

$$f(c_f, c^i_{n-1}, c^i_{n-2}, c^{i-1}_1, c^{i-1}_2) = 0, \tag{30}$$

$$f(c_W, c^1_1, c^1_2) = 0, \tag{31}$$

$$f(c_P, c^N_n, c^N_{n-1}) = 0. \tag{32}$$

If in the first and last equations of (28), for each section, we express the values of c_0^i and c_n^i from the corresponding formulas (29)-(32), we can close the system of differential equations.

Thus, the nonstationary separation process in the cascades can be described by a system of ordinary differential equations (28), satisfying the relations (29)-(32) and the initial conditions

$$c_k^i(0) = c_F \, . \tag{33}$$

For reversible methods of separation the system (28) is supplemented by differential equations which can be obtained without difficulty from (21)-(23). In this case the parameters c_i^*, c_P, and c_W will be unknown functions.

It is inadvisable to solve the resulting system by traditional methods of the Runge—Kutta type, since the largest integration step admissible from the viewpoint of stability of the computation process will be too small.

In the present paper we use a so-called "systemic" method for the numerical solution of differential equations [10], which takes account of the general properties of the system being solved and enables us to use an integration step considerably larger than with the classical methods.

According to this method, the algorithm for solving the system (28) can be represented as follows:

$$c_k(m\Delta\tau + \Delta\tau) = c_k(m\Delta\tau) + \Phi_{kj}(A, \Delta\tau) f_j(m\Delta\tau, c_k), \quad m = 0, 1, 2 \ldots . \tag{34}$$

Here $\Delta\tau$ is the time step; $\Phi(A, \Delta\tau)$ is the stabilizing matrix; $A = \partial f_i/\partial c_j$ is the Jacobi matrix.

In order to construct the stabilizing matrix, we make use of the following recurrence relation:

$$\begin{gathered} \Phi_{q+1} = \Phi_q(2I + A\Phi_q), \qquad q = 0, 1, \ldots, M-1, \\ \Phi_0 = \delta \sum_{\gamma=0}^{r} \frac{(A\delta)^\gamma}{(\gamma+1)!}, \qquad \delta = \frac{\Delta\tau}{2^M}, \end{gathered} \tag{35}$$

where I is the unit matrix.

The use of the "systemic" method enables us to increase the integration step by a factor of 20-30 in comparison with the classical methods and therefore sharply reduces the computation time. The integration step may be $\Delta\tau = 1$, which enables us to calculate the nonstationary process in the separating installation practically to the end after 50-100 steps.

We give below some results of numerical calculations carried out by the proposed method, using the separation of neon isotopes as an example. Figure 1 shows the variation with respect to time of the nonstationary values of the concentration at the product outlet for squared-off cascades with different numbers of sections (curves 1, 2, and 3) and an ideal cascade (curve 4), operating without a stripping part, with a constantly connected calculated product outlet. From this figure it follows that as the efficiency η increases, the kinetic characteristics of a real squared-off cascade merge into the characteristics of an ideal cascade, which agrees completely with the data of [11]. This proves that it is possible to use the ideal-cascade model for calculating nonstationary processes taking place in squared-off cascades.

The calculations showed that in order to reduce the transient time in contracting cascades, it is desirable to have the process take place at the beginning with total reflux and to connect the product outlet some time after the calculated concentration is attained. The reason for this is that when the product outlet is connected in an ideal cascade in the time interval during which the transition process takes place there is a minimum in the kinetic curve (Fig. 2). In constant-width cascades the product outlet should be connected at the time when the calculated concentration is attained, since in this case the concentration value at the product outlet remains practically unchanged. This conclusion confirms the results of [12].

We also investigated the nonstationary process taking place in cascades with a stripping part. The dynamics of such cascades are complicated, since in nonstationary conditions the "zero" point (the point at which the concentration is equal to the input concentration) shifts along the cascade, and this significantly affects the time required for the transition process. In particular, for a constant-width cascade operating with the product and waste outlets disconnected, the shift of the "zero" point may be so large that at the product point we cannot obtain the calculated value of concentration. Therefore, for such cascades the regime of operation with product and waste outlets disconnected should be considered ineffective.

In an ideal cascade the regime of operation of one part of the cascade has little effect on the process in the other part. As a result, there is very little shift in the "zero" point. This enables us to carry out the transition process in a regime with product and waste outlets disconnected. When either of them is connected, we observe the same features as in cascades without stripping part.

NOTATION

ρ, step delay; L, flow between stages; $c = c(s, t)$, concentration of extracted isotope at the s-th stage at time t; ε = coefficient of enrichment of a stage; P, product flow (extraction); W, waste flow; F, input flow; c_P, concentration at product point; c_W, concentration at waste point; c_F, input concentration; c^*, concentration at "junction" point between sections; c_f, concentration at input points; l_W, number of stages in stripping part of the cascade (in units of εs); l_P, number of stages in the cascade (in units of εs); E_i, inventory of i-th phase-reversal device; N, number of sections in the cascade.

LITERATURE CITED

1. G. D. Rabinovich, R. Ya. Gurevich, and I. S. Zakharova, Inzh.-Fiz. Zh., 19, 1052 (1970).
2. G. L. Partsakhashvili, Soobshch. Akad. Nauk GruzSSR, 41, 89 (1966).
3. M. M. Agrest et al., Khim. Prom-st', No. 1 (1967).
4. I. A. Vereninov and Yu. V. Rakitskii, At. Énerg., 32, No. 6 (1972).
5. L. P. Portnov and G. G. Filippov, Teor. Osn. Khim. Tekhnol., 8, No. 5 (1974).
6. G. D. Rabinovich, R. Ya. Gurevich, and G. I. Bobrov, Thermal-Diffusion Separation of Liquid Mixtures [[illegible]sian], Nauka i Tekhnika, Minsk (1971).
7. I. S. Berezin and N. L. Zhidkov, Computational Methods [in Russian], Vol. 2, Nauka, Moscow (1966), Chap. 10.
8. B. P. Demidovich et al., Numerical Methods of Analysis [in Russian], Nauka, Moscow (1967), Chap. 4.
9. I. Babushka et al., Numerical Methods of Solving Differential Equations [Russian translation], Mir, Moscow (1969), Chap. 3.
10. Yu. V. Rakitskii, in: Theory and Technology of Computing Devices. Proceedings of the Leningrad Polytechnic-Institute [in Russian], No. 332 (1973), p. 88.
11. G. A. Sulaberidze and N. I. Laguntsov, Teor. Osn. Khim. Tekhnol., 7, No. 3 (1973).
12. A. M. Rozen, Theory of Isotope Separation in Columns [in Russian], Atomizdat, Moscow (1960).

THEORY OF THERMODIFFUSION SEPARATION ACCORDING TO THE FRAZIER SCHEME

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A theory of a thermodiffusion column with transverse sampling streams is given on the basis of the transport equation for a binary mixture.

Among the different kinds of thermodiffusion apparatus of continuous action, the scheme proposed by D. Frazier in 1958 to connect thermodiffusion columns in which the sampling streams do not pass through but move outside the columns occupies a special place.

The delivery of the supply σ_e and σ_i with concentrations c_0 is accomplished at the upper and lower ends in a plane thermodiffusion column with gap δ, height L, and length B (Fig. 1), where both streams can have the same (Fig. 1a) and opposite (Fig. 1b) directions. Sampling of the product is carried out at the ends opposite to the supply entrance.

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