MULTIPARAMETRIC OPTIMIZATION OF THE PROCESS OF ISOTOPE SEPARATION

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We develop a method for determining the optimal parameters and operating conditions of a separating apparatus. We carry out calculations to minimize the specific losses, using as examples the mass-diffusion and thermal-diffusion methods of separation.

The production of isotopes, especially when it is based on the use of irreversible methods of separation, requires the expenditure of considerable material resources and energy. Therefore, the optimization of separating devices, with a view to reducing the cost per unit of product, is an extremely timely problem.

The method of experimental optimization enables investigators to determine only a limited number of parameters, since the interrelations between the processes taking place in the apparatus are highly complicated. However, the method of multiparametric optimization using electronic computers requires a fairly well-developed theory of the separating element. The present level of the theory enables us to do this for the processes of mass diffusion and thermal diffusion, which are the subject of this article.

In [1], for an estimate of the unit costs of obtaining isotope products in cascade installations based on irreversible separation methods, we proposed the relation

$$Z=\frac{1}{\delta U\eta}\left[P\Phi(c_P)+W\Phi(c_W)-F\Phi(c_F)\right]\left[\frac{a_{\mathrm{app}}(1+k_1)}{t_{\mathrm{c}}}+(a_{\mathrm{E}}+a_{\mathrm{u}})Q_0\right](t+t_{\mathrm{p}})+a_F Ft+a_{\mathrm{m}}\,(t+t_{\mathrm{p}}). \tag{1}$$

It was used in that study for minimizing the costs of obtaining isotopes in a cascade of mass-diffusion elements. However, since at that time there was no satisfactory theory of these apparatuses, our use of the functional (1) was limited to a search for the optimal regime of operation of elements with fixed geometry. The desired optimization function in the case when only one isotope is valuable took the form

$$\begin{gathered}S_{\mathrm{pr}}=\frac{Z}{Pt}=\frac{1}{\delta U\eta}\left[\Phi(c_P)+\frac{c_P-c_F}{c_F-c_W}\,\Phi(c_W)-\Phi(c_F)\,\frac{c_P-c_W}{c_F-c_W}\right]\times\\ \times\left[\frac{a_{\mathrm{app}}(1+k_1)}{t_{\mathrm{c}}}(a_{\mathrm{E}}+a_{\mathrm{u}})Q_0\right]\left(1+\frac{t_{\mathrm{tr}}}{t}\right)+\frac{c_P-c_W}{c_F-c_W}a_F+\frac{a_{\mathrm{m}}}{P}\left(1+\frac{t_{\mathrm{tr}}}{t}\right).\end{gathered} \tag{2}$$

The function Z takes account of the costs (in rubles) of setting up and operating the separating installation, and S_{pr} is the specific cost per unit of isotope product, in rubles per year.

An analogous function, written in a different form, was used in [2] for determining the optimal sampling in an ideal thermal-diffusion cascade operating on a given amount of isotope product.

Since in most separation methods the energy optimum and the apparatus optimum of a cascade do not coincide [3], the choice of the best values of the parameters must be based on a consideration of how the individual types of costs influence the total variation in the cost of isotope production.

It must be recognized that the determination of the operating regime and the choice of the structural parameters solely from the condition of maximum separating capacity or maximum separation factor is one-sided. In the first case we minimize the total number of apparatuses in the cascade, without taking account of the increased energy consumption associated with an increase in the separating capacity itself. Such an approach can be justified only when the energy costs are negligible in comparison with the apparatus costs, i.e., when we have the relation

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$$(a_E + a_u) Q_0 \ll a_{\text{app}} (1 + k_1)/t_{\text{op}}, \tag{3}$$

which under real conditions, as a rule, is not valid for irreversible separation methods. In the second case, the maximum possible enrichment effect is achieved to the detriment of the quantity of enriched product obtained.

It is of practical interest to consider two main operating regimes of cascade installations – a regime with fixed product rate and a regime of operation to obtain a total given amount of isotope product, G_{pr}. The solution of the optimization problem for these two cases has some specific peculiarities. The regime of operation with fixed product rate is characteristic of pilot-plant and industrial cascades based on the use of separation methods in which equilibrium is reached in a relatively short time. The second case is characterized by the fact that the time t of product output may be comparable with the time required for the transient process, which depends on the size of the cascade installation, which is proportional to the size of the sample. The sampling must be regarded as one of the optimization parameters, since to each concrete value of G_{pr} there will correspond its optimum sampling value. This case corresponds, for example, to operation of cascades consisting of liquid thermal-diffusion columns.

In the present paper, for the sake of simplicity, we solve the optimization problem by using the example of a cascade with no waste section, for which the target function reduces to the form

$$S_{\text{pr}} = \frac{\Phi(c_P, c_F)}{\delta U \eta} \left[\frac{a_{\text{app}}(1 + k_1)}{t_c} + (a_E + a_u) Q_0\right]\left(1 + \frac{t_{\text{tr}}}{t}\right) + a_F + \frac{a_{\text{m}}}{P}\left(1 + \frac{t_{\text{p}}}{t}\right), \tag{4}$$

where

$$\Phi(c_P, c_F) = (2c_P - 1) \ln \frac{c_P(1 - c_F)}{c_F(1 - c_P)} - \frac{(c_P - c_F)(1 - 2c_F)}{c_F(1 - c_F)}.$$

We consider the problem of optimization of a cascade by using the example of a mass-diffusion process. The separating capacity δU appearing in formula (4) is:

$$\delta U = \frac{1}{2}(1 - \theta) L' \varepsilon^2 \tag{5}$$

and the quantities L' and ε appearing in it are not themselves optimization parameters, since they are automatically established, depending on the total vapor flow Q_0 and the geometry of the element.

As was shown in [4], the quantity L' is associated with the working and geometric parameters of the element Q_0, T_w, P_w, l_{el}, d_c, and H_d of the system of equations

$$u \Pi H_d = Q_t - L', \tag{6}$$

$$L' = Q_0 \gamma_a \left(1 - \frac{Q_t - L'}{Q_t}\right)\left[1 - \left(1 - \frac{Q_t - L'}{Q_t}\right)^{\frac{1}{q-1}}\right], \tag{7}$$

$$u = \beta \frac{nD_{10}}{nD_{10}^0} \frac{T_0}{T_w} \sqrt{\frac{256 \eta_0 l_c L'}{\pi d_c^4 m_v \left[1 + \left(\frac{m_g}{m_v} - 1\right) \gamma_d\right]}}, \tag{8}$$

$$P_0 = \frac{1}{1 - V_c/V_{\text{el}}} P_w \frac{T_0}{T_w} \left\{\frac{T_w}{T} \frac{h}{H_{\text{el}}} \gamma_0 + \frac{1}{2} \frac{H_u - h}{H_{\text{el}}} \left(1 - \frac{x_d^2}{x_c^2}\right) \left[\gamma_{0\,\text{int}} + \frac{\gamma_{0\,\text{int}} - \gamma_{\text{int}\,0}}{\ln(\gamma_{0\,\text{int}}/\gamma_{\text{int}\,0})}\right] + \frac{H_d}{H_{\text{el}}} \left[\left(1 - \frac{x_d^2}{x_c^2}\right)\left(\gamma_0 + \frac{T_w}{\overline{T}} \gamma_0\right) + \right.\right.$$
$$\left.\left. + \frac{x_d^2}{x_c^2} \left(\overline{\gamma}_{\text{int}} + \frac{\gamma_{\text{int}\,0}}{2}\right)\right]\right\}, \tag{9}$$

$$\lg P_w = 720 - \frac{2760}{T_w}. \tag{10}$$

It should be noted that the perimeter Π of the diaphragm is determined essentially by design considerations and cannot be an optimization parameter.

In addition to the flow of the light fraction, the system (6)-(10) makes it possible to obtain the distributions of flows and concentrations of vapor and gas in the element which are necessary for finding the enrichment coefficient [5]:

$$\varepsilon = \ln\left(\frac{c^+}{1-c^+} \Big/ \frac{c^-}{1-c^-}\right). \tag{11}$$

The values of the concentration of the light component in the enriched and depleted flows, c^+ and c^-, must be determined, according to [6], from equations which take account of the influence of the countercurrent in the element on the separation effect:

$$\frac{dc_u}{dy} = \frac{H}{K} c_u(1-c_u) - \frac{L''}{K}(c_u - c^-), \tag{12}$$

$$c_{u0} = \frac{1}{2}\left[\sqrt{\left(\frac{1-\alpha_0}{\alpha_0}\right)^2 + \frac{4c^-}{\alpha_0}} - \frac{1-\alpha_0}{\alpha_0}\right], \tag{13}$$

$$c_F = \theta c^+ + (1-\theta)c^-. \tag{14}$$

Equations (6)-(10) and (12)-(14), taking account of (11), form a complete system for calculating the variation of the separating characteristics as functions of the design parameters and the working regime of the element, which makes it possible to carry out our search for their optimal values, taking account of formula (4).

The optimization of the separation process was carried out for the case of production of a 95% isotope of neon 22 in a cascade consisting of mercury mass-diffusion elements with a vertical arrangement of an additional condenser. The calculations were carried out by formula (4), making use of the system (5)-(14). The time of the transient process was considered negligible in comparison with the working time of the cascade. The determination of the coefficients which take account of the cost of electric power, coolant, apparatus, etc., was carried out on the basis of handbook data and operating experience with the pilot-plant mass-diffusion cascade described in [7].

The formula (4) for the specific costs is a complex multiparametric function with nonlinear relations. Therefore, the solution of the optimization problem requires using special methods of nonlinear programming. The search for the minimum of the desired function was carried out on an electronic computer by the deformed-polyhedron method [8, 9]. This method is characterized by improved convergence to the optimum when there are deep dips in the target function, by stability of the resulting solution, and by a relatively low cost in machine time.

The target function defined by formula (4) has dimension $M = 5$ (Q_0, l_{el}, d_c, H_d, P_0). Therefore, in searching for the minimum, we constructed a polyhedron with six vertices.

The search began with the construction of a regular polygon (simplex) whose vertices and sides are all equidistant from its center. Then we calculated the values of the function being optimized and selected the vertices with maximum and minimum values of the function. Projecting the vertex with the maximum value of the function being optimized through the center of gravity of the remaining vertices, and replacing its vertices with the improved less-than-maximum value of the target function, we obtained a new polyhedron. The search procedure for finding the vertices with improved values of the target function made use of the rules of reflection, elongation, and compression. In the resulting polyhedron we again determined the vertices with minimum and maximum values. By repeating the process of exclusion of vertices with the maximum values, we determined the minimum of the target function. For convenience in use, the program was made up of separate blocks, in which we calculated the separating characteristics of the apparatus and prepared the initial data for the solution of the optimization problem. The external block was the block for calculating the target function and verifying the optimization search.

In the process of solving the minimization problem for the specific costs, we obtained the optimal values of the design parameters and the working regime of the mass-diffusion elements, given in Table 1.

Another matter of practical interest is the optimization of existing mass-diffusion elements. The solution of this problem permits us, without changing the general dimensions and design of the apparatus, by merely selecting the appropriate parameters for the diaphragm and the capillary, as well as the value of the flow of working vapor, to obtain improvements in the separating properties of the element.

TABLE 1

Q_0, moles/sec	$\ln q$	θ_V	l_{el}, cm	d_c, cm	H_d, cm	P_0, torr	δU, moles/sec
$1{,}40 \cdot 10^{-2}$	1,69	0,40	1,55	0,44	25,4	26	$4{,}12 \cdot 10^{-6}$

TABLE 2

Q_0, moles/sec	$\ln q$	θ_V	l_{el}, cm	d_c, cm	P_0, torr	δU, moles/sec
$1{,}12\cdot10^{-2}$	1,70	0,39	1,13	0,40	27	$3{,}00\cdot10^{-6}$

TABLE 3. Results of the Optimization of an Ideal Thermal-Diffusion Cascade

$P\cdot10^5$, g/sec	$\delta\cdot10^4$, m	ΔT, K	$\overline{T}$, K	n_{seg}	S_{pr} rubles/yr	Remark
2,546	2,50	100	360	1	50,0	$K_w/K_{op} = K_d/K_{op} = 0$ [2]
3,210	1,46	100	360	1	32,8	$K_w/K_{op} = 0$; $K_d/K_{op} = 0{,}19$
1,128	2,83	100	360	12	88,2	$K_w/K_{op} = 0{,}53$; $K_d/K_{op} = 0$
1,343	2,48	100	360	16	73,9	$K_w/K_{op} = 0{,}51$; $K_d/K_{op} \approx 0{,}01$
2,409	1,71	200	386	20	21,7	$(K_w + K_d)/K_{op} = 0{,}42$

We give in Table 2 the results of the calculations for the optimum values of the parameters of an element described in [7], in the case of a fixed $H_d = 15$ cm.

The possible reduction in specific costs is about 80%. This makes it obvious that the optimization carried out on the basis of our mathematical models for a mass-diffusion element [4, 6] can reveal substantial reserves of cost reduction in the production of isotopes, which would be impossible by an experimental examination of a large number of working and geometric parameters.

The problems involved in the optimization of a thermal-diffusion process for separating isotopes will be considered by using the example of a plane ideal cascade consisting of liquid thermal-diffusion columns. We shall assume that the cascade is designed to produce a given amount of product, G_{pr}. In liquid thermal-diffusion columns there will inevitably be parasitic convection caused by the nonuniformity of the temperature of the working surfaces, the impossibility of maintaining a constant working gap, etc. In [10] it was shown that the influence of parasitic mixing decreases as the height of the column decreases. Consequently, in order to minimize the total separating surface of the ideal thermal-diffusion cascade for producing an isotope product of given concentration, we subdivide the cascade into segments of equal length. On the one hand, in order to reduce the influence of the temperature asymmetry, it would be desirable to select the value n_{seg} as large as possible, but on the other hand, for large values of n_{seg} the technological scheme of the cascade becomes more complicated, leading to increased apparatus costs. Thus, the number of subdivisions, n_{seg}, should be regarded as one of the optimization parameters. However, since there are no available data on the influence of n_{seg} on the value of the apparatus costs, we shall limit the number of subdivisions to the number corresponding to the length of liquid thermal-diffusion columns that can be set up in practice.

In order to calculate and minimize the specific costs by formula (4), we used expressions for the specific separating capacity (the separating capacity per unit surface of the cascade) δU, the specific heat flux Q_0, and the transient-process time t_{tr} [10], which, taking account of the parasitic mixing and the longitudinal diffusion, take the form

$$\delta U = \frac{7}{40}\alpha_t^2\frac{\rho D}{\delta}\left(\frac{\Delta T}{\overline{T}}\right)^2\Bigg/\left(1 + \frac{K_d + K_w}{K_{op}}\right), \tag{15}$$

$$Q_0 = \Delta T\lambda/\delta, \tag{16}$$

$$t_{tr} = \frac{\rho\delta}{\delta U}\left[\frac{f+1}{2(f-1)}\ln f - 1\right]. \tag{17}$$

The parasitic mixing is taken into account by the expression

$$\frac{K_w}{K_{op}} = \left(\frac{y_l n_{seg}}{\ln f} - 1\right)\left(1 + \frac{K_d}{K_{op}}\right), \tag{18}$$

where $\exp(y_l)$ corresponds to the separation factor of the cascade segment when there is no parasitic convection. The value of y_l is found from the relation

$$\frac{1+\varkappa}{1-\varkappa}\,\frac{1-2\varkappa+\exp[(1-\varkappa)y_l]}{1+2\varkappa+\exp[-(1+\varkappa)y_l]} = f^{\frac{1}{n_{seg}}} \tag{19}$$

where $\varkappa = 15\bar{T}(\delta T)/[\alpha_T(\Delta T)^2]$ is a parameter characterizing the influence of the parasitic convection and (δT) is the temperature asymmetry over the perimeter of the column, calculated from the results of [11].

In the present study the specific costs were minimized by the method described above with respect to the following parameters: P, δ, ΔT, $\bar{T}$, and n_{seg}, where the limits of variation of the parameters were due either to the technology of manufacture of the thermal-diffusion apparatus or to the conditions of its operation. The calculations showed that the minimum of the specific costs per unit of enriched product, taking account of the mixing due to the parasitic convection and the longitudinal diffusion, corresponds to the maximum temperature drop and minimum value of average temperature; this agrees with the conclusions reached earlier [10] concerning the functional dependence of the separating capacity of an ideal cascade when $K_w = K_d = 0$.

As an example, we shall consider the case of isotope separation in the ideal thermal-diffusion cascade investigated in [2], when the separation factor is $f = 10$, $\alpha_t = 0.04$, the quantity of product obtained is $G_{pr} = 10$ g, $\Delta T = 100$°K, and $\bar{T} = 360$°K. The values of the coefficients of the target function (4) – a_E, a_{app}, etc. – were also calculated on the basis of the data of [2]. The results of the calculations are shown in Table 3. Here we also show the results of the minimization of the specific costs solely on the basis of the size of the sample in [2]. It follows from Table 3 that in the idealized case ($K_w = 0$), optimization with respect to two parameters (P and δ) makes it possible to reduce the specific costs by more than one-third. Since the size of the working gap is reduced, longitudinal diffusion begins to play a substantial role, which is taken into account by the coefficient K_d. However, disregard of parasitic mixing leads to a clear underestimating of the value of the specific costs for obtaining the isotope product.

It follows from the calculations that it would be possible to reduce the cost of the product by increasing the temperature drop across the working gap, which is associated with carrying out the separation process at high pressures, or by increasing the number of segments n_{seg}. In both cases, the reduction in the specific costs is accompanied by a reduction in the optimum size of the working gap in comparison with its size corresponding to the maximum separation factor [2, 11].

In conclusion, it must be emphasized that the above method is also applicable to the multiparametric optimization of installations based on the use of reversible separation methods. In such cases Eq. (4) must be supplemented by the components of the apparatus costs and energy costs which take account of the specific features of the reversible methods, in particular those proportional to the interstage flow in the cascade and also those associated with phase reversal.

NOTATION

P and c_P, W and c_W, F and c_F, flows and concentrations in the sampling, waste, and feed of the cascade, respectively; L', flow of light fraction in a mass-diffusion element; c^+, c^-, mole concentration in the enriched and depleted flows; ε, enrichment coefficient; δU, separating capacity of an element or a unit of surface of the thermal-diffusion column; D_{10}, coefficient of diffusion of the light component into the vapor; P_0, T_0, and P_W, T_W, initial and working pressures and temperatures in a mass-diffusion element; $\ln q = ul_D/nD_{10}$, Peclet diffusion number; $\Phi = (2c - 1)\ln[c/(1 - c)]$, separating potential; η_0, viscosity of the isotope mixture being separated; u, density of flow of the vapor–gas mixture through the diaphragm; n, mole density of the vapor–gas mixture; m_v, m_g, molecular weight of vapor and gas; γ_0, γ_{0u}, mole concentrations of gas in the vapor–gas mixture at the surface of the lower and upper condensers; γ_{ext}, γ_{int}, average concentrations in the external gap and the internal cavity of the element; y_d, average concentration over the diffusion path length; γ_{int0}, gas concentration in the vapor–gas mixture at the boundary between the lower and upper condensers; θ and θ_v, coefficients of separation of the flows of gas and vapor in an element; l_{el}, H_d, Π, effective diffusion resistance, height, and perimeter of the diaphragm; H_{el}, total height of element; H_u, height of upper condenser; x_d, x_c, diameter of diaphragm and condensers; d_c, l_c, diameter and length of capillary at the outlet of the element; Q_0, total flow of vapor in a mass-diffusion element, or total heat flux in a thermal-diffusion column; G_{pr}, given amount of isotope product; α_t, thermal-diffusion constant; D, coefficient of mutual diffusion of the components of the mixture being separated; ρ, λ, density and thermal conductivity of the mixture being separated; f, separation factor; T, ΔT, average temperature and temperature difference between the hot and cold walls of the thermal-diffusion column; K_{op}, K_d, K_w, coefficients of the transfer equation; (δT), temperature asymmetry; $\varkappa$, coefficient taking account of the influence of the temperature asymmetry on the separation effect in the thermal-diffusion column; δ, width of gap in the column; t, working time of the installation with sampling; t_w, time of transient process; t_{op}, time of operation of the separating apparatus; n_{seg}, number of segments of the thermal-diffusion cascade; S_{pr}, specific costs associated with obtaining the isotope product; a_{app}, a_E, a_u, a_F, a_m, k_1, coefficients taking account of the cost of apparatus, energy, coolant, feed, maintenance, and repair of the apparatus, respectively.

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THERMAL CONTACT RESISTANCE IN THERMOPHYSICAL MEASUREMENTS

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UDC 536.2

The author describes the basis for an experimental correction to the thermal contact resistance (TCR) in investigation of thermal conductivity and thermal diffusivity of solids, using specimens in the form of plates. Relations are obtained for thermal deformation of specimens and the contact pressure to compensate for thermal deflection.

The use of a permanent assembly of thermocouples in the contact plates of a thermal measurement cell simplifies the operation of the thermophysical instrument, increases its reliability, and by means of calibration allows error due to parasitic thermocouple emf's to be eliminated. However, there then arises an additional error due to thermal contact resistances (TCR) of the specimen with the thermal measurement cell. In most cases, in investigating the thermal conductivity and diffusivity of materials with $\lambda \geq 0.5$ W/(m•°K) one must introduce a correction for the TCR, determined experimentally on a specimen of known thermal conductivity, or on a metallic specimen whose thermal conductivity is considerably less than the resistance of the test specimens. For a number of practical considerations one usually prefers the second method, which is based on the hypothesis that the TCR depends only on the cleanliness of preparation of the surfaces in contact, the contact pressure, and the type of lubrication, and is independent of the thermal conductivity of the materials in contact.

It is known that heat is transmitted through a contact zone due to conduction by two methods: through the place of immediate (actual) contact of the bodies, and through the medium filling the space between rough protuberances. The conductances of the medium α_m and of the actual contact α_M are in parallel, and therefore the specific conductivity of the contact can be expressed as the sum of the specific conductivities [1]

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