TRANSIENT PROCESS IN AN IDEAL FINE-PARTITION FUNNEL

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The results are shown which have been obtained by solving the differential equation which describes the transient process in an ideal fine-partition funnel.

The funneling of columns for a fine separation of mixture components serves two purposes: firstly, it reduces the energy losses and the capital spent on equipment and, secondly, it shortens the time necessary to reach the conditions at which extraction of a product at a specified rate can begin.

Most effective is an ideal funnel, which is characterized by the relation

$$q=\sqrt{q^*}. \tag{1}$$

While optimization with respect to energy losses can be effected on the basis of a steady-state analysis as shown in [1, 2, 3], one must know the transient performance characteristics of the funnel in order to determine the length of stabilizing time after which extraction of the concentrate can begin.

At present there is no method known by which the transients in an ideal funnel can be calculated. An exception is [2], where the kinetics in a multistage funnel is analyzed for $c \ll 1$. In [4] we find only an orientative estimate of the time Θ_s till extraction can begin, expressed in terms of the inequality:

$$\Theta_s^* < \Theta_s < 2\Theta_s^*, \tag{2}$$

where Θ_s^* is a dimensionless time parameter defined by the initial transfer and, as shown in [3],

$$\Theta_s^* = 4\left[\frac{q+1}{2(q-1)}\ln q - 1\right]. \tag{3}$$

It is well known that a transfer of the concentrated component to the positive end of a separator can, with the same notation as in [4], be expressed in the following manner [5]:

$$j_z = Hc\bar{c} + \sigma c - K\frac{\partial c}{\partial z}, \tag{4}$$

where, according to [4] and [1],

$$H = \frac{\alpha\beta g\rho^2(\Delta T)^2 a^3 B}{6!\eta\bar{T}} = H^* aB = H^* f; \tag{5}$$

$$K = \frac{\beta^2 g^2 \rho^3 (\Delta T)^2 B a^7}{9!\eta^2 D} + aB\rho D \tag{6}$$

for thermodiffusive partition,

$$H = G(\alpha^* - 1) = \rho_n w(\alpha^* - 1) f = H^* f; \tag{7}$$

$$K = Gh \tag{8}$$

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for distillation, and

$$H = G^*m\left\{\exp\left[\frac{(M_2 - M_1)\,\omega^2}{2RT}(r_{\text{in}}^2 - r_{\text{in}}^2)\right] - 1\right\} = H^*f\,, \tag{9}$$

$$K = \frac{G^{*2}m}{2\pi D\rho}\ln\frac{r_{\text{out}}}{r_{\text{out}}} + \pi\rho D\,(r_{\text{in}}^2 - r_{\text{out}}^2) \tag{10}$$

for a countercurrent centrifuge.

As has been noted in [4], Eq. (4) describes also the countercurrent process of chemical exchange and chromatography. In all these three cases optimization of energy and capital expenditures is effected by minimizing the volume of the ideal funnel [1]. This leads to the following expression which determines the shape of an ideal funnel [3]:

$$b\,(y) = \frac{\left[\exp\left(\frac{y_e}{2}\right) - \exp\left(\frac{y}{2}\right)\right]\left[c_0 + \bar{c}_0\exp\left(-\frac{y}{2}\right)\right]}{\exp\left(\frac{y_e}{2}\right) - 1}\,, \tag{11}$$

where b(y) is the ratio of the transverse cross-section area at y to the area across which the initial concentration of the enriched component is sustained, i.e.,

$$b\,(y) = f/f_0\,. \tag{12}$$

Optimal extraction is characterized by the condition:

$$\varkappa_0 \equiv \frac{\sigma}{H_0} = \frac{c_0\bar{c}_0}{2\,(c_e - c_0)}\,, \tag{13}$$

and a steady-state condition corresponding to (13) implies that

$$q_e = \exp\left(\frac{y_e}{2}\right). \tag{14}$$

Bearing in mind that

$$q_e = \frac{c_e\,(1 - c_0)}{c_0\,(1 - c_e)}\,, \tag{15}$$

and taking into account (14), we obtain

$$\varkappa_0 = \frac{1}{2}\,\frac{\bar{c}_0 + c_0\exp\left(\frac{y_e}{2}\right)}{\exp\left(\frac{y_e}{2}\right) - 1} \tag{16}$$

in lieu of (13).

The transient state in a funnel is described by the equation:

$$\mu\frac{\partial c}{\partial \tau} = -\operatorname{div}\vec{j}\,. \tag{17}$$

Since the concentrate component is transferred in the z-direction only, hence by inserting (4) into (17) and considering that

$$\mu = \rho f\,,$$

we find with an introduction of dimensionless variables:

$$\Theta = \frac{H_0^2\tau}{f_0\rho K_0}\,; \quad y = \frac{H_0 z}{K_0}\,, \tag{18}$$

that

$$\frac{\partial c}{\partial \Theta}=\frac{\partial^2 c}{\partial y^2}+\left(\frac{d\ln b}{dy}-\frac{\varkappa_0}{b}-1+2c\right)\frac{\partial c}{\partial y}-\frac{d\ln b}{dy}c\bar{c}. \tag{19}$$

Equation (19) is nonlinear even when b = const, i.e., for a funnel of constant cross section this equation transforms into the equations analyzed in [6, 7, 8].

After inserting into (19) the values of $\varkappa_0$ and b from (11) and (16), we will arrive at the differential equation which describes the transient process in an ideal fine-partition funnel during extraction:

$$\frac{\partial c}{\partial \Theta}=\frac{\partial^2 c}{\partial y^2}-\left[\frac{\exp\left(\frac{y_2}{2}\right)+p\exp\left(\frac{y_e-y}{2}\right)+\exp\left(\frac{y}{2}\right)}{2\left[\exp\left(\frac{y_e}{2}\right)-\exp\left(\frac{y}{2}\right)\right]\left[1+p\exp\left(-\frac{y}{2}\right)\right]}+1-2c\right]$$
$$\times\frac{\partial c}{\partial y}+\frac{\exp\left(\frac{y}{2}\right)+p\exp\left(\frac{y_e-y}{2}\right)}{2\left[\exp\left(\frac{y_e}{2}\right)-\exp\left(\frac{y}{2}\right)\right]\left[1+p\exp\left(-\frac{y}{2}\right)\right]}c\bar{c}, \tag{20}$$

where

$$p=\bar{c}_0/c_0. \tag{21}$$

Equation (20) is of interest when applied to a funnel consisting of countercurrent centrifuges, since a counterflow is possible here only with a continuous supply of fresh material. In rectification or in thermodiffusive partition, in order to shorten the stabilizing time, no extraction should take place until the desired concentration of the enriched product c_e has been reached at the positive end of the funnel.

In this case we let $\varkappa_0 = 0$ in (19) and, taking into account (11), we have

$$\frac{\partial c}{\partial \Theta}=\frac{\partial^2 c}{\partial y^2}-\left\{\frac{\exp\left(\frac{y}{2}\right)+p\exp\left(\frac{y_e-y}{2}\right)}{2\left[\exp\left(\frac{y_e}{2}\right)-\exp\left(\frac{y}{2}\right)\right]\left[1+p\exp\left(-\frac{y}{2}\right)\right]}+1-2c\right\}$$
$$\times\frac{\partial c}{\partial y}+\frac{\exp\left(\frac{y}{2}\right)+p\exp\left(\frac{y_e-y}{2}\right)}{2\left[\exp\left(\frac{y_e}{2}\right)-\exp\left(\frac{y}{2}\right)\right]\left[1+p\exp\left(-\frac{y}{2}\right)\right]}c\bar{c}. \tag{22}$$

The solution to (20) and (22) must satisfy the following boundary conditions:

$$c\,|_{\Theta=0}=c_0;\quad c\,|_{y=0}=c_0; \tag{23}$$

$$\left(\frac{\partial c}{\partial y}-c\bar{c}\right)_{y=y_e}=0. \tag{24}$$

We will now consider the solution to Eq. (22), which, because this equation is nonlinear, has been obtained with the aid of the Minsk-22 digital computer.

Use was made of the finite-difference, stable, and implicit grid with a rate of convergence $O(l + h^2)$. Designating the coefficients in Eq. (22) as follows:

$$\frac{1}{2}\,\frac{\exp(y_i/2)+p\exp\left(\frac{y_e-y_i}{2}\right)}{\left[\exp\left(\frac{y_e}{2}\right)-\exp\left(\frac{y_i}{2}\right)\right]\left[1+p\exp\left(-\frac{y_i}{2}\right)\right]}+1-2c_{ij}=m_{ij},$$

$$\frac{1}{2}\,\frac{\exp\left(\frac{y_i}{2}\right)+p\exp\left(\frac{y_e-y_i}{2}\right)}{\left[\exp\left(\frac{y_e}{2}\right)-\exp\left(\frac{y_i}{2}\right)\right]\left[1+p\exp\left(-\frac{y_i}{2}\right)\right]}c_{ij}\bar{c}_{ij}=n_{ij},$$

we obtained for the node (i, j) the difference equation

$$(m_{ij}h-1)\,lc_{i+1,\,j}+[h^2+l(2-hm_{ij})]\,c_{ij}-lc_{i-1,\,j}+h^2(ln_{ij}-c_{i,\,j-1})=0, \tag{25}$$

where h is the y-step and l is the Θ-step.

Such an equation can be written down for every internal node. The boundary conditions (23) and (24), with (21) taken into account, here become:

$$\frac{1}{2}(c_{-1,\,j}+c_{0,\,j})=\frac{1}{1+p};\quad \frac{c_{n,\,j}-c_{n-1,\,j}}{h}-d_{nj}=0, \tag{26}$$

where

$$d_{n,\,j}=\frac{1}{2}(c_{n,\,j}+c_{n-1,\,j})\left(1-\frac{c_{n,\,j}+c_{n-1,\,j}}{2}\right).$$

In this way, for finding the values c_{ij} at all points we obtained a system of nonlinear algebraic equations (25), (26) with a tridiagonal matrix. This system was linearized over a layer first assumed temporarily and then recalculated by iterations over it.

Computations were performed for c_0 varying from 0.01 to 0.95 and y_e varying from 1 to 20 at different values of the dimensionless time parameter Θ. The computation was ended at those values $\Theta = \Theta_s$ which correspond to the partition coefficient of extraction as defined by Eq. (14).

The relation between Θ_s and $y_e = 2\ln(q)$ is shown in Fig. 1 for various values of the initial concentration. Curve 4 on the same diagram corresponds to Eq. (3). It follows from these curves that the time necessary to reach the desired conditions for extracting the concentrate can be calculated from the initial transfer only if

$$y_e < 6, \tag{27}$$

i.e., when the partition coefficient is greater than 20. It is also evident from the same diagram that the right-hand limit in unequality (2) is not reached at large values of y_e.

As the initial concentration is decreased, the stabilizing time at the same value of the partition coefficient increases and, therefore, the statement in [3] that for an ideal funnel Θ_s is independent of the initial concentration appears false. In rectification, where partition coefficients reach very high values (y_e = 20–40), this point acquires special significance. The data in Fig. 1 confirm the fact established earlier for a column of constant cross section [9], namely that partition becomes more effective as the initial concentration of the enriched product increases.

An analysis of the obtained results shows that, from the instant when extraction begins, the concentration will remain constant with time at the end of the funnel only, while at other sections of the funnel the transient process will continue until

$$q=\exp\left(\frac{y}{2}\right).$$

At the time Θ_s, as can be seen in Fig. 2, the value of the partition coefficient at intermediate sections of a funnel differs from its equilibrium value and, moreover, the initial concentration has no significant effect on this difference – at least for values of y_e satisfying condition (27).

This effect of a concentration lag at intermediate sections was established by Debye [10] for $c \ll 1$.

In connection with this effect, the instant of time when extraction of the concentrate at a calculated rate may begin becomes somewhat indeterminate.

An analysis by Rozen in [2] based on electrical simulation shows that, as one begins to extract an isotope at $\Theta = \Theta_s$, the concentration c_e at the positive end of a column remains almost unchanged. Consequently, the time Θ_s may be considered the time after which operating conditions have been reached.

It is interesting to compare an ideal funnel and a column of constant cross section with regard to the length of the transient time. It may appear, at first glance, that by selecting a column sufficiently long one can shorten the transient time before the desired concentration is reached at the positive end of the column. This is confirmed by the results of numerical computations which have been performed on the basis of the solution given in [8] for a column of finite length and terminating at one end into a reservoir of infinite

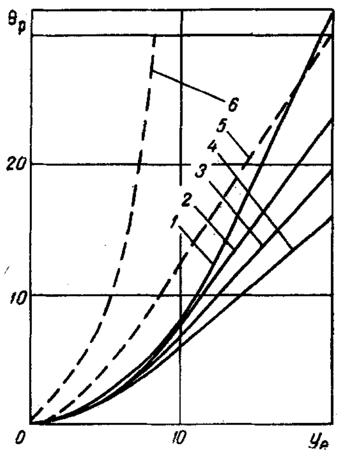

Fig. 1

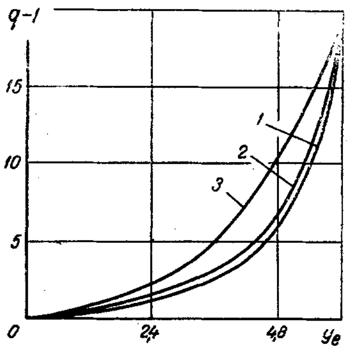

Fig. 2

Fig. 1. Time Θ_s necessary to reach a desired partition level, as a function of $y_e = 2 \ln c\bar{c}_0/c_0\bar{c}$ for an ideal funnel (solid lines) and for an infinitely long column of constant cross section (dashed lines) at various values of initial concentration: 1) $c_0 = 0.05$; 2) $c_0 = 0.5$; 3) $c_0 = 0.95$; 4) according to Eq. (3); 5) $c_0 = 0.5$; 6) $c_0 = 0.05$.

Fig. 2. Partition coefficient q as a function of the funnel length (dimensionless units) at various instants of time, for $y_e = 6$: 1) at the instant when operating conditions are reached (Θ_s) for $c_0 = 0.5$; 2) the same for $c_0 = 0.05$; 3) at steady-state conditions ($\Theta \to \infty$).

volume. Indeed, the transient time before the desired concentration q is reached becomes shorter. As will be shown subsequently, however, this shortening of the time has a limit.

Let us consider the extreme case, $f_0 \to \infty$. According to (13), $\varkappa_0 \to 0$, i.e., such a column may be treated as one which operates with practically no extraction. Let us assume, further, that the column is infinitely long and let us place the origin of coordinates at its positive end. The change in concentration y at this end will then be determined by the equation in [9]:

$$c = \frac{1}{2}\left[1 - \operatorname{erf}\left(\frac{\sqrt{\Theta}}{2}\right)\right] - \left(\frac{1}{2} - c_0\right)\exp\left(-c_0\bar{c}_0\Theta\right)\left\{1 - \operatorname{erf}\left[\left(\frac{1}{2} - c_0\right)\sqrt{\Theta}\right]\right\}, \tag{28}$$

while the concentration at the negative end of the column, infinitely far away, will remain constant and equal to its initial value. The values of

$$q = c\bar{c}_0/c_0\bar{c} \tag{29}$$

have been calculated according to (28) for various values of Θ and c_0.

In comparing a column of constant cross section with the ideal funnel one must, evidently, compare the times necessary to reach the desired value of the partition coefficient as defined by (15) and (29).

The dashed lines in Fig. 1 represent data taken from the diagram in [9] and supplemented according to Eq. (28). An analysis of the curves will lead to the conclusion that in a column of constant cross section the time for reaching a desired concentration is always longer than in the ideal funnel.

NOTATION

$q = c(1 - c_0)/c_0(1 - c)$	is the partition coefficient in the extraction mode;
q^*	is the partition coefficient in the no-extraction mode;
c	is the concentration;
$\Theta = H^2\tau/\mu K$;	
H, K	are the kinetic coefficients;
τ	is the time;

$\mu = \rho f$;	
ρ, β, η, D	are the density, volume expansivity, viscosity, and diffusivity;
a	is the clearance in the thermodiffusive separator;
α	is the thermodiffusion constant;
B	is the gap width in the thermodiffusion separator;
f	is the transverse cross-section area of the column;
G	is the vapor flow rate through the column;
α^*	is the relative volatility;
w	is the vapor flow velocity;
h	is the height of a transfer unit;
m	is the number of centrifuges operating in parallel;
M_2, M_1	are the molecular weights of separated components;
G^*	is the gas flow rate through a centrifuge;
r	is the radius;
R	is the gas constant;
T	is the temperature;
$\bar{T}$	is the mean temperature in the clearance of the thermodiffusion separator;
ΔT	is the temperature difference between the hot and the cold surface;
$\varkappa = \sigma/H$	is the dimensionless extraction parameter;
σ	is the extraction of the concentrate (enriched component);
j	is the specific flow rate of the concentrate in the column;
$b = f/f_0$;	
z	is the vertical coordinate.

Subscripts

0	denotes the value at the origin of coordinates;
s	denotes the operating mode (quasistabilized);
v	denotes the vapor;
out	denotes outer;
in	denotes inner;
e	denotes the value at the condensate extraction point.

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