IDENTIFYING HEAT- AND MASS-TRANSFER CONSTANTS FROM MEASUREMENTS UNDER TRANSIENT CONDITIONS

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Explicit formulas are derived for determining heat- and mass-transfer constants from measurements of transient temperatures (concentrations) in processes which can be described by a general linear parabolic equation.

Many physical transfer processes can be approximately described by the linear parabolic equation

$$\frac{1}{a}\frac{\partial T(x,\ t)}{\partial t}=\frac{\partial^2 T(x,\ t)}{\partial x^2}+\beta_{ef}\frac{\partial T(x,\ t)}{\partial x}+\gamma_{ef}T(x,\ t), \tag{1}$$

where T is a physical variable characterizing the process in question; the subscript "ef" denotes the effective, i.e., the averaged, values of the coefficients in Eq. (1) which in the general case are dependent on T. For example, in examining the propagation of heat in a thin rod with heat transfer on a lateral surface, the coefficient γ_{ef} is proportional to the ratio of the heat transfer coefficient and the thermal conductivity [1]. In the diffusion of an unstable gas or diffusion in the presence of chain reactions [2], γ_{ef} is the ratio of the multiplication factor β^* to the diffusion coefficient D.

We will formulate the problem of identification as the problem of finding the unknown coefficients a, β, and γ on the basis of measurements of transient values of the variable T. Here, it is assumed that the measurements must be made at a sufficiently great number of points in space, for the sake of definiteness of the problem. As is known from the literature, the traditional approach of finding the above constants consists of comparing the specific solution of Eq. (1) obtained on the basis by known values of T (or $\partial T/\partial x$) at the boundaries of a certain region with measurements of T at some point inside this region. Such an approach, however, does not generally permit explicit representation of the sought parameters directly through the measurements because the solution of Eq. (1) is usually expressed through transcendental functions, the arguments of which include these parameters. A method was proposed in [3, 4] for constructing explicit relations to determine thermal diffusivity and thermal conductivity which might be extended to the present case.

Using the integral Laplace transform, we may write the solution of Eq. (1) as follows:

$$T(x,\ s)=A\exp\left[-\left(\frac{\beta}{2}+\sqrt{\frac{\beta^2}{4}-\gamma+\frac{s}{a}}\right)x\right]+B\exp\left[\left(-\frac{\beta}{2}+\sqrt{\frac{\beta^2}{4}-\gamma+\frac{s}{a}}\right)x\right], \tag{2}$$

where the constants A and B are determined on the basis of the character of the interaction of the bounding surfaces with the environment.

Let the conditions of the experiment permit description of an actual process by means of Eq. (1) for a semiinfinite region (model of semiinfinite body). Then the relationship between the values of T at the points $x=0$ and $x=\delta$ in the image space has the form

$$T(\delta,\ s)=T(0,\ s)\exp\left[-\left(\frac{\beta}{2}+\sqrt{\frac{\beta^2}{4}-\gamma+\frac{s}{a}}\right)\delta\right]. \tag{3}$$

It follows from (3) that

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$$\left[\frac{T(0,\ s)}{T(\delta,\ s)}\right]' = \frac{\delta \exp\left[\left(\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} - \gamma + \frac{s}{a}}\right)\delta\right]}{2a\sqrt{\frac{\beta^2}{4} - \gamma + \frac{s}{a}}}, \tag{4}$$

where the differentiation is performed with respect to the transform parameter s. Multiplying (4) by $\sqrt{\left(\frac{\beta}{2}\right)^2 - \gamma + \frac{s}{a}}$ and again differentiating with respect to s, we obtain

$$\left\{\left[\frac{T(0,\ s)}{T(\delta,\ s)}\right]' \sqrt{\frac{\beta^2}{4} - \gamma + \frac{s}{a}}\right\}' = \frac{\delta^2}{4a^2} \frac{\exp\left[\left(\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} - \gamma + \frac{s}{a}}\right)\delta\right]}{\sqrt{\frac{\beta^2}{4} - \gamma + \frac{s}{a}}}. \tag{5}$$

From (5) we have

$$[\varphi' T(\delta,\ s) - 2\varphi T'(\delta,\ s)]\left[\left(\frac{\beta^2}{4} - \gamma\right)a + s\right] + \frac{1}{2}\varphi T(\delta,\ s) = \frac{\delta^2}{4a} T^2(\delta,\ s)\, T(0,\ s), \tag{6}$$

where $\varphi = T'(0,\ s)T(\delta,\ s) - T'(\delta,\ s)T(0,\ s)$.

We will designate $(\beta^2/4 - \gamma)a = z$, $T_1(s) = T(0,\ s)$, $T_2(s) = T(\delta,\ s)$, then

$$z\psi(s) + s\psi(s) + \frac{1}{2}\varphi(s)\, T_2(s) = \frac{\delta^2}{4a}\varphi_1(s), \tag{7}$$

where

$$\psi(s) = \varphi'(s)\, T_2(s) - 2\varphi(s)\, T_2'(s); \quad \varphi_1(s) = T_2^2(s)\, T_1(s). \tag{8}$$

After changing from (7) back into the space of the originals, we obtain

$$z = \frac{\frac{\delta^2}{4a}\varphi_1(T_1,\ T_2) - \psi_1(T_1,\ T_2)}{\psi(T_1,\ T_2)}. \tag{9}$$

Here, we find the functions ψ, ψ_1, and φ_1 from the formulas:

$$\varphi_1(t) = \int_0^t T_2(t-\tau)\int_0^\tau T_2(\tau-\theta)\, T_1(\theta)\, d\theta d\tau,$$

$$\psi(t) = \int_0^t (2t - 3\tau)\, \varphi(\tau)\, T_2(t-\tau)\, d\tau,$$

$$\varphi(\tau) = \int_0^\tau (\tau - 2\theta)\, T_1(\theta)\, T_2(\tau-\theta)\, d\theta,$$

$$\psi_1(t) = \int_0^t (2t - 3\tau)\, \varphi'(\tau)\, T_2(t-\tau)\, d\tau - \frac{1}{2}\int_0^t \varphi(\tau)\, T_2(t-\tau)\, d\tau.$$

Since it is assumed that the parameters a, β, γ, and z are constant within the range of T realized in the experiment, it follows from (9) that

$$\left[\frac{\delta^2}{4a}\varphi_1'(t) - \psi_1'(t)\right]\psi(t) - \left[\frac{\delta^2}{4a}\varphi_1(t) - \psi_1(t)\right]\psi'(t) = 0,$$

from which

$$a = \frac{\delta^2}{4}\, \frac{\varphi_1'\psi - \varphi_1\psi'}{\psi_1'\psi - \psi_1\psi'}. \tag{10}$$

The functions ψ_1', ψ', and φ_1', accordingly, have the forms

$$\varphi_1'(t) = \int_0^t T_2(t-\tau)\int_0^\tau T_2(\tau-\theta)\, T_1'(\theta)\, d\theta d\tau,$$

$$\psi'(t) = \int_0^t (2t - 3\tau)\, \varphi'(\tau)\, T_2(t-\tau)\, d\tau - \int_0^t \varphi(\tau)\, T_2(t-\tau)\, d\tau,$$

$$\psi_1'(t)=\int_0^t (2t-3\tau)\,\varphi''(\tau)\,T_2(t-\tau)\,d\tau-\frac{3}{2}\int_0^t \varphi'(\tau)\,T_2(t-\tau)\,d\tau,$$

$$\varphi'(\tau)=\int_0^\tau (\tau-2\theta)\,T_2(\tau-\theta)\,T_1'(\theta)\,d\theta-\int_0^\tau T_2(\tau-\theta)\,T_1(\theta)\,d\theta,$$

$$\varphi''(\tau)=\int_0^\tau (\tau-2\theta)\,T_2'(\tau-\theta)\,T_1'(\theta)\,d\theta.$$

After the parameter a is determined from Eq. (10), the parameter z can be found from Eq. (9).

To individually find β and γ, we return to (3). In the space of the originals, (3) has the form

$$T_2(\mathrm{Fo})=\exp\left(-\frac{\beta}{2}\,\delta\right)\frac{1}{2\sqrt{\pi}}\int_0^{\mathrm{Fo}} T_1(\tilde{\mathrm{Fo}})\exp\left\{-\left[\frac{z\delta^2}{a}\,(\mathrm{Fo}-\tilde{\mathrm{Fo}})+\frac{1}{4}\,\frac{1}{(\mathrm{Fo}-\tilde{\mathrm{Fo}})}\right]\right\}(\mathrm{Fo}-\tilde{\mathrm{Fo}})^{-3/2}\,d\tilde{\mathrm{Fo}},\tag{11}$$

where $\tilde{\mathrm{Fo}}=a\tau/\delta^2$; $\mathrm{Fo}=at/\delta^2$. From (11) we obtain

$$\beta=\frac{2}{\delta}\,\ln\left[\Phi(\mathrm{Fo})/T_2(\mathrm{Fo})\right],\tag{12}$$

where

$$\Phi(\mathrm{Fo})=\frac{1}{2\sqrt{\pi}}\int_0^{\mathrm{Fo}} T_1(\tilde{\mathrm{Fo}})\exp\left\{-\left[\frac{z\delta^2}{a}\,(\mathrm{Fo}-\tilde{\mathrm{Fo}})+\frac{1}{4}\,\frac{1}{\mathrm{Fo}-\tilde{\mathrm{Fo}}}\right]\right\}(\mathrm{Fo}-\tilde{\mathrm{Fo}})^{-3/2}\,d\tilde{\mathrm{Fo}}.\tag{13}$$

Since a, z, and β are now known, the value of γ can be calculated from the formula

$$\gamma=\{\ln\left[\Phi(\mathrm{Fo})/T_2(\mathrm{Fo})\right]\}^2/\delta^2-\frac{z}{a}\,.\tag{14}$$

In certain practical cases, transfer processes can be described by an equation of type (1) for a plane layer of thickness δ (model of a flat infinite plate). Then the relationship between the values of T at three points through the thickness has the following form in the image space

$$T(x,\ s)=T(\delta,\ s)\exp\left[\frac{\beta}{2}\,(\delta-x)\right]\mathrm{sh}\sqrt{\frac{z+s}{a}}\,x/\mathrm{sh}\sqrt{\frac{z+s}{a}}\,\delta+$$
$$+T(0,\ s)\exp\left(-\frac{\beta}{2}\,x\right)\mathrm{sh}\sqrt{\frac{z+s}{a}}\,(\delta-x)/\mathrm{sh}\sqrt{\frac{z+s}{a}}\,\delta,\tag{15}$$

where δ is the distance between the extreme measurement points.

If $x=\delta/2$, then

$$T(\delta,\ s)=\left[T(\delta,\ s)\exp\left(\frac{\beta}{2}\,\delta_1\right)+T(0,\ s)\exp\left(-\frac{\beta}{2}\,\delta_1\right)\right]\Big/\left(2\mathrm{ch}\sqrt{\frac{z+s}{a}}\,\delta_1\right),\tag{16}$$

where $\delta_1=\delta/2$. The parameters a, β, and γ are most easily determined if measurements of T in two different realizations are available. It follows from (16) that

$$\frac{T_i(\delta,\ s)\exp\left(\frac{\beta}{2}\,\delta_1\right)+T_i(0,\ s)\exp\left(-\frac{\beta}{2}\,\delta_1\right)}{T_i(\delta_1,\ s)}=\frac{T_j(\delta,\ s)\exp\left(\frac{\beta}{2}\,\delta_1\right)+T_j(0,\ s)\exp\left(-\frac{\beta}{2}\,\delta_1\right)}{T_j(\delta_1,\ s)},\tag{17}$$

where the subscripts i and j pertain to the different realizations. Let us designate $\exp\left(\frac{\beta}{2}\,\delta_1\right)=b$, so that we obtain from (17)

$$b^2\left[T_i(\delta,\ s)\,T_j(\delta_1,\ s)-T_i(\delta_1,\ s)\,T_j(\delta,\ s)\right]=T_j(0,\ s)\,T_i(\delta_1,\ s)-T_i(0,\ s)\,T_j(\delta_1,\ s).\tag{18}$$

After changing back to the originals, we determine parameter β from the expression

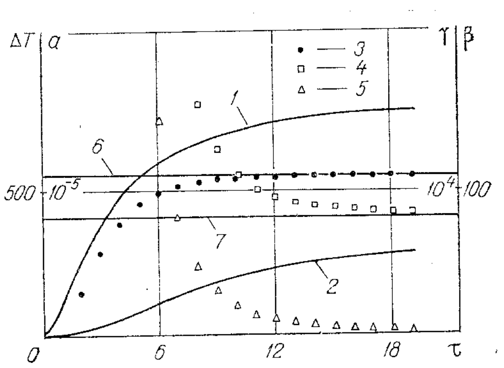

Fig. 1. Results of calculation of the coefficients of the model problem: 1, 2) temperatures at two points of the specimen (K) (distance between measurement points 10 mm); 3, 4, 5) calculated values of a (m^2/sec), γ (m^{-2}), and β (m^{-1}); 6, 7) adopted values of a, γ (value of $\beta = 0$ assumed).

$$\beta = \frac{2}{\delta_1} \ln b; \quad b = [f_1(t)/f_2(t)]^{1/2}, \tag{19}$$

where

$$f_1(t) = \int_0^t [T_j(0,\ t-\tau)\, T_i(\delta_1,\ \tau) - T_i(0,\ t-\tau)\, T_j(\delta_1,\ \tau)]\, d\tau;$$

$$f_2(t) = \int_0^t [T_j(\delta_1,\ \tau)\, T_i(\delta,\ t-\tau) - T_j(\delta,\ t-\tau)\, T_i(\delta_1,\ \tau)]\, d\tau.$$

We can proceed in as follows to determine the parameters a and γ. Let us designate the following in a certain realization, such as the i-th

$$T_1(t) = \left[T_i(\delta,\ t) \exp\left(\frac{\beta}{2}\, \delta_1\right) + T_i(0,\ t) \exp\left(-\frac{\beta}{2}\, \delta_1\right)\right]/2, \quad T_2(t) = T_1(\delta_1,\ t). \tag{20}$$

From (16) we have

$$\frac{T_1(s)}{T_2(s)} = \mathrm{ch} \sqrt{\frac{z+s}{a}}\, \delta_1. \tag{21}$$

Proceeding exactly in this manner, as in the case of a semiinfinite body, we obtain relations of the type (9) and (10) to determine a and z. Since we have found β, a, and z, we can easily calculate the value of the parameter γ.

Thus, using the relations obtained above, we can express the transfer constants in Eq. (1) explicitly through measurements of the transient function T. The integral combinations entering into the theoretical formulas are easily calculated on a computer and do not require the construction of complicated algorithms. Figure 1 shows the results of the calculation of a model problem. As the "experimental" values of the function T, we used the results of calculation of a straightforward problem of heat conduction: the temperatures at two points of a semiinfinite body, with heat exchange on the lateral surfaces and heating from the end. Here, the temperature of the end was assumed to be a constant 2000°K, the ambient temperature was 273°K, the thermal diffusivity $a = 0.04$ m^2/h, the thermal conductivity $\lambda = 40$ W/m·K, the heat-transfer coefficient $\alpha = 1000$ W/m^2·K, the ratio of the perimeter to the cross-sectional area 333 m^{-1}, $\gamma = 8333$ m^{-2}, and $\beta = 0$. It follows from the results shown that the calculated values of a, β, and γ converge fairly quickly with the values adopted in solving the above problem.

It should be noted that, apart from directly using these formulas to determine transfer constants in processes where the contribution of the physical factors associated with these constants is known for certain to be substantial, the formulas can in fact be used to identify an operator of type (1) itself. If data on the measurement error are available, the set of calculated values of the constants a, β, and γ (for a fixed number of time intervals during the realization) can be used, on the basis of a given statistical criterion, to construct an algorithm to check both the linearity of the operator and the amount by which the individual terms of Eq. (1) differ from zero, i.e., within the limits of accuracy of the system of measurements used, information can be obtained regarding the significance of a given physical factor in the process under study.

NOTATION

T, characteristic function of a process (temperature, concentration); x, coordinate; δ, δ_1, distance between measurement points; α, β, γ, transfer constants; Fo, $\tilde{\text{Fo}}$, Fourier numbers; t, τ, θ, time.

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THEORY OF A THERMAL DIFFUSION APPARATUS WITH TRANSVERSE FLOWS

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The article discusses a continuous thermal diffusion apparatus in which supply and removal take place at the ends of the separating slit. The dependence of the shift in concentration on the parameters of the apparatus, the properties of the mixture, and the amount of fluid removed is determined.

All known types of thermodiffusion cascades of constant, stepped, or ideal profile are characterized by the fact that the mixture being separated moves through elements forming a given cascade. The scheme for connecting thermodiffusion columns proposed by Jones and Frazier [1, 2] and shown schematically in Fig. 1a is distinguished by the fact that the mixture is pumped outside the separating part of the column. As can be seen from the figure, the mixture being separated is delivered to the top and bottom ends of the outermost columns and moves along the respective ends until it leaves the cascade. A theory of such a cascade proposed in [3] was constructed on simplified model representations applying to the separation of petroleum products. In connection with the latter, the relations obtained here are approximate.

The present work attempts to avoid the above problems and is based on the use of classical theory [4].

A battery of columns (Fig. 1a) may be represented in an idealized variant as a plane column, the top and bottom parts of which contain channels 2 (indicated by the dashed line in Fig. 1b, c) connected with the separating part of the apparatus 1. The apparatus is divided into a series of narrow columns by vertical barriers 3. It is assumed that diffusion along the x axis in these columns may be ignored, which allows us to regard the problem as being unidimensional within each column. The same assumption is made with regard to diffusion in the top and bottom channels, which is fully justified given the fairly high flow rates typical of the chosen operating regime. It is further assumed that the convective flow entering the channels 2 from the region 1 is ideally mixed along the z axis with the flows passing through the channels.

In any vertical cross section of the apparatus being examined, transfer in the case of a binary mixture is determined by the formula

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