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COUPLED PROBLEMS OF MASS TRANSFER BETWEEN SEMI-INFINITELY LARGE REGIONS DURING A CHEMICAL REACTION OF THE SECOND ORDER

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By the method developed in an earlier study [1], an asymptotic expression (at times $t \to \infty$) is derived here for the rate of mass transfer at the boundary between media when in one of them there takes place a chemical reaction of the second order.

We consider the earlier problem [2, 3] concerning mass transfer in a semi-infinitely large region where a chemical reaction of the second order takes place, viz.,

$$\frac{\partial C_1}{\partial t} - D\frac{\partial^2 C_1}{\partial x^2} + kC_1C_2 = 0, \tag{1}$$

$$\frac{\partial C_2}{\partial t} - D\frac{\partial^2 C_2}{\partial x^2} + kC_1C_2 = 0, \tag{2}$$

$$0 \leqslant x < \infty, \quad 0 < t < \infty;$$

$$C_1|_{x=0} = A = \text{const}; \quad \left.\frac{\partial C_2}{\partial x}\right|_{x=0} = 0;$$
$$C_1|_{x=\infty} = 0; \quad C_2|_{x=\infty} = B = \text{const}; \quad C_1|_{t=0} = 0; \quad C_2|_{t=0} = B. \tag{3}$$

The concentration of substance 1 at the boundary is maintained constant. The plane $x = 0$ is impermeable to substance 2.

We introduce for the analysis two new functions

$$S_1 = C_1; \quad S_2 = B - C_2, \tag{4}$$

so that system (1)-(2) can be rewritten as

$$\begin{aligned} &\frac{\partial S_1}{\partial t} - D\frac{\partial^2 S_1}{\partial x^2} + kS_1(B - S_2) = 0, \\ &\frac{\partial S_2}{\partial t} - D\frac{\partial^2 S_2}{\partial x^2} - kS_1(B - S_2) = 0. \end{aligned} \tag{5}$$

Conditions (3) are transformed in an obvious manner. It is essential, for the application of the given method or solution, that $S_2 = 0$ at $t = 0$ and $x = \infty$.

Adding the two equations (5), we obtain

$$\frac{\partial}{\partial t}(S_1 + S_2) - D\frac{\partial^2}{\partial x^2}(S_1 + S_2) = 0, \tag{6}$$

$$(S_1 + S_2)_{x=\infty} = 0; \quad (S_1 + S_2)_{t=0} = 0. \tag{7}$$

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According to earlier studies [1, 4], problem (6)-(7) with arbitrary boundary conditions at x = 0 can be replaced by the equation

$$\frac{\partial^{1/2}}{\partial t^{1/2}}(S_1+S_2)+\sqrt{D}\,\frac{\partial}{\partial x}(S_1+S_2)=0, \tag{8}$$

where the operation of fractional differentiation is defined by the expression

$$\frac{\partial^{\nu}}{\partial t^{\nu}}f(t)=\frac{1}{\Gamma(1-\nu)}\,\frac{d}{dt}\int_0^t (t-\tau)^{-\nu}f(\tau)\,d\tau,\ \ \nu<1.$$

With expression (8) written for x = 0 and with the boundary conditions as stated originally (3), we write for the mass flux at the boundary

$$-D\frac{\partial C_1}{\partial x}\bigg|_{x=0}=\sqrt{D}\,\frac{\partial^{1/2}}{\partial t^{1/2}}(A+B-C_2|_{x=0})=\sqrt{D}\left(\frac{A+B}{\sqrt{\pi t}}-\frac{\partial^{1/2}}{\partial t^{1/2}}C_2|_{x=0}\right). \tag{9}$$

The values of the quantity $C_2|_{x=\infty}$ in expression (9) is not known at any instant of time. It is obvious from physical considerations, however, that $C_2|_{x=0}=0$ at $t\to\infty$.

We will assume that the halfth-order derivative of any function which decreases as $t\to\infty$ approaches zero faster than does $t^{-1/2}$. This can be easily verified in the case where $C_2|_{x=0}$ decreases faster than does $t^{-\varepsilon}$ (ε = const > 0 being an arbitrary small quantity) as $t\to\infty$, because [1, 4]

$$\frac{\partial^{1/2}}{\partial t^{1/2}}t^{-\varepsilon}=\frac{\Gamma(1-\varepsilon)}{\Gamma\left(\frac{1}{2}-\varepsilon\right)}t^{-\varepsilon-\frac{1}{2}}.$$

At $t\to\infty$, therefore, the last term in expression (9) can be omitted and the expression for the rate of mass transfer at the boundary can be written in the final form as

$$-D\,\frac{\partial C_1}{\partial x}\bigg|_{x=0}=\sqrt{\frac{D}{\pi t}}(A+B). \tag{10}$$

This expression is identical to that obtained earlier [2, 3] under the assumption that $k\to\infty$ (a momentary reaction spreading as a front). It can be demonstrated that the analytical solution to the original problem, at any time t, is

$$-D\,\frac{\partial C_1}{\partial x}\bigg|_{x=0}=D^{1/2}(\pi t)^{-1/2}A\cdot F(Akt,\ Bkt).$$

Therefore, the asymptotic expressions for $t\to\infty$ and $k\to\infty$ are equivalent.

Expression (10) has been derived here in a much simpler way than earlier [2], this method being applicable to a large class of problems in the theory of mass transfer. One of such problems will be solved here. The proposed method has also a substantial drawback, however; it requires that the diffusion coefficients for substances 1 and 2 within the reaction space be equal.

Let us then proceed to the problem of mass transfer between semi-infinitely large regions. We assume that the initial distribution of substance 1 (concentration A) over the region $-\infty<x<0$ is uniform. At instant of time t = 0 "the barrier is removed" and substance 1 diffused into the region $0\leqslant x<\infty$, where it reacts with substance 2 which is already there (initial concentration B) and does not cross the boundary. The problem is to find the mass flux of substance 1 through the boundary at time $t\to\infty$.

The diffusion of substance 1 in the left-hand half space is described by the equation

$$\frac{\partial C_1}{\partial t}-D'\,\frac{\partial^2 C_1}{\partial x^2}=0, \tag{11}$$

and its diffusion in the right-hand half space is described by the system of equations (1)-(2). The set of initial and boundary conditions is

$$C_1|_{x=-\infty}=A;\quad C_1|_{t=0,\ x<0}=A;\quad C_1|_{x=\infty}=0;$$
$$C_1|_{t=0,\ x>0}=0;\quad C_2|_{x=\infty}=B;\quad C_2|_{t=0,\ x>0}=B;$$
$$\frac{\partial C_2}{\partial x}\bigg|_{x=+0}=0;\quad \psi C_1|_{x=-0}=C_1|_{x=+0};$$

$$D'\frac{\partial C_1}{\partial x}\Big|_{x=-0} = D\frac{\partial C_1}{\partial x}\Big|_{x=+0}. \tag{12}$$

Using the expressions in [1] or [4] for Eq. (11) describing the process in the left-hand half space, one can obtain the relation between quantities C_1 and $\partial C_1/\partial x$ in the form

$$\frac{\partial^{1/2}}{\partial t^{1/2}}(A - C_1) - \sqrt{D'}\frac{\partial}{\partial x}(A - C_1) = 0 \tag{13}$$

(this relation has been written for the function $A - C_1$, because its value at $x = -\infty$ at $t = 0$ is zero).

Writing expression (13) for $x = -0$ and expression (8) for $x = +0$, we obtain, after elimination of the first derivatives (12) with respect to x, an equation for $C_1|_{x=0}$:

$$\sqrt{D'}\left[\frac{A}{\sqrt{\pi t}} - \frac{\partial^{1/2}}{\partial t^{1/2}} C_1|_{x=-0}\right] = \sqrt{D}\left[\frac{B}{\sqrt{\pi t}} + \frac{\partial^{1/2}}{\partial t^{1/2}}(C_1|_{x=+0} - C_2|_{x=+0})\right].$$

Performing here the operation $\partial^{-1/2}/\partial t^{-1/2}$ yields

$$C_2|_{x=+0} = [\psi^{-1}(D'/D)^{1/2} + 1]\, C_1|_{x=+0} + B - A(D'/D)^{1/2}. \tag{14}$$

It becomes obvious, from physical considerations, that $C_2|_{x=+0}$ approaches a constant value at $t \to \infty$ and that three situations are possible here: 1) $C_2|_{x=+0} = 0$; 2) $C_2|_{x=+0} = \delta$ $(0 < \delta < B)$; 3) $C_2|_{x=+0} = B$.

Assuming situation 1) or 2) leads to absurd conclusions. For certain relations between the parameters expression (14) yields $C_1|_{x=+0} < 0$. We thus must assume situation 3), which is consistent with the physical aspects of the final stage of the process. After substance 1 at the boundary has been consumed, the concentration of substance 2 returns to its initial level. Then expression (14) yields at $t \to \infty$

$$C_1|_{x=+0} = \frac{\sqrt{D'}}{\psi^{-1}\sqrt{D'} + \sqrt{D}} A. \tag{15}$$

We will now determine the mass flux of substance 1 through the boundary on the basis of relations (13) and (15), viz.,

$$-D'\frac{\partial C_1}{\partial x}\Big|_{x=-0} = \sqrt{D'}\frac{\partial^{1/2}}{\partial t^{1/2}}(A - C_1) = \sqrt{D'}\left\{\frac{A}{\sqrt{\pi t}} - \frac{\partial^{1/2}}{\partial t^{1/2}}\left[\frac{\psi^{-1}\sqrt{D'}}{\psi^{-1}\sqrt{D'} + \sqrt{D}}\cdot A + f(t)\right]\right\},$$

where $f(t) > 0$ is a decreasing function. By analogy to the preceding problem, we have $(\partial^{1/2}/\partial t^{1/2})f = o[(\partial^{1/2}/\partial t^{1/2})\mathrm{const}]$ at $t \to \infty$. The sought expression for the mass flux is then

$$-D'\frac{\partial C_1}{\partial x}\Big|_{x=-0} = \frac{\sqrt{D'D}}{\psi^{-1}\sqrt{D'} + \sqrt{D}}\cdot\frac{A}{\sqrt{\pi t}}. \tag{16}$$

Accordingly, at $t \to \infty$ the rate of mass transfer is determined only by diffusion and does not depend on the reaction rate constant. It is to be noted that solution of the original problem for $k = 0$ (diffusion without chemical reaction) yields expressions (15) and (16), which are valid for every t.

Thus, solution of the coupled problem with loss of substance 1 in the region $-\infty < x < 0$ yields a qualitatively different result than solution of system (1)-(3) with a constant concentration of substance 1 at the boundary. The chemical factor, which increases the rate of mass transfer, is effective only during a short initial period of time t.

An analogous phenomenon, namely transition of the process from the kinetic mode to the diffusion mode at $t \to \infty$, has been established earlier [5] in the case where the chemical reaction takes place at the surface and one of the reactants (or both) diffuses from the semi-infinitely large region.

NOTATION

A and B, initial concentrations of substances 1 and 2, respectively, C_1 and C_2, concentrations of substances 1 and 2, respectively; D, diffusion coefficient for both substances within the reaction space; D', diffusion coefficient for substance 1 in the region where the reaction does not take place; $\partial^\nu/\partial t^\nu$, fractional-differentiation operator; k, reaction rate constant; f and F, arbitrary functions; S_1 and S_2, functions linearly related to the concentrations; x, space coordinate; t, time; and ψ, distribution factor.

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RETRIEVAL OF THE BOUNDARY CONDITIONS FROM THE TEMPERATURE MEASUREMENTS AT POINTS INSIDE A SYSTEM OF PLANE DOUBLE-LAYER BODIES

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A reverse heat-conduction problem is reduced to integrating a system of ordinary differential equations by the method of smoothing splines.

In many specific practical engineering problems there arises the situation where determining the temperature and the thermal flux at external surfaces in systems of plane double-layer bodies requires measurement of the temperature as a function of time at internal points of the system [1]. We will consider the rather general formulation of reverse boundary-value problems of heat conduction for double-layer plates with an ideal thermal contact at the joint. For obtaining correct solutions to the reverse heat-conduction problems we will use the solution to the Cauchy problem [2, 3] and the method of smoothing splines [4].

The heat-conduction equation in a Cartesian system of coordinates, independent for each plate, will be written as [5]

$$\frac{\partial T_k}{\partial \tau} = \varepsilon_k \frac{\partial^2 T_k}{\partial X^2}, \quad 0 \leqslant \tau < \infty, \quad 0 \leqslant X \leqslant X_k, \tag{1}$$

where k = 1, 2 is the consecutive number of each layer, $X = x/R_0$, $\tau = a_0 t/R_0^2$, $\varepsilon_k = a_k/a_0$, $X_k = R_k/R_0$, a_0 and R_0 are arbitrary values of, respectively, the thermal diffusivity and the geometrical dimension, and R_k is the thickness of the k-th layer.

The conditions of ideal contact and the initial conditions will be stipulated as

$$T_1|_{X=X_{p,1}} = T_2|_{X=X_{p,2}}, \tag{2}$$

$$\pm \frac{\lambda_1}{R_0} \left.\frac{\partial T_1}{\partial X}\right|_{X=X_{p,1}} = \frac{\lambda_2}{R_0} \left.\frac{\partial T_2}{\partial X}\right|_{X=X_{p,2}}, \tag{3}$$

$$T_k|_{\tau=0} = \varphi_k(X), \tag{4}$$

where in expression (3) the plus sign corresponds to systems of coordinates in series and the minus sign corresponds to systems of coordinates in opposition, $\varphi_k(X)$ in expression (4) characterizing a nonuniform temperature distribution.

We assume that the heat transfer between the surface of the first plate layer and the ambient medium is subject to a boundary condition of the second kind

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