APPROXIMATE METHOD FOR SOLVING UNSTEADY NONLINEAR MASS TRANSFER PROBLEMS

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Let us consider a general nonlinear differential equation

$$Ly = F\left(t, \mathbf{x}, y, f\left(t, \mathbf{x}, y\right)\right), \tag{1}$$

in which L is, as a rule, an arbitrary linear operator; F is an arbitrary function of $t, \mathbf{x}, y, f$; $f(t, \mathbf{x}, y)$ is a nonlinear function of variable y; $\mathbf{x} = \{x_1, ..., x_n\}$ is the coordinate vector. The function F can include integrals of $f(t, \mathbf{x}, y)$ and derivatives of y with respect to coordinates $\{x_1, ..., x_n\}$.

This type of equation with appropriate initial and boundary conditions is widely used in problems of physicochemical hydrodynamics and chemical engineering, and its solution is strongly complicated due to the nonlinearity of f. Therefore, the idea to develop an approximate method of solving general equation (1) using the analytical or low-error approximate solutions to its linear case together with iterative algorithms and interpolation techniques is of current interest [1].

Let us replace $f(t, \mathbf{x}, y)$ with a constant value $\langle f \rangle$, which is obtained by averaging $f(t, \mathbf{x}, y)$ over some domain of t and $\mathbf{x}$, and find a solution to the simplified problem

$$Ly = F(t, \mathbf{x}, y, \langle f \rangle), \tag{2}$$

assuming that Eq. (2) with the initial and boundary conditions related to Eq. (1) has an exact analytical, or low-error approximate, solution. $\langle f \rangle$ is generally a function of $\mathbf{x}$ and t, and can be determined by solving the integral equation

$$\langle f \rangle = \frac{1}{tS} \int_0^t \int_S f\left(\tau, \mathbf{x}, y[\tau, \mathbf{x}, \langle f \rangle]\right) \delta S \, d\tau \tag{3}$$

using the iterative algorithm

$$\langle f \rangle^{(i+1)} = \frac{1}{tS} \int_0^t \int_S f\left(\tau, \mathbf{x}, y\left[\tau, \mathbf{x}, \langle f \rangle^{(i)}\right]\right) \delta S \, d\tau, \tag{4}$$

which virtually represents the method of successive approximations. Here, S is the length, or square area, or volume, depending on the dimension of the problem under study. The initial, or boundary, value or the value obtained for the preceding time, or coordinate, interval can be used as $\langle f \rangle^{(0)}$.

Thus, for example, when the time dependence of function y is to be found, Eq. (2) is solved for the time point t; that is, for the end point of the interval $[0, t]$ for which the value of $\langle f \rangle$ was determined. When the relation between $\langle f \rangle$ and t cannot be obtained as an explicit analytical solution to Eq. (3), it can be found by determining the values of $\langle f \rangle$ for several (3 or 4) values of t from Eq. (3) with the help of iterative algorithm (4), and then by using the method of asymptotic interpolation [2] to build the whole curve and find the constant coefficients in the interpolation formula.

As many one-dimensional unsteady problems of mass and heat transfer described by Eq. (2) have exact analytical solutions, they are best suitable for testing the above approximate method.

The above end-point interpolation method using the average values of a nonlinear term or factor to solve the nonlinear mass transfer problem can be illustrated by solving the problem with a variable molecular diffusion coefficient D, which is a function of the solution concentration c. In chemical engineering processes, the dependence of D on c can considerably affect the rate of mass transfer. The study of this effect is complicated by the fact that there is no universal relation to describe the dependence of D on c for liquids [1].

For dilute salt and other solutions, the experimental data on the dependence of D on c can satisfactorily be described by the relation [3]:

$$D = D_0(1 - b\sqrt{c}), \tag{5}$$

where *b* is a constant coefficient.

The equation describing the unsteady one-dimensional mass transfer by diffusion in a process where D is governed by (5) can be written as

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial y}\left[D_0\left(1 - b\sqrt{c}\right)\frac{\partial c}{\partial y}\right]. \tag{6}$$

Its solution will be sought for the following initial and boundary conditions:

$$\begin{aligned} &t = 0, \quad 0 \le y \le H, \quad c = 0 \\ &t > 0, \quad y = 0, \quad c = c_*; \quad y = H, \quad \partial c / \partial y = 0. \end{aligned} \tag{7}$$

The numerical solution to the problem (6)-(7), which will be used to estimate the accuracy of the approximate method, can be obtained using the standard mathematical package *pdepe* built into *Matlab*.

The problem (6)-(7) in dimensionless form with the diffusion coefficient D averaged over the time and coordinate is written as

$$\frac{\partial C}{\partial \tau} = \langle D\rangle \frac{\partial^2 C}{\partial Y^2}, \ \langle D\rangle = \frac{1}{\tau Y}\int_0^{\tau}\int_0^{Y}\left(1 - B\sqrt{C\left[Y_1, \tau_1, \langle D\rangle\right]}\right) dY_1 d\tau_1, \tag{8}$$

$$\begin{aligned} &\tau = 0, \quad 0 \le Y \le 1, \quad c = 0; \\ &\tau > 0, \quad Y = 0, \quad c = 1; \quad Y = 1, \quad \partial c / \partial x = 0; \end{aligned} \tag{9}$$

where $C = c/c_*$, $Y = y/H$, $\tau = D_0 t / H^2$, $B = b\sqrt{c_*}$.

The problem (8)-(9) has an exact analytical solution [1]:

$$C = 1 + \frac{4}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^{m+1}}{2m+1}\exp\left[-\frac{\pi^2}{4}(2m+1)^2\langle D\rangle\tau\right]\cos\left[\frac{\pi}{2}(2m+1)(1-Y)\right]. \tag{10}$$

To compare the numerical and approximate solutions, we will use the experimental relation $D = D_0(1 - 0{,}55\sqrt{c})$ recommended for some monovalent salt solutions with a molar concentration $c \le 0.1M$ [1].

Figures 1-2 illustrate the variation of the dimensionless concentration with the dimensionless coordinate and time. The dependence of $\langle D\rangle$ on coordinate *Y* was described by the interpolation equation

$$\langle D\rangle = (1 - B)\exp(-a_1 Y^p) + (1 - \exp(-a_2 Y^q)).$$

The dependence of $\langle D\rangle$ on time τ was described by the interpolation equation

$$\langle D\rangle = \left[1 + a_1\left(1 - \exp\left[-a_2\tau^r\right]\right)\right]^{-1}.$$

Here, a_1, a_2, p, q, r are positive constant coefficients.

It is seen that the end-point interpolation method with constant (averaged) values of the diffusion coefficient, which uses the varying interval of averaging, describes well the concentration profile along the coordinate over its whole range (Fig. 1). At the same time, the method in which the averaging is done only for a constant (entire) interval yields a

significant error, overestimating the values of concentration for the intermediate values of coordinate. Note that Eq. (10) for the $D=D_0(1-0.55\sqrt{c_*})$ case can satisfactorily describe the concentration profile only within a small region near the interface, considerably underestimating the values of concentration as the distance from the interface increases.

The profile of concentration versus time is described well by both the approximate method with a varying interval of averaging and the method with a constant interval of averaging (Fig. 2). Eq. (10) for the $D=D_0$ case considerably overestimates the value of concentration from the very beginning of the process.

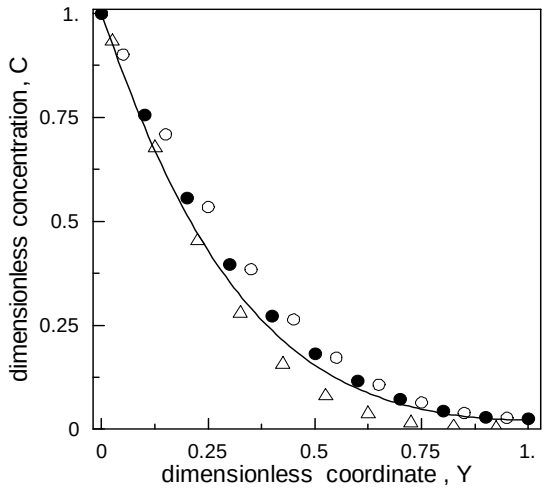

Fig. 1. Concentration profile along the coordinate ($\tau = 0.1$): line – numerical solution; filled circles – approximate method with a varying interval of averaging; unfilled circles – approximate method with a constant interval of averaging; triangles – equation (10) for the $D=D_0(1-0.55\sqrt{c_*})$ case.

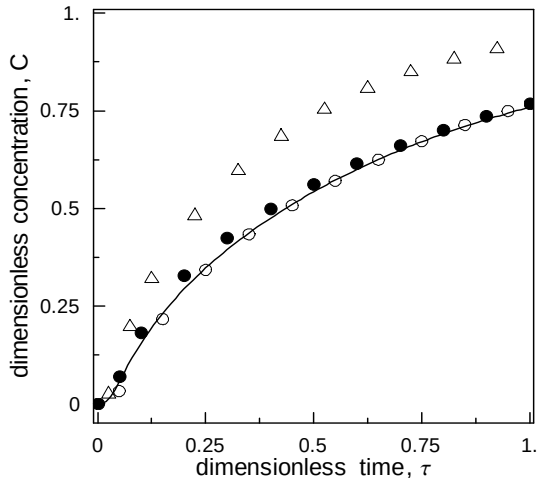

Fig. 2. Dependence of concentration on time ($Y = 0.5$): line – numerical solution; filled circles – approximate method with a varying interval of averaging; unfilled circles – approximate method with a constant interval of averaging; triangles – equation (10) for the $D=D_0$ case.

The above results imply that the use of averaged values of nonlinear terms or factors along with the end-point interpolation technique in solving the nonlinear mass transfer problems can make it possible to utilize the exact or low-error approximate analytical solutions obtained for the particular linear cases of these problems, in studying the relationships of nonlinear mass transfer. This approach can be of particular importance when the direct application of linear analytical solutions to study of nonlinear mass transfer processes is impossible because of their high error.

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2. A.V. Vyaz'min, I.A. Denisov, A.D. Polyanin, Theoretical Foundations of Chemical Engineering, 2001, Vol. 35, No. 1.
3. R.C. Reid, J.M. Prausnitz, B.E. Polling, The properties of gases and liquids, McGraw-Hill, N.Y., 1987.