COMPUTATION OF SOME COEFFICIENTS IN EQUATIONS OF COMBINED TRANSFER USING THE STRAIGHT-LINE METHOD

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The application of numerical methods to finding the coefficients in systems of partial differential equations of heat and mass exchange is shown on a specific example.

With the development of the theory of the transfer of energy and matter there has arisen the problem of deducing the coefficients of heat and mass exchange from experimental data. The coefficients in the equations which form the basis of the theory are important physical thermal characteristics of the materials under consideration and hence numerous works have been devoted to the construction of procedures for their determination [1-9]. In such works the formulas used in carrying out the computations are invariably based on solutions obtained by analytical methods [10]. There are a number of problems, however, in which it is extremely difficult to obtain solutions in an analytic form. Such problems arise, for example, when industrial processes are simulated using phenomenological theory. Hence it is necessary to develop sufficiently adaptable, simple, and reliable numerical methods for determining these coefficients (one such procedure was presented in [11]).

The procedure presented in this article consists of a combination of the straight-line method and the method of the least squares, applied to a transformed system of ordinary differential equations. Since in processing experimental data integral relations give more reliable results than differential relations, because of the much higher accuracy of numerical integration in comparison with numerical differentiation, the least-squares method is applied to the equivalent system of integral equations [12].

As an object of our investigations we took the mathematical model of the industrial process of drying grains in a dense and boiling uniform flow, the model is obtained on the basis of [13] by means of several idealizations and assumptions which can easily be understood from the formulation of the boundary-value problem below (the conventional notation is used, see also [13]):

$$\frac{\partial u}{\partial \tau} + w\,\frac{\partial u}{\partial x} - a_m(t)\left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\,\frac{\partial u}{\partial r}\right) = 0,$$

$$\frac{\partial t}{\partial \tau} + w\,\frac{\partial t}{\partial x} + \frac{A(v)}{c'\gamma'}(t - t_c) - \frac{\rho}{c'}\left(\frac{\partial \bar{u}}{\partial \tau} + w\,\frac{\partial \bar{u}}{\partial x}\right) = 0,$$

$$\frac{\partial u}{\partial r}(\tau,\ x,\ R) = \begin{cases} -\dfrac{B(t,\ v)}{a_m(t)}(u_R - u_p), & u_R \leqslant u_g, \\ -\dfrac{B(t,\ v)}{a_m(t)}(u_g - u_p), & u_R > u_g, \end{cases}$$

$$\frac{\partial u}{\partial r}(\tau,\ x,\ 0) = 0,$$

$$u(\tau,\ 0,\ r) = u^0(\tau,\ r),\quad t(\tau,\ 0) = f_1(\tau),$$

$$u(0,\ x,\ r) = u_0(x,\ r),\quad t(0,\ x) = f_2(x). \tag{1}$$

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Since in (1) $\bar{u}(\tau, x) = \frac{2}{R^2} \int_0^R rudr$ it is easy to obtain the differential relation

$$\frac{\partial \bar{u}}{\partial \tau} + w \frac{\partial \bar{u}}{\partial x} = \begin{cases} -\frac{2B(t, v)}{R}(u_R - u_p), & u_R \leqslant u_g \\ -\frac{2B(t, v)}{R}(u_g - u_p), & u_R > u_g \end{cases} \tag{2}$$

Of the parameters appearing in (1), some (c', γ', a_m, ρ) can be considered as known [5, 6]; also, in practice, the initial conditions can be considered as specified. It remains to find suitable functions A(v) and B(t, v) and also to estimate the degree to which the model corresponds to the industrial process under consideration. We begin with the steady-state equations of the drying process obtained for $\partial u/\partial \tau = 0$ and $\partial t/\partial \tau = 0$:

$$\begin{gathered} \frac{\partial u}{\partial x} = \frac{a_m(t)}{w}\left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r}\right), \\ \frac{\partial t}{\partial x} = \frac{A(v)}{c'\gamma' w}(t_c - t) - \frac{2\rho B(t, v)}{c' w R}(u_R - u_p), \\ \frac{\partial u}{\partial r}(x, R) = \begin{cases} -\frac{B(t, v)}{a_m(t)}(u_R - u_p), & u_R \leqslant u_g, \\ -\frac{B(t, v)}{a_m(t)}(u_g - u_p), & u_R > u_g, \end{cases} \\ \frac{\partial u}{\partial r}(x, 0) = 0, \ u(0, r) = u_0(r), \ t(0) = t_0. \end{gathered} \tag{3}$$

The first stage of the search consists in applying the straight-line method to the system (3). We write down the finite-difference relations:

$$\left(\frac{\partial u}{\partial r}\right)_k \approx \frac{u_{k+1} - u_{k-1}}{2h}, \tag{4}$$

$$\left(\frac{\partial^2 u}{\partial r^2}\right)_k \approx \frac{u_{k+1} - 2u_k + u_{k-1}}{h^2}. \tag{5}$$

Since $r_k = kh$ and

$$(\Delta u)_k = \left(\frac{\partial^2 u}{\partial r^2}\right)_k + \frac{1}{r_k}\left(\frac{\partial u}{\partial r}\right)_k, \tag{6}$$

we obtain

$$(\Delta u)_k \approx \frac{1}{2kh^2}[(2k+1)u_{k+1} - 4ku_k + (2k-1)u_{k-1}]. \tag{7}$$

At the boundary (the straight line with k = n) we have:

$$\begin{gathered} (\Delta u)_n = \left(\frac{\partial^2 u}{\partial r^2}\right)_n + \frac{1}{r_n}\left(\frac{\partial u}{\partial r}\right)_n, \\ u_{n-1} = u_n - h\left(\frac{\partial u}{\partial r}\right)_n + \frac{h^2}{2}\left(\frac{\partial^2 u}{\partial r^2}\right)_n - \ldots, \\ \left(\frac{\partial^2 u}{\partial r^2}\right)_n \approx \frac{2}{h}\left[\left(\frac{\partial u}{\partial r}\right)_n - \frac{u_n - u_{n-1}}{h}\right], \\ (\Delta u)_n \approx \frac{2}{h}\left[\left(\frac{\partial u}{\partial r}\right)_{r=R} - \frac{u_n - u_{n-1}}{h}\right] + \frac{1}{R}\left(\frac{\partial u}{\partial r}\right)_{r=R}. \end{gathered} \tag{8}$$

A similar problem was considered in [14] for a capillary porous ball with constant temperature of the surrounding medium. The numerical calculations show sufficiently rapid convergence of the straight-line method with respect to the coordinate r. By setting h = R/4 the system of equations (3) for the case

$u_R \leq u_g$ can be transformed into

$$\frac{du_1}{dx} = \frac{a_m(t)}{wR^2}(24u_2 - 24u_1),$$

$$\frac{du_2}{dx} = \frac{a_m(t)}{wR^2}(20u_3 - 32u_2 + 12u_1),$$

$$\frac{du_3}{dx} = \frac{a_m(t)}{wR^2}\left(\frac{56}{3}u_4 - 32u_3 + \frac{40}{3}u_2\right),$$

$$\frac{du_4}{dx} = -\frac{9B(t,\ v)}{wR}(u_4 - u_p) + \frac{32\, a_m(t)}{wR^2}(u_3 - u_4),$$

$$\frac{dt}{dx} = \frac{A(v)}{c'\gamma' w}(t_c - t) - \frac{2\rho\, B(t,\ v)}{c' wR}(u_4 - u_p)$$

with the initial conditions

$$u_i(0) = u_0,\ t(0) = t_0,\ i = 1,\ 2,\ 3,\ 4. \tag{9}$$

In the second stage smoothed empirical functions must be introduced into the system of equations (9) or into the corresponding integral equations; in this way a vector of residuals is formed and from this system the unknown coefficients are obtained. The approximate values of the parameters are obtained by solving the system of normal equations obtained according to the method of least squares.

Since the data on industrial grain-drying tests did not include any information on the distribution of the field of moisture content according to the size of the particle it was not possible under such conditions to find the diffusion coefficient of moisture. Hence the quantity $a_m(t)$ was approximated on the basis of laboratory experiments [5, 6]:

$$a_m = 0.662 \cdot 10^{-12} t^2.$$

Setting $u_4 \approx \bar{u}$ in the first approximation and adopting for the coefficients A and B the empirical relationships

$$A = av(x),\quad B = bv(x)\, t(x), \tag{10}$$

we convert the last differential equation of the system (9) into integral form

$$t(x) = t_0 + \alpha_1 \int_{x_0}^{x} v(\xi)\,[t_c(\xi) - t(\xi)]\, d\xi - \alpha_2 \int_{x_0}^{x} v(\xi)\, t(\xi)\, [\bar{u}(\xi) - u_p]\, d\xi, \tag{11}$$

where $\alpha_1 = a/c'\gamma' w$, $\alpha_2 = 2\rho b/c' wR$. We substitute for the functions t(x) and u(x) in the identity (11) by corresponding empirical dependences $\tilde{t}(x)$ and $\tilde{u}(x)$, for the given sequence $x = x_1,\ x_2,\ \ldots,\ x_n$ ($n \gg S$ is the number of parameters to be determined) and obtain the system:

$$\tilde{t}(x_i) = t_0 + \alpha_1 \int_{x_0}^{x_i} v(\xi)\,[t_c(\xi) - \tilde{t}(\xi)]\, d\xi - \alpha_2 \int_{x_0}^{x_i} v(\xi)\, \tilde{t}(\xi)\, [\tilde{u}(\xi) - u_p]\, d\xi + \delta(x_i), \tag{12}$$

where $\delta(x_i)$ is the residual, $i = 1,\ 2,\ 3,\ \ldots,\ n$. Using the method of least squares the coefficients α_1 and α_2 can be found by minimizing the function

$$\Phi(\alpha_1,\ \alpha_2) = \sum_{i=1}^{n} \delta^2(x_i). \tag{13}$$

The derivatives $\partial\Phi/\partial\alpha_1$ and $\partial\Phi/\partial\alpha_2$ are calculated and set equal to zero; two equations for the unknown α_1 and α_2 are obtained:

$$\sum_{i=1}^{n} \Big\{ \tilde{t}(x_i) - t_0 - \alpha_1 \int_{x_0}^{x_i} v(\xi)\,[t_c(\xi) - \tilde{t}(\xi)]\, d\xi$$

$$+ \alpha_2 \int_{x_0}^{x_i} v(\xi)\, \tilde{t}(\xi)\, [\tilde{u}(\xi) - u_p]\, d\xi \Big\} \int_{x_0}^{x_i} v(\xi)\,[t_c(\xi) - \tilde{t}(\xi)]\, d\xi = 0,$$

$$\sum_{i=1}^{n}\Big\{\bar{t}(x_i)-t_0-\alpha_1\int_{x_0}^{x_i}v(\xi)[t_c(\xi)-\bar{t}(\xi)]\,d\xi$$

$$+\alpha_2\int_{x_0}^{x_i}v(\xi)\,\bar{t}(\xi)\,[\bar{u}(\xi)-u_p]\,d\xi\Big\}\int_{x_0}^{x_i}v(\xi)\,\bar{t}(\xi)\,[\bar{u}(\xi)-u_p]\,d\xi=0. \quad (14)$$

In view of the size of the error (of the order of 5-10%) in the smoothing of industrial experiments the procedure of least squares is replaced by a simpler method: $\delta(x_i)$ are set equal to zero in Eqs. (12), the system (12) is averaged for two groups of points, and the sought coefficients are obtained by solving two linear algebraic equations. In case of the step-by-step drying ($u_p = 0.1$; $100°C \le t_c \le 180°C$; 0.2 m/sec $\le v \le$ 0.6 m/sec) of a dense moving stratum of thickness 0.2 m, the empirical coefficients are equal to

$$A = 0.266\,v(x),$$
$$B = 0.858\cdot 10^{-8}\,v(x)\,t(x), \quad (15)$$

while in the case of oscillating conditions in a boiling stratum of the same thickness ($100°C \le t_c \le 200°C$; $v \approx 1.6$-1.8 m/sec)

$$A = 1.22,\ B = 3.5\cdot 10^{-8}t. \quad (16)$$

Equations (15) and (16) provide the zero approximation of the sought parameters in the sense that for $u_4(x)$ the value $\bar{u}(x)$ is taken. However, a solution of the system (9) with the values of A and B thus established ensures that the integrals $\int_{x_0}^{x_i}\bar{u}(x)dx$ and $\int_{x_0}^{x_i}u_4(x)dx$ are sufficiently close and hence there is no need for iterations.

The degree of correspondence of the model to the real process was estimated according to maximal mean deviations of the regression curves for the experimental values: $\max_x|\Delta t(x)| = 7\ °C$, $\max_x|\Delta u(x)| = 0.0066$; in view of the nonuniformity of the heating and drying of the material under the conditions normally prevailing in industry, the magnitude of the obtained errors is fully acceptable.

The straight-line method together with various other procedures for solving systems of algebraic equations can also be recommended in other cases, for example, in the determination of the heat- and mass-transfer coefficients using standard bodies. Then the formulation of the adjoint boundary-value problem does not present any additional difficulties compared with the boundary-value problem of the 3rd kind under consideration.

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