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COMPREHENSIVE DETERMINATION OF POTENTIAL-DEPENDENT HEAT- AND MASS-TRANSFER CHARACTERISTICS OF DISPERSE MATERIALS

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A method is proposed for parametric identification of a mathematical model of coupled heat and mass transfer (HMT) in a disperse medium.

The heat- and mass-transfer characteristics of disperse media generally depend on the temperature and concentration of the substances distributed in the solid phase, which makes it necessary to account for type I nonlinearity [1] in the corresponding inverse problems.

The methods and equipment that are developed should provide not only for comprehensive determination of the HMT characteristics of disperse media, but also for the solution of the more complicated problem – recording of the dependence of the sought characteristics on the temperature of the test material and the concentration of the substance distributed in it.

The analysis conducted in [2] showed that the methods and equipment currently used in laboratory practice for comprehensive determination of the HMT characteristics of disperse materials do not fully meet the above requirements and are in need of improvement. They are not sufficiently accurate and lack the proper theoretical and metrological underpinnings. Substantial methodological errors are introduced by the linear mathematical models (MM) used in place of nonlinear models and the simplifications made to nonlinear models in the derivation of the formulas. Another shortcoming of the methods is the need to measure temperature and local concentration at several points of the test specimen, which complicates the measuring equipment and diminishes its reliability.

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The proposed method makes it possible to comprehensively determine the dependence of the sought HMT characteristics on temperature and concentration on the basis of measurements of temperature and concentration over time at just one specimen point.

The below formulas constitute a mathematical model of unidimensional coupled HMT in a disperse medium for moderate temperatures and heating rates, when the phase transformation criterion can be ignored [3]

$$\frac{\partial U}{\partial \tau} = \frac{\partial}{\partial x}\left[a_m(T,\ U)\frac{\partial U}{\partial x}\right] + \frac{\partial}{\partial x}\left[a_m^T(T,\ U)\frac{\partial T}{\partial x}\right], \tag{1}$$

$$C(T,\ U)\gamma_0\frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left[\lambda(T,\ U)\frac{\partial T}{\partial x}\right],\ \ x>0,\ \tau>0,\ \gamma_0=\text{const}. \tag{2}$$

It is difficult to identify the given nonlinear MM, i.e., to determine the parameters of Eqs. (1) and (2) as a function of the HMT potentials T and U. However, the problem can be simplified on the basis of physical considerations. Numerous investigations in heat and mass transfer [4] have established that the dependence of the heat capacity of a moist material C on temperature T in the processes being examined can be ignored, while the dependence of C on moisture content U can be reliably expressed by the equation

$$C(U) = C_0 + C_q U;\ C_0,\ C_q\ \text{— const}. \tag{3}$$

The heat capacity of a dry material C_0 and that of the liquid distributed inside it C_q can be determined relatively simply by established methods [5]. We thus assume that the values of C_0, C_q, and γ_0 are known beforehand and that the problem consists of determining the functional dependence of the following HMT characteristics on T and U: $a_m(T, U)$, $a_m^T(T, U)$, $\lambda(T, U)$, $a(T, U)$.

To identify these parameters of the disperse medium being analyzed, we organize the physical model in such a way that as to ensure satisfaction of the boundary conditions:

$$\begin{gathered} U(x,\ 0) = U_0,\ T(x,\ 0) = T_0;\ U(0,\ \tau) \neq U_{\text{en}}\ T(0,\ \tau) = T_{\text{en}}; \\ \frac{\partial U}{\partial x}(x,\ \tau) \to 0,\ \frac{\partial T}{\partial x}(x,\ \tau) \to 0\ \text{where}\ x \to \infty, \\ U_0,\ T_0,\ U_{\text{en}}\ T_{\text{en}}\text{— const};\ U_0 \neq U_{\text{en}};\ T_0 \neq T_{\text{en}} \end{gathered} \tag{4}$$

i.e., we will use test specimens — which during the tests can be regarded as semiinfinite bodies — that have a uniform distribution of temperature T_0 and concentration U_0. At the initial moment of time $\tau = 0$, we organize heat and mass transfer by the specimen surface $x = 0$ with the environment, which has the temperature T_{en} and mas content φ_{en}. This transfer occurs at a rate which precludes external diffusion resistance [3].

We will assume that at a certain fixed distance $x_0 \neq 0$ from the surface of the body $x = 0$ we can experimentally determine, as a function of time, the temperature $T(x_0, \tau)$ and the local concentration $U(x_0, \tau)$ of the substance distributed in the body. We will show that in this case the sought characteristics can be determined as a function of temperature T and concentration U.

We note that the inverse problems of heat conduction and HMT are often ill-conditioned in the sense of the term used by Adamar [6].

To solve ill-conditioned problems, from the general set of solutions we select a set M of correct solutions such that:

1) we know beforehand that a solution exists and that it belongs to the set M;

2) this solution is unique;

3) infinitely small variations of the input parameters not leading to a solution from the set M correspond to infinitely small variations of the solution. If such a set can be isolated, then the problem will be considered correct in the sense of the term used by Tikhonov.

In studying the Tikhonov correctness of mathematical physics problems, the existence of a solution and its membership in the correct set M are postulated in the formulation of the problem, i.e., the set M is chosen so that it is clear from previous physical considerations that the solution belongs to M. The uniqueness of the solution also follows from physical considerations. Thus, for the problem to be correct in the sense of Tikhonov, it is sufficient that the set M be compact, since this will ensure satisfaction of condition (3) by virtue of Tikhonov's theorem [6].

In the problem (1), (2), (4) being considered, the temperature T and moisture content U are bounded functions $T(x, \tau) \in [T_0, T_{en}]$, $U(x, \tau) \in [U_0, U_{en}]$. Moreover, these functions do not change discontinuously inside the body. Thus, their derivatives are also bounded functions. Meanwhile, the set M of uniformly bounded functions, possessing uniformly bounded derivatives, is compact in the space of continuous functions by virtue of Arcel's theorem [7]. These conditions guarantee that the solution of the inverse HMT problem will belong to a correct compact set. Thus, the problem being considered is correct in the sense of Tikhonov.

It should also be noted that the set M_1 of monotonically increasing (decreasing) and uniformly bounded functions can be taken as the correct set for the inverse HMT problem being examined, since these very conditions are realized in the physical model [the temperature and moisture content inside the body are monotonically increasing or decreasing functions, depending on the differences $(T_{en} - T_0)$ and $(U_{en} - U_0)$]. In this case, the set M_1 is compact in the space of quadratically integrable functions L_2 [7].

By making the substitution $\xi = x/2\sqrt{\tau}$, we reduce problem (1), (2), (4) in partial derivatives to a problem involving ordinary derivatives [8]:

$$-2\xi\frac{d\bar U}{d\xi}=\frac{d}{d\xi}\left[\tilde a_m(\xi)\frac{d\bar U}{d\xi}\right]+\frac{d}{d\xi}\left[\hat a^T_m(\xi)\frac{d\bar T}{d\xi}\right],$$

$$-2\xi\tilde C(\xi)\gamma_0\frac{d\bar T}{d\xi}=\frac{d}{d\xi}\left[\tilde\lambda(\xi)\frac{d\bar T}{d\xi}\right],\ \xi>0,$$

$$\bar U(\infty)=U_0,\ \bar U(0)=U_{en},\ \bar T(\infty)=T_0,\ \bar T(0)=T_{en},$$

$$\bar T\equiv\bar T(\xi)\equiv T(\xi,\ 1/4),\quad \bar U\equiv\bar U(\xi)\equiv U(\xi,\ 1/4).$$

Comparing $\frac{\partial U}{\partial x}=\frac{1}{2\sqrt{\tau}}\frac{\partial\bar U}{d\xi}$, $\frac{\partial T}{\partial x}=\frac{1}{2\sqrt{\tau}}\frac{d\bar T}{d\xi}$ respectively, with $\frac{\partial U}{\partial\tau}=-\frac{x}{4\tau^{3/2}}\frac{d\bar U}{d\xi}$ and $\frac{\partial T}{\partial\tau}=-\frac{x}{4\tau^{3/2}}\frac{d\bar T}{d\xi}$, we obtain

$$\frac{\partial U}{\partial x}=-\frac{2\tau}{x}\frac{\partial U}{\partial\tau},\tag{5}$$

$$\frac{\partial T}{\partial x}=-\frac{2\tau}{x}\frac{\partial T}{\partial\tau}.\tag{6}$$

It should be noted that

$$\frac{\partial}{\partial x}\left[a_m(U,\ T)\frac{\partial U}{\partial x}\right]=\frac{1}{4\tau}\left[\left(\frac{\partial a_m}{\partial\bar U}\frac{d\bar U}{d\xi}+\frac{\partial a_m}{\partial\bar T}\frac{d\bar T}{\partial\xi}\right)\frac{d\bar U}{\partial\xi}+a_m\frac{d^2\bar U}{d\xi^2}\right],$$

$$\frac{\partial}{\partial\tau}\left[a_m(U,\ T)\frac{\partial U}{\partial x}\right]=-\frac{x}{4\tau^{3/2}}\left[\left(\frac{\partial a_m}{\partial\bar U}\frac{d\bar U}{\partial\xi}+\right.\right.$$

$$\left.\left.+\frac{\partial a_m}{\partial\bar T}\frac{d\bar T}{d\xi}\right)\frac{d\bar U}{d\xi}\frac{1}{2\sqrt{\tau}}+a_m\frac{d\bar U}{d\xi}\frac{1}{x}+\frac{a_m}{2\sqrt{\tau}}\frac{d^2\bar U}{d\xi^2}\right],$$

from which

$$\frac{\partial}{\partial x}\left[a_m(U,\ T)\frac{\partial U}{\partial x}\right]=-\frac{2\tau}{x}\frac{\partial}{\partial\tau}\left[a_m(U,\ T)\frac{\partial U}{\partial x}\right]-\frac{a_m}{2\sqrt{\tau}}\frac{d\bar U}{d\xi}\frac{1}{x}.$$

Considering that

$$-a_m\gamma_0\frac{\partial U}{\partial x}=j_m^U, \tag{7}$$

we find

$$\frac{\partial}{\partial x}\left[a_m(U,\ T)\frac{\partial U}{\partial x}\right]=\frac{1}{\gamma_0}\left(\frac{2\tau}{x}\frac{\partial j_m^U}{\partial\tau}+\frac{j_m^U}{x}\right). \tag{8}$$

Similarly,

$$\frac{\partial}{\partial x}\left[a_m^T(U,\ T)\frac{\partial T}{\partial x}\right]=\frac{1}{\gamma_0}\left(\frac{2\tau}{x}\frac{\partial j_m^T}{\partial\tau}+\frac{j_m^T}{x}\right), \tag{9}$$

$$\frac{\partial}{\partial x}\left[\lambda(U,\ T)\frac{\partial T}{\partial x}\right]=\frac{2\tau}{x}\frac{\partial q}{\partial\tau}+\frac{q}{x}, \tag{10}$$

where

$$j_m^T=-a_m^T\gamma_0\frac{\partial T}{\partial x}, \tag{11}$$

$$q=-\lambda\frac{\partial T}{\partial x}. \tag{12}$$

Considering that the flux of the substance j_m in the investigated body is the sum of two components: the diffusion flux j_m^U and the thermodiffusion flux j_m^T [4]:

$$j_m(x,\ \tau)=j_m^U+j_m^T=-\gamma_0\left(a_m\frac{\partial U}{\partial x}+a_m^T\frac{\partial T}{\partial x}\right). \tag{13}$$

Using Eqs. (5) and (6), we find that

$$a_m^T(U,\ T)=\left[\frac{x_0 j_m(x_0,\ \tau)}{2\tau\gamma_0}-a_m(U,\ T)\frac{dU(x_0,\ \tau)}{d\tau}\right]\left[\frac{dT(x_0,\ \tau)}{d\tau}\right]^{-1}. \tag{14}$$

Similarly, with allowance for (6) and (10), we find from (12) and (2) that

$$\lambda(U,\ T)=\frac{x_0 q(x_0,\ \tau)}{2\tau}\left[\frac{dT(x_0,\ \tau)}{d\tau}\right]^{-1}, \tag{15}$$

$$a(U,\ T)=\frac{\lambda(U,\ T)}{C(U)\gamma_0}=\frac{x_0^2}{2\tau}\left[\frac{\tau}{q(x_0,\ \tau)}\frac{dq(x_0,\ \tau)}{d\tau}+1\right]^{-1}. \tag{16}$$

With allowance for (3) and (8)-(10), we find from (1)-(2) that

$$\gamma_0\frac{\partial U}{\partial\tau}=\frac{2\tau}{x}\frac{\partial j_m}{\partial\tau}+\frac{j_m}{x}, \tag{17}$$

$$(C_0+C_q U)\gamma_0\frac{\partial T}{\partial\tau}=\frac{2\tau}{x}\frac{\partial q}{\partial\tau}+\frac{q}{x}. \tag{18}$$

Solving (17) and (18) as first-order differential equations for $j_m(x_0,\ \tau)$ and $q(x_0,\ \tau)$, we obtain

$$j_m(x_0,\ \tau)=\frac{x_0\gamma_0}{2\sqrt{\tau}}\left\{\frac{U(x_0,\ \tau)-U_0}{\sqrt{\tau}}+\frac{1}{2}\int_{\tau_U}^{\tau}[U(x_0,\ \nu)-U_0]\,\nu^{-3/2}d\nu\right\}, \tag{19}$$

$$q(x_0,\ \tau)=\frac{x_0\gamma_0}{2\sqrt{\tau}}\left\{C_0\left[\frac{T(x_0,\ \tau)-T_0}{\sqrt{\tau}}+\frac{1}{2}\int_{\tau_T}^{\tau}[T(x_0,\ \nu)-T_0]\,\nu^{-3/2}d\nu\right]+C_q\int_{\tau_T}^{\tau}U(x_0,\ \nu)\frac{dT(x_0,\ \nu)}{d\nu}\nu^{-1/2}d\nu\right\}, \tag{20}$$

where τ_U and τ_T are the moments of time at which the concentration and temperature in the section x_0 first deviate from the initial values U_0 and T_0. The constants of integration $\sqrt{\tau_U/\tau}j_m(x_0, \tau_U)$ and $\sqrt{\tau_T/\tau}q(x_0, \tau_T)$ in (19) and (20) can be ignored due to their smallness, since, first of all, $\tau \gg \tau_U$, $\tau \gg \tau_T$ and, secondly the derivatives $dU/d\tau(x_0, \tau_U)$ and $dT/d\tau(x_0, \tau_T)$ are nearly equal to zero, i.e., $j_m(x_0, \tau_U) \approx 0$, $q(x_0, \tau_T) \approx 0$. The latter follows from (5)-(7) and (11)-(13). Our numerical experiments validated this simplification.

It follows from (14), (15), and (16) that:

$$a_m^T(U, T) = \left\{\frac{x_0^2}{4\tau^{3/2}}\left[\frac{U(x_0, \tau) - U_0}{\sqrt{\tau}} + \frac{1}{2}\int_{\tau_U}^{\tau}[U(x_0, \nu) - U_0]\nu^{-3/2}d\nu\right] - a_m(U, T)\frac{dU(x_0, \tau)}{d\tau}\right\}\left[\frac{dT(x_0, \tau)}{d\tau}\right]^{-1}, \tag{21}$$

$$\lambda(U, T) = \frac{x_0^2\gamma_0}{4\tau^{3/2}}\left[\frac{dT(x_0, \tau)}{d\tau}\right]^{-1}\left\{C_0\left[\frac{T(x_0, \tau) - T_0}{\sqrt{\tau}} + \frac{1}{2}\int_{\tau_T}^{\tau}[T(x_0, \nu) - T_0]\nu^{-3/2}d\nu\right] + C_q\int_{\tau_T}^{\tau}U(x_0, \nu)\frac{dT(x_0, \nu)}{d\nu}\frac{d\nu}{\sqrt{\nu}}\right\}, \tag{22}$$

$$a(U, T) = \frac{x_0^2}{4\tau^{3/2}}\left\{\left[1 + \frac{C_q}{C_0}U(x_0, \tau)\right]\left[\frac{dT(x_0, \tau)}{d\tau}\right]\right\}^{-1}\left\{\frac{T(x_0, \tau) - T_0}{\sqrt{\tau}} + \frac{1}{2}\int_{\tau_T}^{\tau}[T(x_0, \nu) - T_0]\nu^{-3/2}d\nu + \frac{C_q}{C_0}\int_{\tau_T}^{\tau}U(x_0, \nu)\frac{dT(x_0, \nu)}{d\nu}\frac{d\nu}{\sqrt{\nu}}\right\}. \tag{23}$$

To calculate $a_m^T(U, T)$ from Eq. (21), it is necessary to first determine the diffusion relation $a_m(U, t)$. To do this, we conduct a series of tests under isothermal conditions at different temperatures T_i, $i = 1, 2, \ldots, n$, where n is the number of points of the subdivision of the temperature interval we are interested in. The relation $a_m(U, T_i)$ is calculated from the equation

$$a_m(U, T_i) = \frac{x_0^2\left\{\frac{U(x_0, \tau) - U_0}{\sqrt{\tau}} + \frac{1}{2}\int_{\tau_U}^{\tau}[U(x_0, \nu) - U_0]\nu^{-3/2}d\nu\right\}}{4\tau^{3/2}\frac{dU(x_0, \tau)}{d\tau}}, \tag{24}$$

obtained in a manner similar to the above in the course of solving problem (1)-(2), (4) with $T_{en} = T_0 = T_i$.

The studies conducted in [3] show that at heat-carrier temperatures less than 100°C, thermodiffusion can be ignored in calculations of the kinetics of drying of capillary-porous materials. This simplifies the initially chosen mathematical model by excluding the term $\frac{\partial}{\partial x}\left[a_m^T(U, T)\frac{\partial T}{\partial x}\right]$ (i.e., $a_m^T = 0$) from Eq. (1). In this case, the characteristics λ, a, and a_m are determined from a single test in accordance with Eqs. (22), (23), and

$$a_m(U, T) = \frac{x_0^2\left\{\frac{U(x_0, \tau) - U_0}{\sqrt{\tau}} + \frac{1}{2}\int_{\tau_U}^{\tau}[U(x_0, \nu) - U_0]\nu^{-3/2}d\nu\right\}}{4\tau^{3/2}\frac{dU(x_0, \tau)}{d\tau}}. \tag{25}$$

An estimate of the accuracy of the above method of determining HMT characteristics performed in accordance with [9, 10] showed that the systematic error of determination of the sought characteristics from theoretical relations (21)-(25) is 8% for thermal conductivity, 6% for diffusivity, and 9% for diffusion. In the determination of thermodiffusion, the error of calculation of the characteristics is significantly affected by the contribution of the thermodiffusion flux to the overall mass flow. A reduction in this contribution is accompanied by an increase in the thermodiffusion error, which in the best case is on the order of 15-20%.

The proposed method was tested on several friable and solid materials in the mass transport of both moisture and of different solvents. The absence of materials with standard characteristics of coupled HMT and the substantial differences in the numerical values of the sought characteristics obtained by different authors for the same given material make it necessary to evaluate the reliability of the method and results by analyzing the adequacy of the chosen model to the physical HMT process realized in a test. The data obtained on the HMT characteristics of the investigated materials was used as a basis for calculating theoretical curves depicting the change in specimen temperature and concentration as a result of numerical solution of a direct nonlinear problem of coupled HMT with the conditions realized in an independent experiment. Comparison of the theoretical and experimental curves of change in temperature and concentration in different sections of the specimens showed that their differerence did not exceed the errors of measurement of the respective field quantity. This is evidence of the accuracy of the proposed method and the reliability of the results obtained for the HMT characteristics of the investigated materials.

NOTATION

T, temperature of the medium, K; U, concentration of substances distributed in the medium, kg/kg; a_m, diffusion, m^2/sec; a_m^T, thermodiffusion, $m^2/(sec \cdot K)$; C, C_0, C_q, specific heat capacity of the medium, the medium at U = 0, and the substance distributed in the medium, $J/(kg \cdot K)$; γ_0, density of the dry material, kg/m^3; λ, thermal conductivity, $W/(m \cdot K)$; a, diffusivity, m^2/sec; j_m^U, j_m^T, j_m, density of the diffusion, thermodiffusion, and total fluxes of the substances, $kg/(m^2 \cdot sec)$; q, heat flux, W/m^2; x, space coordinate; τ, time.

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