БЪЛГАРСКА АКАДЕМИЯ НА НАУКИТЕ BULGARIAN ACADEMY OF SCIENCES
ТЕОРЕТИЧНА И ПРИЛОЖНА МЕХАНИКА THEORETICAL AND APPLIED MECHANICS
София, 1990, год. XXI, № 4 Sofia, 1990, Year XXI, No 4

An Algorithm for Numerical Solution of One Class of Inverse Problems for Diffusion with Memory

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The molecular diffusion in porous materials realizes simultaneously with some physicochemical processes. There have been proposed some generalized transient equations, accounting the latter processes [1], [2]. It is shown [3], [4] they can be considered as special cases of transient equations for materials with memory.

The determination of the parameters of the generalized transient equations, which values are usually not enough known, is of practical interest. The subject of the present paper is the numerical solution of one class of inverse problems for diffusion with memory, when the concentration gradient history of the diffusing component is accounted by an exponential memory function. In this case the investigations could be referred to the generalized models of Luikov [1] and the models for diffusion and first-order reaction [5], [6].

The experimental determination of the moisture concentration profiles at different moments of the concrete masstransfer process (for example drying) is connected with a precise measurement equipment. With the purpose to develop an effective method for parameters identification it is expedient to consider such inverse problems, which are based on the data from simplified experiments. An example for such an experiment is the mass measuring of the samples during the moisture transfer under consideration (drying or moisture saturation).

The aim of the present investigation is to propose a numerical method for automatic determination of the model parameters (connected with the class of problems under consideration) based on descrete experimental data for the sample mass as a function of time. We will use the numerical algorithm for solution of the corresponding boundary problem, developed in [7].

Statement of the inverse problem of diffusion with memory. Numerical algorithm for its solution

We set the problem to evaluate the parameters D, K_1 and K_2, connected with the model equation for diffusion with memory:

$$(1)\qquad \frac{\partial c}{\partial t} = -D \operatorname{div} \operatorname{grad} c + D \int_0^t K_1 \exp[-(K_1+K_2)(t-t')] \operatorname{div} \operatorname{grad} c(t')\, dt' \quad \text{in } V$$

under the following boundary and initial conditions:

(2) $$c/_s = c^0(t)$$

(3) $$c/_{s=0} = c_0 = \text{const.}$$

and under the assumption that the values of the functional $\Delta M(t)$ are known for $t=t_i$, $i=0, 1, \ldots, N$, where

(4) $$\Delta M = \int_V (c - c^\infty)\,\mathrm{d}v \quad \left(\text{or} \quad \Delta M = \int_V (c - c_0)\,\mathrm{d}v\right).$$

With c, c^∞, $c^0(t)$ and ΔM we denote correspondingly the moisture concentration, its equilibrium value, the known functional dependence of the boundary moisture concentration on t and the mass of moisture in the considered sample, taking part in the masstransfer from the moment t to the steady state moment t^∞ (or from the initial state to the moment t).

We want the known values $\Delta M(t_i)$ to be approximated by the corresponding model values ΔM_i, derived from (1)-(4), to a sufficiently good desired accuracy, i. e. to minimize $\|\Delta M_i - \Delta\tilde{M}_i\|$ within such accuracy, where $\|\cdot\|$ is a selected norm.

Supposing the experimental data for ΔM_i are normally distributed, the determination of D, K_1 and K_2 could be done by the least square method, minimizing the quadratic form*:

(5) $$F(D, K_1, K_2) = \sum_{i=1}^{N} (f_i - \tilde{f}_i)^2,$$

where

(6) $$f_i = \frac{\Delta M_i}{\Delta_{\max} M}.$$

The determination of $\tilde{f}_i$ is done numerically in two steps:

1. Following the algorithm for the boundary problem (1)-(3) solution [7], we calculate the values of the function $\tilde{c} = (c - c)/(c_0 - c^\infty)$ at the nodes of the finite element mesh, introduced for the domain V, for every $T_i = \frac{t_i}{t^\infty}$.

2. The model values $\tilde{f}_i$ are evaluated from (4) and (6), using the FE approximation of $\tilde{c}: \{C\}_i \{N\}_i$.

The flowchart of the algorithm for numerical determination of the model parameters is presented in Fig. 1 and Fig. 2. On its base a program is developed in the case of a two-dimensional diffusion. The algorithm is tested by program realizations on EC1061 using experimental data for the mass of the cement stone samples, measured during their drying at constant temperature 105°C [8]. We have used the following approximation at the boundary condition $c^0 = \text{const.}$ The zero values, obtained for K_1 and K_2, can be explained with the week effect of the sorption processes, realizing very fast at 105°C. It is used 20 min processor time at 3% accuracy of minimizing the form (5).

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* We propose the following procedure of data processing for the considered series of samples:

1. Normalizing of the experimental data for every sample with $\Delta_{\max} M_i = M(0) - M(t^\infty)$ (or with $M(t^\infty) - M(0)$, referred to $T_i = t_i/t^\infty$.

2. Averaging of the normed data f_i for the series of samples.

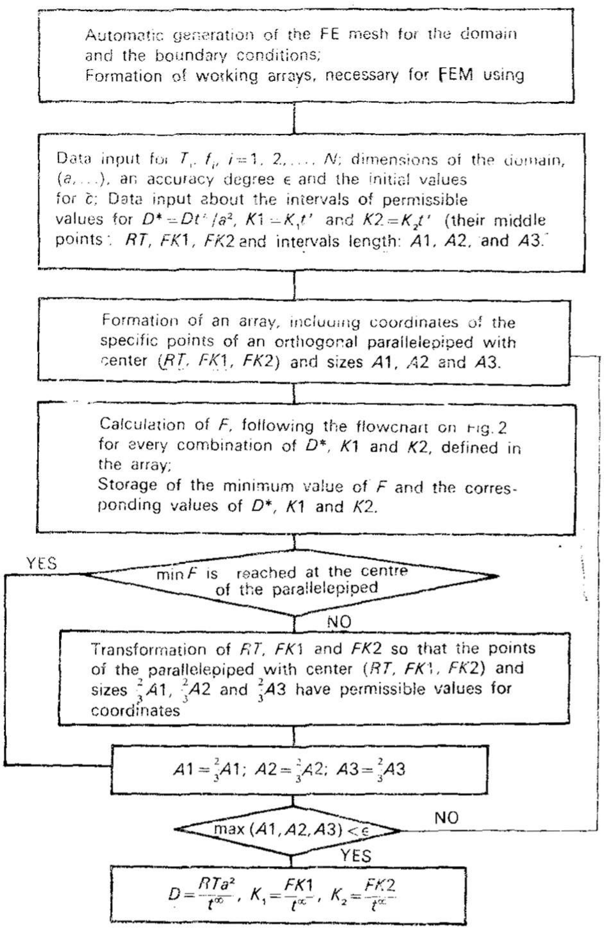

Fig. 1

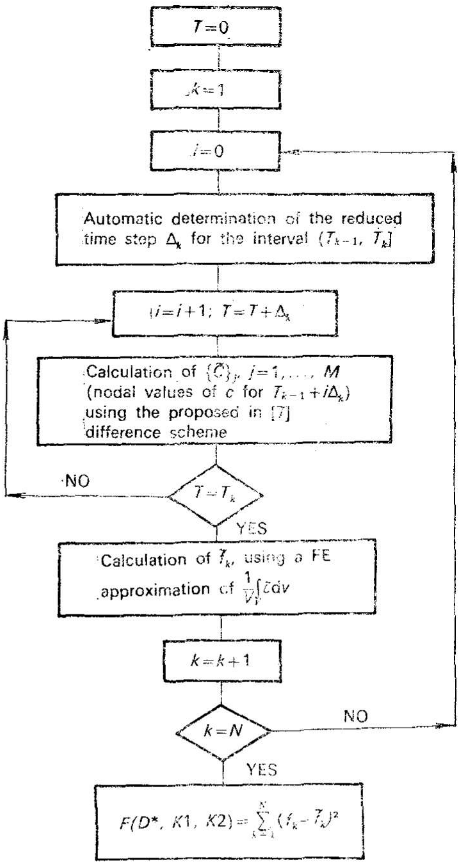

Fig. 2

Conclusions

The proposed algorithm can be used for determination of the model parameters, connected with an isothermal moisture transfer process. Simultaneously the applicability of the considered generalized transfer equation can be tested for different masstransfer processes of diffusion type.

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Received 2. 09. 1988