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SOLUTION OF INVERSE PROBLEMS OF THE MECHANICS OF REACTIVE MEDIA

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The general inverse problem of heat and mass transfer in a porous reactive material is reduced to a set of particular problems by using splitting of the problem according to chemical and physical processes. A brief exposition is given of the methods for solving these particular inverse problems.

I. To raise the accuracy of computations in the mechanics of reactive media, more and more complex formulations of the problem are utilized at this time [1]. The complication proceeds in the direction of a more complete and detailed accounting of the structure and manifold of physicochemical transformations, extensive propagation of the conjugate as well as the two- and three-dimensional formulations of the problems. In all cases the extensive introduction into practice is repressed by the absence of information about the thermophysical coefficients, the thermokinetic constants of heterogeneous and homogeneous chemical reactions, and the flow characteristics on the surface of the streamlined reactive body. The characteristics mentioned can be determined as a result of solving inverse problems.

The following scheme is proposed for investigating complex inverse problems: 1) the most complete mathematical model is written on the basis of an analysis of a physicochemical model of the processes; 2) the most essential factors are exposed, say, on the basis of an analysis of dimensionalities and similarity, time expenditures of the researcher and the computer are taken into account and a more optimal, compromise mathematical model is constructed; 3) a search of available literature data is conducted, laboratory tests are planned and performed on specimens of the materials being investigated under conditions as close as possible to the full-scale conditions in order to determine the unknown characteristics and to obtain information to estimate the adequacy of the mathematical model; 4) appropriate particular inverse problems are posed and solved; 5) the direct problem is solved by using the obtained transfer coefficients and thermokinetic constants; the solution obtained is compared with full-scale and model experimental data.

As an example, let us consider the mathematical model of heat and mass transfer processes in a porous reactive material (glass-plastic) in a one-dimensional nonstationary formulation

$$\frac{\partial}{\partial t}(\rho_1\varphi_1) = -\rho_1\varphi_1 k_1 \exp\left(-\frac{E_1}{RT}\right), \tag{1}$$

$$\frac{\partial}{\partial t}(\rho_2\varphi_2) = \alpha_1\rho_1\varphi_1 k_1 \exp\left(-\frac{E_1}{RT}\right) - \rho_2\varphi_2 k_2 \exp\left(-\frac{E_2}{RT}\right), \tag{2}$$

$$\frac{\partial}{\partial t}(\rho_3\varphi_3) = \alpha_2\rho_2\varphi_2 k_2 \exp\left(-\frac{E_2}{RT}\right),\ \rho_4\varphi_4 = \text{const}, \tag{3}$$

$$\frac{\partial}{\partial t}(\rho_5\varphi_5) + \frac{\partial}{\partial y}(\rho_5\varphi_5 v) = (1-\alpha_1)\rho_1\varphi_1 k_1 \exp\left(-\frac{E_1}{RT}\right) + (1-\alpha_2)\rho_2\varphi_2 k_2 \exp\left(-\frac{E_2}{RT}\right), \tag{4}$$

$$\rho_5\varphi_5\left(\frac{\partial c_\alpha}{\partial t} + v\frac{\partial c_\alpha}{\partial y}\right) = \frac{\partial}{\partial y}\left(\rho_5\varphi_5 D_\alpha \frac{\partial c_\alpha}{\partial y}\right) - c_\alpha R_5 + R_{5\alpha},\ \alpha = 1,\ 2, \tag{5}$$

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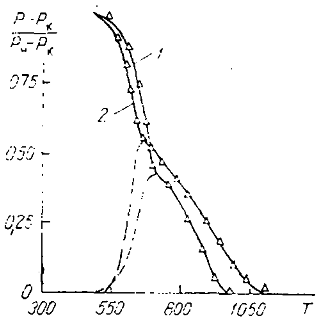

Fig. 1

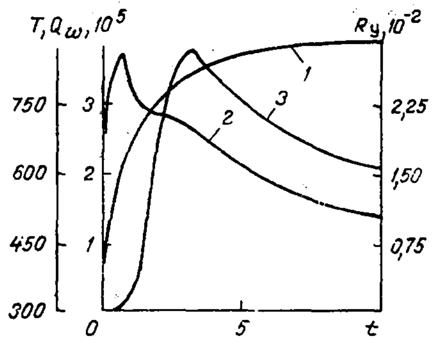

Fig. 2

Fig. 1. Relative weight loss for specimens of the materials VPR-10 + IFED (1) and VPR-10 + EKhD (2) for q = 0.085 K/sec; points are computed values. T, K.

Fig. 2. Initial temperature T_w (1) and heat flux Q_w (2) and mass entrainment rate R_e (3) restored from the solution of the pseudo-inverse problem as a function of the time t. T, K; Q_w, W/m^2; R_e, kg/(m^2·sec); t, sec.

$$\frac{\partial P}{\partial y} = -\frac{\mu v}{k}, \tag{6}$$

$$\left(\sum_{i=1}^{5} \rho_i\varphi_i C_{pi}\right)\frac{\partial T}{\partial t} + \rho_5\varphi_5 C_{p5} v\frac{\partial T}{\partial y} = \frac{\partial}{\partial y}\left(\sum_{i=1}^{5}\lambda_i\varphi_i\frac{\partial T}{\partial y}\right) - q_1\rho_1\varphi_1 k_1\exp\left(-\frac{E_1}{RT}\right) + q_2\rho_2\varphi_2 k_2\exp\left(-\frac{E_2}{RT}\right) + q_R R_h\exp(-R_h y), \tag{7}$$

$$P = \frac{\rho_5 RT}{M},\ \frac{1}{M} = \sum_\alpha \frac{c_\alpha}{M_\alpha},\ \sum_\alpha c_\alpha = 1,\ \sum_{i=1}^{5}\varphi_i = 1. \tag{8}$$

The system (1)-(8) is written for moderate heating times and temperatures of up to approximately 1000°C. The sequential scheme of two pyrolysis reactions, the filtration of gaseous products, the conductive and convective heat transfer, the diffusion of gaseous components (the "fuel-oxidizer" scheme) and heat absorption in a glass-plastic according to the Bouger law is taken into account.

To solve specific problems this system of equations should be supplemented by appropriate initial and boundary conditions, and the coefficients of the mathematical model are determined in the form of constants or of certain approximate dependences.

II. Using the method of splitting the problem according to physical and chemical processes, inverse problems of different types may be set up. Thus, if the characteristic times of the heat conduction, diffusion, and filtration processes are much less than the characteristic time of pyrolysis [1, 2]

$$t_e = \frac{r_0^2}{a} \ll t_p,\ t_D = \frac{r_0^2}{D} \ll t_p,\ t_f = \frac{r_0^2}{u_*} \ll t_p, \tag{9}$$

i.e., the process proceeds under homothermal conditions, then (1)-(3) describing the pyrolysis of glass-plastics for a known time dependence of the temperature are separated out of equations (1)-(8), and an inverse kinetic problem can be formulated for this process: Determine the kinetic constants from time dependences of the specimen temperature and weight known from experiment. The algorithm for the solution of such a problem was constructed by minimization of the residual

$$\delta = \sum_{i=1}^{N} W_i (P_i - P_i^e)^2,\ P = gV\sum_{i=1}^{4}\rho_i\varphi_i \tag{10}$$

by a quasigradient method by using scaling of the variables [2].

Results of solving the inverse problem and comparison with experiment by thermal decomposition on a derivatograph are given in the table and in Fig. 1 for the materials VPR-10 + IFED and VPR-10 + EKhD. It is seen that agreement is good enough between the experimental and computed values of the specimen weights. The accumulation of the intermediate

TABLE 1. Kinetic Constants of the Thermal Decomposition of Glass-Plastics Based on VPR-10

Binder	Experiment conditions		k, 1/sec	E/R, K	α
	q, K/sec	T, K			
IFED	0,085	373—1023	$0,122\cdot 10^5$	10670	0,48
			0,334	5480	0
EKhD	0,085	373—1073	$0,527\cdot 10^7$	13050	0,59
			$0,526\cdot 10^{-1}$	4000	0

pyrolysis product — pyrosol — is extracted by dashed line in the figure. The first stage is endothermal in nature while the second is associated with the formation of a coke residue and is exothermal.

Similar results are also obtained for other heating times and materials. It should be noted that as the heating time increases the kinetic constants also change, as was noted in [3, 4] and generalized in [5]. Consequently, to utilize the kinetic constants under conditions of a sharp distinction from experiment, they must be corrected. Some of the methods are given in [5].

Among the inverse problems of chemical kinetics are also problems on determining the thermokinetic constants of heterogeneous chemical reactions. Problems on determining the activation energy and the preexponential of the oxidation reaction of the carbon-graphite material EG-0 and polymethylmetacrylate are solved. The existence and uniqueness of the solution of these problems are proved [2].

III. Inverse boundary value problems of heat and mass transfer are formulated as follows: On the basis of known initial conditions, boundary conditions on the internal body surface Y_3, and an additional condition about the temperature on the external heated body surface $Y_1(t)$ or at a certain interior point Y_2, restore such important heat and mass transfer characteristics as the heat flux and mass entrainment rate was well as the field of all the desired functions in the whole domain of integration $D\{Y_1(t) \le y \le Y_3,\ 0 \le t \le t_K\}$ on the surface $Y_1(t)$. The function $Y_1(t)$ is considered known. When the temperature on the body surface is given as the additional condition, the problem is called pseudo-inverse. A simpler mathematical model of the physicochemical processes than (1)-(8) was used in its solution: heat transfer by radiation and heterogeneous chemical reactions were not taken into account, the material was modeled by a four-component porous reactive medium consisting of the original polymer binder, a coke residue, a gas phase, and a filler, respectively. Adiabaticity, nonpenetration, and the derivative of the gas density with respect to the space coordinate equal to zero were used as boundary conditions on the surface Y_3. The permeability coefficient was determined from the Kozeni—Karman formula and the dynamic viscosity from the Sutherland formula. The solution of the pseudo-inverse problem was performed numerically by IIM [6] for a material similar in its properties to a glass-plastic with an epoxy-phenolic binder. The iteration process of the search for the desired functions in a new time layer was terminated upon satisfaction of given accuracy or the maximal number of iterations. The initial surface temperature T_W as well as the heat flux Q_W and the rate of mass entrainment R_e found from solving the inverse heat and mass transfer problem are presented in Fig. 2.

When the temperature at a certain interior point of the body is given instead of the temperature on the reactive body surface and the heat flux at this point is different from zero, a direct numerical method and a regularizing algorithm on the basis of a Tkhonov method [7] were used to solve the inverse problem. A generalized heat conduction equation given in a domain with moving boundaries was used to describe the heat transfer process in the body. Stability of the solution of the inverse heat conduction problem was achieved when using the direct numerical method by step regularization and smoothing of the initial temperature by spline functions or by the Tikhonov method. Selection of the regularization parameter when solving the inverse heat conduction problem by using the regularizing algorithm was realized by the residual principle. The following changes [8] were introduced in the known algorithm from [7] to obtain a stable solution of the inverse heat conduction problem when using the original temperature given with error. Firstly, the solution of the direct heat conduction problem was realized in the residual method by using IIM in the whole domain D. Secondly, the heat flux coming into the body was determined from solution of the direct heat conduction problem by an analytic formula obtained on the basis of IIM. This algorithm is well recommended for the processing of the heat flux sensor readings. Its detailed numerical investigation was performed in [8].

IV. The next type of inverse heat and mass transfer problem are coefficient inverse problems. They are realized if the characteristic filtration time is much less than the characteristic heat conduction time $t_f \ll t_e$ and are formulated as follows. Determine thermophysical characteristics of the reactive material λ, ρC_p by means of known initial conditions, boundary conditions on the exterior and interior surfaces of the material and by the known temperature at inner points of the body. The specimen heating modes can be arbitrary but assuring specimen heating in the temperature band of interest. To simplify the computations the specimen is selected in such a shape that heat propagation therein would be one-dimensional. Conditions were here conserved that assure a unique solution of the inverse problem [2, 9, 10]. A parametric representation of the thermophysical characteristics desired was used. A direct numerical method and an iteration algorithm based on the method of conjugate gradients with coordiante transformation [2] were used to determine the approximation parameters. In the first case the mathematical model of the process consisted of one heat conduction equation with effective thermophysical characteristics, and in the second, of a system of heat and mass transfer equations. In contrast to [11], a difference approximation of the partial derivatives of the functional with respect to the parameters was used when using the iteration algorithm, which was caused by the difficulty in determining the gradient of the functional in terms of the solution of the conjugate problem. The approximation and numerical differentiation of the experimental temperature in the direct numerical method were conducted by using cubic B-splines. Stability of the solution in this method was achieved because of step regularization and utilization of an iteration regularizing algorithm from [2] for the solution of the system of linear algebraic equations to determine the approximation parameters. Instability of the solution in the gradient method of parametric optimization was eliminated because of the selection of the ultimate amount of iterations consistent with the known integral error of the original data. The results of the numerical investigation of the inverse coefficient heat conduction problem are presented in [2].

When the structure of the multiphase reactive medium and the thermophysical coefficients of its components are known, formulas obtained on the basis of the theory of the generalized heat conduction and the additivity principle [1] were used to determine the heat conduction coefficients and the specific heats of the medium during the solution of the direct and pseudoinverse heat and mass transfer problems.

As a rule, the method of splitting a complex problem according to chemical and physical processes and in this connection simplified problem formulations are utilized in the solution of inverse heat and mass transfer problems. However, the effective thermokinetic and thermophysical coefficients influence each other, consequently, algorithms for their simultaneous determination have been proposed recently which would permit taking account of the mutual influence of the coefficients. The efficiency of these algorithms is confirmed by the solution of model examples.

NOTATION

y, spatial coordinate; t, time; T, temperature; ρ, density; P, pressure, v, velocity; φ, volume fraction; c, mass concentration; M, molecular weight; D, effective diffusion coefficient; R_5, mass rate of formation of gaseous pyrolysis products; R_k, coefficient of radiation attenuation in the Bouger law; R_e, mass entrainment rate; k, permeability coefficient; μ, dynamic viscosity; λ, heat-conduction coefficient; C_p, specific heat; k_1, E_1, q_1, k_2, E_2, q_2, preexponential, the activation energy, and the thermal effects of the first and second reactions, respectively; q_R, magnitude of the radiation flux absorbed by the material; q, specimen heating time; α_1, α_2, reduced stoichiometric numbers; R, universal gas constant; Q, heat flux; t_e, t_D, t_f, t_p, characteristic times of the heat conduction, diffusion, filtration and pyrolysis processes; a, thermal diffusivity coefficient; u_*, characteristic filtration rate; P_i^e, P_i, experimental and theoretical values of the specimen weight; W_i, statistical weight; g, free-fall acceleration; V, specimen volume; $Y_1(t)$, Y_3, coordinates of the external and internal body surfaces; Y_2, coordinate of an interior point of the body with a known temperature. Subscripts: 1, initial binder; 2, 3, intermediate and condensed pyrolysis products; 4, inert filler; 5, gas phase; α, number of the gaseous component; H, initial state; K, final state; w, surface $Y_1(t)$. IIM, iteration-interpolation method.

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SOLUTION OF A TWO-DIMENSIONAL HEAT-CONDUCTION PROBLEM FOR A GEOMETRICALLY COMPLEX DOMAIN BY AN INTEGROINTERPOLATION METHOD

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A methodology is proposed for the construction of an algorithm to solve heat transfer problems for spatial domains of complex geometric shape.

The creation of a new engineering operating under high-temperature loading or intensive cooling conditions is associated with carrying out a large amount of special temperature investigations of materials and structures. Such operations are a constant necessity for many branches of industry, consequently, thermal computation methods are also perfected simultaneously with the rise in the demands on engineering systems. Computational algorithms based on one-dimensional formulations of heat transfer problems are most widespread. If a notable fraction of algorithms arrived earlier at analytic methods of solution, then numerical methods have acquired greater weight at this time in connection with the development of computer technology. These methods possess a substantial advantage resulting from the possibility of their utilization for different formulations of problems, for instance, with any nonlinearities taken into account.

However, when studying fine physical processes associated with structure heating, it is already not always sufficient to utilize a one-dimensional heating model Hence, a large quantity of researches has appeared devoted to methods and algorithms for the solution of heat transfer problems in multidimensional formulations.

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