

CONSTRUCTION AND IDENTIFICATION OF MATHEMATICAL MODELS
OF HEAT TRANSFER AND MASS TRANSFER IN CAPILLARY-POROUS
BODIES

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An engineering approach to the construction, identification, and use of mathematical models of heat and mass transfer is proposed for the selection of optimal regimes for the heating of capillary-porous bodies.

Most technological processes for treating capillary-porous bodies occur at high temperatures, a situation that results in intensive external and internal transfer of heat and mass. Examples of this type of a process are the drying of foods and other products, thermal treatment of construction materials, etc. The main problem in developing a new process or improving an existing one is the selection of the working parameters (ambient temperature, type of heat exchange, time and rate of heating), which provide for good quality of production, minimal expenditure of energy, high efficiency, safety, and environmental control. Selection of the optimal regime for high-temperature heating of capillary-porous bodies encounters difficulties stemming from the following factors. Firstly, heat and mass transfer, as a rule, are accompanied by phase transitions and chemical transformations on the surface and interior of the material. Thus, drying of the products is accompanied by the intensive evolution of moisture, while thermal treatment of construction materials leads to evaporation and hydration of the binding materials. Secondly, capillary-porous bodies have a high porosity. These two factors, taken together, cause appreciable change in the structure of the material during heating.

It is common to use a system of differential equations based on the theory of irreversible processes for constructing a mathematical model of heat and mass transfer in capillary-porous bodies; the system of equations for coupled heat and mass transfer proposed by A. V. Lykov [1] is most commonly used. The use of this system will not always yield correct results since the system does not account for structural changes that occur in a body during heating. A consequence of these changes is that the characteristics of the material entering into the equations are functions of the process rather than physical constants. As an illustration, we refer to the data of several authors. The thermophysical and mass-exchange properties of the hardening claydite concrete were investigated in [2]. As a result it was obtained that the coefficient of thermal conductivity changes by a factor of four, and the coefficient of diffusion of moisture changes by more than a factor of ten during the heating process. The coefficient of thermal conductivity λ of the special concrete was measured in [3]. In the process of hardening, the value of λ at first increases from 1 to $11 \text{ W} \times \text{m}^{-1} \times \text{K}^{-1}$ and then decreases sharply to $0.5 \text{ W} \times \text{m}^{-1} \times \text{K}^{-1}$. Apparently, such a noticeable change in the values of heat and mass exchange characteristics is related to new structural formations inside the material.

Since the characteristics of the capillary-porous body depend on changes in the structures of the material and, therefore, are functions of the heating process and transfer potentials, and the kinetics of the structurization is complicated and unknown in most cases, they cannot be determined except experimentally; the experimental conditions should correspond to specific regimes existing in practice. Strictly speaking, characteristics obtained in one regime must not be used for the theoretical analysis of the other one. Therefore, a great many laborious experiments are required.

Two more difficulties in using the system of equations of the coupled thermal mass transfer should be noted. The first is that due to variability of characteristics, the equations become

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substantially nonlinear, so that it is difficult to analyze the process, even with the help of modern computers. The second difficulty derives from the fact that a number of thermal and mass-exchange characteristics, which are determined experimentally with high error, enter into the system (thermal, about 10%, and mass exchange, up to 30-40%). Therefore, the accuracy of the final result is small, regardless of the method of solution.

Thus, the use of the system of equations of coupled thermal mass exchange for the analysis and selection of optimal conditions for heating the capillary-porous bodies is limited and requires additional grounds for each particular case.

Below, we offer an approach to the analysis of heat and mass exchange in capillary-porous bodies, based on two assumptions: 1) as experiments show, temporal and spatial dependencies of the transfer potentials (temperature, moisture content) are monotonic in nature and are mainly determined by the working parameters of the heating process; 2) in order to describe the processes of heat and mass transfer, we require a compromise between the experimental data, reflecting the real properties of materials, and the theory, which allows the data to be analytically connected with the heating regime.

The essence of the offered approach is as follows. In the first stage of the investigation, a mathematical model is formulated on the basis of preliminary information on the specifics of the process in the material under study (a special experiment is performed if required). The model should meet the following requirements: it should reflect only those phenomena which make the greatest contribution to the heat and mass transfer; 2) equations describing the model should contain the minimal number of parameters subject to experimental determination; 3) the equations themselves should be relatively simple, allowing us to analyze the influence of each factor on the entire process based on a numerical experiment.

In the second stage, the equations (or a system of equations) of heat and mass transfer are solved, and analytical expressions for calculating the potential fields for the transfer are found. It should be noted that these equations cannot be considered as an adequate mathematical description of the actual process. Solutions obtained in the given case constitute certain functions which approximate more complicated dependencies, not known with full details, between the heating regime and phenomena occurring inside the material. Methods have been developed for solving the inverse problems for determining the transfer coefficients which enter into the equations. In fact, these coefficients are parameters of the approximating model rather than properties of the material.

In the third stage, experiments with a specified capillary-porous body of real configuration are performed with the limiting (lax and strict) values and mean values of the working parameters. In the experiments, the potential fields for the transfer are measured, and then the parameters of the model are determined on the basis of the solution of the inverse problem.

In the last, fourth stage, the parameters determined for the limiting regimes are averaged. Proceeding from the averaged values, the potential fields of the transfer are calculated for the limiting and mean regimes. Then the results of the calculations are compared to the experimental data. If the discrepancy is negligible and meets the practical needs, then such a model can be used for describing the processes of heat and mass transfer in the investigated region, as well as for analysis and search of the optimal values of the working parameters. In case of appreciable discrepancies between the calculated and experimental data, the model calls for correction and improvement. If this does not lead to a positive result or complicates the model unduly, the approach should be replaced by other possible ways of solving the problem. This condition constitutes a criterion of applicability of the proposed method.

The approach described above can be formulated briefly in the following way. In Fig. 1, a conventional input value X (temperature of heating, intensity of heat exchange, etc.) is plotted along the x axis, and a conventional output value Y (temperature or humidity of the surface or center of the body, temperature gradient, the maximal temperature differential, etc.) is plotted along the y axis. The limiting and mean values of the input parameter are designated, respectively, by X_A , X_B , and X_C . The proposed method consists in finding the function $Y = f(X)$, which approximates a relationship between the output and input values in the interval $[X_A; X_B]$, the coefficients of this approximating function being determined experimentally.

The proposed method has been used for solving three practical problems: finding the optimal regime of high-temperature thermal treatment of claydite concrete [4]; determining the parameters of a chemical reactor producing maleic anhydride [5]; and describing the

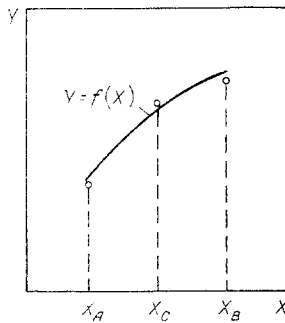


Fig. 1. Dependence of the output value Y on the working parameter X. By convention, the experimental data is represented by dots.

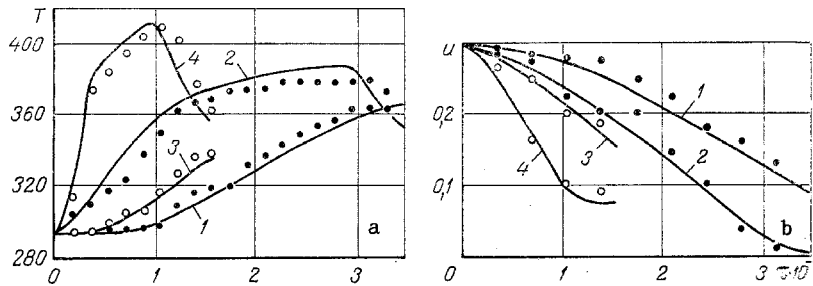


Fig. 2. Temperature T (a) and moisture content u (b) versus time τ for central (1, 3) and surface (2, 4) layers of the claydite concrete under lax (1, 2) and strict (3, 4) conditions of thermal treatment. Dots represent the experimental data, and curves represent results of calculation. T, K; u, kg/kg; τ , sec.

kinetics of the high-temperature drying of milled peat in tube dryers [6].

In investigating the processes of heat and mass transfer in claydite concrete, a simple model is used, which is based on the following assumptions: mass exchange produces only a negligible effect on the formation of the thermal field; moisture transfer is due to the temperature gradients and moisture content; the internal heat source and drainage of moisture due to the reaction of hydration of the concrete make a negligible contribution to the common balance of heat and mass; the transfer coefficients are constant; and the concrete slab can be approximated by an infinite slab. The parameters of the model under consideration are the coefficients of thermal conductivity a and diffusion of moisture a_m , thermogradient coefficient δ , relative coefficients of heat exchange at the lower (closed) and upper (open) surfaces h_1 and h_2 , and coefficient of mass efficiency α_m . For the determination of the listed characteristics, the experiments were performed under conditions of strict (the heating rate $b = 4.44 \times 10^{-2}$ K/sec, temperature of the isothermal aging $T_i = 433$ K, aging time $\tau_i = 7.2 \times 10^3$ sec) and lax ($b = 1.11 \times 10^{-2}$ K/sec, $T_i = 393$ K, $\tau_i = 2.16 \times 10^4$ sec) regimes. The values of the coefficients obtained are for the strict regime: $a = 7.5 \times 10^{-7}$ m²/sec, $a_m = 6.3 \times 10^{-7}$ m²/sec, $\delta = 1.3$ K⁻¹, $h_1 = 32$ m⁻¹, $h_2 = 25$ m⁻¹, $\alpha_m = 2.8 \times 10^{-8}$ sec/m; and for the lax regime: $a = 6.4 \times 10^{-7}$ m²/sec, $a_m = 4.7 \times 10^{-7}$ m²/sec, $\delta = 0.7$ K⁻¹, $h_1 = 28$ m⁻¹, $h_2 = 19$ m⁻¹, $\alpha_m = 2.2 \times 10^{-8}$ sec/m.

The temperature and moisture content fields are calculated from the averaged values of the parameters ($a = 7.0 \times 10^{-7}$ m²/sec, $a_m = 5.5 \times 10^{-7}$ m²/sec, $\delta = 1.0$ K⁻¹, $h_1 = 30$ m⁻¹, $h_2 = 22$ m⁻¹, $\alpha_m = 2.5 \times 10^{-8}$ sec/m). As is seen from Fig. 2, the experimental and calculated results for the limiting regimes qualitatively are in good agreement; satisfactory quantitative agreement is also observed (the maximal discrepancy is about 20%). A comparison of experimental and calculated data for the mean regime gave similar results. Therefore, the dependencies, obtained on the basis of the considered model, approximate adequately the experimental data

over the entire range of working parameters and can be used for selecting the optimal regime of the thermal treatment.

NOTATION

λ , a , thermal conductivity and thermal diffusivity, respectively; a_m , moisture diffusion coefficient; δ , thermogradient coefficient; α , heat-treated coefficient; $h = \alpha/\lambda$, relative heat transfer coefficient; α_m , coefficient of mass efficiency; τ , time; T , temperature; u , moisture content; b , heating rate; T_i , temperature of isothermal aging; τ_i , aging time.

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