

INVESTIGATION OF THE HEAT-TRANSFER
CHARACTERISTICS IN DECOMPOSING HEAT-
SHIELD MATERIALS

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A derivation is given for the general equations of heat and mass transfer in decomposing heat-shield material on the basis of using the Umov transfer equation. A simplified system of equations is presented which contains the functional thermophysical characteristics. The functional thermophysical characteristics are determined in a numerical example for the case when the functionality is due to thermal decomposition of the material according to the Arrhenius law.

At present, principally decomposing material of the bonded plastics type are used in heat shields operating under intensive thermal load conditions. Complex and multistage physicochemical transformations occur in these materials under high-temperature heating, which alter the structure, chemical composition, and physical properties of the material substantially, and exert significant influence on the heat transfer within the coating. Models based on using the mass-, energy-, and momentum-conservation laws with different simplifying assumptions [1-4] are ordinarily used to describe mathematically the heat- and mass-transfer processes in decomposing materials, and, as a rule, the questions of the practical determination of the physical characteristics used in these equations hence remain open.

On the basis of using the Umov equation, the derivation of the general heat- and mass-transfer equations in a decomposing heat-shield material is given in this paper. Simplified equations are presented which have been obtained by introducing the functional thermophysical characteristics. The method of determining the functional thermophysical characteristics, which is based on solving the inverse problem, is examined in the example of a numerical experiment.

Let us assume that the decomposing heat-shield material can be considered as a homogeneous porous medium consisting of a gaseous phase and a solid phase, where each phase consists of a definite number of mutually reacting components. To obtain the fundamental conservation equations, let us, analogously to [5], use the Umov equation of substance transfer,

$$\frac{\partial C}{\partial t} + \text{div}(CV_C) = -\text{div}(j_C) + I_C, \quad (1)$$

where C , V_C , j_C , I_C are, respectively, the concentration, velocity of convective transfer, diffusion flux, and intensity of the volume sources of the substance.

The mass-conservation equation of the i -th gaseous component is obtained from (1) by using the following relationships:

$$C = m\rho_{1i}, \quad V_C = V_1 \cdot \frac{s}{m}, \quad j_C = sj_{1i}, \quad I_C = \omega_{1i},$$

$$\frac{\partial}{\partial t}(m\rho_{1i}) + \text{div}(s\rho_{1i}V_1) = \text{div}(sj_{1i}) + \omega_{1i}. \quad (2)$$

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Summing (2) over all i -components and taking account of the relationships

$$\rho_1 = \sum_{i=1}^N \rho_{1i}, \quad \sum_{i=1}^N j_{1i} = 0, \quad \omega_1 = \sum_{i=1}^N \omega_{1i},$$

we obtain the mass-conservation equation for the gaseous phase:

$$\frac{\partial}{\partial t} (m\rho_1) + \operatorname{div} (s\rho_1 \mathbf{V}_1) = \omega_1. \quad (3)$$

The mass-conservation equation for the solid phase can be obtained analogously:

$$\frac{\partial}{\partial t} [(1-m)\rho_{2i}] + \operatorname{div} [(1-s)\rho_{2i} \mathbf{V}_2] = -\operatorname{div} [(1-s)j_{2i}] + \omega_{2i}, \quad (4)$$

$$\frac{\partial}{\partial t} [(1-m)\rho_2] + \operatorname{div} [(1-s)\rho_2 \mathbf{V}_2] = \omega_2, \quad (5)$$

$$\rho_2 = \sum_{i=N+1}^{N+M} \rho_{2i}, \quad \omega_2 = \sum_{i=N+1}^{N+M} \omega_{2i}.$$

Here \mathbf{V}_2 is the mean mass flow rate of the solid phase, the velocity of material shrinkage, or deformation because of the thermal stresses, pressure, external forces, etc.

To derive the momentum-conservation equation of the gas phase, let us use the relationships

$$C = m\rho_1 \mathbf{V}_1, \quad \mathbf{V}_C = \frac{s}{m} \mathbf{V}_1, \quad j_C = s_1 p, \quad I_C = m\rho_1 F_1, \quad (6)$$

$$\frac{\partial}{\partial t} (m\rho_1 \mathbf{V}_1) + \operatorname{div} (s\rho_1 \mathbf{V}_1 \mathbf{V}_1) = \operatorname{grad} (s_1 p) + m\rho_1 F_1,$$

where p is the pressure, s_1 is a coefficient [6] reflecting the magnitude of the surface through which the pressure pulse is transmitted (for the case when the porous material is a system of linear capillaries $s_1 = s$), and F_1 is the fictitious mass resistance force during gas filtration in the porous medium.

The equation of solid-phase motion cannot be written down, since the processes associated with displacement of the solid carcass, including the shrinkage, have still been investigated only slightly. Hence, we shall consider the velocity \mathbf{V}_2 a given quantity.

Let us use the equation of state in the form

$$p = \rho_1 R T_1 \quad (7)$$

to obtain the connection between the pressure and density of the gas phase. The energy-conservation equation for the gas phase is obtained from (1) with the following relationships taken into account:

$$\begin{aligned} C &= m\rho_1 \left(U + \frac{1}{2} \mathbf{V}_1 \mathbf{V}_1 \right), \quad \mathbf{V}_C = \frac{s}{m} \mathbf{V}_1, \quad h = U + \frac{p}{\rho} = \int_0^T c_p dT, \\ j_C &= -s\lambda_1 \operatorname{grad} T_1 + s \sum_{i=1}^N h_{1i} j_{1i} + \mathbf{H}_{R,1} + s p \mathbf{V}_1, \\ I_C &= \alpha (T_2 - T_1) + m\rho_1 F_1 \mathbf{V}_1 + \sum_{i=1}^N h_{1i}^* \omega_{1i}, \\ \frac{\partial}{\partial t} \left[m\rho_1 \left(h_1 + \frac{1}{2} \mathbf{V}_1 \mathbf{V}_1 \right) \right] + \operatorname{div} \left[s\rho_1 \left(h_1 + \frac{1}{2} \mathbf{V}_1 \mathbf{V}_1 \right) \mathbf{V}_1 \right] &= \\ &= \frac{\partial}{\partial t} (m\rho) + \operatorname{div} (s\lambda_1 \operatorname{grad} T_1) - \operatorname{div} \left(s \sum_{i=1}^N h_{1i} j_{1i} \right) - \\ &\quad - \operatorname{div} (\mathbf{H}_{R,1}) + \alpha (T_2 - T_1) + m\rho_1 F_1 \mathbf{V}_1 + \sum_{i=1}^N h_{1i}^* \omega_{1i}, \end{aligned} \quad (8)$$

where \mathbf{H}_R is the integrated radiant energy flux (relative to the wavelengths), α is the volume coefficient of heat exchange between the solid and gas phases, and h_{1i}^* is the enthalpy of the i -th gaseous component at the temperature T_2 .

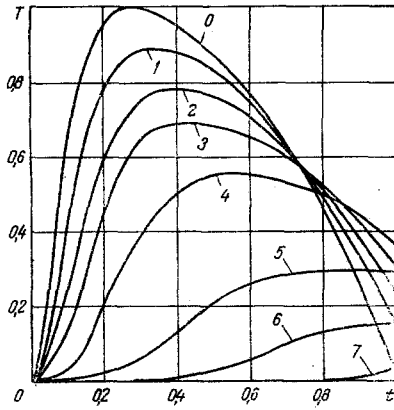


Fig. 1. Time dependence of the temperature at the points x_0-x_7 ($x_0 = 0$; $x_1 = 0.04$; $x_2 = 0.08$; $x_3 = 1.12$; $x_4 = 0.2$; $x_5 = 0.4$; $x_6 = 0.6$; $x_7 = 1$).

The energy-conservation equation for the solid phase is derived analogously:

$$\frac{\partial}{\partial t} [(1-m)\rho_2 h_2] + \text{div} [(1-s)\rho_2 h_2 \mathbf{V}_2] = \text{div} [(1-s)\lambda_2 \text{grad } T_2] - \text{div} (\mathbf{H}_{R,2}) - \alpha(T_2 - T_1) - \sum_{i=1}^N h_{1i}^* \omega_{1i}. \quad (9)$$

The transfer equations (2)-(9) obtained are fundamental for a reacting multicomponent porous medium. In investigating specific problems, this system must be supplemented by the chemical-kinetics and radiation-transfer equations, by expressions for the diffusion fluxes, and the rate of shrinkage of the solid carcass, and values of the physical characteristics entering into the complete system of equations must be given.

Estimates of the order of the terms in (2)-(9) [7] show that under the assumption that $m = s = s_1$ and $m\rho_1 h_1 \ll (1-m)\rho_2 h_2$, the system of equations (2)-(9) can be reduced to the following simplified form in solving one-dimensional problems associated with the intensive heating of heat-shield materials (10-100 deg/sec):

$$\frac{\partial}{\partial x} (m\rho_1 V_1) = \omega_1 = -\omega_2, \quad (10)$$

$$\frac{\partial}{\partial t} [(1-m)\rho_2] = \omega_2, \quad (11)$$

$$\frac{\partial}{\partial t} [(1-m)\rho_2 h_2] = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right). \quad (12)$$

The decomposition velocity ω_2 at an arbitrary point x during thermal destruction of the material is determined principally by the law of temperature variation at this point and can be computed by using the chemical-kinetics equations. Then the solutions of (10)-(11) are

$$m\rho_1 V_1 = \int_x^1 \omega_2(T(\tau), t, \xi) d\xi, \quad (0 \leq \tau \leq t, V_1|_{x=1} = 0), \quad (13)$$

$$(1-m)\rho_2 = (1-m)\rho_2|_{t=0} + \int_0^t \omega_2(T(\tau), t) d\tau, \quad (0 \leq \tau \leq t), \quad (14)$$

and (12) can be written as follows:

$$\frac{\partial}{\partial t} (\Phi T) = \frac{\partial}{\partial x} \left(F \frac{\partial T}{\partial x} \right) - \frac{\partial}{\partial x} (\Psi T), \quad (15)$$

where $\Phi[T(x, \tau)]$, $F[T(x, \tau)]$ are functionals of $T(\tau)$ and $\Psi[T(\xi, \tau), x]$ is a functional of $T(\xi, \tau)$, ($0 \leq \tau \leq t$, $0 \leq x \leq \xi \leq 1$).

If convective heat transfer of the gas phase is neglected, we can then obtain from (10)-(12)

$$G[T(x, \tau)] \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} F \left[T(x, \tau) \frac{\partial T}{\partial x} + Q[T(x, \tau)] \right], \quad (16)$$

$$G[T(x, \tau)] = (1-m)\rho_2 c_{p,2}, \quad Q[T(x, \tau)] = -(h_2 - h_1)\omega_2.$$

Here, in contrast to the nonlinear heat-conduction equation where the thermophysical characteristics are functions of the temperature, the expressions in the square brackets are functionals of $T(\xi, \tau)$. The general sense of the introduction and practical utilization of functional thermophysical characteristics exists under the assumption that they can be described by sufficiently simple mathematical expressions and then determined on the basis of experimental data by means of solutions of the appropriate inverse problems. It should be noted that the approach formulated can be used successfully to investigate individual processes taking place in the heat and mass transfer of decomposing materials such as nonisothermal kinetics, microstructural analysis, etc.

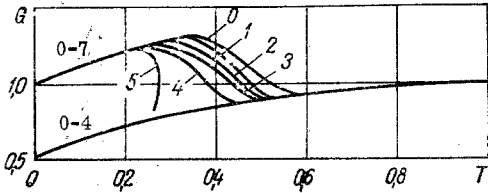


Fig. 2. Change in the functional G at the points x_0-x_7 .

An example of a one-time determination of two functional thermophysical characteristics by solving the inverse problem is presented below to illustrate the proposed approach to solving heat-transfer problems in decomposing materials.

The one-dimensional problem described by (16) under the assumption that $Q[T(x, \tau)] = 0$ was considered:

$$G[T(x, \tau)] \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} F[T(x, \tau)] \frac{\partial T}{\partial x}, \quad (17)$$

$$(0 \leq \tau \leq t \leq 1, \quad 0 \leq x \leq 1),$$

$$T(x, 0) = 0, \quad T(0, t) = T_w(t), \quad \left. \frac{\partial T}{\partial x} \right|_{x=1} = 0,$$

$$T_w(t) = \begin{cases} 16t(0.5 - t), & (0 \leq t \leq 0.25), \\ \frac{16}{9}t(0.5 + t(0.5 - t)), & (0.25 < t \leq 1), \end{cases}$$

$$G = \eta \cdot (1 + a_1 T) + (1 - \eta)(a_2 + a_3 T + a_4 T^2),$$

$$F = \eta(a_5 + a_6 T) + (1 - \eta)(a_7 + a_8 T + a_9 T^2),$$

$$\eta = \exp \left(- \int_0^t a_{10} \exp \left(- \frac{a_{11}}{T(\tau) + 0.15} \right) d\tau \right),$$

$$a_1 = 1; \quad a_2 = 0.5; \quad a_3 = 1.1; \quad a_4 = -0.6; \quad a_5 = 0.15;$$

$$a_6 = 0.65; \quad a_7 = 0.08; \quad a_8 = 0.16; \quad a_9 = 0.36;$$

$$a_{10} = 3 \cdot 10^5; \quad a_{11} = 5.$$

The functionals G and F have been selected dependent on both the temperature and the degree of material decomposition η ; the functional dependence on the heating prehistory is taken into account in the expression for η , which is written as the solution of the Arrhenius equation for a first-order reaction. The problem (17) was solved on an electronic computer by using an implicit difference scheme. Shown in Fig. 1 is the time-variation in the temperature at two boundary (x_0, x_7) and six interior (x_1-x_6) points of the material. The temperature change in the values of the functionals G and F for the points (x_0-x_7) is represented in Figs. 2 and 3. The values of the functionals G and F during heating first grew along the upper lines in Figs. 2 and 3, then went over to the lower curves and reached some maximum values along them, and later diminished along these curves.

By the definition of the functionals G and F , the time change in the temperature at the points x_0-x_7 was considered known in solving the inverse problem [7].

In order to diminish the correlation between the parameters a_1-a_{11} , the functionals G, F were given the following form during the search:

$$G = \bar{\eta}[(1 - T) + T p_1 p_6] + (1 - \bar{\eta})[(2T - 1)(T - 1) p_2 - 4T(T - 1) p_3 + T(2T - 1) p_4],$$

$$F = \bar{\eta}[(1 - T) p_5 + T p_8] + (1 - \bar{\eta})[(2T - 1)(T - 1) p_7 - 4T(T - 1) p_9 + T(2T - 1) p_{10}].$$

$$\bar{\eta} = \exp \left[- \int_0^t p_{10} \exp \left(- p_{11} \left(\frac{1}{T(\tau) + 0.15} - 2 \right) \right) d\tau \right].$$

New parameters p_1-p_{11} , related to the parameters a_1-a_{11} by the expressions

$$p_1 = \frac{1 + a_1}{p_6}, \quad p_2 = a_2, \quad p_3 = a_2 + \frac{1}{2} a_3 + \frac{1}{4} a_4,$$

$$p_4 = a_2 + a_3 + a_4, \quad p_5 = a_5, \quad p_6 = a_5 + a_6,$$

$$p_7 = a_7, \quad p_8 = a_7 + \frac{1}{2} a_8 + \frac{1}{4} a_9, \quad p_9 = a_7 + a_8 + a_9,$$

$$p_{10} = a_{10} \exp(1 - 2a_{11}), \quad p_{11} = a_{11}$$

TABLE 1. Results of Solving the Inverse Problem

Parameter	Initial value	Result of the search	Exact value
p_1	5,0	2,50110	2,5
p_2	1,5	0,50006	0,5
p_3	1,5	0,91072	0,9
p_4	1,5	0,99154	1,0
p_5	0,4	0,15783	0,15
p_6	0,4	0,79851	0,8
p_7	0,2	0,08204	0,08
p_8	0,2	0,25309	0,25
p_9	0,2	0,59863	0,6
p_{10}	150,0	13,62081	13,61999
p_{11}	10,0	5,01374	5,0

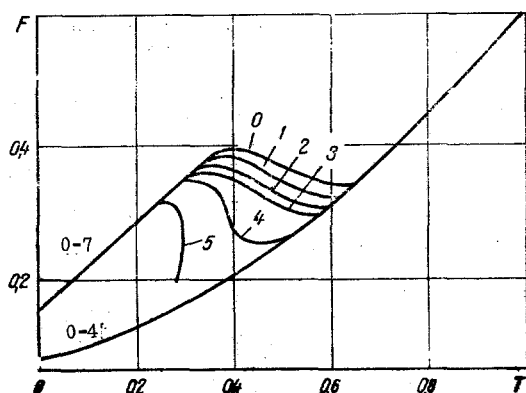


Fig. 3. Change in the functional F at the points x_0-x_7 .

steepest descent in the rate of convergence and the random search method even more, was used as the method to search for the parameters p_1-p_{11} . The values of the partial derivatives $\partial J/\partial p_k$ needed were calculated by using first differences.

Presented in Table 1 are exact values of the parameters p_1-p_{11} , their initial values, and results of solving the search problem. As is seen, the solution of the inverse problem during processing the numerical experiment has been obtained with sufficiently high accuracy, which indicates the possibility of determining confident functional characteristics for real materials.

NOTATION

a , parameter; C , concentration of substance; c , specific heat; F , a functional, the filtration resistance force; G , a functional; H , radiant-energy flux; h , enthalpy; I , source; J , quality criterion; j , diffusion flux; m , volume porosity; p , pressure; Q , a functional; R , gas constant; s , surface porosity, coefficient; T , temperature; t , time; U , internal energy; V , velocity; x , space coordinate; α , heat-transfer coefficient; ξ , space coordinate; η , degree of decomposition; λ , heat-conduction coefficient; ρ , density; τ , time; ω , rate of formation of the chemical component; Φ , Ψ , functionals. Subscripts: 1 refers to gas phase, parameter number; 2 refers to solid phase, parameter number; C refers to substance; i refers to number of the chemical component, thermocouple number; j refers to number of a time point; k refers to parameter number; M refers to number of a solid-phase component; N refers to number of a gas-phase component; p refers to specific heat at constant pressure; R refers to radiant energy; w refers to surface temperature; exp refers to experimental results; the asterisk is defined in (8); the bar above the symbols refers to the effective value.

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