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COMPLEX MODEL OF INTERACTION OF COMPOSITES WITH RADIATION AND A GAS FLOW

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A complex mathematical model of interaction of composite polymer materials (CMs) with radiations of different nature and a gas flow is developed. The model permits allowance for a set of such physicochemical phenomena as volumetric radiation absorption, pyrolysis of the organic components of the material, filtration of gaseous pyrolysis products in the pores of the subsurface layer, and the corresponding change in the composition and properties of the material in the subsurface layer. Based on the model, a computational system for calculating the parameters of interaction of CM products with radiation and a gas flow is created in accordance with advanced principles of object-oriented programming.

Mathematical modeling of the processes of interaction of CM products with radiations of different nature in simultaneous "blowing" of their surfaces by a gas flow that fits adequately a real-life prototype is a pressing problem in modern technology.

A generalized scheme of interaction of CM with a concentrated radiation flux and a gas flow is presented in Fig. 1. The scheme shows the following basic phenomena and processes in the subsurface layer of the structure and in the zone of interaction of the boundary layer of the gas flow that washes its surface with damage (ablation) products. (The numbers correspond to the positions of the figure):

1. Unsteady warmup of CM (formation of a temperature field variable throughout the volume of the plate and with time). Formation of plastic and carbonized layers.
2. Heat release in the volume due to the absorption of external-radiation energy.
3. Absorption or release of heat in the subsurface layer in pyrolysis of organic (polymer) components of CM and secondary reactions of pyrolysis products (including that resulting from photochemical reactions that occur in the presence of the ultraviolet component in the spectrum of penetrating radiation).
4. Formation of porosity in the subsurface layer due to the gas release in pyrolysis and deformation of the skeleton (expansion or shrinkage).
5. Deformation of the skeleton of the plastic layer under the action of a pressure difference between the pore space and the ambient medium that leads to the expansion or shrinkage of the subsurface layer.
6. Flow of pyrolysis gases to the heated surface along communicating pores and fractures of the carbonized layer (CL) accompanied by heat and mass transfer with the skeleton. Injection of the gases into the boundary layer of the external gas flow.
7. Formation of the stressed state in the CL skeleton under the action of the pressure and friction of the gas flow, the recoil momentum of a light-erosion plasma generated near the CM surface, the resistance of a porous skeleton to the flow of pyrolysis gases, and inertia overloads and vibration.
8. Penetration of the external radiation through open pores and fractures deep into the carbonized layer (channeling or the tunnel effect).

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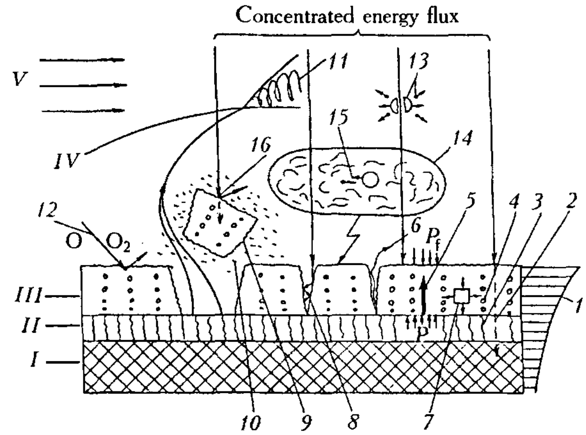

Fig. 1. Generalized scheme of interaction of CM with a concentrated radiation flux and a hot gas flow: *I*) undecomposed material; *II*) plastic layer; *III*) carbonized layer; *IV*) boundary layer; *V*) incoming gas flow.

9. Separation and removal of parts of the carbonized layer by the gas flow (mechanical mass removal).

10. Sublimation of material from the carbonized layer surface and from the surface of separated pieces in the process of their motion in the wall layer of the light-errosion plasma.

11. Gasdynamic, thermal, and chemical interactions of the incoming gas flow with the products of light-erosion damage and ablation of CM.

12. Chemical interaction of oxidizing components of the gas mixture with the carbon of the surface with recombination of oxidant atoms that depends on the catalytic nature of the surface.

13. Dissociation and ionization of the gas mixture in the concentrated flux of radiant energy through it.

14. Formation of an electron avalanche in the light-erosion plasma – optical breakdown accompanied by shock waves in the wall gas flow.

15. Heat transfer between the electron and ion components of the light-erosion plasma that have significantly different temperatures.

16. Absorption and scattering of radiant energy by the light-erosion plasma laden with condensed particles.

A mathematical description of heat and mass transfer and mechanical processes in the structure of CM under the joint action on them of radiation and heat and power loads is proposed based on mathematical concepts developed in heat and mass transfer theory, the mechanics of deformable porous media, and the mechanics and physics of a deformable rigid body [1-7]. Assumptions are made on the equality of the temperatures of the porous-medium skeleton and the gas (vapor) that fills the pores, the smallness of the intrinsic radiation of material as compared to the external radiation, etc.

With allowance for the assumptions made, the energy equation is represented in the form

$$(1-\varphi)\,\rho' c' \frac{\partial T}{\partial t} = \mathrm{div}\,(\lambda\,\mathrm{grad}\,T) + \sum_{i=1}^{3} m_i'' c_p'' \frac{\partial T}{\partial x_i} + \mathrm{div}\, q_{\mathrm{rad}} + \omega_{\mathrm{x\text{-}rad}} - \rho_0\,(1-K)\,Q\,\frac{\partial \chi}{\partial t}\,, \tag{1}$$

$$t > 0\,;\quad x_{i\mathrm{w}}(t) \le x \le x_{i\mathrm{cold}}\,;\quad x_{i\mathrm{w}} = x_{i0} \pm \int_{x_{i0}}^{x_{i\mathrm{fill}}} e_i\,dx_i - \int_0^t v_{\mathrm{y}i}\,dt\,,$$

while the equation of conservation of mass of the gas (vapor) that moves in the pores is represented as

$$\operatorname{div}(-\Gamma \operatorname{grad} \Phi) = \rho_0 (1 - K) \frac{\partial \chi}{\partial t}. \tag{2}$$

Equations (1) and (2) are solved under the boundary conditions:

$$T(x_i, 0) = T_0(x_i); \tag{3}$$

$$\alpha_f (T_f - T_w) - \sum_{\gamma=1}^{\Gamma} Q_\gamma \dot{m}_\gamma = -\lambda \frac{\partial T}{\partial n}\bigg|_{n=n_w(t)-0}; \tag{4}$$

$$\Phi|_{n=n_w(t)-0} = \Phi_0; \tag{5}$$

$$T|_{x_i=x_{i\text{bound}}-0} = T|_{x_i=x_{i\text{bound}}+0}, \quad \lambda \frac{\partial T}{\partial x}\bigg|_{x_i=x_{i\text{bound}}-0} = \lambda \frac{\partial T}{\partial x}\bigg|_{x_i=x_{i\text{bound}}+0}; \tag{6}$$

$$\Phi|_{x_i=x_{i\text{bound}}-0} = \Phi|_{x_i=x_{i\text{bound}}+0}, \quad \Gamma \frac{\partial \Phi}{\partial x_i}\bigg|_{x_i=x_{i\text{bound}}-0} = \Gamma \frac{\partial \Phi}{\partial x_i}\bigg|_{x_i=x_{i\text{bound}}+0}; \tag{7}$$

$$\alpha_e (T_{\text{cold}} - T_e) + A_{\text{eff}} \sigma (T_{\text{cold}}^4 - T_e^4) - \sum_{\delta=1}^{\Delta} Q_\delta \dot{m}_\delta = -\lambda \frac{\partial T}{\partial n}\bigg|_{n=n_{\text{cold}}-0}; \tag{8}$$

$$\Phi|_{n=n_{\text{cold}}-0} = \Phi_0. \tag{9}$$

To close the system of equations (1) and (2) with boundary conditions (3)-(9), we employed the following relations for the parameters that appear in them.

In connection with the fact that the skeleton of a porous CM in the general case is two-component and consists of a filler and the condensed residue of a binder (matrix), its density and heat capacity are determined as

$$\rho' = [\mu_{\text{fill}}/\rho_{\text{fill}} + (1 - \mu_{\text{fill}})/\rho_m]^{-1}, \quad c' = c_m (1 - \mu_{\text{fill}}) + c_{\text{fill}} \mu_{\text{fill}}. \tag{10}$$

The condensed residue, in turn, consists of a polymer and its coke, the relation between which changes during the pyrolysis. Then for its density and heat capacity we can employ the analogous formula

$$\rho_m = [\mu_b/\rho_b + (1 - \mu_b)/\rho_{\text{cond}}]^{-1}, \quad c_m = c_{\text{cond}} (1 - \mu_{\text{cond}}) + c_b \mu_b. \tag{11}$$

To calculate the current values of the weight fraction of the polymer in the binder by employing a single-step scheme of the process of pyrolysis, we can obtain a formula of the form

$$\mu_b = (1 - \chi)/(1 - \chi + K_b \chi). \tag{12}$$

The current value of the weight fraction of the filler or reinforcing material in the skeleton is determined by the formula

$$\mu_{\text{fill}} = \bar{\mu}_{\text{fill}} / (\bar{\mu}_{\text{fill}} + \bar{\mu}_{\text{b}} + \bar{\mu}_{\text{cond}}) . \tag{13}$$

The current values of the weight fractions of the polymer and its coke in CM are calculated by the formulas

$$\bar{\mu}_{\text{b}} = (1 - \chi)(1 - \bar{\mu}_{\text{fill}}) , \quad \bar{\mu}_{\text{cond}} = \chi K_{\text{b}} (1 - \bar{\mu}_{\text{fill}}) . \tag{14}$$

At the upper level, consideration is given to a two-component composition that consists of a matrix with the thermal conductivity λ_{m} and a reinforcing filler in the form of filaments or fabric with thermal conductivity λ_{fill} and volume fraction φ_{fill} directed parallel to the heated surface. From analyzing the literature on the thermal physics of inhomogeneous media it follows that, to calculate the effective thermal conductivity of this composition in the lateral direction, for example, in the case of CMs reinforced by filaments we can use the following formula:

$$\lambda = \lambda_{\text{m}} \left[1 + \frac{\varphi_{\text{fill}}}{(1 - \varphi_{\text{fill}})/2 + 1/(\lambda_{\text{fill}}/\lambda_{\text{m}} - 1)} \right] , \tag{15}$$

$$\lambda_{\text{m}} = \lambda' (1 - \varphi_{\text{m}})^{1.5} M_{\text{cont}} + \lambda'' \varphi_{\text{m}}^{0.25} , \tag{16}$$

$$\varphi_{\text{m}} = 1 - (1 - \varphi_{\text{m}}^{0}) [1 - \chi (1 - K_{\text{b}})] \rho_{\text{m}}^{0} / \rho_{\text{m}} . \tag{17}$$

At the lower structural level, consideration is given to a two-component skeleton of a porous matrix that consists of alternating layers of a polymer and its cokes, the relation between which changes during physicochemical transformations. For the thermal conductivity of this structure, the formulas

$$\lambda' = \lambda_{\text{b}} \varphi_{\text{b}} + \lambda_{\text{cond}} (1 - \varphi_{\text{b}}) , \tag{18}$$

$$\varphi_{\text{b}} = (1 - \chi)/(1 - \chi + \chi K_{\text{b}} \rho_{\text{m}} / \rho_{\text{cond}}) \tag{19}$$

hold true.

The conductive thermal conductivity of the pyrolysis gases that fill the pores is determined from their composition, which in turn is found from thermodynamic calculations. For practical use, we can recommend a linear approximation of its temperature dependence

$$\lambda'' = 5 \cdot 10^{-4} + 8 \cdot 10^{-5} T . \tag{20}$$

The density of the luminous-radiation flux that penetrates into the structure as a function of the transverse coordinate can be represented in the form

$$q_{\text{rad}} = q_{\text{e}} [1 - R(x)] \exp(-k_{\Sigma}(x) x) ,$$
$$R = R_0 + (R_{\text{cond}} - R_0) \chi , \quad k_{\Sigma} = k_{\Sigma.0} + (k_{\Sigma.\text{cond}} - k_{\Sigma.0}) \chi . \tag{21}$$

The power of the energy release in the volume of the material due to the absorption of radiation in the x-ray spectrum is determined from the prescribed value of the energy density of x-ray radiation (XR) incident onto the surface of the structure U, J/m^2 in the time Δt, sec and the distribution of the mass absorption coefficient of XR (F, m^2/kg) along the mass coordinate (m, kg/m^2) calculated by the special procedure. Using these data the distribution of the energy release due to the absorption of XR across the thickness of the obstacle is calculated by means of an explicit dependence:

$$\Delta Q(x) = UF(m)\,\rho_i(x)\,. \tag{22}$$

The power of the energy release in the volume of obstacle material under the assumption of a linear dependence of U on time is calculed by the formula

$$\omega_{\text{x-rad}}(t) = \begin{cases} 0 & \text{for } t < t_1\,, \\ \dfrac{\Delta Q(x)}{t_2 - t_1} & \text{for } t_1 \le t \le t_2\,, \\ 0 & \text{for } t > t_2\,. \end{cases} \tag{23}$$

In the general case, the CM shell can be exposed (simultaneously with irradiation) to internal and external heatings. Its convective heat transfer with the gas flow can be complicated by the following factors:

a) loading of the flow with the particles of the condensed phase;

b) variability of the velocity along the surface and its curvature and roughness;

c) injection of gases from the surface;

d) chemical reactions of the injected gases with the gases of the flow that washes the surface.

The theoretical and experimental investigations performed showed that, for engineering practice, a sufficient degree of accuracy is ensured with certain simplicity by the approximate approach to calculating convective heat transfer that is based on the adoption of the principle of superposition in relation to the above complicating factors. According to this approach, one employs as the main calculated dependence the widely known Avduevskii criterial formula for the Stanton number on a smooth impermeable plate in flow of a dust-free gas:

$$\text{St}_0 = 0.0296\text{Re}^{-0.2}\,\text{Pr}^{-0.6}\left(\frac{I_{\text{w}}}{I_{\text{f}}}\right)^{0.39}\left(1 + \frac{k-1}{2}\,r\text{M}^2\right)^{0.11}. \tag{24}$$

To allow for the effect of the above factors on the heat and mass transfer coefficient, the empirical corrections K_i

$$\frac{\alpha}{c_p} = \text{St}_0\,\rho_{\text{f}}\,u_{\text{f}} \prod_{i=1}^{I} K_i \tag{25}$$

are introduced.

For an approximate calculation of the emittance of the hot gas flow that washes the surface, we can use the regression relation [11]

$$\varepsilon_{\text{f}} = 0.229 + 0.0616d + 0.00011T_{\text{f}} - 0.3684\mu_{\text{condph}} + 0.00502p_{\text{f}} + 0.00338L\,. \tag{26}$$

The solution of the system of differential equations (1)-(2) with boundary conditions (3)-(9) and closing relations (10)-(26) is obtained for the computational scheme "unbounded multilayer plate" by the finite difference method. To allow for the substantial nonlinearity of the equations due to the coefficients and the parameters of the boundary conditions as functions of the initial temperature, iterations on each time layer are used in numerical realization of a computational algorithm. The program is developed for modern IBM-compatible computers in accordance with advanced principles of object-oriented programming.

The developed algorithms and programs were tested by comparison of the results obtained using them with analytical solutions of the following boundary problems:

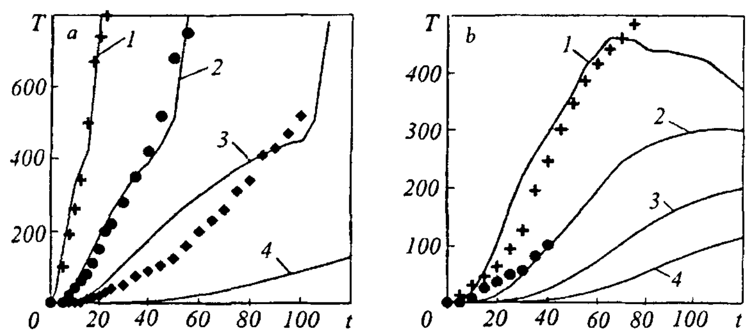

Fig. 2. Calculated (curves) and experimental (points) dependences of temperature on time at different distances from the heated surface of a specimen of rubber-like material and glass-reinforced plastic upon irradiation with a flux of constant density 1120 kW/m^2 (a) and of variable density (b): a) 1) x = 1.5 mm; 2) 3.2; 3) 4.9; 4) 10; b) 1) x = 1.8 mm; 2) 3.9; 3) 5.9; 4) 7.9. T, °C; t, sec.

1) unsteady "symmetric" and "asymmetric" warmups of a single-layer plate with constant thermophysical characteristics of the material for a constant intensity of heat transfer with the ambient medium;

2) unsteady warmup of a semi-infinite mass with constant thermophysical characteristics of the material for a constant intensity of heat transfer with the ambient medium;

3) steady-state warmup of a multilayer plate with strongly differing thermophysical characteristics of the materials for different intensities of heat transfer on the surfaces.

The created computational system was checked by comparison of the results of calculations performed using it with experimental data*) (see Fig. 2).

Figure 2a presents the results of calculating the unsteady warmup of a double-layer plate that consists of rubber-like material (of thickness 16 mm) and glass-reinforced plastic (of thickness 3 mm). Under experimental conditions, its surface was affected by a time-constant luminous-radiation (LR) flux with a density of 1120 kW/m^2. The coefficient of LR absorption by the pyrolysis products was taken to be 0.5. The reflection factor was $R = 0$, while the coefficient of the absorption by material was $k_\Sigma \to \infty$ (the radiant heat transfer in the pores of the carbonized layer was allowed for in the Rosseland approximation by introducing the corres-

TABLE 1. Thermophysical Characteristics of Rubber-Like Thermal Protective Material 51-2135 as Functions of Temperature

T, °C	φ	ρ', kg/m^3	c', J/(kg·K)	χ	λ_Σ, W/(m·K)
0	0.017	1170.0	1420.0	0	0.250
152	0.017	1190.7	1549.9	0	0.271
302	0.032	1189.7	1777.7	0.025	0.311
452	0.096	1185.0	1958.5	0.132	0.370
602	0.538	1093.0	1601.2	0.888	0.121
752	0.591	1053.7	1407.9	0.987	0.191
902	0.597	1048.0	1417.7	0.998	0.591
1052	0.599	1049.6	1456.4	1.000	0.715
1202	0.602	1057.2	1500.5	1.000	0.859
1352	0.604	1064.8	1541.6	1.000	1.030
1502	0.612	1085.3	1580.1	1.000	1.229
1652	0.621	1111.8	1616.3	1.000	1.460
1802	0.630	1138.5	1650.5	1.000	1.725

*) Experimental data are obtained with the participation of B. I. Sevast'yanov and V. V. Panin.

TABLE 2. Time Dependence of the Radiant Heat Flux Density

t, sec	0	10	20	25	35	45	60	65	120
$q \cdot 10^4$, W/m^2	0	5	10	20	40	60	75	0	0

ponding radiant component into the total thermal conductivity). The thermophysical characteristics of rubber-like material decomposed in heating as functions of the temperature and the degree of decomposition employed in the calculations are given in Table 1.

The total thermal effect of thermal decomposition of this material is $0.81 \cdot 10^6$ J/kg. Since the glass-reinforced-plastic substrate was heated slightly under experimental conditions, the thermophysical characteristics of its material were taken to be constant in the calculation: $\rho = 1820$ kg/m^3, $c = 1100$ J/(kg·K), and $\lambda = 0.37$ W/(m·K).

Apart from the calculated dependences of the temperature on time at different distances from the heated surface, Fig. 2a gives the corresponding experimental data. Satisfactory agreement of the calculations with experiment is evident.

Figure 2b compares the calculation and the experimental data for experiments on irradiation of double-layer specimens of a similar structure with LR with a time-variable flux density (see Table 2).

The calculations were performed for the same initial data as in the previous case. The figure shows that, in spite of the significant difference of the level of LR intensity and the character of irradiation of the specimens from the first case, in the second case, the calculations are also in satisfactory agreement with experiment for the same initial data on the characteristics of materials.

The results of an experimental check of the variants of the mathematical model for the case of the interaction of CM with hot gas flows are presented in [9, 10].

Thus, testing and experimental check of the algorithms and programs developed confirmed the legitimacy of the assumptions made in the mathematical modeling of the interaction of composites with radiation and a gas flow.

NOTATION

φ, porosity, volume fraction; ρ, density; c and c_p, heat capacity; T, temperature; t, time; λ, thermal conductivity; m, mass velocity; x_i, coordinates; q, energy-flux density; ω, volumetric heat-source power; K, coke number; Q, thermal effect; χ, degree of completeness of thermal decomposition; e, volumetric expansion (shrinkage) deformation; v_{rem}, rate of surface mass removal; $\Gamma(T) = kM''/2\varphi\mu''R_{\text{un}}T$, tensor of modified permeability factors of the porous medium; M'', molecular mass; R_{un}, universal gas constant; $\Phi = (\varphi p)^2$, parameters of intrapore pressure; p, pressure; α, convective heat transfer coefficient; n, normal to the structure surface; A_{eff}, coefficient of radiant heat transfer between the surface and the ambient medium; σ, Stefan–Boltzmann constant; μ, weight fraction; M_{cont}, parameter of contact resistance between the structural elements of material; R, reflection factor of the surface heated by radiation; k_Σ, effective (total) absorption coefficient; ε, emissivity factor; d, average diameter of particles of the condensed phase; $\mu_{\text{cond.ph}}$, weight fraction of the condensed phase; L, characteristic dimension; t_1 and $t_2 = t_1 + \Delta t$, instants of the beginning and end of action of XR on the considered element of the structure; $\text{St}_0 = (\alpha/c_p)_0/\rho_f u_f$, Stanton number; $(\alpha/c_p)_0$, coefficient of heat transfer on a smooth impermeable plate; ρ_f, gas density near the surface; u_f, velocity in the flow core; $\text{Re} = (\rho_f u_f x)/\mu_w$, Reynolds number; μ_w, gas viscosity at surface temperature; Pr, Prandtl number at surface temperature; I_w and I_f, enthalpies of the gases near the surface and in the flow core; M, Mach number; k and r, adiabatic exponent and restoration factor; x, distance from the leading edge of the plate to the calculated cross section. Subscripts and superscripts: $'$, skeleton of the porous medium; $''$, gas that fills the pores; w, outer surface of the structure; f and e, external and internal flows; 0, initial state; bound, boundary between the layers; γ and δ, numbers of chemical reactions on the outer and inner surfaces; fill, filler; m, matrix (condensed residue of the polymer portion of material); b, initial polymer (binder); cond, condensed residue; eff, effective; rem, removal; rad, radiant; cold, cold.

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