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MATHEMATICAL SIMULATION OF THE PROCESS OF COMBUSTION OF SLIGHTLY GASEOUS POROUS COMPOSITIONS

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A one-dimensional model of combustion of slightly gaseous porous compositions is considered. Using this model an analysis of the dependence of the combustion characteristics on the basic parameters such as the mass ratio of the "gas-free" and "volatile" components in the starting composition, initial porosity, position of the gas liberation source relative to the reaction front of the "gas-free" component, and degree of sample hermetic sealing is performed for different exothermicity and endothermicity levels of the chemical processes taking place.

Because of the presence of various admixtures [1, 2] of a partially gasifying reaction product or an artificially introduced gassy component [3], the combustion of SHS compositions and the combustion of pyrotechnic systems with a large condensed residue [4] are accompanied by gas seepage. The gas formed due to phase transformation of a portion of the components or chemical reaction moves through pores under a pressure difference. In the process of combustion of such slightly gaseous systems (SGS) a complex conductive-filtrational mechanism of heat transfer is realized.

Much research has been done in the last decade on the process of the propagation of heat waves in disperse media [5]. Study of the laws governing the combustion of SGS, started as long ago as the 1960s [4, 5], has recently been extended [7, 8] in connection with the development of a variety of practical applications of SHS processes of SGS (for example, the production of porous materials and articles).

The process of combustion initiated on a cylindrical sample from the end face by a "glowing wall" and the exchange of heat by this sample with the external medium through the side surface can be described, on the assumption of a one-temperature model, by the following system of differential equations:

the macrokinetics of transformation

$$\frac{\partial \eta}{\partial t} = (1 - \eta) k_B \exp(-E_B/RT), \tag{1}$$

$$\frac{\partial a}{\partial t} = (1 - a) k_L \exp(-E_L/RT) \tag{2}$$

for the "gas-free" (with condensed products), Eq. (1), and "volatile" (with gaseous products) components, Eq. (2); the initial gas and that formed as a result of reaction (2) filter in accordance with the Darcy law

$$\mathbf{v} = k_f \operatorname{grad} P. \tag{3}$$

the equation of state that connects pressure with the density ρ_g and molecular weight μ_g

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$$P = RT\rho_g/\mu_g. \tag{4}$$

the mass conservation law

$$\frac{\partial \rho_s}{\partial t} + \operatorname{div}(\rho_g \pi \mathbf{v}) = 0. \tag{5}$$

the energy equation

$$\frac{\partial H}{\partial t} = \operatorname{div}(\lambda_s \operatorname{grad} T) - \operatorname{div}(c_g \rho_g \pi \mathbf{v} T), \tag{6}$$

where the heat content

$$\begin{aligned} H = [c_g\rho_g\pi + c_B\rho_B(1-\pi_0)\nu + c_L\rho_L(1-\pi_0)(1-\nu)(1-a)]T + \\ + Q_B\rho_B(1-\pi_0)\nu(1-\eta) + Q_L\rho_L(1-\pi_0)(1-\nu)(1-a). \end{aligned} \tag{7}$$

the initial conditions

$$\pi = \pi_0; \quad \eta = \eta_0; \quad a = a_0; \quad T = T_0; \quad P = P_0. \tag{8}$$

the boundary conditions at end faces impermeable for gas ($x = 0, l$) and at a heat-insulated end face ($x = l$)

$$\begin{aligned} &x = 0 \quad T(0, r, t) = T_w, \quad \frac{\partial P}{\partial x}(0, r, t) = 0; \\ &x = l \quad \lambda_s \frac{\partial T}{\partial x}(l, r, t) = 0, \quad \frac{\partial P}{\partial x}(l, r, t) = 0; \end{aligned} \tag{9}$$

and at the side surface

$$\begin{aligned} &r = R_0 \quad \lambda_s \frac{\partial T}{\partial r}(x, R_0, t) = -\alpha(T - T_{in}), \\ &\frac{\partial P}{\partial r}(x, R_0, t) = \mu(P_{in} - P), \end{aligned} \tag{10}$$

where α and μ are proportionality factors. There are the following symmetry conditions on the axis:

$$r = 0 \quad \lambda_s \frac{\partial T}{\partial r}(x, 0, t) = 0, \quad \frac{\partial P}{\partial r}(x, 0, t) = 0. \tag{11}$$

One can consider noninsulated and open end faces.

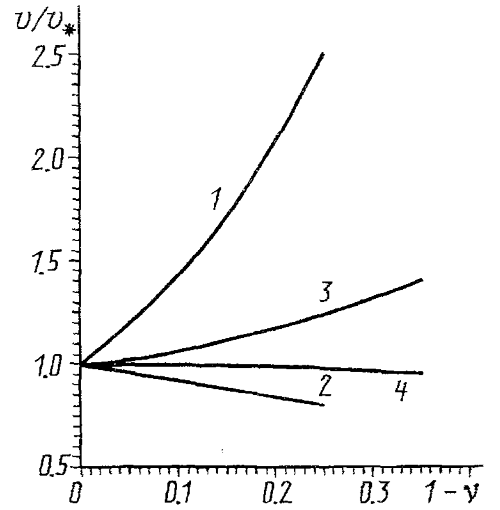
Variations in the volume, thermophysical parameters, and coefficient of filtration and phase transformations are not considered in the model suggested. It is assumed that the porosity and density of the composition change in the process of gasification:

$$\pi = \pi_0 + (1 - \pi_0)(1 - \nu)a; \tag{12}$$

$$\rho_s = \rho_g\pi + \rho_B(1 - \pi_0)\nu + \rho_L(1 - \pi_0)(1 - \nu)(1 - a). \tag{13}$$

The model represents only the basis of real SGSs and can be transformed if needed.

To simplify the computational algorithm, the numerical experiment was conducted for a one-dimensional (averaged over the radius) version of the problem at hand. The results obtained correspond to steady state regimes of combustion. We investigated the effect of various factors (the quantity of the gassy component, position of the



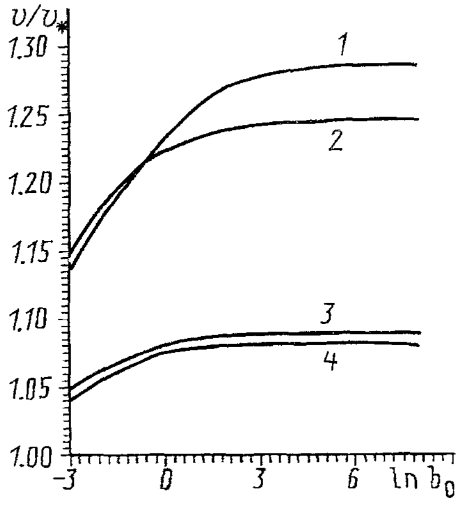


Fig. 1. Combustion rate vs the quantity of a gasifying additive TF = 3 (15): 1) $\gamma_B = 0.18$; $\beta_B = 0.161$; $Q_L/Q_B = 1.5$; $kF = 1\cdot 10^4$; $b_0 = 1.44\cdot 10^{-4}$; 2) 0.18; 0.161; -0.3; $1\cdot 10^4$ and $1.44\cdot 10^{-4}$; 3) 0.206; 0.191; 0.5; 44.5, and $5.6\cdot 10^2$; 4) 0.206; 0.191; 0.5; 44.4, and $1.44\cdot 10^{-4}$.

Fig. 2. Combustion rate vs the degree of hermetic sealing ($\gamma_B = 0.206$; $\beta_B = 0.191$; $kF = 44.4$; $c_L/c_B = 1$; $\lambda_s/\lambda_B = 1$; TF = 3; $\pi_0 = 0.25$; $(1-\nu) = 0.8$): 1, 2, 4) $c_g/c_B = 1$; 3) 0.33; 1, 2, 3) $\rho_L/\rho_B = 1$; 4) 0.15; 1) $Q_L/Q_B = 1.5$; 2, 3, 4) -0.1).

gasification source, initial porosity of the composition, and degree of hermetic sealing of the burning sample) on the front structure and the rate of its displacement.

It is shown (Fig. 1) that the rate of combustion increases with increase in the quantity of gassy additive if the reaction of the transformation of the gassy component is exothermal (curve 1) and decreases if the process is endothermal (curve 2). Here v_* is the dimensionless rate of combustion for $(1 - \nu) = 0$. The gases evolved in the zone of warming promote additional convective heating of the initial composition when they filter in the direction of the motion of the combustion front and lower the temperature of the composition when they filter opposite to the direction of the combustion front. If the gas filters through a side surface, the process of combustion becomes more intense. In fact, in the presence of radial filtration the expenditures of heat for warming the gas up to the combustion temperature diminish and this leads to an increase in the rate of combustion (compare curve 3 with curve 4 in Fig. 1). However, the increase in the combustion rate with a decrease in the degree of hermetic sealing is not unlimited. Starting with a certain value of the parameter b_0 the motion of the gases in the longitudinal direction ceases (Fig. 2). All the gases escape through the side surface. The combustion rate does not change (v_* is the dimensionless rate of combustion of an obturated sample ($b_0 = 0$)). The parameter b_0 that characterizes the degree of hermetic sealing in the problem considered depends on the dimensionless parameter γ, thermal diffusivity coefficient $a_B = \lambda_B/c_B\rho_B$, radius of the burning sample R_0, and adiabatic rate of combustion of the "gas-free" component u_B:

$$b_0 \simeq \left(\frac{\gamma_a}{u}\right)^2_B \frac{2}{R_0}. \tag{14}$$

An increase in b_0 means that the outflow of gases through the side surface of the sample increases (the degree of hermetic sealing decreases). The larger the density of the "volatile" component, the stronger is the dependence of the rate of combustion on b_0 (curve 2 compared to curve 4 in Fig. 2). The greater the heat capacity of the gases formed (curve 1 as against curve 3 in Fig. 2), the larger are the values of b_0 at which the dependence of the combustion rate on the degree of hermetic sealing will exist.

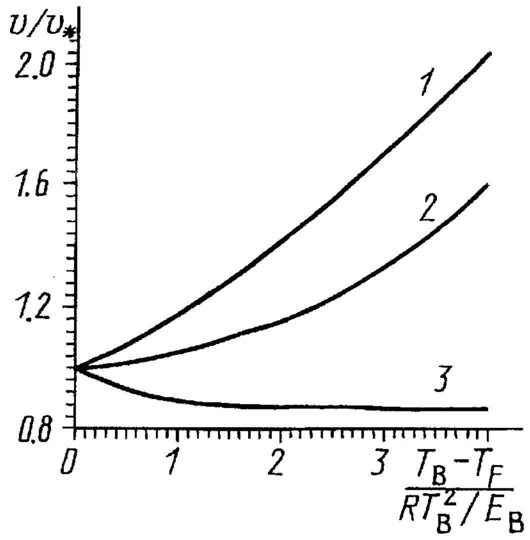


Fig. 3. Combustion rate vs the "place" of gasification: 1) $\gamma_B = 0.206$; $\beta_B = 0.191$; $Q_L/Q_B = 1.5$; kF = 44.4; $b_0 = 5.6\cdot 10^2$; 2) 0.206; 0.191; -0.1; 44.4, and $5.6\cdot 10^2$; 3) 0.18; 0.161; -0.3; $1\cdot 10^4$, and $1.44\cdot 10^{-4}$.

The "position" of intense gasification can be conveniently characterized with respect to the zone of transformation of the "gas-free" component by the dimensionless parameter

$$TF = \frac{T_{gB} - T_f}{RT^2_{gB}/E_B}. \tag{15}$$

Here E_B and T_{gB} are the energy of activation and the temperature of combustion of the "gas-free" component, respectively; T_f is the temperature corresponding to the maximum of the rate of gas evolution in the front. If the parameter (15) is equal to zero, gasification occurs in the zone of the reaction of the "gas-free" component. An increase in the parameter (15) means that the "place" of gasification recedes from the reaction zone. The dependence of the combustion rate on the "place" of gasification is presented in Fig. 3. In the case of the exothermal reaction of gasification (curve 1) and the endothermal reaction under the conditions of side filtration (curve 2) the rate of combustion increases with increase in the paramater (15). In the case of the endothermal reaction of gasification and absence of side filtration because of intense cooling of the reaction zone of the "gas-free" component by gases arriving from a low-temperature gasification zone, the rate of combustion can decrease (curve 3).

No matter how large the degree of the exothermicity of the gasification process or of the hermetic sealing of the gassy composition is, an increase in the initial porosity of the latter leads to intensification of the combustion process.

NOTATION

ρ_g, gas density; μ_g, molecular weight of the gas; H, heat content; π_0, initial porosity; ν, fraction of the condensed phase in the SGS; $(1 - \nu)$, fraction of the "volatile" component; v_{fl}, dimensionless rate of combustion; b, γ, parameters; a_B, thermal diffusivity coefficient; R_c, radius of the burning sample; T_f, temperature corresponding to the maximum of the gas evolution rate in the front.

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