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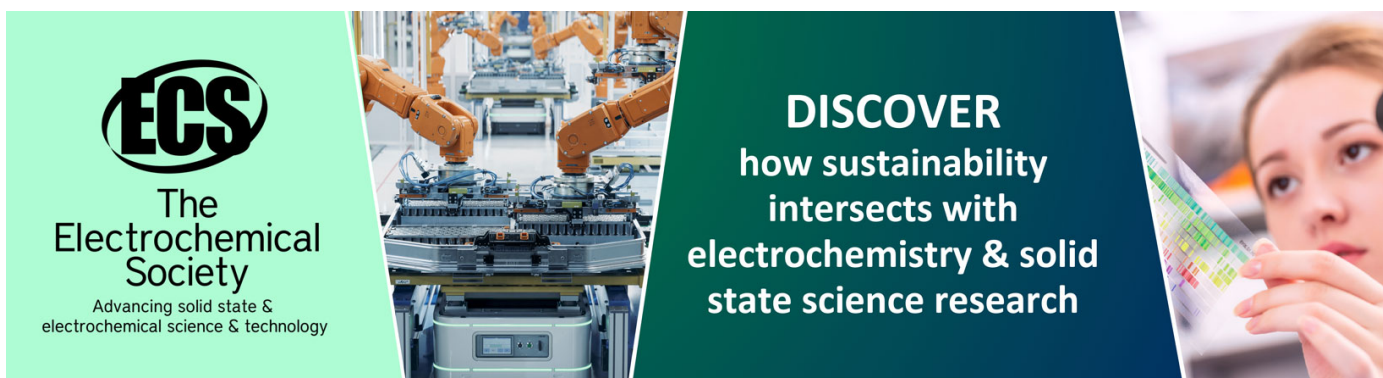
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Macrokinetics of combustion of layered compositions with a low-melting inert layer

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Abstract. The paper represents a mathematical model for the gasless combustion of a layered composition. The inner layer of the composition consists of an inert low-melting metal. Other layers consist of a highly exothermic gasless mixture. Metal of the inner layer melts during the combustion of adjacent layers. The melt under the influence of surface tension forces spreads in porous combustion products of the gasless mixture to form a composite material. The capillary flow of melt in porous channels is limited by the temperature of the carcass equal to the melting point. The results have shown that the time required for a combustion wave to propagate through an inert layer depends on its thickness and thermal conductivity. The modes of combustion synthesis are determined for layered composite materials. The dynamics of the structure formation of composite materials is considered depending on the thickness of the inner metal layer and the coefficient of external heat exchange.

1. Introduction

Synthesis of layered compositions is one of the promising directions in the area of SHS [1]. To conduct this process, an initial layered structure should include different reacting mixtures to initiate combustion in parallel or perpendicular to the plane of coupled layers. In addition to the thermal and chemical interaction between the layers of the composition, there are accompanying processes of melting, crystallization and capillary wetting. Strong and weak exothermic layers are combined to conduct synthesis by the «chemical furnace» method. To obtain composite materials in the combustion mode, a sample is prepared from a mixture of reacting and inert powders. The synthesis product is a material that consists of reaction products enclosed in an inert material matrix. The limitation of this method is to meet necessary and sufficient conditions for the self-propagating mode of synthesis. The structure of the material synthesized depends on the ratio between the dimensions of inert and reacting layers, the adiabatic combustion temperature, the thermophysical characteristics of materials, the parameters of phase transition, and the conditions for heat exchange with the environment [2]. The obtaining of a composite material with a gradient structure by the SHS method is based on the melting of an inner layer and spreading a metal melt in the porous structure of outer layers due to the action of capillary forces. The melt penetration depth that determines the structure of the composite depends on the size of pores, surface tension, phase transition parameters and temperature distribution. The required structure of the synthesized product can be obtained by changing the ratio between the layers of the composition.



2. Mathematical model and results

We consider a sample formed by two layers of a combustible mixture, between which is a layer of low-melting inert metal. Figure 1 shows the regions that can appear during the synthesis and formation of a final product.

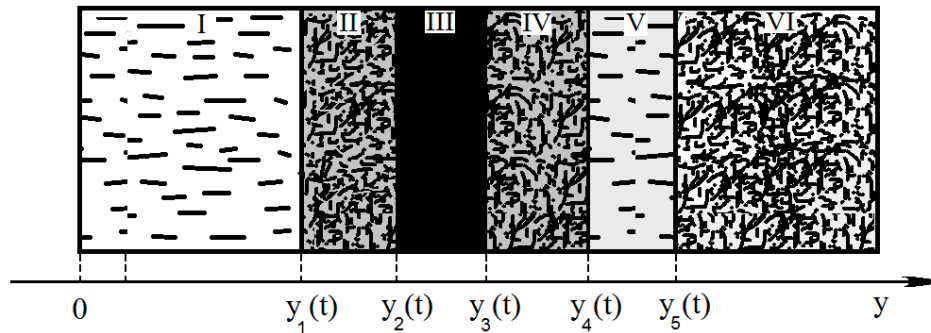


Figure 1. Scheme of the sample: I is combustion products of a gasless mixture, II is a composite material, III is a layer of metal, IV is a composite material, V is combustion products of a gasless mixture, VI is a green mixture.

The mathematical formulation of the problem concerning the synthesis a multilayer composite material in the gasless combustion mode is reduced to the system of equations as follows. The heat conduction equation (1) and the equation of chemical kinetics (2) are considered in region I ($0 < y_1(t)$), in front of the layer of inert material, where the refractory product F is synthesized:

$$(1-m)\rho_2 c_2 \frac{\partial T_2}{\partial t} = \frac{\partial}{\partial y} \left(\lambda_2 \frac{\partial T_2}{\partial y} \right) + (1-m)Q\rho_2 \frac{d\alpha}{dt} - \chi_e(T_2 - T_0), \quad (1)$$

$$\frac{d\alpha}{dt} = k(T_2)f(\alpha) \quad (2).$$

In the equations (1) and (2), T_2 is the temperature of the reacting mixture; T_0 is the initial and ambient temperature; t is the time; $f(\alpha)$ is the kinetic law that is used in the form $f(\alpha)=1-\alpha$ in the calculations; α is the conversion depth (mass fraction of the product in the reacting mixture); $k(T_2)=k_0 \exp(-E/RT_2)$, k_0 , and E are the reaction rate constant, the pre-exponential factor and the activation energy of chemical reaction; Q is the thermal effect of reaction; c_2 , ρ_2 , λ_2 are the heat capacity, density and thermal conductivity of the mixture; m is the porosity; χ_e is the coefficient of external heat exchange; R is the gas constant.

In the general case, a reacting mixture and a melt spreading in it are in region II ($y_1(t) < y < y_2(t)$). The heat balance equations in the mixture and the melt are given by:

$$(1-m)c_2\rho_2 \frac{\partial T_2}{\partial t} = \lambda_2 \frac{\partial^2 T_2}{\partial y^2} + (1-m)\rho_2 Q \frac{\partial \alpha}{\partial t} - \chi(T_2 - T_1) - \chi_e(T_2 - T_0), \quad (3)$$

$$m\rho_1[c_1 + Q_L\delta(T_1 - T_L)] \left[\frac{\partial T_1}{\partial t} - V_- \frac{\partial T_1}{\partial y} \right] = \lambda_1 \frac{\partial^2 T_1}{\partial y^2} + \chi(T_2 - T_1) - \chi_e(T_1 - T_0), \quad (4)$$

where T_1 is the temperature of the inert substance; V_- is the melt rate in the region $y_1(t) < y_2(t)$; $\delta(T_1 - T_L)$ is the Dirac delta function; ρ_1 , c_1 , λ_1 is the density, heat capacity and thermal conductivity of metal; T_L and Q_L are the temperature and heat of metal during melting. The rate of the capillary spread of a melt is determined by the formula:

$$V = \frac{dl}{dt} \approx \frac{\sigma d_c}{8\mu l}, \quad (5)$$

where σ is the coefficient of surface tension; d_c is the diameter of the capillary; μ is the viscosity of the melt; l is the length of the path traveled by the melt in the capillary or the penetration depth of the melt into the porous carcass.

A melt or a solid metal can exist in region III ($y_2 < y < y_3(t)$). The motion law of the boundary y_3 is determined by the total melt rate $y_3(t) = (V_- + V_+)m_0t$, where V_+ is the rate of the liquid phase in pores in the right part of the sample. In this region the heat conduction equation has the form

$$\rho_1[c_1 + Q_L \delta(T_1 - T_L)] \frac{\partial T_1}{\partial t} = \lambda_1 \frac{\partial^2 T_1}{\partial y^2} - \chi_e (T_1 - T_0). \quad (6)$$

In region IV ($y_3(t) < y < y_4(t)$), where the melt spreads towards the cold boundary in the pores of the reacting mixture, the heat conduction equations for the two-phase medium have the form (3) and (4), and the kinetics equation has the form (2). In the heat conduction equation for the melt (4), the velocity V_- should be replaced by the flow rate in the opposite direction $-V_+$. It should be noted that V_- and V_+ , despite the fact these values are determined from equation (5), differ in absolute value, since the start (completion) time for the melt spreading through pores in the left and right of the sample is different.

Finally, in regions V and VI ($y_4(t) < y < y_5(t)$, $y_5(t) < y < \infty$, $y_5(t)$ is the coordinate of combustion front), where there are the combustion products and a fresh mixture, the melt is absent, and the temperature and depth of conversion are determined by equations (1) and (2).

The ignition source (heated wall) is modeled at the left boundary of the sample: $y = 0$: $T_2 = T_w$ ($t < t_w$), $\partial T_2 / \partial y = 0$ ($t > t_w$). At the moving boundaries $y_1(t)$ and $y_3(t)$, the conditions that reflect the interphase heat exchange $\partial T_1 / \partial y - \chi(T_1 - T_2) = 0$ and $\partial T_1 / \partial y - \chi(T_2 - T_1) = 0$ are given for the temperature of the liquid phase. The coupling conditions $T_1 = T_2$, $\lambda_1 \partial T_1 / \partial y = (1 - m) \lambda_2 \partial T_2 / \partial y$ are given at the interlayer boundaries $y = y_2$ and $y = y_3(t)$ before spreading the melt through pores in the left and right parts of the sample. Initial conditions are as follows: $t = 0$, $T_1 = T_2 = T_0$, $\alpha = 0$.

The mathematical formulation was reduced to a dimensionless form by using the following quantities:

$$\begin{aligned} Td &= \frac{cRT_*^2}{QE}, \quad \theta_1 = \frac{(T_1 - T_*)E}{RT_*^2}, \quad \theta_2 = \frac{(T_2 - T_*)E}{RT_*^2}, \quad \theta_L = \frac{(T_L - T_*)E}{RT_*^2}, \quad \theta_0 = -Td^{-1}, \quad Ar = \frac{RT_*}{E}, \quad \xi = \frac{y}{y_*}, \\ y_* &= \sqrt{\frac{\lambda_{20} t_*}{c\rho}}, \quad t_* = \frac{cRT_*^2}{QEK(T_*)}, \quad K(T_*) = k_0 \exp(-E / RT_*), \quad \tau = \frac{t}{t_*}, \quad \tau_w = \frac{t_w}{t_*}, \quad \Lambda = \frac{\lambda_1}{\lambda_{20}}, \quad C = \frac{c_1 \rho_1}{c_2 \rho_2}, \\ A_{cap} &= \frac{c_2 \rho_2 d_c \sigma}{4\mu \lambda_{20}}, \quad Ph = \frac{Q_L}{QTd}, \quad \lambda_2 = \lambda_{20} (1 - m)^n, \quad \alpha_e = \frac{\chi_e y_*}{\lambda_{20}}, \quad \alpha_i = \frac{\chi y_*}{\lambda_{20}}, \quad L_{i0} = \frac{y_i(0)}{y_*}, \quad L_2 = \frac{y_2}{y_*}. \end{aligned}$$

The parameter A_{cap} determining the rate and depth of penetration of the melt into adjacent porous layers is the ratio between the characteristic time of the capillary flow and the time of conductive heat transfer. Depending on the characteristic pore size, the thermophysical properties of a porous medium and the viscosity of the liquid phase, the value A_{cap} can vary in a wide range. In the limiting case $A_{cap} = 0$, the melt does not spread in pores. We restrict the parametric study of the problem to dimensionless quantities that determine the structure of the composite material: A_{cap} , m , L_i , Λ , α_e .

Depending on the parameters of the metal layer, the combustion of the sample can be conducted in two ways using different critical conditions. In the first case, the sample reacts completely with a certain delay time to overcome a layer and with a sharp increase in the combustion rate at the moment of ignition in the right part. In the second case, the combustion wave does not propagate through the layer. Under the adiabatic conditions $\chi_e = 0$, only the first case takes place, i.e. the combustion wave

propagates through the inertial layer irrespective of the parameters. To consider heat transfer, there is a need in critical conditions to conduct the combustion of the sample in a different way. These conditions depend on the size and physical and chemical parameters of the inert layer. For a low-melting inert component ($\theta_L \approx 0$), an increase in the number of the phase transition Ph which characterizes the heat of melting leads to the increase in the delay time and the stop of combustion near the critical conditions. A decrease in the melting temperature narrows the heating zone in the inert layer, while the loss of heat required for the combustion wave to overcome a barrier is reduced.

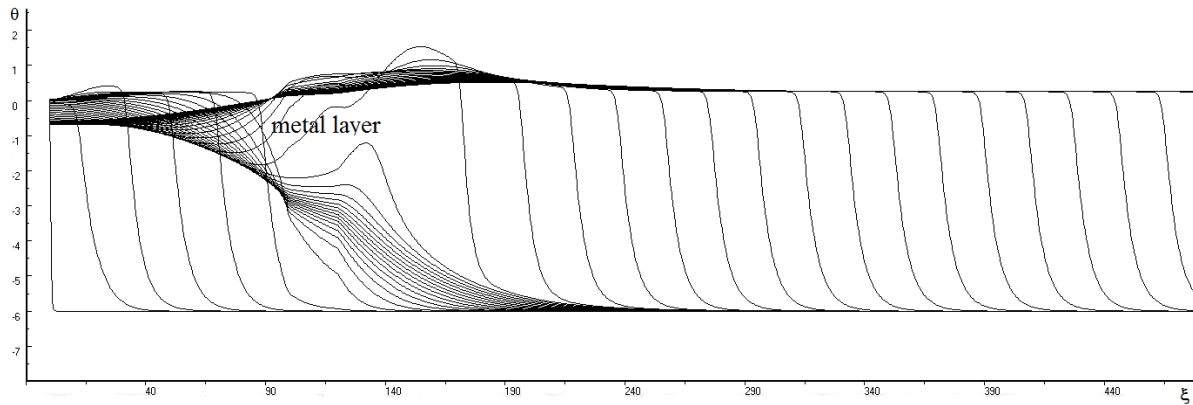


Figure 2. Temperature distributions (temperature distribution lines are given with a time step of $\Delta\tau = 100$).

The combustion mode (before and after the inert layer) is determined by the parameters of the active medium (figure 2). The parameters of the inert layer determine only the time when a wave starts propagating in the stable mode with the combustion characteristics corresponding to the active medium. The delay time is directly proportional to the thickness of the layer y_L . The longer the delay time of front for spreading through inert layer is, the greater the heating zone in the active part of the sample behind it. Influence of the melt spreading in pores on igniting and overcoming an inert barrier by the combustion wave is insignificant.

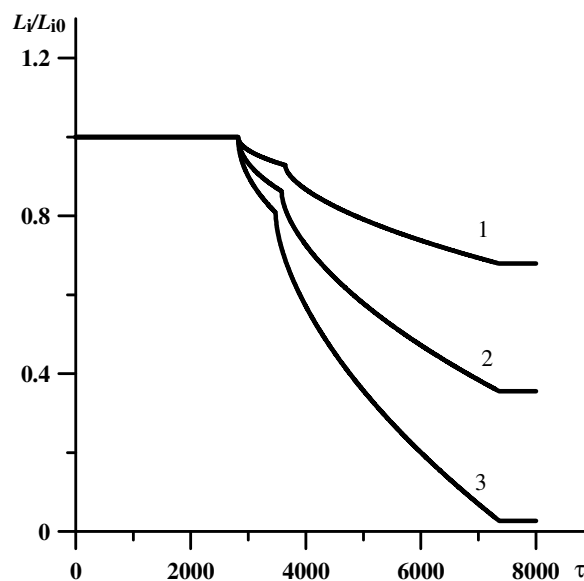


Figure 3. Relative thickness of the inner layer in the non-adiabatic combustion mode.

Propagation of the combustion wave in the layered composition depends on thermal, chemical and hydrodynamic factors. The action of thermal factors is determined by the intensity of heat exchange, the melting temperature of an inert layer, the thermal conductivity and heat capacity of substances in a mixture. Chemical factors include the rate, kinetics, and thermal effect of chemical reactions. Hydrodynamic factors determine the rate and depth of penetration of the melt into pores and depend on the structural parameters m and A_{cap} . These factors determine the peculiarities of the structure formation of composite materials. Experimental studies [3] on the interaction of tungsten foil with a Ni-Al-based melt in the SHS mode confirm the results of modeling.

Under non-adiabatic conditions $\chi_e \neq 0$, a layered structure may be formed with an inert layer, the thickness of which is less than the initial value y_L . figure 3 illustrates the thickness of the inert layer as a function of the parameter of a capillary flow A_{cap} . A decrease in the temperature of the porous carcass below the melting point leads to the stop of the capillary flow and crystallization of the melt. The metal in the inner layer III (figure 1), not penetrating in pores, remains in the form of a layer that separates the layers of the composite material.

3. Conclusion

Thus, during the combustion of a three-layer system, various production processes can be conducted: penetration, surface welding. The results of modeling for the combustion of a three-layer sample in a two-dimensional formulation with simultaneous ignition of all layers of the system are given in [4]. The method for regulating the structure of the final product is to vary the thickness of the inner layer, the porosity, the dispersion (changing the effective diameter of capillaries and the thermal conductivity), the ratio of reagents, additional heating or cooling of a layered system, and replacement of metal foil with a layer of powder to reduce thermal conductivity.

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