MODELING OF COMBUSTION SYNTHESIS IN MULTILAYER GASLESS SYSTEM

by

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A combustion model for a flat layered composition has been developed, where chemically active layers alternate with inert metallic layers with high thermal conductivity. The heat exchange between the layers was specified by the conjugate boundary conditions. A numerical study of gasless combustion of a multilayer system with heat-conjugated layers of two types was performed. Optimal layer sizes and parameters of the layer system were obtained to provide the maximum burning rate of the layer package. The effect of increasing the burning rate was found to be associated with heat recovery and an increase in the effective thermal conductivity of the system. The concentration limits of combustion were determined depending on the volume content of the inert element. Replacing the system of inert layers with that of low-calorie mixture layers leads to a model for synthesis of inorganic materials in the "chemical furnace" mode.
Key words: *heat transfer, gasless combustion, layered system*

Introduction

To increase the efficiency of high temperature synthesis of complex systems that are not capable of independent combustion, a method has been developed for forming a sample as a package of thermally conjugated layers with different thermal and physical characteristics [1]. For auxiliary layers – heat donors (DL), as a rule, high-calorie metal-thermite compositions with a high combustion temperature are used. Thermal energy from the DL enters the main synthesis layer (SL) for additional heating of the reactants and reaction products. The heating rate in the inner layer due to its thermal isolation is very high and exceeds the heating rate in radiation furnaces. Experimental studies of the synthesis of layered materials in a mode of frontal combustion are presented in [2-11]. In [12, 13] a mathematical modeling of combustion of a sample in the form of a strip of finite size, consisting of two layers with different chemical activity, was performed – a *chemical furnace* mode. The dependence of the synthesis rate on the ratio of the mixture volumes in a flat sample and their properties was calculated. It was shown that depending on the ratio between the layer sizes, the combustion mode of the inner layer changed from the frontal combustion to the inductive one. A model for the solid-phase exothermic reaction propagation in a layer between inert materials with different thermal and physical properties was proposed in [14].

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The focus of the study in this paper is the gasless combustion of a system of conjugated alternating layers with different thermophysical characteristics. Layers of one kind were chemically active. Layers of the other type were inert, made of metal with high thermal conductivity. The main objective of the study was to determine the minimum burning time of such a layered system for certain volume contents of its components, thickness and the number of layers. The aim of the study is to find an optimal ratio of the high temperature layers and the heat-conducting i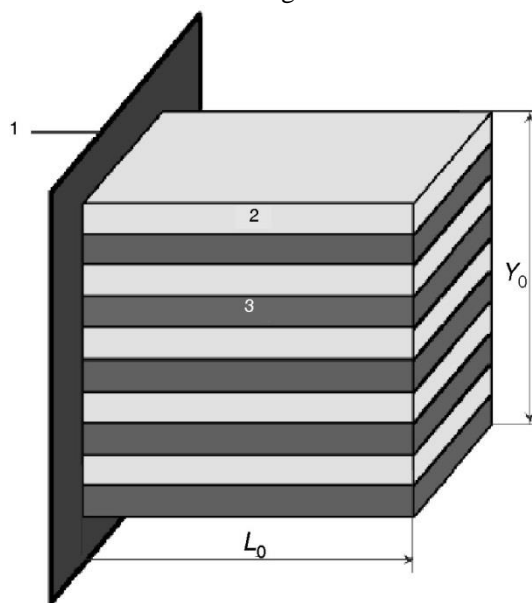nert ones. It was shown in [15] that introduction of a heat-conducting element into a sample of a cylindrical form of a gas-free composition leads to a significant increase in the burning rate due to heat recovery from the reaction product zone to the preheat zone.

The paper addresses a system of conjugated layers containing heat-conducting elements, *i. e.* layers made of a material with high heat-conducting properties (Cu, Ag, *etc.*). The system is an alternation of inert and active layers with different thermophysical parameters, with a total thickness of Y_0 and a sample length of L_0, fig. 1. Active layers 2 in their characteristics correspond to the gas-free composition $Ti + 2B$, and layers 3 are made of Cu. Ignition is carried out due to short-term simultaneous contact of all the system layers with a heated surface (1). The sample surface opposite the ignition plane is assumed to be thermally insulated. The contact time of the system with the heated surface is fixed.

Figure1. The sample structure;
1 – heated surface, 2 and 3 – layers with different thermophysical parameters

Mathematical model for gasless combustion of a layered system

The mathematical model of combustion of a layered composition in dimensionless variables has the following form:
− the heat conduction equation for the active layer:

$$c(\xi)\frac{\partial \theta_1}{\partial \tau} = \frac{\partial}{\partial \xi}\left[\lambda(\xi)\frac{\partial \theta_1}{\partial \xi}\right] + \lambda(\xi)\frac{\partial^2 \theta_1}{\partial z^2} \quad (\xi_{i-1}<\xi<\xi_i-\xi_0) \tag{1}$$

− the heat conduction equation for inert layer:

$$c(\xi)\frac{\partial \theta_2}{\partial \tau} = \frac{\partial}{\partial \xi}\left[\lambda(\xi)\frac{\partial \theta_2}{\partial \xi}\right] + \lambda(\xi)\frac{\partial^2 \theta_2}{\partial z^2} + \frac{1}{\gamma}\frac{\partial \eta}{\partial \tau} \quad (\xi_i<\xi<\xi_i+\xi_0) \tag{2}$$

− the equation of chemical conversion:

$$\frac{\partial \eta}{\partial \tau} = \gamma(1-\eta)\exp\frac{\theta_2}{1+Ar\theta_2} \quad (\xi_i<\xi<\xi_i+\xi_0) \tag{3}$$

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where i is the layer pair number ($i = 1$-N), N – the total number of layer pairs, ξ_i – the lateral co-ordinate of the inert layer, and ξ_0 – the active layer thickness.

Boundary conditions:

$$\tau \leq \tau_{\text{ign}} : \theta_k(0,\xi,\tau) = 0; \ \ \tau > \tau_{\text{ign}} : \frac{\partial \theta_k(0,\xi,\tau)}{\partial z} = 0; \ \ \xi = \xi_i, \ \xi = \xi_i + \xi_0 : \theta_1 = \theta_2, \ \Lambda\frac{\partial \theta_1}{\partial \xi} = \frac{\partial \theta_2}{\partial \xi}$$

$$\frac{\partial \theta_2(z,Y,\tau)}{\partial \xi} + \alpha_t \left[\theta_2(z,Y,\tau) - \theta_0\right] = 0; \ \ \frac{\partial \theta_k(L,\xi,\tau)}{\partial z} = 0; \ \ \theta_k(z,\xi,0) = \theta_0, \ \ \eta(z,\xi,0) = 0 \ (k = 1,2)$$

A symmetric sample was considered and the following condition was set for the axis of symmetry:

$$\frac{\partial \theta_1(z,0,\tau)}{\partial z} = 0$$

Dimensionless parameters of the problem:

$$\gamma = \frac{c_2 R T_*^2}{QE}, \ \ \text{Ar} = \frac{R T_*}{E}, \ \ \theta_k = \frac{(T_k - T_*)E}{R T_*^2}, \ \ \theta_0 = \frac{(T_0 - T_*)E}{R T_*^2}, \ \ \Lambda = \frac{\lambda_1}{\lambda_2}, \ \ C = \frac{c_1 \rho_1}{c_2 \rho_2}$$

$$\alpha_t = \frac{\alpha x_*}{\lambda_2}, \ \ t_* = \frac{c_2 R T_*^2}{QE k_0}\exp\left(\frac{E}{R T_*}\right), \ \ z = \frac{x}{x_*}, \ \ \xi = \frac{y}{x_*}, \ \ \tau_{\text{ign}} = \frac{t_{\text{ign}}}{t_*}$$

$$x_* = \sqrt{\frac{\lambda_2 t_*}{c_2 \rho_2}}, \ \ Y = \frac{Y_0}{x_*}, \ \ \xi = \frac{y_0}{z_*}, \ \ L = \frac{L_0}{x_*}$$

where L_0 is the sample length, Y_0 – the sample thickness, $T_* = T_0 + (Q/c_2)$ – the scale temperature, T_0 – the ambient temperature and the initial sample temperature, η – the depth of conversion, c_k – the specific heat, λ_k – the coefficient of thermal conductivity, ρ_k – the density, Q – the thermal effect of the reaction, t – the time, x and y are co-ordinates, k_0 – the pre-exponential factor in the reaction rate constant, E – the activation energy, R – the universal gas constant, and α – the heat transfer coefficient from the sample surface to the environment.

Numerical results

The problem was solved by the co-ordinate-wise splitting method using an implicit scheme with constant space and time steps, $h = 0.5$ and $\Delta\tau = 0.25$, respectively, and fixed sample sizes $L = 300$, $Y = 75$.

The burning time of the sample decreases with introduction of high-conducting layers into the sample compared with combustion of a homogeneous sample, fig. 2. The effect of increasing the burning rate is due to the heat recovery from the reaction product zone to the preheat zone by the inert layers with high thermal conductivity. Another parameter that affects the burning rate is the thickness of the heat-conducting layers. The highest burning rate of the layered sample was achieved at $N = 3$, which corresponds to a greater *homogenization* of the sample than in the case of $N = 1$. The thickness of the inert layer becomes much less than the thickness of the heated layer and the time for its preheat is significantly reduced. On the other hand, with an increase in the number of layers, the concentration limit for combustion occurs at a much lower dilution of the active mixture with an inert substance than for a three-layer sample (fig. 2, $N = 1$). This reduces the concentration limits of combustion of the

layer composition with the increase in the number of layer pairs. The critical content of the inert substance for the case $N = 1$, which separates the combustion and extinction modes, is approximately 47%, and for $N = 3$ it reaches 39%.
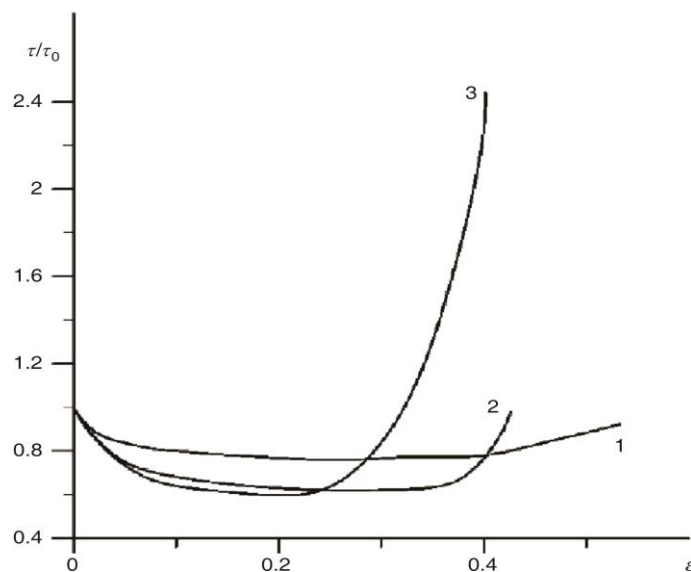

Figure 2. The dependence of the sample burning time on the volume content of inert substance $\varepsilon = 1 - (\xi_0 N)/Y$ and the number of layer pairs N: $1 - N = 1$, $2 - N = 2$, $3 - N = 3$; $\lambda_1/\lambda_2 = 30$, Ar = 0.1, $\theta_0 = -6$ (τ_0 is the burning time of a homogeneous sample)

The temperature fields characterizing the structure of the combustion wave for $\varepsilon = 0.3$ with a different number of layers are shown in fig. 3.
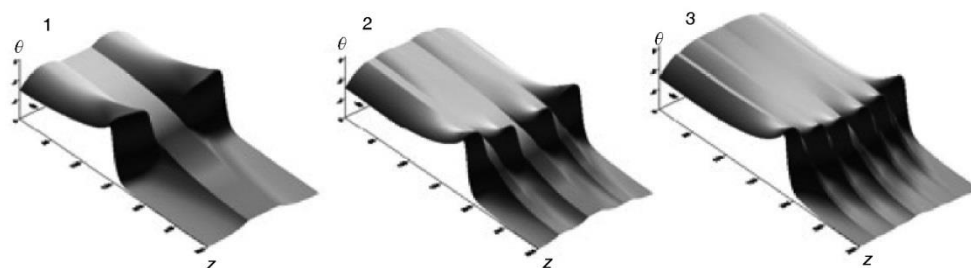

Figure 3. The temperature field; $1 - N = 1$, $2 - N = 2$, $3 - N = 3$; $\theta_0 = -6$, $\tau = 800$

The temperature gradients at $N = 1$ in the direction of the ξ axis are much larger than for the cases $N = 2$ and $N = 3$. With an increase in the number of layers, the temperature field becomes homogeneous. In the preheat zone of the combustion wave, there is an essential temperature difference between the inert and active layers. Inert layers, due to their high thermal conductivity, transfer the heat from the reaction product zone of the active layers to the low temperature region. The introduction of inert heat-conducting layers makes it possible to increase the effective coefficient of thermal conductivity of the layer system. The higher is

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the thermal conductivity of the inert substance, the more pronounced is the effect of heat recovery in the gasless combustion of the layered composition.

Acknowledgment

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