Flame spreading in an oxidant flow above burning surface of material

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1 Introduction

The condensed fuel burning in an oxidant gas flow occurs in investigations of various processes, for example: burning of fuel in hybrid engines; interaction of hypersonic flying vehicles with the atmosphere; spreading of flame over the fuel surface. To model these processes, it is necessary to simulate the flame propagation above the burning surface of material numerically. In the case of flame propagation in a closed region, where the influence of adjacent walls cannot be neglected, for example, in hybrid engines, the three-dimensional numerical simulation of this problem should be carried out. It allows to identify the non-stationary and asymmetric character of the process. Also, the numerical calculation needs verification by using the experimental data and analytical solutions. The experimental results are given by large-scale project on combustion in microgravity like as “Saffire” [1]. The analytical solutions can be obtained within the frame of boundary layer approximation and assumption of diffusion flame [2, 3]. A large number of papers have been devoted to investigations of boundary layers with combustion, the results of which have been generalized in [4-9]. However, the available data are very contradictory. Thus, for example, the results of measurements of the characteristics of heat and mass transfer in the boundary layer differ by more than an order of magnitude [10]. This problem requires a deeper analysis and the formulation of new different studies. A diffusion combustion model was widely used in the description of burning material surface in the flow of oxidant. The theory of diffusion combustion was developed in the classical Schwab and Zel'dovich works [11, 12], F.A. Williams [5] and the other papers [13-15].

In this paper, the results of numerical studies of flame propagation in weightlessness above the burning surface of material including unsteady-state transition stage are presented. A mathematical model is developed accounting for the peculiarities of diffusion combustion of fuel in the airflow. Three dimensional unsteady-state simulations of chemically reacting gas mixture above thermochemical destructing surface are performed. The numerical scheme is verified using the analytical solution [2]. As example, the processes in the combustion chamber of a hybrid engine are considered.

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2 Flame propagation over a flat surface

The numerical simulation of three-dimensional flow of a mixture gas with chemical reactions over a flat surface is presented (**Fig. 1**). To create an effective numerical model, two ways of determining the heat removal are considered, and a comparison with the analytical solution obtained with frame of the boundary layer approximation [2] is represented.

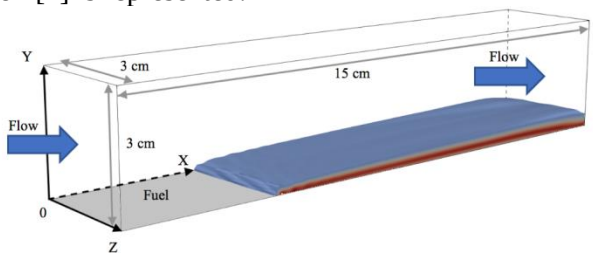

Figure 1. The scheme of the flame propagation over a flat surface.

The system of governing equations in the tensor representation has the following forms [16]:

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot \left(\rho_k \mathbf{u} - D_{eff} \nabla \frac{\rho_k}{\rho} \right) = \dot{\omega}_k , \quad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u} - \boldsymbol{\tau} \right) + \nabla p = 0 , \; \boldsymbol{\tau} = -\frac{2}{3}\rho K \mathbf{I} + \mu_{eff} \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} \nabla \cdot \mathbf{u}\mathbf{I} \right), \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left(\rho E \mathbf{u} + p\mathbf{u} - \lambda_{eff} \nabla h - \mu_{eff} \nabla K - \boldsymbol{\tau} \cdot \mathbf{u} \right) = 0 , \quad (3)$$

where $\rho = \sum_{k=1}^{N} \rho_k$ - density of the mixture, $\mathbf{u} = (u, v, w)$ - velocity, p - pressure, K - turbulence energy, ω_k - mass velocity of component formation, τ - stress tensor (k=1 stands for oxidant, k=N stands for fuel, the rest components represent intermediate reagents, reaction products and inert components).

The total internal energy of a unit mass of the mixture E is consisting from internal energy of components, kinetic and turbulent energy. The effective transport coefficients μ_{eff}, D_{eff}, λ_{eff} in equations (1)-(3) are expressed in terms of the turbulent μ_f and molecular μ viscosities of the mixture [16].

To determine the heat flux and mass flow, two formulas are used for numerical calculations. In the first case the heat flux has the following form [16]:

$$q_w = \left[\rho c_p (T - T_w) u_T \right] \Big/ \left[\mathrm{Pr}_T \left(\max\{U^+, U/u_T\} + P\{\mathrm{Pr}/\mathrm{Pr}_T\} \right) \right], \quad (4)$$

Where U - flow velocity near the wall, u_T - characteristic friction velocity, U^+=U/u_T - dimensionless velocity, T_w - interface temperature, Pr - Prandtl number, Pr_T - turbulent Prandtl number, $P(\mathrm{Pr}/\mathrm{Pt}_T)$=9.24((Pr/Pr$_T$)$^{3/4}$-(Pr/Pr$_T$)$^{1/4}$) - experimental determined function. The velocity in the vicinity of the wall in a turbulent sub-layer based on the Prandtl hypothesis on the turbulent viscosity takes the dimensionless form [17,18] $U^+ = \ln(\tilde{\mathrm{E}} y^+) / \kappa_v$, where y - coordinate characterizing distance from the wall, y^+=$\rho u_T y/\mu$ - dimensionless coordinate, κ_v=$\kappa/(1+\Xi v_w^+)$, κ=0.41 - Carman constant, v_w^+= v_w/u_T - dimensionless regression rate, Ξ=3.11+0.61·ln y^+, E=9.793.

Then the mass flow can be written as

$$(\rho v)_w = q_w \Big/ \left(c_f (T_w - T_f) + h_L \right), \quad (5)$$

where T_f - fuel temperature, h_L - specific heat of phase transition, c_f - fuel heat capacity.

In the second case the formula for heat flux are based on the analytical solutions for turbulent regime [2]:

$$q_w = -\tau_w \left[c_{pe}(T_e - T_w) + u_e^2/2 + Y_{1e}(\Phi_N \Delta H + \Delta C_p T_w) \right] / u_e , \qquad (6)$$

where u_e, T_e, Y_{1e}, c_{pe} is the velocity, temperature, oxidizer concentration and heat capacity in the external flow respectively, Φ_N - stoichiometric ratio. Turbulence is simulated based on the model [18].

The friction stress on the wall τ_w is determined from the joint solution of the following equations

$$(\rho v)_w = -B\tau_w / u_e = -0.0296 \cdot \rho u_e \ln(1+B) \cdot \mathrm{Re}^{-1/5}, \ \mathrm{Re} = \rho u_e x / \mu ,$$

$$B = \left[c_{pe}(T_e - T_w) + u_e^2/2 + Y_{1e}(\Phi_N \Delta H + \Delta C_p T_w) \right] / \left[c_f (T_w - T_f) + h_L \right]. \qquad (7)$$

The computational domain shown in **Fig. 1** is a parallelepiped with sides 15cm*3cm*3cm. The surface of the solid fuel coincides with the z0x plane. The other walls are rigid. The problem is solved in 3-D version to find the non-stationary asymmetric effects, which don not show up in one- or two-dimensional simulation. It allows to model the unevenness and asymmetry of the flame propagation until the steady-state conditions are established. In the left-hand side, the inlet jet penetrates the box. The inlet air parameters are the following: temperature T=1156 K, velocity v=1067 m/s, pressure p=7.4 bar. At the right-hand side, a free outlet conditions are set. At initial instant, the box is filled with the air at temperature T=1000 K and pressure p=1 bar. The fuel is hydroxilterminated polybutadiene HTPB used in a standard hybrid rocket configuration.

We regard the obtained analytical solution [2] and two numerical schemes: the first one uses the heat flux and mass flow determined by formulas (4) and (5), the second one is based on the equations (6) and (7). To determine the heat removal and the characteristic constants correctly, we compare these three solutions. **Fig.2** shows the dependence of the regression rate v_f on the distance from the flame tip (X) for steady flame over fuel layer. It can be seen that the curves have a significant difference only near the tip of the flame and then the graphs practically coincide. The analytical solution has the following form

$$v_f = 0.0296 \cdot \rho u_e \ln(1+B) \cdot \mathrm{Re}^{-1/5} / \rho_f \qquad (8)$$

It means that this solution ("Analitical" on **Fig.2**) and numerical solution based on formulas (6), (7) ("Numerical 1" on **Fig.2**) have singularity at zero. Also, the formula (8) was obtained under the assumption of a diffusion combustion regime, and as shown in [2] the region near the flame tip corresponds to kinetic regime and the solution should be formulated using the Arrhenius law in this zone. After that, the main role is played by diffusion and it is necessary to use the formula (8). The detected deviation of numerical and analytical solution is an expected disagreement, because the analytical diffusion combustion model does not work properly in the tip, while developed numerical model works within the whole range of parameters. Although in the initial section the curves do not coincide by the reasons described above, the further coincidence indicates the correctness of the numerical model and the advisability of using this scheme ("Numerical 2" on **Fig.2**).

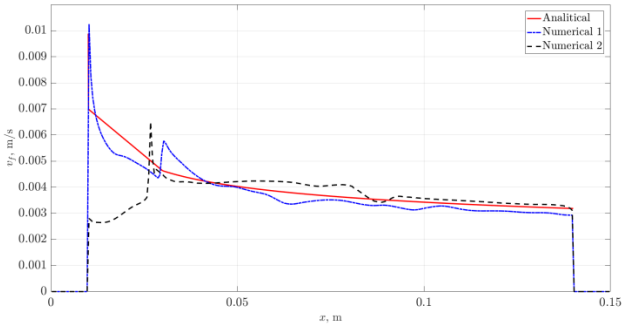

Figure 2. Analytical and numerical solutions for regression rate of HTPB fuel.

Fig. 3 illustrates the three-dimensional numerical simulation of the evolution of gas temperature in a given volume with three-dimensional structure of flame propagation above the solid fuel surface after ignition. The gas temperature distribution more than 1400 K is demonstrated. The flame "fingers" of different lengths are formed, while one of the flame "fingers" is pulled forward and reaches the end of the region, the other "fingers" don't move far away from the main front. After that, the flame front becomes stable. These "fingers" make the flow essentially unsymmetrical. That testifies the fact, that performing unsteady state simulations one should not rely heavily on symmetries. The combustion zone occupies only the region near the walls, which is typical for diffusion flame stabilized over the fuel surface (**Fig. 3**). The surface blowing with supersonic speed is characterized by the shock wave formation near the flame tip.

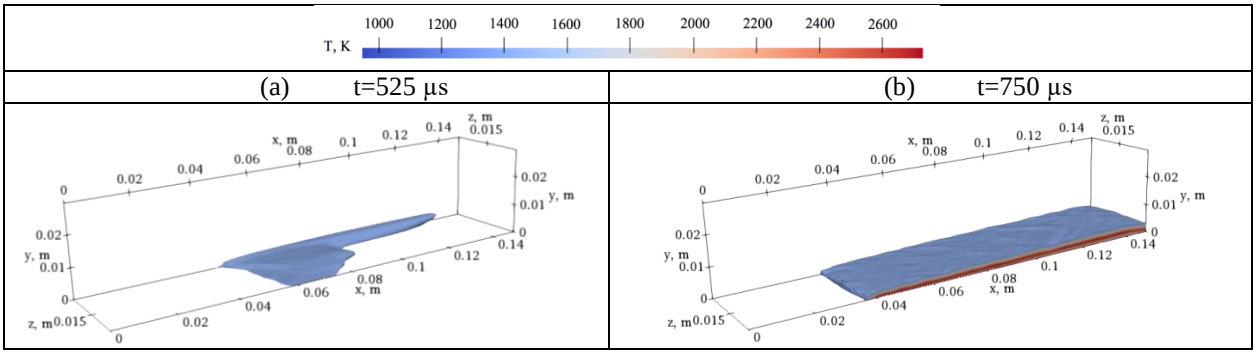

Figure 3. The evolution of gas temperature for the problem of flame propagation over a flat surface in 3-D.

3 Solid fuel surface burning in the hybrid rocket engine

The numerical simulations of three-dimensional flow in combustion chamber of hybrid rocket are performed. To represent this process, it is used the verified numerical model described in the previous paragraph.

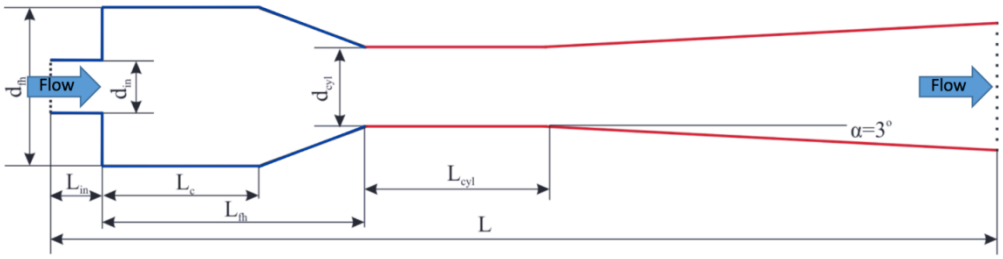

Figure 4. Schematic view of the computational domain. Cross-section along *z* axis.

The dark blue color in **Fig. 4** indicates the rigid walls of the combustion chamber. The red color illustrates the surface of solid fuel. On the left side, the supersonic inlet jet penetrates the combustion chamber. The air parameters are the following: temperature T=1156 K, mass flux *m* =0.184 kg/s, Mach number M=1.6. On the right side, a free outlet conditions are set. Linear dimensions of the chamber are the following: L=180 mm, L_{in}=10 mm, L_c=30 mm, L_{fh}=50 mm, L_{cyl}=35 mm, d_{in}=10 mm, d_{fh}=30 mm, d_{cyl}=15 mm. The chamber at initial instant is filled in by air at temperature T=300 K and pressure p= 1 bar.

Fig. 5 illustrates the evolution of gas temperature within the chamber of a hybrid motor. On starting the engine, a heated supersonic jet penetrates the chamber causing formation of a shock wave, which on reflecting from the walls finally forms a barrel structure of shock waves illustrated in **Fig. 5a** by periodical

variation of temperature. At the same time ignition takes place near fuel surface at the beginning of solid fuel layer. The successive process demonstrates flow stabilization; combustion zone occupies only the region near the walls, which is typical for diffusion flame stabilized in the combustion chamber (**Figs. 5c**). On further penetration of jet and igniting fuel layers (**Figs. 5a, 5b)** the asymmetry of flame propagation in the combustion chamber is observed. That testifies the fact, that performing unsteady state simulations one should not rely heavily on symmetries.

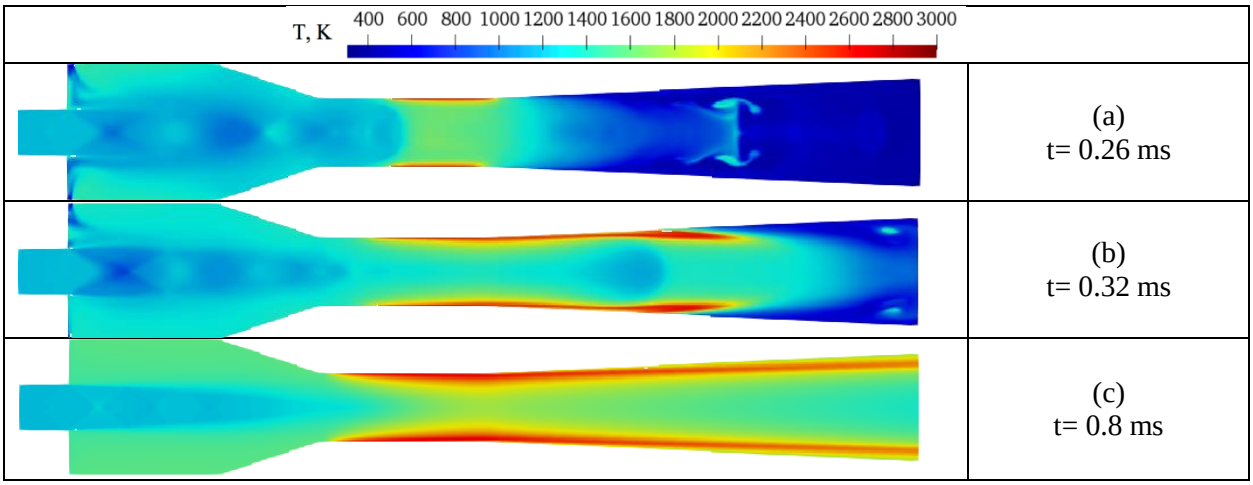

Figure 5. Temperature maps within the chamber for different times.

4 Conclusions

To create an effective numerical model, two ways of determining the heat removal are considered, and a comparison with the analytical solution obtained within the frame of the boundary layer approximation is represented. In the initial section the solutions do not coincide due to kinetic regime being established near the flame tip, the further coincidence indicates the correctness of the numerical model and the advisability of using this scheme. The three-dimensional numerical simulation of the flame propagation over the solid fuel surface shows that uneven process after ignition. The flame "fingers" of different lengths are formed. After that, the flame front becomes stable. The problem is solved in 3-D version to find the non-stationary asymmetric effects, which do not show up in one- or two-dimensional simulation. The numerical simulations of three-dimensional flow in combustion chamber of hybrid rocket are performed. To represent this process, it is used the verified numerical model. The asymmetry of flame propagation in the combustion chamber is observed. That testifies the fact, that performing unsteady state simulations one should not rely heavily on symmetries. The successive process demonstrates flow stabilization; combustion zone occupies only the region near the walls, which is typical for diffusion flame stabilized in the combustion chamber. The supersonic regime is not established until the fuel vapor occupies all the chamber section. Then central part becomes free from fuel vapor, and finally fuel vapor is concentrated only near the solid fuel surface below the diffusion flame zone. The ignition of fuel is characterized by a decrease in molar fraction of butadiene on the condensed fuel surface in the center of the combustion chamber.

Acknowledgments

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