Zero-dimensional thermochemical model of pulsed jet combustion

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A zero-dimensional thermochemical model of PJC system is proposed. The model incorporates the consideration of mixing of the burned and fresh gases with further chemical reaction in vortices. It yields a reasonable rate of pressure rise depending on the parameters of the turbulent jet plume.

Introduction

The concept of Pulsed Jet Combustion (PJC) proposed by Oppenheim [1] for internal combustion engines, refines the open chamber - direct injection - stratified charge concept. The combustion process, once started in prechamber, is then extinguished at efflux from the orifice between the prechamber and the cylinder head space. Later on, combustion revives in the turbulent vortices created by the high-speed jet. The PJC concept implies that active radicals in the burning vortices maintain a sufficiently high temperature during mixing with the fresh gas and gives rise to multiple ignition sources. The latter fact is of essential significance, since the combustion process becomes apparently distributed rather than propagating in the mode of a turbulent diffusion flame.

Thus, the PJC concept is based on the idea of a two-step combustion process:

- the first step provides a high-speed turbulent jet of combustion products containing active radicals;
- the second step is reignition followed by sustained formation of multiple ignition sites in vortices.

The paper describes an idealized (i.e., adiabatic) zero-dimensional thermochemical model for the two-step combustion in the PJC system.
Formulation

The combustion system under study consists of the main chamber of volume $V^0$ and the prechamber of volume $V_p$. Prior to ignition, the former is filled with a homogeneous fuel-air mixture with specified molar concentrations of components, $y_{ak}$, while the latter is filled with a homogeneous mixture of different composition with concentrations $y_{pk}$. Initial temperature and pressure in the system are $T^0$ and $p^0$.

The diameter of the orifice between the prechamber and the main chamber is $D^0$. After ignition in the prechamber, a turbulent plume is created in the main chamber by the jet of combustion products. The plume is composed of multiple vortices of various sizes. Combustion is resumed in the vortices due to the mixing of the high-temperature combustion products with the cold fresh mixture. The vortices grow in size by engulfing new portions of fresh mixture and thermal expansion due to the chemical reaction. The combustion process terminates when the entire mixture has burned out.

To model the combustion process in the system, the following simplifying assumptions have been adopted:

- the prechamber mixture burns under constant volume conditions;
- combustion products have a thermodynamically equilibrium composition;
- expansion of prechamber combustion products is isentropic;
- both fuel-air mixture and combustion products obey the equation of state of a perfect gas;
- pressure is uniform throughout the system;
- heat losses to the walls are negligible;
- mixing and reaction of the fresh mixture with combustion products proceed simultaneously;
- vortices are spherical and similar in size;
- vortices, once having appeared, do not disappear or multiply;
- chemical reaction is of one-step Arrhenius type.

The $j$-th vortex is characterized by the following properties, the vortex diameter $d_j$ (or volume $v_j$), the entrainment velocity across the vortex boundary $u_p$, the vortex mass $m_p$, the vortex temperature $T_p$, and the molar concentration of the $k$-th component. The process of engulfing the fresh mixture is modeled by the equation
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\[ dm_j = \dot{m}_j dt = \chi \rho d_f^2 \rho_0 u_0 dt. \] (1)

Henceforth, the suffix 0 denotes unburned mixture properties, \( t \) is time, \( \rho \) is the density, \( \chi \) is the coefficient introduced here for taking into account the engulfing of burned gas from neighbouring vortices. For a set of similar vortices we assume that \( \chi = (V_l - V_b) / V_l \), where \( V_l \) is the volume of burned gas.

Chemical conversion in a vortex is governed by the net reaction rate of Arrhenius type with the rate constant \( k_0 \).

Within the framework of the assumptions adopted, the equations for pressure, volume and average temperature of the \( f \)-th vortex are:

\[ dp = D_0 \left[ \frac{R_0 T_0}{p} \sum_j \dot{m}_j - \sum_j \frac{h_{0j} \dot{m}_j}{C_j} + \sum_j \sum_{k=1}^{n_j} \frac{\mu_k N_j h_{jk} dV_{ijk}}{C_j} + \sum_j \sum_{k=1}^{n_j} \frac{\mu_k y_{jk} (h_{jk} - C_{pk} T_j) dN_{ijk}}{C_j} \right]. \]

\[ dv_j = C_j \left[ \frac{\sum_{k=1}^{n_j} \mu_k y_{jk} C_{pk}}{R} - 1 \right] v_{j} \dot{p} - \sum_{k=1}^{n_j} \frac{\mu_k N_j h_{jk} dV_{ijk}}{C_j} + \sum_{k=1}^{n_j} \frac{\mu_k y_{jk} (h_{jk} - C_{pk} T_j) dN_{jk}}{C_j} \right]. \] (2)

\[ dT_j = \frac{v_{j} \dot{p}}{R N_j} + \frac{p dV_{j}}{R N_j} \frac{T_j dN_{j}}{N_j}, \]

where

\[ C_j = p \sum_{k=1}^{n_j} \frac{\mu_k y_{jk} C_{pk}}{R}, \quad h_{jk} = h_{0k} + C_{pk} (T_j - 298), \quad T_0 = \left( \frac{p}{p_0} \right)^{k} T_0. \]

\[ D_0 = \frac{(\xi - 1) n_j R_0 T_0}{p^2} - \sum_j \left( \frac{\sum_{k=1}^{n_j} \mu_k y_{jk} C_{pk}}{R} - 1 \right) \frac{v_{j}}{C_j}. \]

In the above equations, \( R_0 \) is the gas constant of the fresh mixture, \( R \) is the universal gas constant, \( h \) is the enthalpy, \( m \) is the mass, \( n_j \) is the number of components in the gas, \( \mu_k \) is the molecular mass, \( C_{pk} \) is the specific heat at constant pressure, \( h_{0k} \) is the component formation enthalpy, \( N_j \) is the number of moles in the \( f \)-th vortex, \( \xi = (\gamma - 1) / \gamma \) with \( \gamma \) being the specific heat ratio of the unburnt gas.

Results and discussion

As an example, combustion of a stoichiometric methane-air mixture is considered under the following conditions: \( p^0 = 10^5 \text{ Pa}, V_l = 3 \times 10^{-4} \text{ m}^3, V_b = 3 \times 10^{-6} \text{ m}^3, T^0 = 332 \text{ K}. \) The entrainment velocity \( u_0 \) was assumed constant \( u_0 = u_0, \) the initial size of vortices \( d_f(t = 0) = d(t = 0) = D^0. \)
The reaction equation is taken in the form [2]

$$\frac{d([\text{CH}_4])}{dt} = -k_A [\text{CH}_4][\text{O}_2]^{0.5}$$

(3)

where

$$k_A = 4.8 \cdot 10^9 \rho (0.987 \cdot 10^{-5})^{0.7} \exp \left( \frac{-12200}{T} \right),$$

[\text{CH}_4] and [\text{O}_2] are the concentrations of methane and oxygen in mole/(cm³-K).

To close the set of governing equations the following equations of balance for \text{CH}_4, \text{O}_2, \text{N}_2, \text{CO}_2, \text{and H}_2\text{O} concentrations are used:

$$dN_j = Adn_j,$$

$$dy_{\text{CH}_4} = \left( \frac{x_{\text{CH}_4}}{\mu_{\text{CH}_4}} - y_{\text{CH}_4} A \right) \frac{dn_j}{N_j} - k_A M_j^{1/2} y_{\text{CH}_4} y_{\text{O}_2}^{1/2} dt,$$

$$dy_{\text{O}_2} = \left( \frac{x_{\text{O}_2}}{\mu_{\text{O}_2}} - y_{\text{O}_2} A \right) \frac{dn_j}{N_j} + 2k_A M_j^{1/2} y_{\text{CH}_4} y_{\text{O}_2}^{1/2} dt,$$

$$dy_{\text{N}_2} = \left( \frac{x_{\text{N}_2}}{\mu_{\text{N}_2}} - y_{\text{N}_2} A \right) \frac{dn_j}{N_j},$$

(4)

$$dy_{\text{CO}_2} = -\left( \frac{y_{\text{CO}_2}}{N_j} \right) A dn_j + k_A M_j^{1/2} y_{\text{CH}_4} y_{\text{O}_2}^{1/2} dt,$$

$$dy_{\text{H}_2\text{O}} = \left( \frac{y_{\text{H}_2\text{O}}}{N_j} \right) A dn_j + 2k_A M_j^{1/2} y_{\text{CH}_4} y_{\text{O}_2}^{1/2} dt,$$

$$A = \frac{x_{\text{CH}_4}}{\mu_{\text{CH}_4}} + \frac{x_{\text{O}_2}}{\mu_{\text{O}_2}} + \frac{x_{\text{N}_2}}{\mu_{\text{N}_2}}$$

where $M_j = 10^3 N_j / V_j$ is the molar concentration of mixture in the $j$-th vortex, $x_i$ denotes the mass concentrations of the $k$-th component in the burned mixture. The balance equations (4) indicate that species concentrations in the $j$-th vortex vary due to mixing and chemical conversion.

The set of governing equations was solved numerically using the standard Runge-Kutta method. The STANJAN code [3] was used to estimate equilibrium compositions and thermochemical parameters.

At fixed geometry and thermodynamic initial conditions, for a specified fuel-air mixture, the solution of Eqs. (1) to (4) contains a single dimensionless governing parameter $\alpha = t_{cha} / (D^3 / u_0)$, where $t_{cha} = (k_A(M_j)^{0.5})^{-1}$ is the characteristic chemical time, $D^3 / u_0$ is the
characteristic time of turbulent mixing. Our calculations revealed that the dependence of pressure \( p/p_0 \) on the dimensionless time \( t_{u0}/d \) shows a bifurcation behavior at \( \alpha = \alpha_* = 1.9 \cdot 10^{-7} \). At \( \alpha < \alpha_* \), the solution of the problem is represented with a good approximation by a unique curve 1 in figure 1, whereas at \( \alpha > \alpha_* \), mixture ignition fails, and \( p/p_0 = 1 \) (curve 2 in figure 1). Curve 3 in figure 1 corresponds to the almost critical case, \( \alpha = 0.995\alpha_* \). The absence of heat loss in the model results in monotonous pressure increase to the thermodynamic value. Qualitatively, the predicted pressure vs time dependence corresponds with the experimental findings of [1].

![Graph](image)

**Fig. 1.** Predicted pressure histories in the constant-volume adiabatic PJG system depending on the dimensionless parameter \( \alpha = t_{u0}(D_p/n)^{1/4} \). Curve 1 represents solutions with \( \alpha < \alpha_* \), curve 2 with \( \alpha > \alpha_* \), curve 3 with \( \alpha = 0.995 \alpha_* \), where \( \alpha_* = 1.9 \cdot 10^{-7} \) is the critical value of \( \alpha \).

Figure 2 shows the dependencies of temperature on the dimensionless time \( t_{u0}/d \). Curves 1 and 5 show the histories of burned and unburned gas temperature, respectively, at \( \alpha = 0.12\alpha_* \). For this case, curve 4 shows the evolution of the average temperature in the combustion chamber. Curves 2 and 3 correspond to the temperature of burned gas at almost critical values of curve 2 for \( \alpha = 0.995\alpha_* \), curve 3 for \( \alpha = 1.005\alpha_* \). Noteworthy is the behavior of curve 2 at the beginning of the process. Temperature of burned gas escaped from the prechamber decreases first due to engulfing cold fresh mixture. However, mixing of the combustion products with the increasing amount of fresh mixture results in conditions favoring auto-ignition and temperature grows sharply. Further temperature rise proceeds approximately along the unique curve 1. Curve 6 shows the history of the unburned gas temperature under conditions \( \alpha > \alpha_* \). The fresh mixture does not change its temperature during the whole process.
**Fig. 2.** The dependencies of temperature on the dimensionless time $tu/d$. Curve 1: burned gas temperature, $\alpha = 0.12\alpha_\infty$. Curves 2 and 3: burned gas temperature at $\alpha = 0.995\alpha_\infty$ and $\alpha = 1.005\alpha_\infty$. Curve 4: average temperature in the combustion chamber, $\alpha = 0.12\alpha_\infty$. Curve 5: unburned gas temperature, $\alpha = 0.12\alpha_\infty$. Curve 6: unburned gas temperature, $\alpha > \alpha_\infty$.

**Fig. 3.** The dependencies of density on dimensionless time $tu/d$ at $\alpha = 0.12\alpha_\infty$. Curves 1 and 3 show the evolution of unburned and burned gas density, respectively. Curve 2 corresponds to the average density in the combustion chamber.

Figure 3 shows the dependencies of density on dimensionless time $tu/d$ for the case with mixture ignition, $\alpha = 0.12\alpha_\infty$. Curves 1 and 3 show the evolution of unburned and burned gas density, respectively. Curve 2 corresponds to the average density in the combustion chamber. Clearly, the average density is $\rho^0$, which is consistent with the assumption of constant volume combustion.
Fig. 4. The history of methane content in the combustion chamber. Curve 1: $\alpha = 0.12 \alpha_e$. Curve 2: $\alpha = 0.995 \alpha_e$. Curve 3: $\alpha = 1.005 \alpha_e$.

Fig. 5. The dependence of the vortex size on time. Curve 1 shows the evolution of vortex size in the reactive medium, $\alpha = 6 \cdot 10^{-3} \alpha_e$. Curve 2 corresponds with the vortex growth in the absence of chemical reaction, $\alpha >> \alpha_e$. 
Figure 4 shows the history of methane content in the combustion chamber, with \((CH_4)^0\) denoting the initial mass of methane. Curve 1 represents the case \(\alpha < \alpha_c\) (\(\alpha = 0.12\alpha_c\)), and curves 2 and 3 correspond to near critical values of \(\alpha\), for curve 2: \(\alpha = 0.995\alpha_c\), for curve 3: \(\alpha = 1.005\alpha_c\).

Figure 5 illustrates the role of chemical energy release in the growth of vortex size. Curve 1 shows the evolution of vortex size in the reactive medium at \(\alpha = 6 \cdot 10^{-3}\alpha_c\), while curve 2 corresponds with the vortex growth in the absence of chemical reaction (\(\alpha >> \alpha_c\)). In the latter case, a vortex grows due to engulfing the fresh mixture. In the case of reactive medium, the effect of thermal expansion is dominant. The decrease in the vortex growth rate at late stages of the process is evidently caused by the decrease in the amount of unburned mixture.

**Conclusion**

A zero-dimensional thermochemical model of PJC system has been proposed. The model yields the rate of pressure rise depending on the parameters of the turbulent jet plume. Further improvement of the model with due regard for vortices size distribution and heat loss is projected to better represent the real conditions. The model is planned to be used for studying NO\(_x\) formation in PJC system.

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**References**