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## THERMOCHEMICAL MODEL OF A TWO-STAGE COMBUSTION PROCESS IN THE CONCEPT OF PULSED JET COMBUSTION

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### 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 give 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  $V^\circ$  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,  $y_{0k}$ , while the latter is filled with a homogeneous mixture of different composition with concentrations  $y_{pk}$ . Initial temperature and pressure in the system are  $T^\circ$  and  $p^\circ$ .

The diameter of the orifice between the prechamber and the main chamber is  $D^\circ$ . 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  $u_j$ , the vortex mass  $m_j$ , the vortex temperature  $T_j$ , and the molar concentration of the  $k$ -th component. The process of engulfing the fresh mixture is modelled by the equation

$$dm_j = \dot{m}_j dt = \chi \pi d_j^2 \rho_0 u_{j0} dt. \quad (1)$$

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  $\chi = (V^\circ - V_b)/V^\circ$ , where  $V_b$  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  $k_A$ .

Within the framework of the assumptions adopted, the equations for pressure, volume and average temperature of the  $j$ -th vortex are:

$$\begin{aligned}
 dp &= D_0^{-1} \left[ \frac{R_0 T_0}{p} \sum_j dm_j - \sum_j \frac{h_0 dm_j}{C_j} \right. \\
 &\quad \left. + \sum_j \sum_{k=1}^{n_f} \frac{\mu_k N_j h_{jk} dy_{jk}}{C_j} + \sum_j \sum_{k=1}^{n_f} \frac{\mu_k y_{jk} (h_{jk} - C_{pk} T_j) dN_j}{C_j} \right], \\
 dv_j &= C_j^{-1} \left[ - \left( \sum_{k=1}^{n_f} \frac{\mu_k y_{jk} C_{pk}}{R} - 1 \right) v_j dp - \sum_{k=1}^{n_f} \mu_k N_j h_{jk} dy_{jk} \right. \\
 &\quad \left. - \sum_{k=1}^{n_f} \mu_k y_{jk} (h_{jk} - C_{pk} T_j) dN_j + h_0 dm_j \right], \\
 dT_j &= \frac{v_j dp}{R N_j} + \frac{p dv_j}{R N_j} - \frac{T_j dN_j}{N_j},
 \end{aligned} \tag{2}$$

where

$$\begin{aligned}
 C_j &= p \sum_{k=1}^{n_f} \frac{\mu_k y_{jk} C_{pk}}{R}, \quad h_{jk} = h_k^o + C_{pk} (T_j - 298), \quad T_0 = \left( \frac{p}{p_0} \right)^\xi T^o \\
 D_0 &= \frac{(\xi - 1) m_0 R_0 T_0}{p^2} - \sum_j \left( \frac{\sum_{k=1}^{n_f} \mu_k y_{jk} C_{pk}}{R} - 1 \right) \frac{v_j}{C_j}.
 \end{aligned}$$

In the above equations,  $R$  is the gas constant,  $h$  is the enthalpy,  $m$  is the mass,  $n_f$  is the number of components in the gas,  $\mu_k$  is the molecular mass,  $C_{pk}$  is the specific heat at constant pressure,  $h_k^o$  is the component formation enthalpy,  $N_j$  is the number of moles in the  $j$ -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:  $p^o = 10^5$  Pa,  $V^o = 3 \cdot 10^{-4}$  m<sup>3</sup>,  $V_p = 3 \cdot 10^{-6}$  m<sup>3</sup>,  $T^o = 332$  K. The entrainment velocity  $u_{0j}$  was assumed constant  $u_{0j} = u_0$ , the initial size of vortices  $d_j(t = 0) = d(t = 0) = D^o$ .

The reaction equation is taken in the form [2]

$$\frac{d[\text{CH}_4]}{dt} = -k_A[\text{CH}_4][\text{O}_2]^{0.5} \quad (3)$$

where

$$k_A = 4.8 \cdot 10^6 T (p \cdot 0.987 \cdot 10^{-5})^{0.2} \exp\left(-\frac{12200}{T}\right),$$

$[\text{CH}_4]$  and  $[\text{O}_2]$  are the concentrations of methane and oxygen in mole/( $\text{cm}^3 \cdot \text{K}$ ).

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

$$\begin{aligned} dN_j &= Adm_j, \\ dy_{\text{CH}_4j} &= \left(\frac{x_{\text{CH}_4}}{\mu_{\text{CH}_4}} - y_{\text{CH}_4j}A\right) \frac{dm_j}{N_j} - k_A M_j^{1/2} y_{\text{CH}_4j} y_{\text{O}_2j}^{1/2} dt, \\ dy_{\text{O}_2j} &= \left(\frac{x_{\text{O}_2}}{\mu_{\text{O}_2}} - y_{\text{O}_2j}A\right) \frac{dm_j}{N_j} - 2k_A M_j^{1/2} y_{\text{CH}_4j} y_{\text{O}_2j}^{1/2} dt, \\ dy_{\text{N}_2j} &= \left(\frac{x_{\text{N}_2}}{\mu_{\text{N}_2}} - y_{\text{N}_2j}A\right) \frac{dm_j}{N_j}, \\ dy_{\text{CO}_2j} &= -\frac{y_{\text{CO}_2j} Adm_j}{N_j} + k_A M_j^{1/2} y_{\text{CH}_4j} y_{\text{O}_2j}^{1/2} dt, \\ dy_{\text{H}_2\text{O}j} &= -\frac{y_{\text{H}_2\text{O}j} Adm_j}{N_j} + 2k_A M_j^{1/2} y_{\text{CH}_4j} y_{\text{O}_2j}^{1/2} dt, \\ A &= \frac{x_{\text{CH}_4}}{\mu_{\text{CH}_4}} + \frac{x_{\text{O}_2}}{\mu_{\text{O}_2}} + \frac{x_{\text{N}_2}}{\mu_{\text{N}_2}}, \end{aligned} \quad (4)$$

where  $M_j = 10^3 N_j / V_j$  is the molar concentration of mixture in the  $j$ -th vortex,  $x_k$  denotes the mass concentration 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) contain a single dimensionless governing parameter  $\alpha = t_{ch} / (D^\circ / u_0)$ , where  $t_{ch} = (k_A M_j(0)^{0.5})^{-1}$  is the characteristic chemical time,  $D^\circ / u_0$  is the characteristic time of turbulent mixing. Our calculations revealed that the dependence of pressure  $p/p^\circ$  on the dimensionless time  $tu_0/d$  shows a bifurcation behavior at  $\alpha = \alpha_* = 1.9 \cdot 10^{-3}$ . At  $\alpha < \alpha_*$  the solution of the problem is represented with a good approximation by a unique curve 1 in Fig. 1, whereas at  $\alpha > \alpha_*$  mixture ignition fails, and  $p/p^\circ = 1$  (curve 2 in Fig. 1). Curve 3 in Fig. 1 corresponds to the almost



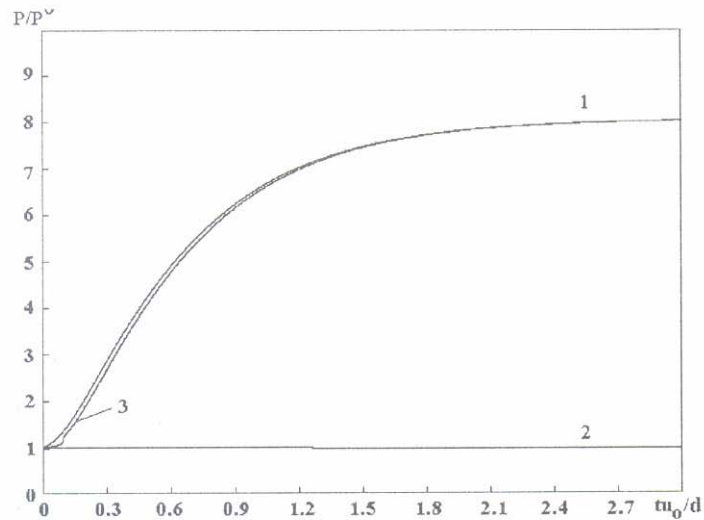


Figure 1: Predicted pressure histories in the constant-volume adiabatic PJC system depending on the dimensionless parameter  $\alpha = t_{ch}(D^0/u_0)^{-1}$ . Curve 1 represents solutions with  $\alpha < \alpha_*$ , curve 2 with  $\alpha > \alpha_*$ , curve 3 with  $\alpha = 0.995\alpha_*$ , where  $\alpha_* = 1.9 \cdot 10^{-3}$  is the critical value of  $\alpha$ .

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]. The model allows to study the effect of turbulence and mixture composition on pressure history in the PJC system as well as  $\text{NO}_x$  formation.

### 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  $\text{NO}_x$  formation in PJC system.

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### 3D MODELING OF PULSED JET COMBUSTION

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#### Introduction

The concept of Pulsed Jet Combustion (PJC), proposed by Oppenheim [1] as an alternative mode of energy release in stratified-charge internal combustion engines, shows a number of practical advantages. Based on the fundamental ideas of Gussak, Semenov and Zel'dovich concerning the role of active radicals in the torch mechanism of ignition and flame propagation, the PJC concept implies a staged combustion process:

- the flame generated in a prechamber is extinguished by shear at efflux from the orifice between the prechamber and the main chamber;
- combustion is spontaneously reinitiated in the main chamber in the core of the hot turbulent jet.

According to [1], further chemical transformations in the main chamber occur in a fireball, i.e. via distributed combustion sustained by multiple pockets of high concentration of active radicals. Of prime importance are the entrainment processes resulting in the fireball growth.

It should be emphasized that the fireball mode of combustion differs in principle from turbulent propagating flame mode. The latter is characterized by laminar-like average structure with certain characteristic thickness of the turbulent reaction zone. The turbulent propagating flame mode is assumed in the most stratified charge concepts.