SPONTANEOUS COMBUSTION REGIMES IN IC ENGINES

One of the basic principles of classical combustion theory is the assumption that the combustible mixture is uniform and temperature or concentration gradients are negligible. In effect, the existence of spatial nonuniformities is usual for the overwhelming majority of technical devices. Under conditions close to self-ignition these nonuniformities may give rise to fast spontaneous flames and combustion instability. This review confines itself to available information on spontaneous flames in IC engines including experimental evidences of knocking operation and, mainly, theoretical treatments of the accompanying problems.

1. INTRODUCTION

Combustion regimes arising under conditions close to reactive mixture self-ignition are of growing interest nowadays. To first mentions of specific fast flames (‘spontaneous flames’) one should attribute papers of Voinov [22] and Sokolik [18]. When investigating ‘knocking’ combustion in IC engines they observed incipience of localized hot spots in preflame zone with subsequent escape of fast transonic or supersonic flames from those spots. The velocity of these flames was found to vary significantly in space and time. Voinov [22] has suggested an idea that the propagation mechanism of such flames consists in successive self-ignition of preconditioned mixture layers. To his conviction such spontaneous flames give rise to shock and detonation waves in a knocking engine.

Further experimental studies [8,18] revealed detailed features of the phenomenon and substantiated close connection between spontaneous flames and explosion onset. Since spontaneous flame can propagate without oriented motion of the matter [11], it may exist under conditions when laminar or turbulent flames are impossible. For example, spontaneous flame can propagate in a very narrow gap [13] or through a small orifice. Erosion of IC cylinder wall may be attributed to this kind of combustion waves. Another specific feature of spontaneous flames is their strictly oriented propagation resulted from unisotropic local

* Institute of Chemical Physics Moscow - RUSSIA
distributions of temperature and/or mixture concentration.

Thus, phenomenologically, a realistic self-ignition process reveals the following features:
- it proceeds inhomogeneously (in hot spots)
- it's propagation is oriented
- its propagation velocity is time dependent
- a spectrum of propagation velocities is continuous
- it is accompanied with gasdynamic effects

In a classical theory of thermal and chain explosions these features are not taken into account. A combustible mixture is assumed uniform with local temperature and species concentration gradients being neglected. However, in many applications the above features may become important.

Zeldovich et al [25] were the first who studied spontaneous flames theoretically. At present there exists a voluminous literature on theoretical study of spontaneous combustion regimes both in homogeneous [11, 4-6, 9-12, 15, 23-25] and heterogeneous [17, 11, 16] media.

The most important consequence of spontaneous flame origin and propagation is a possibility of strong shock or detonation initiation. This may become a case when the following two requirements are met:
- a reactive mixture is preconditioned for localized self-ignition
- a proper ignition delay gradient is formed in the vicinity of an ignition site

The latter condition is required for ensuring coupling between spontaneous flame and accompanying pressure waves. Coupling results in shock wave and, subsequently, detonation wave formation [11, 26].

Zeldovich et al [26] have classified explosion processes arising spontaneously in a reactive mixture with concentration or temperature nonuniformities. They distinguished the following types of explosion evolution:
1) spatially uniform constant volume explosion;
2) direct detonation initiation. Detonation arises gradually inside or outside a nonuniformity and propagates steadily in a rest of mixture;
3) detonation initiation with a shock precursor. Detonation arises outside a nonuniformity behind a shock precursor generated at earlier stages of explosion;
4) oscillatory explosion processes. A reactive shock wave forms inside a nonuniformity and decays outside it giving rise to secondary explosions and secondary shock waves.

Zeldovich et al [26] have shown also that there exists a critical (minimum) size of a nonuniformity for a given mixture which makes it
possible direct detonation initiation. The study of Zeldovich et al [26] was based on a simplified approach making use of a one-step Arrhenius type reaction and neglecting transport processes.

The aim of this paper is to generalize the classification of Zeldovich et al [26] by studying gasdynamic patterns arising in nonuniformly preheated hydrogen-oxygen mixture with due regard for detailed chemical kinetics and transport processes.

2. FORMULATION

Consider a volume of dimension $L$ containing initially quiescent stoichiometric $H_2 - O_2$ mixture at pressure $p_0$. A spatial domain of characteristic dimension $X_i$ with nonuniform temperature distribution $T(x)$ is assumed to exist in the volume. For modeling wave patterns generated in the system due to the nonuniform initial conditions we adopt the following assumptions:

- the problem is treated one-dimensionally;
- the combustion is laminar;
- the combustion gases obey the perfect gas law;
- the volume is confined by adiabatic, non-catalytic, impermeable wall.

The basic equations used for solving the problem in LaGrangian formulation are as follows

\[
\frac{\partial p}{\partial t} + \rho \frac{\partial w}{\partial x} = 0; \quad \frac{\partial y_j}{\partial t} + \frac{\partial (\rho y_j v_j)}{\partial x} = \frac{\omega_j}{\rho}, \quad j = 1, \ldots, N
\]

\[
\frac{\partial T}{\partial t} - \frac{1}{\rho c_p} \frac{\partial T}{\partial x} + \frac{1}{\rho c_p} \sum_{j=1}^{N} \rho y_j v_j c_p \frac{\partial T}{\partial y} = \frac{1}{\rho c_p} (\lambda T_p \frac{\partial T}{\partial y})
\]

\[
\frac{4 \rho \eta}{3 c_p} \frac{\partial w}{\partial x} + \frac{1}{\rho c_p} \sum_{j=1}^{N} \omega_j h_j = 0
\]

\[
\frac{\partial w}{\partial t} + \frac{\partial p}{\partial x} - \frac{4}{3} \frac{\partial}{\partial y} \left( \rho \eta \frac{\partial w}{\partial y} \right) = 0
\]

\[
p - \rho^0 \rho T \sum_{j=1}^{N} \frac{Y_j}{m_j} = 0; \quad \frac{\partial x}{\partial y} = \frac{1}{\rho}
\]

where $0 \leq \psi \leq \psi_{max}$ is LaGrangian coordinate, $x$ Eulerian coordinate, $t$ time, $p$ density, $w$ mass velocity, $T$ temperature, $y_j$ mass fraction of species $j$, $N$ number of species, $v$ diffusion velocity of species $j$, $m_j$
molecular mass of species $j$, $\dot{\omega}_j$ molar rate of formation of species $j$, $c_{pj}$ specific heat of species $j$ at constant pressure, $c_p$ specific heat of the mixture at constant pressure, $\lambda_T$ thermal conductivity, $\eta$ dynamic viscosity, $h_j$ specific enthalpy of species $j$, $R^0$ universal gas constant.

The set of equations (1) is supplemented by initial conditions

$$T(0, \psi) = T^0(\psi); \quad y_j(0, \psi) = y_{j0}, \quad J = 1, \ldots, N$$
$$p(0, \psi) = p_0; \quad w(0, \psi) = 0$$

and boundary conditions

$$\frac{\partial T(t, 0)}{\partial \psi} = 0; \quad \frac{\partial T(t, \psi_{max})}{\partial \psi} = 0$$
$$\frac{\partial y_j(t, 0)}{\partial \psi} = 0; \quad \frac{\partial y_j(t, \psi_{max})}{\partial \psi} = 0 \quad J = 1, \ldots, N$$
$$\frac{\partial p(t, 0)}{\partial \psi} = 0; \quad \frac{\partial p(t, \psi_{max})}{\partial \psi} = 0$$
$$w(t, 0) = 0; \quad w(t, \psi_{max}) = 0$$
$$x(t, 0) = 0; \quad x(t, \psi_{max}) = X_{max}$$

where index 0 denotes values at $t = 0$.

Temperature distribution $T(0, x)$ in a nonuniformity is taken monotonous in the form

$$0 \leq x \leq \delta \quad T = T_m \quad \text{(peak value)}$$
$$\delta < x < X_T \quad \text{cubic polynomial interpolating between } T_m \text{ and } T_e$$
$$X_T < x < L \quad T = T_e \quad \text{(ground value)}$$

The function $T^0(\psi)$ is then derived by using the last equation of Eqs. (1).

In order to observe wave patterns outside a nonuniformity we specify $L \geq 2X_T$. The reaction mechanism for $H_2 - O_2$ mixture and transport coefficients are taken from [14]. The problem (1)-(4) is solved numerically by the method described in detail in [23].

3. ESTIMATION OF INITIAL CONDITIONS

For estimating initial values of $T_m, T_e, p_0$, and $X_T$ at which one can expect spontaneous onset and amplification of shock waves in a stoichiometric $H_2 - O_2$ mixture we make use of the coupling criterion [11, 26]

$$u_s \approx u_g$$

Here $u_s$ is the spontaneous flame velocity, $u_g$ the characteristic gasdynamic velocity. A local value of $u_s$ is defined by Zeldovich [27] as
\[ u_s = |\text{grad} \ t_i|^{-1} \]  \hspace{1cm} (6)

where \( t_i \) is the local induction time of mixture self-ignition. A characteristic gasdynamic velocity is

\[ u_g = \left( \frac{\gamma p_0}{\rho_0} \right)^{1/2} \]  \hspace{1cm} (7)

To obtain an explicit relationship between the basic parameters of the problem in the frame of Eq. (5) we use the local induction time written in the form

\[ t_i = A[H_2]^a[O_2]^b \exp(E/RT) \]  \hspace{1cm} (8)

where \([H_2]\) and \([O_2]\) are the molar concentrations of hydrogen and oxygen respectively, \(a\) and \(b\) the exponents, \(E\) the effective activation energy. Combination of Eqs. (6) and (8) gives

\[ u_s = \left( - \frac{t_i (E/RT^2)}{\text{grad}T} \right)^{-1} \]  \hspace{1cm} (9)

This expression introduced into Eq. (5) with due regard for Eq. (7) gives an estimate of the temperature gradient:

\[ \text{grad}T = \left( \frac{RT^2}{E} \right) \left( \frac{\gamma p}{\rho} \right)^{1/2} \]  \hspace{1cm} (10)

Assuming \( T \) above the autoignition limit at a given value of \( P_0 \) (say, \( P_0 = 0.1 \text{ MPa}, \ T = 1000 \text{ K} \) [2, 21]) one obtains for a stoichiometric \( H_2 - O_2 \) mixture [20]: \( \gamma \approx 1.354 \), \( P_0 = \rho_0 / RT \approx 0.144 \text{ kg/m}^3 \), where \( \gamma \) is the ratio of specific heats. Ignition delay data of [17] give for the above example \( E = 18240 \pm 2870 \text{ kal/mole}, \) and the induction time about 50 \( \mu \text{sec} \) (for the average \( E \) value). Ignition delay data of [3] give for the same example \( E = 17200 \text{ kal/mole}, \ t_i = 160 \mu \text{sec}. \) As a result, \( \text{grad}T = (750 - 2200) \text{ K/m.} \) Choosing \( \chi_T = 1 \text{ cm} \) as a characteristic size of temperature nonuniformity we come finally to the following set of basic parameters:

\[ P_0 = 0.1 \text{ MPa}; \ T_e = 1000 \text{ K}; \ X_T = 1 \text{ cm}; \ T_m \approx (1010 - 1020) \text{ K} \]

A parameter \( \delta \) entering Eq. (4) is used for ensuring adiabatic conditions at the wall. In calculations \( \delta = 0.2 \text{ cm} \) was assumed.

4. RESULTS OF CALCULATIONS

The correctness of the reaction scheme given in [14] was first confirmed by comparing predicted induction times with available measurements. At \( T_e = T_m = 1000 \text{ K}, \ P_0 = 0.1 \text{ MPa} \) the predicted induction time of a stoichiometric \( H_2 - O_2 \) mixture is 99.4 \( \mu \text{sec} \), which is close to the measured value [3, 17].

At very small temperature increments \( \Delta T = T_m - T_e \leq 1 \text{ K} \) almost constant volume explosion has been observed in calculations with \( \chi_T = 1 \)
cm, $T_c = 1000$ K, $p_c = 0.1$ MPa.

Figure 1 shows pressure history in the mixture with a temperature nonuniformity of size $X_T = 1$ cm with $T_m = 1010$ K, $T_o = 1000$ K ($\Delta T = T_m - T_o = 10$ K), $p_o = 0.1$ MPa. As is clearly seen, a detonation wave arises spontaneously outside the nonuniformity. The detonation wave propagates at the velocity $\approx 2560$ m/s which is rather close to the thermodynamic value 2519 m/s, calculated by Vasiliev et al [20] for the outlined conditions. A calculated temperature of combustion products $\approx 3200$ K which corresponds with the thermodynamic value 3136 K, calculated by Vasiliev et al [20]. At time $t \approx 100$ $\mu$s the reaction in front of the detonation wave becomes apparent. The overpressure in a shock wave emanating from the nonuniformity is about $\Delta p \approx 0.4$ MPa. Clearly the explosion process under consideration should be attributed to the second type in classification of Zeldovich et al [26]. Similar results were obtained at $\Delta T = 30$ K other conditions being equal. The overpressure in a shock wave emanating from the nonuniformity increased in the latter case up to $\Delta p_i \approx 0.6$ MPa.

Further increase in peak temperature up to $T_m = 1100$ K ($\Delta T = 100$ K) results in decreasing the shock overpressure at the

Fig.1 Time-dependent pressure profile in stoichiometric $H_2-O_2$ mixture with a temperature nonuniformity: $T_m = 1010$ K; $T_o = 1000$ K, $p_o = 0.1$ MPa, $X_T = 1$ cm.

Fig.2 Time-dependent pressure profile in stoichiometric $H_2-O_2$ mixture with a temperature nonuniformity: $T_m = 1100$ K; $T_o = 1000$ K, $p_o = 0.1$ MPa, $X_T = 1$ cm.
edge of nonuniformity to $\Delta p_e \approx 0.4$ MPa (Fig.2). Also evident is the change of explosion dynamics. After emanating from the nonuniformity a shock wave decays. Apparent amplification of the shock wave at $t \approx 40 \mu s$ is a result of its reflection from the opposite wall at $x = 2$ cm. Shock attenuation is caused by growing difference between reaction induction times at $T = T_m$ and $T = T_e$. The explosion process under consideration should be attributed to the fourth type in the classification of Zeldovich et al [26].

Increasing peak temperature to $T_m = 1400$ K ($\Delta T = 400$ K) as in Fig.3 we observe further decrease in shock overpressure to $\Delta p_e \approx 0.16$ MPa at the edge of the nonuniformity. A reaction front lags behind a shock and propagates in the mode of laminar flame. A shock wave may play the role of shock precursor which preconditions the mixture downstream a flame front.

Therefore the explosion processes of the third type may be expected. Explosion process of the third type was observed numerically in [23,26]. A secondary explosion downstream the flame front, amplification of a secondary shock wave and, finally, the onset of the C-J detonation were detected. The shock overpressure at the edge of a nonuniformity was about 0.1 MPa.

Fig.3 Time-dependent pressure profile in stoichiometric $H_2 - O_2$ mixture with a temperature nonuniformity: $T_m = 1400$ K; $T_e = 1000$ K, $p_o = 0.1$ MPa, $X_T = 1$ cm.

5. CONCLUSION

The detailed study of explosion dynamics in a nonuniformly preheated mixture confirms the classification of Zeldovich et al [26]. A coupling criterion (Eq.(4)) gives good estimates for predicting the range of parameters giving rise to spontaneous onset of severe explosion processes.
6. Acknowledgment

The author would like to express his thanks to Prof. P. Roth and Dipl.-Ing. A. Mack from the Duisburg University for their useful cooperation.

7. References