Auto-ignition in near-wall boundary layer as a cause of deflagration to detonation transition

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Presented is the detailed study of the effect of non-isentropic processes in the near-wall boundary layer on mixture auto-ignition behind a precursor shock wave during Deflagration to Detonation Transition. The spontaneous flame arising in the boundary layer has been shown to propagate at the velocity close to local sound velocity. In this case one can expect the strong coupling between the localized chemical energy release and the accompanying pressure waves. The concept under study can be used for understanding the phenomenon of ‘explosion in explosion’.

Introduction

Deflagration to detonation transition (DDT) in most gaseous combustible mixtures is known to take place in sufficiently long ducts. Despite extensive studies of the DDT phenomenon, universal theory is still lacking. Zel’dovich [1] was one of the pioneers in explaining DDT by shock-flame interaction. Manson [2] reported the results of thermodynamic calculations of flame and shock velocities pertaining to DDT. The limits of DDT were calculated within the framework of a simplified one-dimensional model ignoring the non-isentropic processes behind the shock wave [3].

Oppenheim [4] has demonstrated experimentally that the detonation wave arises suddenly after ‘explosion in explosion’ somewhere between the flame and the sequence of shock waves. So far, there has been no adequate quantitative explanation for the phenomenon of ‘explosion in explosion’. Experimental observations show that a localized explosion, if occurs, does not necessarily give rise to detonation. What conditions are then required for the onset of detonation? Oppenheim analyzed the thermodynamic parameters of the shock-compressed gas in multiple shocks under conditions pertaining to DDT. It has been found that the pressure $p$ and temperature $T$ of the critical particle (fluid particle located in the center of ‘explosion in explosion’, [4]) appear to be outside the explosion limits. Moreover, the induction time integral for the critical fluid particle
\[ I = \int_{\tau_0}^{p} \frac{d\tau}{\tau(p,T)} \]  

has been found to vary from $5 \cdot 10^{-4}$ to $4 \cdot 10^{-2}$, depending on the empirical formula used for steady state induction time $\tau(p,T)$. This implies that shock compression itself does not provide conditions favoring autoignition of the critical particle.

Wolański [5] has suggested possible explanation of 'explosion in explosion' based on the analysis of non-isentropic processes behind the leading shock. Kinetic energy dissipation at the duct wall can result in local temperature increase thus locally enhancing chemical energy release.

This paper reports a detailed study of the effect of the non-isentropic processes on mixture autoignition behind a shock wave. As a starting point, the laminar boundary layer behind a single shock wave is considered.

Formulation

Consider propagation of a single plane shock wave in a duct filled with a combustible gas mixture. The shock velocity is assumed to be constant. Fluid particles entering the wall boundary layer decelerate, and their temperature increases. Based on the known velocity distribution in the boundary layer, one can estimate the temperature profile using the energy conservation equation. Depending on the thermal boundary conditions at the duct wall, the temperature maximum can be reached at a finite distance from the wall, or at the wall itself if adiabatic conditions are specified. The difference in gas temperature drastically affects the autoignition induction process for fluid particles. The induction time is expected to depend on the distance from a fluid particle to the wall and differs considerably from the value found for the critical particle in [4].

The mathematical model for the effect under study is based on the following simplifying assumptions:

1. plane shock wave;
2. two-dimensional planar steady flow;
3. laminar boundary layer;
4. constant thermophysical properties;
5. adiabatic confinement;
6. negligible pre-ignition self-heating of combustible mixture, as compared with the temperature increase due to kinetic energy dissipation;
7. single-step chemical reaction.

In the coordinates attached to the shock, the gas velocity ahead of the shock is $D$, while behind the shock the free stream has the constant longitudinal velocity $U_\infty$ and a variable
transverse velocity component. The latter arises due to the curvature of a realistic shock wave and can be determined from the solution of the shock wave - boundary layer interaction problem [6]. The corresponding gas temperatures in the undisturbed and shocked free-stream gas are $T_0$ and $T_w$ where subscripts ‘0’ and ‘$\infty$’ denote the conditions prior and after shock arrival, respectively.

The profile of the longitudinal velocity $u$ has been found in [7] for a range of the shock Mach numbers. For a shock wave of moderate intensity, it can be approximated with a good accuracy, using the solutions obtained in [7], as a piece-linear function of coordinates: $u = u(x,y)$.

Then, the mass conservation equation

$$\frac{\partial}{\partial x}(pu) + \frac{\partial}{\partial x}(pv) = 0,$$  \hspace{1cm} (2)

yields the transversal velocity component $v$. The procedure outlined was used to calculate the flow velocity distribution.

Temperature was estimated using the Crocco integral for a compressible boundary layer. Under the conditions

$$\frac{dp}{dx} = 0, \hspace{1cm} Pr = 1, \hspace{1cm} \gamma = \text{const}, \hspace{1cm} \nu^2 \ll u^2,$$

the gas temperature at the wall is [8]

$$T = T_w \eta \left( 1 + \gamma r M^2 \frac{(\gamma - 1)(1 - w^2)}{2U^2} \right),$$  \hspace{1cm} (3)

where $U$ and $w$ denote the longitudinal velocity components of particle in the free stream and in the boundary layer, respectively, in the laboratory coordinate system, $M$ is the local Mach number of the shock-compressed gas, $\gamma$ is the specific heat ratio, $r$ is the temperature recovery coefficient, $\eta$ is the coefficient introduced for taking into account thermal boundary conditions at the duct wall, $Pr$ is the Prandtl number.

A 7% decrease in initial reactant concentration is introduced as a criterion for autoignition. This was found to correspond approximately to condition $I = 1$ (see equation (1)) for the kinetic parameters specified below. The equation for the reaction rate with the initial condition is

$$\frac{da}{dt} = -ka^2 \exp \left( -\frac{E}{RT} \right), \hspace{1cm} a(0) = 1,$$  \hspace{1cm} (4)

where $a = [A]/[A]_0$ denotes the dimensionless reactant concentration (e.g., the oxidizer), $k$ is the pre-exponential factor, $E$ is the activation energy, $R$ is the gas constant.

If the initial and boundary conditions are specified, one can obtain the histories of gas variables along the trajectory of a fixed gas particle and, finally, find the ignition location and induction time.
Results

The problem formulated above was solved numerically for a model combustible mixture with the following properties:

\[
\gamma = 1.36, \quad \nu = 10^{-5} \text{ m}^2/\text{s}, \quad E = 40 \text{ kcal/mole}, \quad k = 10^{10} \text{ s}^3, \quad \eta = 1, \quad r_i = 1, \\
p_0 = 10^5 \text{ Pa}, \quad T_0 = 300 \text{ K}, \quad \alpha_0 = 538.5 \text{ m/s}, \\
M_2 = 3.5, \quad U_\infty = 427 \text{ m/s}, \quad D = 1885 \text{ m/s}, \quad M = 1.53, \\
p_i = 14.3 \cdot 10^3 \text{ Pa}, \quad \rho_i = 2.15 \text{ kg/m}^3.
\]

Fig. 1. The trajectories of fluid particles 2 to 11 in the laminar boundary layer behind a shock wave of \( M = 3.5 \). Free stream particle 1 is located outside the plot scale. \( \delta \) is the thickness of the boundary layer. Dark circles show position of particle ignition.

Ten particles (particles 2 to 11) entering the boundary layer and a single particle (particle 1) moving in a free stream were examined. Table 1 shows the predicted particle parameters. Clearly, the induction time for particle 1 is larger than for particles 2–11. Note, that the transverse velocity in the post-shock gas affects considerably the particle induction process, despite the fact that \( \nu \ll \mu \). Particle trajectories are shown in figure 1, with particle ignition position marked by dark circles. Free stream particle 1 is located outside the plot scale.

Figures 2 and 3 show the plots of temperature and reactive species concentration versus distance to the shock wave. Particle 11 exhibits the largest rate of temperature increase and, therefore, ignites first. Ignition site of particle 1 is located outside the plot scale.
Fig. 2. The plots of temperature vs distance to the shock wave for 11 fluid particles. Dark circles show particle position and temperature at the moment of ignition.

Fig. 3. The plots of reactive species concentration vs distance to the shock wave for 11 fluid particles. Dark circles show particle position at the moment of ignition. Ignition criterion $\alpha_{ig} = 0.93$. 
Properties of particles entering the boundary layer.

<table>
<thead>
<tr>
<th>Particle No.</th>
<th>$y$ [m]</th>
<th>$\tau$ [s]</th>
<th>$x_{i0}$ [m]</th>
<th>$T_{i0}$ [K]</th>
<th>$a_i$ [m/s]</th>
<th>$K(\tau)$</th>
<th>$\omega_{i0}$ [m/s]</th>
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<tr>
<td>1</td>
<td>free stream</td>
<td>7.48 $\cdot$ 10^{-3}</td>
<td>3.190</td>
<td>966</td>
<td>952.7</td>
<td>1.00</td>
<td>–</td>
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<tr>
<td>2</td>
<td>12 $\cdot$ 10^{-3}</td>
<td>198 $\cdot$ 10^{-4}</td>
<td>0.141</td>
<td>1278</td>
<td>1096</td>
<td>0.87</td>
<td>419</td>
</tr>
<tr>
<td>3</td>
<td>11 $\cdot$ 10^{-3}</td>
<td>171 $\cdot$ 10^{-4}</td>
<td>0.126</td>
<td>1288</td>
<td>1100</td>
<td>0.88</td>
<td>556</td>
</tr>
<tr>
<td>4</td>
<td>10 $\cdot$ 10^{-3}</td>
<td>149 $\cdot$ 10^{-4}</td>
<td>0.113</td>
<td>1297</td>
<td>1104</td>
<td>0.89</td>
<td>591</td>
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<tr>
<td>5</td>
<td>9 $\cdot$ 10^{-3}</td>
<td>128 $\cdot$ 10^{-4}</td>
<td>0.100</td>
<td>1302</td>
<td>1106</td>
<td>0.88</td>
<td>619</td>
</tr>
<tr>
<td>6</td>
<td>8 $\cdot$ 10^{-3}</td>
<td>109 $\cdot$ 10^{-4}</td>
<td>0.088</td>
<td>1310</td>
<td>1109</td>
<td>0.88</td>
<td>631</td>
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<td>7</td>
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<td>12 $\cdot$ 10^{-3}</td>
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<td>1320</td>
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<td>0.89</td>
<td>556</td>
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<tr>
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<td>74 $\cdot$ 10^{-4}</td>
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<td>0.89</td>
<td>615</td>
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<tr>
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<td>0.041</td>
<td>1357</td>
<td>1129</td>
<td>0.89</td>
<td>727</td>
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</table>

Fig. 4. The dependence of the induction integral on time for 11 fluid particles. Dark circles show the values of the induction integral at the moment of particle ignition. Ignition criterion $\omega_{i0} = 0.93$

Figure 4 shows the dependence of induction integral (1) on time. Clearly, the ignition criterion $\omega_{i0} = 0.93$ results in induction integral close to 1 for all fluid particles under consideration. The predicted value of the induction time integral (1) for particle 1, taken at the moment of ignition of particle 10, is 5$\times$10^{-4}. It correlates, by the order of magnitude, with the respective data of [4] for a critical particle at the moment of its explosion. Thus, the boundary layer effect explains the discrepancy between the predictions of [4] and experimental findings.
Fig. 5. The predicted time-distance diagram for 11 fluid particles moving behind a shock wave of $M = 3.5$. Particle 1 represents free stream conditions. Particles 2 to 11 enter the near-wall laminar boundary layer at different height. Dark circles show time and position of particle ignition. Ignition site of particle 1 is located outside the plot scale.

Figure 5 shows the predicted time-distance diagram for 11 fluid particles. The line connecting dark circles will evidently represent the path of the spontaneous flame propagating in the post-shock flow.

Let us estimate the ratio $u_{sp}/a_l$, where $u_{sp}$ is the spontaneous flame velocity [8] and $a_l$ is the local sound velocity. The value of $u_{sp}$ can be approximated as

$$u_{sp} = \frac{1}{|\text{grad} \tau|} = \frac{\Delta \tau}{\Delta x}^{-1}.$$  \hspace{1cm} (5)

It follows from Table 1 that $u_{sp}/a_l$ is of the order of unity. This fact indicates that the amplification of pressure waves initiated by ignition events inside the boundary layer can occur by the Zel'dovich mechanism [9]. The Zel'dovich mechanism provides an explanation of the nature of strong shock or detonation waves onset [10] and, therefore, could be the reason for 'explosion in explosion'.

**Discussion**

A further improvement of the model should take into account the effects of transport processes on the fluid particle ignition, turbulent fluctuations in the boundary layer, and multiple shock compression.

Under non-adiabatic conditions, instead of eq. (3) one can use the similarity relation [2]

$$\frac{T_s - T_w}{T_{s,\infty} - T_w} = \frac{w}{U}$$  \hspace{1cm} (5)

$$\frac{T_s - T_w}{T_{s,\infty} - T_w} = \frac{w}{U}$$
where $T_s$ and $T_w$ are, respectively, the stagnation and wall temperature. The exact solution of [7] for the laminar boundary layer can be replaced by the $1/7$th power law for velocity distribution in the turbulent boundary layer (TBL), i.e.

$$\frac{w}{U} = \left(\frac{y}{\delta}\right)^{1/7} \quad (6)$$

where $\delta$ is the boundary layer thickness. The combination of Eqs. (5) and (6) allows one to obtain the profile of average static temperature in TBL, replacing Eq. (3). It can be shown that at $M > \sqrt{\frac{2}{\gamma-1}} \left(1 - \frac{T_w}{T_s}\right)$ the static temperature attains a maximum value inside TBL, which is dependent of $M$, $\gamma$, and $T_w$. Hence, non-isentropic processes are expected to effect ignition in TBL under non-adiabatic conditions.

The account of multiple shock compression of reactive mixture will evidently decrease the characteristic Mach number at which the effects under consideration become significant.

Conclusion

Kinetic energy dissipation in a compressible boundary layer behind a shock wave is shown to considerably affect autoignition of a reactive mixture. The particles entering a boundary layer have been shown to exhibit substantially shorter induction time than in the free stream, which provides the explanation for the discrepancies between simplified 1D simulations and experimental findings. The predicted spontaneous flame velocity has been shown to be close to the local sound velocity. According to the Zel'dovich mechanism, in this case one can expect the strong coupling between the localized chemical energy release and the accompanying pressure waves which can be used as a basis for the further studies of the ‘explosion in explosion’ phenomenon.

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References