Estimations of the Critical Conditions for Ignition, Deflagration-to-Detonation Transition and Detonation

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1 The initiation problem

Determination of critical initiation energy for detonation and combustion modes is the global problem from scientific and practical points of view (ecology and explosion safety). According to the current classification, a combustible mixture can be excited by three basic methods:
- weak initiation (or ignition) when only laminar burning is excited (with propagation velocities at the level of tens of centimeters per second);
- strong (direct) initiation when a self-sustained DW is formed quickly in an immediate vicinity of the initiator and then propagates over mixture with a velocity at the level of several kilometers per second;
- intermediate case where the mixture is ignited at the initial stage and then the flame front is accelerated owing to natural or artificial reasons up to velocities at the level of a hundred meters per second (visible velocity). Under certain conditions, even the deflagration-to-detonation transition (DDT) can occur.

In the latter case, the type of symmetry is of principal importance for the DDT: expanding (cylindrical or spherical) waves or quasi-plane waves (propagating in a straight tube). In expanding waves without any artificial effects, the main mechanism of acceleration is autoturbulization of the flame. The issue of the possibility of spontaneous DDT in expanding waves is still under discussion and has no clear experimental evidence. In addition to flame autoturbulization interaction with the side walls plays an important role for plane waves in tubes, and it is well known that the DDT is principally possible (especially for active fuel–oxygen mixtures).

The direct (strong) initiation of detonation wave (DW) in gaseous mixture and the spark initiation of combustion wave (CW) have some similar features: overdriven wave near the discharge filament, decaying of wave at removing from discharge kernel, the critical stage of self-initiation of mixture,… after which the detonation or combustion process is formed successfully or its are quenched. The forming of DW or CW is observed when the additional chemical energy release at self-initiation processes is sufficient to compensate the under-liberation of energy (from point of view of spatial and temporal factors). Using such similarity it can be proposed the uniform point of view on initiation of DW and CW.

2 The criterion of detonation initiation

The next criterion of the initiation of detonation process is offered: the critical initiation energy is equal to the work performed by the extending detonation products on path length equals to the characteristic size of multifront DW - longitudinal cell size $b$. Starting point is chosen to be equal to the diffraction radius of DW (which is the critical point of self-reinitiation process at DW-diffraction on right angle) in the moment of
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The collision of an axial rarefaction waves up to an axis of a gas charge. The formulas for the critical initiation energies for plane, cylindrical and spherical detonation waves are obtained.

\[
E_{\delta} = \int_{R_{\delta}+b}^{R_{\delta}+b} P_C J 4\pi r^2 dr = 4\pi P_C J [3R_0^3 b + 3R_0 b^2 + b^3] =
\]

\[
\rho_0 D_0^3 b^3 4\pi \pi C_J [2.4tg^2 \varphi (d_\delta / a)^2 + 2.7tg \varphi (d_\delta / a) + 1] / (\gamma_0 M_0^3) = B_1 \rho_0 D_0^3 b^3,
\]

\[
E_{2\delta} = \int_{R_{2\delta}+b}^{R_{2\delta}+b} P_C J 2\pi r dr = \pi P_C J [2R_0 b + b^2] =
\]

\[
\rho_0 D_0^3 b^2 \pi \pi C_J [1.8tg \varphi (l_\delta / a) + 1] / (\gamma_0 M_0^3) = B_2 \rho_0 D_0^3 b^2,
\]

\[
E_\mu = \int_{R_{\mu}}^{R_{\mu}} P_C J d r = P_C J b = \rho_0 D_0^3 b \pi \pi C_J / (\gamma_0 M_0^3) = B_3 \rho_0 D_0^3 b,
\]

where \( D_0 \) and \( M_0 \) - velocity and Mach number of Chapman-Jouguet (CJ) DW, \( \rho_0 \) and \( \gamma_0 \) - density and adiabatic index of an investigated mixture, \( R_{\delta} \) - the critical diffraction radius for different cases of symmetry, \( P_C J = \pi \pi C_J P_0 \) - pressure of DW-products, \( a = b \cdot tg \varphi \) - transverse size of a DW cell.

The common formula – \( E_{\varphi} = B_\varphi \rho_0 D_0^3 b^r \).

The calculating results are well correlated with experimental data. On Fig.1 the critical mass of HE-charge on \( H_2 \)-concentration is demonstrated for DW-initiation in \( H_2 \)-air mixtures: symbols – experimental data, solid and dashed lines (the model of multi-points initiation and formula of given paper) correspond to calculated data.

### 3 The criterion of ignition

The similar criterion of spark initiation of burning process is offered also: the critical burning energy is equal to the work performed by the extending combustion products on path length equals to the characteristic thickness of flame front. The starting point is chosen to be equal to the one half of the critical diameter \( d_\delta \) of combustion quenching (which is the critical point of self-reinitiation process of CW). The Peclet criteria for limiting combustion regimes \( Pe^{*}=d_q/b_{th}=\text{const}=65 \) was used for estimation, \( b_{th} \) – the characteristic thermal size of reaction zone of flame front. The next formulas for the critical initiation energies of combustion process for plane, cylindrical and spherical cases are proposed.

\[
E_{\varphi} = \int_{R_{\varphi}+b_{\delta}}^{R_{\varphi}+b_{\delta}} P_0 4\pi r^2 dr = 4/3 \cdot \pi P_0 [3/4 \cdot d_\varphi^2 b_{\delta} + 3/2 \cdot d_\varphi b_{\delta}^2 + b_{\delta}^3] \equiv \pi P_0 (Pe^{*})^3 b_{\delta}^3,
\]
The common formula is the next: \[ E_{n*} = R_v^\gamma P_0 (P_e^*)^{\gamma - 1} b_{th}^\gamma. \]

The calculating results (solid and dashed line for detonation and combustion critical initiation on Fig. 2) demonstrate the correlation with known experimental data (symbols). Figs. 1-2 are typical for another mixtures.

4 The DDT-criterion

In problems of explosion hazard of combustible systems, it is extremely important to model reliably the entire scenario of explosion evolution: ignition of the mixture and development of a low-velocity laminar flame, acceleration of burning owing to natural or artificial turbulization, subsequent formation of compression waves by an expanding flame and formation of the leading shock wave (SW), SW amplification, and an adiabatic flash in the compressed mixture, which leads (under favorable conditions) firstly to DW formation in the region of the compressed and heated gas and then, after the detonation wave catches up with the leading shock wave, to DW propagation over the initial mixture.

When the mixture is ignited, the flame-propagation velocity (normal burning velocity) is much lower than the maximal velocity of deflagration; hence, the final state of combustion products in the laminar flame front accurately corresponds to the combustion mode at a constant pressure.

Influence of compression waves before flame front leads to situation, when the initial state ahead of the flame front starts to move upward along the shock adiabatic line (more exactly, along Poisson’s adiabatic curve at low amplitudes of the waves), whereas the final state either remains almost unchanged or starts to move downward along the deflagration branch of adiabatic line for reaction products (with energy-release). The straight line connecting these new states, which was almost horizontal for the laminar flame, becomes inclined and its slope continues to increase. A moment will come with increasing SW intensity when this straight line will reach the point correspond to explosion in constant volume, which is the closest point of the transformation of the mixture from the initial state to adiabatic line with energy-release for the final reaction products. In this situation two solutions arise for the state at the shock adiabatic line: one corresponds to the combustion mode with the final state at the deflagration branch, and the other corresponds to the detonation mode with the final state at the detonation branch. Such a situation is assumed to be a necessary DDT condition in the present paper.

The equation for the shock adiabatic line (curve 1 in Fig. 3) can be written as

\[ \pi_1 = \frac{2\gamma}{\gamma + 1} \cdot \frac{2\sigma}{(\gamma + 1) - (\gamma - 1)\sigma} - \frac{\gamma - 1}{\gamma + 1}, \]

and the equation of the straight line (curve 2 in Fig. 3) passing through the points of states of instantaneous combustion in a constant volume (\( V = V_0 = \text{const} \)) and combustion at a constant pressure (\( P = P_0 = \text{const} \)) is

\[ \pi_{II} = \pi_V = \frac{\pi_V - 1}{1/\sigma - 1} (1/\sigma - 1), \]

\( (\pi = P/P_0, \sigma = \rho/\rho_0, \text{ and } \gamma \text{ is the ratio of specific heats}). \) The combined solution determines the point of intersection of these curves. This intersection point can be reached from the initial state with the help of an SW whose amplitude is determined by the relation
$M_{\text{min}}^2 = \frac{(\gamma + 1)\pi^* + (\gamma - 1)}{2\gamma} = \frac{\gamma + 1}{2\gamma} \cdot \pi V_0$, 

because $\pi^* = \pi V$.

The last relation allows one to estimate the minimum Mach number of the shock wave that converts the initial state of the mixture to this compressed state (curve 4 in Fig. 3) from which the initial mixture can equiprobably transform to reaction products either in the flame front or in the detonation wave (curve 3 in Fig. 3 is the Michelson straight line from the initial state to the Chapman–Jouguet state). Actually, this is the condition for the DDT, namely, the DDT for expanding waves. For waves propagating in a straight tube, the state at the intersection point $\pi^*$ can occur in the case of reflection from the wall, which corresponds to a different minimum SW amplitude for the DDT in a tube. The data for a number of known mixtures are listed in Table 1: velocity of sound in the initial mixture, pressure $P$ and degree of compression $\sigma$ for typical processes of deflagration and detonation (identified by the subscripts), and minimum Mach number for the DDT behind an incident ($M_{\text{inc}}$) and reflected ($M_{\text{ref}}$) waves. For all mixtures, fairly accurate values of the minimum Mach number are obtained: $M_{\text{min}} = 0.56M_0$ for expanding waves and $M_{\text{min}} = 0.33M_0$ for plane waves propagating in a constant-section straight tube ($M_0$ is the Mach number of an ideal Chapman–Jouguet wave).

<table>
<thead>
<tr>
<th>Mixture</th>
<th>$c_0$ m/s</th>
<th>$P_{\text{CJ}}$</th>
<th>$\sigma_{\text{CJ}}$</th>
<th>$P_{\text{V}}$</th>
<th>$\sigma_{\text{V}}$</th>
<th>$P_{\text{def}}$</th>
<th>$\sigma_{\text{def}}$</th>
<th>$\pi^*$</th>
<th>$M_{\text{inc}}$</th>
<th>$M_{\text{ref}}$</th>
<th>$M_{\text{CJ}}$</th>
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<tbody>
<tr>
<td>C2H2+2.5O2</td>
<td>330</td>
<td>33.83</td>
<td>1.84</td>
<td>17.07</td>
<td>0.07</td>
<td>0.48</td>
<td>0.036</td>
<td>18.2</td>
<td>3.95</td>
<td>2.1</td>
<td>7.34</td>
</tr>
<tr>
<td>C2H2+air (st)</td>
<td>347</td>
<td>19.11</td>
<td>1.82</td>
<td>9.77</td>
<td>0.12</td>
<td>0.48</td>
<td>0.062</td>
<td>10.6</td>
<td>3.05</td>
<td>1.8</td>
<td>5.38</td>
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<tr>
<td>C2H4+3O2</td>
<td>328</td>
<td>33.43</td>
<td>1.85</td>
<td>16.87</td>
<td>0.07</td>
<td>0.48</td>
<td>0.036</td>
<td>17.8</td>
<td>7.24</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2H4+air (st)</td>
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<td>18.35</td>
<td>1.81</td>
<td>9.38</td>
<td>0.12</td>
<td>0.48</td>
<td>0.064</td>
<td>10.1</td>
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<td>2H2+O2</td>
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<td>0.49</td>
<td>0.062</td>
<td>10.4</td>
<td>3.0</td>
<td>1.8</td>
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<td>0.15</td>
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<td>0.076</td>
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<td>CH4+2O2</td>
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<td>14.84</td>
<td>0.08</td>
<td>0.49</td>
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<tr>
<td>CH4+air (st)</td>
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<td>0.13</td>
<td>0.47</td>
<td>0.069</td>
<td>9.6</td>
<td>2.9</td>
<td>1.75</td>
<td>5.09</td>
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</table>

The parameters of the mixture were computed by the “SAFETY” Code.

5 Conclusions

The formulas for estimation of critical ignition energy and critical energy of detonation initiation were proposed. These formulas are based on the concept of critical layer of combustible mixture for excitation of combustion or detonation regimes. Also the estimation was proposed for the critical Mach number of the shock wave that can ensure the deflagration-to-detonation transition (DDT): $M_{\text{min}} = 0.56M_0$ for expanding waves and $M_{\text{min}} = 0.33M_0$ for plane waves propagating in a constant-section straight tube ($M_0$ is the Mach number of an ideal Chapman–Jouguet detonation wave). The condition $M > M_{\text{min}}$ ensures the DDT mode, whereas only laminar or turbulent burning without the DDT is observed for lower Mach numbers. The estimation is based on the equiprobable transition from the compressed state of the initial mixture both to the detonation and to the deflagration branch of the adiabat of reaction products (with respect to the initial state of the combustible mixture).

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