Chapter 6. Detonation

ON THE ZEL’DOVICH THEORY OF DETONABILITY LIMITS

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Zel’dovich theory of detonability limits proved still to be a basis for relevant studies of gaseous and multi-phase detonations. An analysis of existing theoretical approaches indicates that the dominant role in attaining detonability limits is played by kinetic energy dissipation which effects both convection and chemical energy release behind the detonation front. If the dissipation mechanism is weakly coupled with convection and chemistry, there should exist a continuous spectrum of detonation velocities. At strong coupling, detonability limits are to be manifested.

Introduction

In 1940, Ya. B. Zel’dovich has published the paper ‘To the Theory of Detonation Propagation in Gaseous Systems’ [1] which can be considered as the key stone for the modern theory of detonability limits.

Since the discovery of the detonation phenomenon by Berthelot and Vieille, it is known that a steady self-sustained propagation of detonation waves in tubes is possible only within a certain range of explosive mixture composition, i.e. between fuel-lean and excessively fuel-rich one. Marginal values of fuel concentration were referred to as ‘concentration limits of detonability’. It was found experimentally that the concentration limits are dependent of tube diameter, shape of tube cross section, characteristic pressure and temperature, as well as inert diluents. Moreover, the limits are affected by introduction of mechanical obstructions (e.g. wall roughness, dispersed particles) and additives exhibiting phase transition (e.g. water fog, film, or foam), by imposing electric fields, and even by elasticity of tube walls.

In the pre-Zel’dovich theories, the concentration limits of detonability were explained by increasingly incomplete burnout of explosive mixture in a detonation wave, resulting in sharp decrease in detonation propagation velocity at marginal fuel concentrations. Such theories were based on a concept of ‘available chemical time’ which was supposed to truncate chemical energy release in a detonation wave.

Zel’dovich was the first who has taken into consideration momentum and energy losses intrinsic to confined reactive flows. In his theory, concentration limits of detonability are attained due to competition between the rates of chemical energy release and losses. At the marginal fuel concentration losses prevail and chemical energy
release appears to be insufficient to support self-sustaining propagation of a detonation wave. In this theory, the ‘available chemical time’ arises naturally.

There are two principal points distinguishing the Zel’dovich theory. The first is that incomplete burnout of explosive mixture is caused by momentum and energy losses in the reaction zone. All these factors together contribute to decrease in the detonation velocity when approaching detonability limits. The second is that there exists a finite deficit of the detonation velocity at the limit. By other words, detonation velocity attains the lower limiting value rather than decreases continuously as could be expected from the early theories.

In [1], Zel’dovich considered momentum and energy losses due to skin friction at and heat transfer to the tube wall. The theory was later modified in [2–4] to incorporate realistic expressions for losses and cover the evolution of an explosive mixture from the initial state prior compression in a lead shock wave to the final state of stagnant and cooled combustion products. In [4–7], the theory was extended qualitatively to tubes with rough walls. It was shown that mechanical obstructions can significantly widen detonability limits due to transition from the bulk ignition and reaction mechanism in the detonation wave to the mechanism of reflection-induced localised ignition with further turbulent flame propagation [2]. Quantitative applications of the theory for tubes with smooth walls were undertaken in [8, 9] and for tubes with rough walls in [10].

A principal approach of Zel’dovich to the problem of detonability limits was used in [11, 12] where a theory is suggested which incorporates momentum losses due to divergence of reactive flow streamlines in the wall boundary layer behind a lead shock wave. Predictions provided by this theory [13] exhibit similar qualitative and quantitative features as those based on the original idea of Zel’dovich.

An interesting extension of the Zel’dovich theory was suggested in [14–16]. Instead of momentum and kinetic energy losses due to skin friction at tube walls, the authors of [14–16] consider bulk dissipation of turbulence behind the detonation front. Again, qualitative and quantitative results [16] are similar to those discussed above.

The theory is applicable to detonations of multi-phase systems exhibiting interphase exchange of mass, momentum and energy [10].

In general, when analysing the available quantitative results of theory applications, an interesting implication can be revealed. It appears that momentum losses play the dominant role in the theory. Analysis in [4, 10, 16] indicates that even in tubes with smooth walls the effect of skin friction is always more pronounced than that of heat transfer to the tube wall. For detonations in rough tubes heat losses can be neglected as compared with kinetic energy dissipation due to enhanced drag [4–6]. In theories [11–16] basically momentum loss is considered, however governed by different loss mechanisms. These observations imply that kinetic energy dissipation is responsible for detonability limit. In this paper, a simple substantiation to this fact is presented on the basis of 1-D conservation equations.
The Role of Kinetic Energy Dissipation

We will show that the kinetic energy dissipation in the reaction zone of a detonation wave results in the detonation velocity decrease. This factor can result in approaching detonability limit.

A simple form of the energy conservation equation for the flow behind the steady self-sustained detonation front propagating at the CJ detonation velocity $D_{CJ}$ is

$$h_2 - h_1 + \frac{u_2^2}{2} - \frac{u_1^2}{2} = q,$$

where $h$ is the static enthalpy, $u$ is the velocity in the frame of reference attached to the lead shock, $q$ is the chemical energy release, indices 1 and 2 correspond to the properties at the lead shock and at the CJ plane, respectively.

Equation (1) indicates that the chemical energy release is consumed to increase the static enthalpy and kinetic energy of the flow. Based on the strong shock approximation, it is easy to estimate the relative distribution of chemical energy release among those components:

$$\frac{h_2 - h_1}{q} = \frac{2(2 - \gamma)}{\gamma + 1},$$

$$\frac{u_2^2/2 - u_1^2/2}{q} = \frac{(\gamma - 1)(2\gamma - 1)}{\gamma + 1},$$

where $\gamma$ is the specific heat ratio (assumed constant).

Let us assume that a part of kinetic energy $\delta(u^2/2)$ is dissipated into heat. In terms of Eqs. (2) this can be written as

$$\frac{h_2' - h_1'}{q'} = \frac{2(2 - \gamma)}{\gamma + 1} + \Delta,$$

$$\frac{u_2'^2/2 - u_1'^2/2}{q'} = \frac{(\gamma - 1)(2\gamma - 1)}{\gamma + 1} - \Delta,$$

where prime denotes the disturbed solution, $\Delta = \delta(u^2/2)/q'$. As a result of such redistribution of energy, one can expect variation of parameters in the CJ-plane. First, we will show that the CJ-condition $u_2'/c_2' = 1$ does not exist any more at a given detonation velocity $D_{CJ}$ ($c_2$ is the sound velocity at the CJ-plane). Indeed, if $q' = q$, $h_1' = h_1$ and $u_1' = u_1$, the perturbed values of flow velocity and sound speed at the
CJ-plane are given by

\[ u'_2 = u_2 \sqrt{1 - \frac{\delta(u^2/2)}{u'_2/2}}, \]

\[ c'_2 = c_2 \sqrt{1 + \frac{(\gamma - 1)\delta(u^2/2)}{c'_2^2}}. \]

By definition \( u_2 = c_2 \), therefore Eq. (4) gives \( u'_2/c'_2 < 1 \). This means that the steady solution is violated. Since the disturbed flow becomes subsonic, the rarefaction wave enters the reaction zone and decreases the detonation velocity. Let us find the arising deficit in the detonation velocity. Introducing the normalised detonation velocity deficit as

\[ \sigma = \frac{D_{CJ}^2 - D'^2}{D_{CJ}^2} \]

and applying approximation of strong shock, we obtain the analogs of Eqs. (4):

\[ u'_2 = u_2 \sqrt{1 - \frac{\delta(u^2/2)}{u'_2/2} - \frac{\sigma(u^2/2)}{u'_2/2} \frac{(\gamma - 1)(2\gamma - 1)\Delta q}{\gamma + 1 \frac{u'_2/2}{u'_2/2}}}, \]

\[ c'_2 = c_2 \sqrt{1 + \frac{(\gamma - 1)\sigma h_1}{c'_2} - \frac{(\gamma - 1)(2 - \gamma)\Delta q}{\gamma + 1 \frac{c'_2^2}{c'_2^2}}}, \]

where \( \Delta q = q - q' \) is the energy loss due to incomplete burnout of mixture at the CJ-point. The CJ-condition \( u'_2/c'_2 = 1 \) is satisfied if

\[ \sigma = \frac{\gamma - 1}{2} \left[ \frac{\delta(u^2/2)}{u'_2/2} + \frac{\gamma(\gamma - 1)}{\gamma + 1 \frac{u'_2/2}{u'_2/2}} \right] \]

or, in terms of the detonation velocity:

\[ D' = D_{CJ} \sqrt{1 - \frac{(\gamma + 1)^2 \delta(u^2/2)}{\gamma - 1 \frac{D_{CJ}^2}{D_{CJ}^2}} - \frac{\gamma(\gamma - 1)}{\gamma + 1 \frac{D_{CJ}^2}{D_{CJ}^2}} \frac{\Delta q}{D_{CJ}^2}}. \]

Clearly, any mechanism of kinetic energy dissipation results in the detonation velocity deficit.

When deriving Eq. (6) we did not specify any particular function for the dissipation \( \delta(u^2/2) \). Clearly, if \( \delta(u^2/2) \) is decoupled from flow properties and the mechanism of chemical energy release is insensitive to decrease in the detonation velocity, then
theoretically, depending on dissipation, there exists a continuous spectrum of detonation velocities from $D_{CJ}$ to the sound velocity in the fresh mixture.

In this concern, detonation in rough tubes can be considered as an example with dissipation nearly decoupled from the flow. As is known [4–7], the ignition and reaction propagation mechanisms in this case are weakly sensitive to the detonation velocity. Therefore, the reaction zone lengths appear to be nearly insensitive to the latter. In addition, the rate of kinetic energy dissipation is determined by the drag coefficient of mechanical obstructions in a tube. In a wide range of flow Reynolds numbers, the drag coefficient is known to be constant and dependent only on obstructions shape.

Experimentally, by introducing mechanical obstructions, one can continuously diminish the detonation velocity in a specified mixture by a factor of 3 and even more (see, for example, relevant references in [10]).

If the mechanism of kinetic energy dissipation is significantly coupled with the flow, one can expect the existence of detonability limits. Below, we present a simple example to this.

Let us consider the case when kinetic energy dissipation is provided by skin friction at a smooth wall. It can be easily shown that for a tube of circular cross section in this case

$$\delta(u^2/2) \approx \frac{4(l/d)\tau_w}{\rho_0} = f(D'),$$

where $d$ is the tube diameter, $\rho_0$ is the initial density of the explosive mixture, $\tau_w$ is the mean shear stress in the reaction zone, $l$ is the reaction zone length. Clearly, the dissipation is strongly coupled with the flow, in particular due to dependence on the reaction zone length. Since the latter is exponentially dependent on temperature behind the lead shock, it appears that at a certain detonation velocity deficit Eq. (6) has no solution for $D'$ any more.

By taking into account the dependencies of all governing parameters on $D'$ we obtain the following equation for $D'$ instead of Eq. (6):

$$D'^2 = D_{CJ}^2 - \alpha \exp \left( \frac{\beta}{D'^2} \right)$$

(7)

where $\alpha$ is some algebraic function of $D'$, $\beta = (\gamma + 1)E/2(\gamma - 1)$ with $E$ being the reaction activation energy. The exponential term can be approximated in the form

$$\exp \left( \frac{\beta}{D'^2} \right) \approx \exp \left( \frac{\beta}{D_{CJ}^2} \right) \exp \left[ -\frac{\beta(D'^2 - D_{CJ}^2)}{D_{CJ}^4} \right]$$

which allows to rewrite Eq. (7) as follows

$$m = \phi \exp^m,$$

(8)

where $\phi = \beta \alpha \exp(\beta/D_{CJ}^2)/D_{CJ}^4$, and $m$ is the new variable $m = -\beta(D'^2 - D_{CJ}^2)/D_{CJ}^4$. Differentiating $m$ over $\phi$ gives

$$\frac{dm}{d\phi} = \frac{e^m}{1 - m},$$

$$m = \phi \exp^m,$$
and, obviously, \( m \) should be less than unity. The limiting value of \( D' \) in this case is given by condition \( m = 1 \), or

\[
D'^2 = D^2_{CJ} \left( 1 - \frac{2(\gamma - 1)D^2_{CJ}}{(\gamma + 1)^2 E} \right)
\]

Since \( 2(\gamma - 1)D^2_{CJ}/(\gamma + 1)^2 = RT_1 \), where \( R \) is the gas constant and \( T_1 \) is the temperature at the lead shock of CJ detonation, we come to the well-known Zel'dovich formula for the tolerable drop in the detonation velocity:

\[
\sigma = \frac{RT_1}{E}
\]

which can be written in a usual form after expanding in a series for large activation energy asymptotics

\[
\frac{D_{CJ} - D'}{D_{CJ}} = \frac{RT_1}{2E}.
\]

Similar solutions can be obtained for some other dissipation functions determined by momentum loss due to lateral expansions of the reaction zone and inert mass addition due to interphase mass transfer [17].

**Conclusion**

It is shown that the kinetic energy dissipation in the detonation wave can result in the detonation velocity decrease and attaining detonability limits. Depending on the mechanism of momentum loss (e.g., drag force, turbulence generation and dissipation, expansion, shock reflections, etc.) detonation velocity deficit differs. In principle, if the dissipation mechanism is weakly coupled with the flow (as is the case with detonations in rough tubes) the theory predicts a continuous spectrum of detonation velocities. In case of strong coupling between the kinetic energy dissipation and flow properties (as is the case with detonations in smooth tubes) there exists a finite tolerable drop in the detonation velocity manifesting detonability limit.

Of particular importance is to find out whether the above considerations are relevant to multi-dimensional nonideal detonations. Nowadays, people very often argue against 1-D theory. However, the application of 1-D theory always implies knowledge of combustion mechanism and the averaged momentum and energy loss. The paramount role is played, of course, by the adopted combustion mechanism. When 1-D model is applied with an inadequate combustion mechanism or doubtful expressions for momentum and energy loss, the predictions can be really poor. If, however, a researcher implements a well-founded model based on experimental evidences and findings from relevant multi-dimensional computations, the predictions can be improved significantly. In many cases of practical importance, the Zel'dovich theory of detonability limits proved to be the only available tool for engineering applications.
References


