Detonation velocity in poorly mixed gas mixtures

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Abstract. The technique for computation of the average velocity of plane detonation wave front in poorly mixed mixture of gaseous hydrocarbon fuel and oxygen is proposed. Here it is assumed that along the direction of detonation propagation the chemical composition of the mixture has periodic fluctuations caused, for example, by layered stratification of gas charge. The technique is based on the analysis of functional dependence of ideal (Chapman-Jouget) detonation velocity on mole fraction (with respect to molar concentration) of the fuel. It is shown that the average velocity of detonation can be significantly (by more than 10%) less than the velocity of ideal detonation. The dependence that permits to estimate the degree of mixing of gas mixture basing on the measurements of average detonation velocity is established.

1. Introduction

The velocity of detonation wave front is one of the most important and significant characteristic of explosive substance [1]. For explosive gases there are well-proven techniques (for example, described in [2]) for computation of parameters of steady-state ideal (without energy losses due to friction and heat exchange) detonation frequently called the Chapman-Jouget detonation [3]. The above-mentioned techniques are based on the assumption concerning chemical equilibrium of the composition of detonation combustion products (detonation products). The equilibrium computations are in good agreement with experimental data. Particularly, this concerns the velocity of detonation front \( D \) accurately measured in experiments.

The velocity of detonation \( D \) mainly depends on chemical composition of explosive gas constituting the mixture of gaseous fuel and oxidizer, which is usually oxygen or air. Taking into account only the value \( D \), it is easy to estimate the values of other parameters of detonation products such as pressure, density, mass velocity and sound velocity [4].

It is evident that the constancy of value \( D \) in practice is available only in case of ideal mixing of gas mixture. When detonation wave propagates in a poorly mixed mixture with fluctuations of chemical composition, it is properly to speak of the average velocity of detonation \( \bar{D} \) because the velocity of detonation front will also undergo fluctuations. The question to what extent \( \bar{D} \) may differ from the velocity of detonation \( D \) in ideally mixed mixture remains open.

Such a problem is of interest because it concerns explosion safety problems, development and modernization of different technical devices with detonation products as working material [5, 6]. In such devices with continuous or pulse (pulsating) operation, the explosive gas mixture is formed...
under conditions of flow supply of fuel and oxidizer through two independent channels. It is evident that this does not provide complete mixing of all mixture components.

To estimate the degree of mixing influence on detonation parameters, a simplified scheme of computations is proposed in [7]. The computations imply that the mixture with inhomogeneous chemical composition is the system of elementary volumes uniformly distributed in space. Each volume consists of three parts: ideally mixed mixture, pure fuel and pure oxidizer. Here, pure components do not take part in chemical reaction since they are inert gas. By the degree of mixing we mean the fraction of ideally mixed mixture \( \beta \) in elementary volume. By [7], the change of detonation velocity \( D \) of inhomogeneous-composition mixture from \( D_0 \) can be expressed in the form of approximation formula: \( D_\beta / D = \sqrt{\beta} \), where \( D \) is the detonation velocity in an ideally mixed mixture.

In [8], by using the same assumptions and more accurate equilibrium computations of detonation in mixtures based on hydrocarbon fuels for values \( \beta = 0.6 \pm 1 \), this dependence was refined: \( D_\beta / D = \beta^{0.295 \pm 0.005} \). However, as the author of this work points out, the model of poorly mixed mixture used in computation is somewhat artificial since the division of elementary volume of the mixture into three parts, which are enormously different in properties, is sufficiently rough. It is more correct to consider the model when the first part of elementary volume contains the mixture of given composition, the second part contains a somewhat fuel-enriched explosive mixture and the third one contains a somewhat lean explosive mixture.

2. Statement of the problem

Let a plane detonation wave propagate along the coordinate axis \( x \) over (in) the explosive mixture consisting of gaseous hydrocarbon fuel (denote it by \( C_yH_z \)) and oxygen \( O_2 \). The chemical composition of the mixture can be described as

\[
n C_yH_z + (1-n)O_2,
\]

where \( n \) is a mole fraction (a relative molar concentration) of fuel in the mixture. In the case when this mixture is stoichiometric, \( n \) will equal to the value \( n_{st} = 4/(4y + z + 4) \).

For mixtures of type (1), the technique detailed in [2] makes it possible to compute the velocity of ideal detonation \( D \) while \( 0 < n < n_{st} \), and the products of chemical reaction do not contain pure carbon C, i.e., when oxygen is still sufficient in the mixture to oxygenate C to carbon monoxide CO. It follows from (1) that the limiting value of the mole fraction of fuel is \( n_{max} = 2/(y + 2) \). Thus, in what follows we shall assume that within the interval \( 0 < n < n_{max} \), the functional dependence \( D = D(n) \) is known. Note that the detonation velocity \( D \) coincides with sound velocity in a pure oxidizer (in this case, oxygen) as \( n \to 0 \).

Suppose that the gas mixture is poorly mixed and there are periodic fluctuations of the mole fraction of fuel \( n \) along the axis \( x \). To describe the propagation of detonation wave in such a system, we divide the domain occupied by a gas mixture into elementary volumes located in sequence.

Let a longitudinal (along the axis \( x \)) dimension of these volumes be equal to \( L \) and coincide with spatial period of pulsations \( n \). Then to describe the propagation of the mole fraction of fuel \( n = n(x) \), it suffices to give this propagation inside one elementary volume. According to recommendations in [8], such a distribution can be represented as piecewise constant function

\[
n(x) = \begin{cases} 
(1 + \lambda)n, & \text{at } 0 \leq x < L/3 \\
n, & \text{at } L/3 \leq x < 2L/3 \\
(1 - \lambda)n, & \text{at } 2L/3 \leq x \leq L
\end{cases}
\]  

(2)

where dimensionless parameter \( \lambda \) \( (\lambda \geq 0) \) characterizes the amplitude of fluctuations of gas-mixture chemical composition. Thus, at \( \lambda = 0 \), the mixture will be assumed to be ideally mixed. It follows from (1) and (2) that fluctuations \( n \) must result in conformal changes of relative mole oxygen fraction
within the range from \((1-n-\lambda n)\) to \((1-n+\lambda n)\) inside the elementary volume. Note that (2) satisfies the condition
\[
\bar{n} = \frac{1}{L} \int_0^L n(x) dx = n,
\]
where \(\bar{n}\) is the average value of molar concentration of fuel inside the elementary volume and here deviations of \(n(x)\) with respect to \(n\) do not exceed the amplitude value \(\lambda n\) for the fluctuations of chemical composition.

Combining dependences (2) and \(D = D(n)\), for poorly mixed gas mixture \((\lambda > 0)\), it is possible to estimate the average detonation velocity \(\bar{D}\) at length \(L\) by using an evident relation:
\[
\frac{1}{\bar{D}} = \frac{1}{L} \int_0^L \frac{dx}{D}.
\]

When varying the mole fraction of fuel \(n\), such an approach permits to construct functional dependence \(\bar{D} = \bar{D}(n)\) within the interval \(0 < n < \bar{n}\), where \(\bar{n} = n/(1+\lambda)\). The latter relation is conditioned by the constraints of the used model since the value \(n\) must not exceed \(n_\ast\) at different degrees of mixing of gas mixture. However, these constraints are not so principal since it is always possible to use known results of detonation computations at \(n > n_\ast\) (see, for example, [9]) performed by using the computer program “Safety” [10].

3. Results of computations

The confirmation of estimate of \(\bar{D}\) is performed for detonation in fuel-oxygen mixture (FOM) based on methane \(nCH_4 + (1-n)O_2\) with spatial fluctuations of its chemical composition according to (2) under standard initial conditions: pressure is \(p_0 = 1\) atm and temperature is \(T_0 = 298.15\) K. For this mixture \(n_\ast = 1/3\) and the limiting value for the mole fraction of fuel is \(n_\ast = 2/3\).
The velocity of ideal detonation \( D \) (solid line) and the average velocity of detonation \( \overline{D} \) (dashed line) of poorly mixed mixture \( nCH_4 + (1-n)O_2 \) versus the mole fraction of methane \( n \) at different values of dimensionless parameter \( \lambda \): Curve 1 — \( \lambda = 0.1 \); 2 — \( \lambda = 0.2 \); 3 — \( \lambda = 0.3 \).

Figure 1 presents the computational dependences of ideal detonation velocity \( D = D(n) \) and average detonation velocity \( \overline{D} = \overline{D}(n) \) obtained by using (4) for different degrees of mixing of fuel and oxidizer. It is evident that at any value of the mole fraction of fuel \( n \) the average velocity of detonation (Curves 1-3) is less than the velocity of ideal detonation (shown by a solid line in the figure). At \( n < 0.3 \), the deviations of \( \overline{D} \) from \( D \) are slight (less than 1%) even in the case of relatively large fluctuations of chemical composition of mixture \( \lambda = 0.1 + 0.3 \). However, in the domain \( n_d < n < n_* \), the difference between \( \overline{D} \) and \( D \) becomes rather essential. This is due to the fact that within a specified range of molar concentrations of methane, function \( D(D(n)) \) behaves nonmonotonically and has a characteristic maximum approximately at \( n = 0.5 \) when the velocity of ideal detonation \( D \) reaches the value of 2635 m/s. Note that in the vicinity of the extremum of \( D \) (Curves 1-3) is less than the velocity of ideal detonation (shown by a solid line in the figure).

Table 1. Detonation velocity in poorly mixed gas mixtures

| Mixture              | \( n \) | \( D \), m/s | \( \overline{D}/D \) |
|----------------------|-------|-------------|-----------------|
| \( nCH_4 + (1-n)O_2 \) | 0.5   | 2635        | 0.997 0.989 0.974 0.954 0.923 0.886 |
| \( nC_3H_8 + (1-n)O_2 \) | 0.5   | 2934        | 0.998 0.967 0.949 0.930 0.913 0.890 |
| \( nC_4H_8 + (1-n)O_2 \) | 0.29  | 2609        | 0.999 0.995 0.989 0.979 0.967 0.953 |
| \( nC_4H_{10} + (1-n)O_2 \) | 0.23  | 2601        | 0.999 0.996 0.991 0.984 0.975 0.964 |

In practical use of FOM detonation, it is domain \( n_d < n < n_* \), where the nonmonotonical behavior of dependence \( D = D(n) \) is most pronounced, that is the most demanded. Therefore, the deficiency of detonation velocity \( \Delta D/D = 1 - \overline{D}/D \) observed in experiments may serve as a ground for the fact that the gas mixture is poorly mixed.

Figure 2 presents the computational results \( \Delta D/D \) depending on the amplitude of fluctuations of mole fuel fraction \( \lambda n \) for values \( n \) shown in the table. It is seen that computational data are well grouped near the curve (dashed line), which can be described by the approximation formula

\[
\Delta D/D = (1.5\lambda n)^{1.5}.
\]

Dependence (5) makes it possible to solve an inverse problem, namely: basing on the measurements of detonation velocity, to estimate the degree of mixing of mixture \( \overline{D} \) that can be defined as \( \overline{D} = 1 - \lambda n \).
Figure 2. The estimate of deficiency of detonation velocity $\Delta D/D$ versus the amplitude of fluctuations of mole fuel fraction $\lambda n$ for different FOMs. Points: 1 — mixture $nCH_4 + (1-n)O_2$; 2 — mixture $nC_2H_4 + (1-n)O_2$; 3 — mixture $nC_2H_6 + (1-n)O_2$; 4 — mixture $nC_4H_{10} + (1-n)O_2$. Dependence (5) is shown by a dashed line.

4. Conclusion
The influence of periodic chemical-composition fluctuations of different intensity degree on the average detonation velocity in poorly mixed oxygen explosive mixtures based on hydrocarbon fuels is numerically investigated. There exists a range of relative molar fuel concentrations, which admit considerable deviations (to the smaller side) of the value of such a velocity from the detonation velocity of ideally mixed mixture. This is due to the fact that the computational dependence of ideal detonation velocity on the mole fuel fraction behaves nonmonotonically and has a characteristic maximum. For poorly mixed gas mixtures, the approximation formula describing the correlation between the average detonation velocity and the amplitude of fluctuations of chemical composition is obtained.

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