Detonation onset in acetylene – oxygen mixture

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1 Abstract

Detonation of acetylene mixed with oxygen in various proportions is studied using mathematical modeling and experimental combustion chamber. Simplified kinetics of acetylene burning was compiled from various sources, it includes 11 reactions with 9 components. Defragration to detonation transition is obtained in a cylindrical tube with a portion of obstacles modeling Shchelkin spiral; the transition takes place in this portion for a wide range of initial mixture composition. Modified ka-omega turbulence model is used to simulate flame acceleration in the Shchelkin spiral portion of the system. The sizes of the detonation chamber and the turbulent spiral ring portion are similar to those used in the experiments. The results are compared with experiments and with theoretical data on Chapman – Jouguet detonation velocity.

2 Introduction and Problem Statement

Onset of detonation being very dangerous for classical RAM engines could, however, serve the basis for creating new generation of engines - pulse detonating engines (PDE) [1]. Thermodynamic efficiency of Chapmen-Jouget detonation as compared to other combustion modes is due to the minimal entropy of the exhaust jet. Based on this efforts have been made during the past several decades to show that proper utilization of the operation cycle does result in improved performance. However, there are several issues in developing this technology, which represent scientific and technological challenges. The success in resolving these problems will determine the implementation of pulse detonation propulsion [2].

The control of detonation onset is of major importance in pulse detonating devices. The advantages of detonation over constant pressure combustion bring to the necessity of promoting the deflagration to detonation transition (DDT) and shortening the pre-detonation length. For this issue the problems of detonation onset and deflagration to detonation transition should be simulated quite accurately, because these processes strongly depend on inlet conditions, mixture composition and geometrical characteristics of combustion chamber [3].

A scheme of the detonation chamber used in experiments [4] is shown on the fig. 1.

In our simulations, we did not calculate the process of filling the gas chamber with acetylene and oxygen, neither we regarded the nitrogen diluting the mixture. Instead, we regarded a fully premixed

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non-moving gas in the chamber, which consisted of the ignition portion, the spiral portion, and the tube portion. The whole system was closed, and had smooth internal walls, except for the spiral portion. We used the following sizes in our calculations:

D = 24.4 mm – diameter of the detonation chamber; L = 1240 mm – total length of the chamber;

 $L_{ign} = 100$ mm - length of the ignition portion; $L_{spir} = 300$ mm - length of the spiral portion.

The turbulent spiral ring had the following features: thickness 3.5 mm, pitch 7.1 mm, thus giving the blockage ratio of 49.8%, as in the experimental setup.



Figure 1. Detonation chamber used in experiments.

The ignition was simulated by introducing energy into a small portion of the system during a relatively short period; the location of the ignitor was at 70 mm from the left closed edge of the system (where the nitrogen valve is depicted on the fig. 1). Radius of the portion where the energy was introduced was 2

mm, and the energy flux was $2 \cdot 10^{11} W/m^3$ during $10^{-5} s$, resulting in about 64 mJ of ignition energy. The energy release was enough to ignite the mixture, but the corresponding shock was not intensive to lead to instant detonation setup. Therefore, the detonation was obtained each time via DDT process in the Shchelkin spiral portion of the chamber.

3 Mathematical Model

The gas dynamic model consists of the equations of mass balance of components, momentum balance, and energy balance. It is accomplished with 3 PDE for turbulent parameters, and multiple algebraic equations of state, of transport, of turbulent model, and of the kinetic model. The last describes mass transition between components in chemical processes, and the corresponding energy release and consumption.

The gas dynamic model is as follows:

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{u}) + \nabla \cdot \mathbf{I}_k = \mathbf{e}_k, \quad k = 1, \dots, N; \quad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p) = \nabla \cdot \boldsymbol{\tau}$$
(2)

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left(\rho E \mathbf{u} + p \mathbf{u}\right) + \nabla \cdot \mathbf{J} = \nabla \cdot \left(\mathbf{\tau} \cdot \mathbf{u}\right) + \boldsymbol{\mathcal{G}}$$
(3)

Here, ρ_k is partial density of k-th species (total N components in gas mixture), \mathbf{u} is the mean velocity vector, \mathbf{I}_k is the diffusion vector, $\boldsymbol{\mathscr{B}}_k$ is the rate of the species origination in chemical processes (mass per volume unit), ρ is density of the mixture, p is pressure, $\boldsymbol{\tau}$ is stresses tensor

deviator, \mathbf{J} is conductive energy flux, E is total energy including internal, kinetic and chemical parts. The last term $\mathbf{\Phi}$ is the intensity of external energy modeling the ignitor.

The gas dynamic model (1) – (3) includes the features from the turbulence model, in particular, the $(2 \circ K/2)$

spherical part of the turbulence stresses tensor, which is equal to $(-2\rho K/3)\mathbf{U}$ by definition, is being added to pressure (with an opposite sign). Also, the total energy includes an additional term: turbulent kinetic energy, which is equal to K.

The turbulence model includes 2 equations of the Wilcox ka-omega model [6], accomplished with the third equation modeling turbulent viscosity lag [5]. The model stands both for full-developed turbulence, and for the turbulence setup. The viscosity lag equation enables to better modeling of transient processes.

$$\frac{\partial \rho K}{\partial t} + \nabla \cdot \left(\rho K \mathbf{u}\right) = \nabla \cdot \left[\left(\mu + \sigma^* \mu_T\right) \nabla K\right] + P_T - \beta^* \rho K \omega_{;}$$
(4)

$$\frac{\partial \rho \omega}{\partial t} + \nabla \cdot \left(\rho \omega \mathbf{u}\right) = \nabla \cdot \left[\left(\mu + \sigma \mu_T\right) \nabla \omega\right] + \alpha \frac{\omega}{K} P_T - \beta \rho \omega^2; \qquad (5)$$

$$\frac{\partial \mu_T}{\partial t} + \nabla \cdot \left(\mu_T \mathbf{u} \right) = A \left(\rho \frac{K}{\omega} - \mu_T \right).$$
(6)

Here, K is kinetic energy of turbulence, μ is dynamic molecular viscosity of the mixture, μ_T is turbulent viscosity, P_T is turbulent production term, ω is turbulence dissipation rate; σ , σ^* , α , β , β^* and A are parameters of the model that either depend algebraically on flow parameters and turbulent Reynolds Re_T and Mach M_T numbers [6], or stay constant. Those turbulence model relations look as follows:

$$\beta^{*} = \frac{9}{100} \cdot \frac{1+680\chi_{k}^{2}}{1+400\chi_{k}^{2}} \cdot \frac{5/18 + (\text{Re}_{T}/8)^{4}}{1+(\text{Re}_{T}/8)^{4}} \left(1 + \frac{3}{2}F(M_{T})\right);$$

$$\alpha = \frac{13}{25} \cdot \frac{0.1 + \text{Re}_{T}/2.7}{1+\text{Re}_{T}/2.7} \cdot \frac{1+\text{Re}_{T}/6}{\beta/3 + \text{Re}_{T}/6};$$

$$\beta = \left(\frac{9}{125} - \frac{9}{100} \cdot \frac{5/18 + (\text{Re}_{T}/8)^{4}}{1+(\text{Re}_{T}/8)^{4}} \cdot \frac{3}{2}F(M_{T})\right) \cdot \frac{1+70\chi_{\omega}}{1+80\chi_{\omega}};$$

$$A_{T} = \frac{35}{100} \cdot \frac{0.01 + \text{Re}_{T}}{1+\text{Re}_{T}};$$

$$\sigma = \sigma^{*} = \frac{1}{2}, \quad \text{Re}_{T} = \frac{\rho K}{\omega \mu}, \quad M_{T}^{2} = \frac{2K}{a^{2}}, \quad F(M_{T}) = \max\left\{0, \left(M_{T}^{2} - 0.0625\right)\right\};$$

$$\chi_{k} = \max\left\{0; \frac{1}{\omega^{3}} \frac{\partial K}{\partial x_{j}} \frac{\partial \omega}{\partial x_{j}}\right\}, \quad \chi_{\omega} = \left|\frac{\Omega_{ij}\Omega_{jk}S_{ki}}{(0.09\omega)^{3}}\right|.$$
(7)

Here, S_{ij} are components of the deformation velocity tensor, and Ω_{ij} are components of the rotation tensor; both tensors are symmetric and antisymmetric parts of the velocity gradient. Diffusion and energy conduction are modeled in accordance with a Boussinesque turbulent model for fluxes

The initial conditions for gas dynamic equations stand for non-moving uniform gas mixture with low level of turbulence (zero turbulence is invalid in ka-omega turbulence model). The turbulence parameters initial state is determined by initial kinetic turbulent energy K_0 , and initial turbulent Reynolds number, which is in fact relation between steady-state eddy viscosity and molecular viscosity [8]. The boundary conditions stand for conditions on a smooth impermeable adiabatic wall with no adsorption of components and no catalytic reactions. This results in zero normal velocity component,

and zero normal gradient of temperature and mass shares of components at the wall. The conditions on tangential velocity component and on turbulent parameters are based on the theoretical profiles of those parameters in the vicinity of a smooth wall (so called wall laws) [9]:

The heat capacity at constant pressure, and enthalpy, and entropy of the gas mixture are calculated on the basis of their values for components dependent on temperature T, and partial molar density of each \mathbf{V}

component X_k . The viscosity mixture depends of species concentrations X_k and components viscosity $\mu_k(T)$ non-linearly [9].

The full kinetic model of acetylene consists of hundreds of reactions with hundreds of components. On the other hand, acetylene is a high-energetic fuel, and the mixture must contain radical components. We composed a short kinetic mechanism from various sources. It consists of the following parts.

1. Acetylene oxidation. The reaction governing the decay of acetylene is set as [10] proposed: $C2H2+O2 \rightarrow 2CO+2H$, but its kinetics is changed as to fit with the experimental results [11],

which read: $C2H2 + O2 \rightarrow products$; with overall intensity coefficient $k = 4.6 \cdot 10^{15} T^{-0.54} \exp(-45000/RT)[C2h2][O2]$

2. CO oxidizing as in Watanabe – Otaka model [12] as described in [13], with 2 changes: reversibility of CO oxiation, and no hydrogen oxidation (because it is deetailed further):

 $CO + 0.5O2 \rightleftharpoons CO2$ $k = 3.98 \cdot 10^{14} \exp(-40000/RT)[CO][O2]^{0.25}[H2O]^{0.5}$

 $CO + H_2O \rightleftharpoons CO_2 + H_2$ $k = 2.75 \cdot 10^{12} \exp(-20000/RT)[CO][H_2O]$

3. Hydrogen, and short radicals exchange and recombination kinetics is taken from Maas & Pope work [14]. Exchange:

 $H + O2 \rightleftharpoons OH + O$ $k = 2.00 \cdot 10^{14} \exp(-8455/T)[H][O2]$

 $O + H_2 \rightleftharpoons OH + H$ $k = 5.06 \cdot 10^4 T^{2.67} \exp(-3163/T)[O][H_2]$

 $OH + H2 \rightleftharpoons H2O + H$ $k = 1.00 \cdot 10^8 T^{1.6} \exp(-1660/T)[OH][H2]$

 $2OH \rightleftharpoons H2O + O_{k} k = 1.50 \cdot 10^{9} T^{1.14} \exp(-48.1/T) [OH]^{2}$

Recombination/dissociation:

 $2H + M \rightleftharpoons H2 + M$, $k = 1.80 \cdot 10^{18} T^{-1} [H]^2 [M]$

$$2O + M \rightleftharpoons O2 + M$$
 $k = 2.90 \cdot 10^{17} T^{-1}[O]^2[M]$

 $H + OH + M \rightleftharpoons H_2O + M$, $k = 2.20 \cdot 10^{22} T^{-1}[H][OH][M] (cm, mol, K)$.

4. Another recombination/dissociation reaction, which accelerate water vapor release is taken from [15]: $O + H + M \rightleftharpoons OH + M$ $k = 4.71 \cdot 10^{18} T^{-1} [H] [O] [M]$ (cm, mol, K).

The third-body component in recombination and dissociation reactions is based on Chaperon coefficients from [16]:

[M] = 6.5[H2O] + 0.4[O2] + 0.4[N2] + 0.75[CO] + 1.5[CO2] + 3.0[C2H2] + 1.0[others]

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4 **Results**

Fig.2 shows details of detonation onset in the spiral region for the mixture with equivalence ratio 2.5. This mixture composition corresponds to maximal value of Chapman Jouget detonation velocity. Shown spiral portion from 200 to 300 mm from the left edge (the spiral size from 100 to 400 mm) Upper part of each color map: pressure field, lower part: concentration of CO2, this parameter traces the flame front fairly because its concentration grows higher as the cold mixture ignites but then the carbon monoxide decomposes into CO+O2 due to high temperature behind the flame front.

As the flame propagates, the pressure grows in the system, and the flame accelerates. The pressure field shows numerous shocks produced by the spiral elements. Transfer to detonation takes place between 0.838 and 0.848 ms after local explosion between the rings near the wall in the vicinity of the axis of the system, after the flame consumes the unburned portion of gas seen in this location at 0.838 ms. First the shape of the detonation wave is almost hemi-spherical (0.848 ms), then it flattens (0.857 ms). The level of pressure behind the wave is above 20 bars.



Figure 2. Numerical simulation of detonation onset in the spiral section of the tube. Upper part of each color map: pressure field, lower part: concentration of CO2.

It is seen from Fig. 3 that for lean mixtures (lower equivalence ratio) the flame velocity in short tube is higher in cases when the calculated curve does not correspond to detonation but traces accelerated deflagration. Flame velocity here is taken as average on the base of 500 - 800 mm from the system left edge. The flame velocity shown on the figure in case of detonation is calculated as in the experiments; by time difference between rapid pressure increase at 600 and 700 mm locations from the left edge of the system. Numerical simulations show maximal velocity in the range of equivalence ratios from 1.0 up to 3.0.



Figure 3. Combustion wave velocity variation versus mixture equivalence ratio: simulations, experiments and C-J detonation.

Deflagration to detonation transition in acetylene mixed with oxygen in various proportions is obtained in a cylindrical tube with a section of obstacles modeling Shchelkin spiral both experimentally and in numerical simulations. Numerical simulation showed that detonation onset takes place in the unburned pocket of gas surrounded by hot reaction products as soon as ignition occurs in this pocket.

Depending on the mixture equivalence ratio different deflagration to detonation transition scenarios happened. For mixture equivalence ratios $1.0 < \phi < 2.5$, onset of detonation took place in the zone of obstacles, and then the detonation wave propagated along the tube. For lean mixtures accelerated turbulent flame was observed. For rich mixtures ($\phi \approx 4.0$) a galloping combustion regime was observed, which resulted the onset of detonation in longer tube, while in a shorter one it did not take place due to predetonation distance limitation.

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