Three-dimensional simulation of combustion, detonation and deflagration to detonation transition processes

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Abstract. The paper presents results of numerical and experimental investigation of mixture ignition and detonation onset in shock wave reflected from inside a wedge. Contrary to existing opinion of shock wave focusing being the mechanism for detonation onset in reflection from a wedge or cone, it was demonstrated that along with the main scenario there exists a transient one, under which focusing causes ignition and successive flame acceleration bringing to detonation onset far behind the reflected shock wave. Several different flow scenarios manifest in reflection of shock waves all being dependent on incident shock wave intensity: reflecting of shock wave with lagging behind combustion zone, formation of detonation wave in reflection and focusing, and intermediate transient regimes. Comparison of numerical and experimental results made it possible to validate the developed 3-D transient mathematical model of chemically reacting gas mixture flows incorporating hydrogen – air mixtures.

1 Introduction

Self-sustaining waves can propagate in meta-stable media; energy needed to support such waves is released by the wave itself. As a rule, two regimes of propagation exist, subsonic and supersonic; the difference is based on the different mechanisms of medium activation. Processes of transition between those regimes are less studied up to now, in comparison with pure subsonic or supersonic modes. Control of detonation onset is necessary in perspective pulse detonation engines using hydrogen-air mixtures in the working cycle, which are under development now. In our studies we'll use hydrogen fuel because, on one hand, it is a very perspective fuel making the engine exhaust much cleaner than that for hydrocarbon combustion [1,2], and on the other hand, chemical kinetics for hydrogen – air mixtures combustion are well developed [3-8]. The advantages of a constant volume combustion cycle as compared to constant pressure combustion in terms of thermodynamic

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efficiency has focused the search for advanced propulsion on detonation engines [9-10]. The thermodynamic efficiency of Chapman – Jouguet detonation as compared with slow combustion modes is due to the minimal entropy of the exhaust jet [10]. The present investigation is focused on initiation of detonation within limited in size spatial structures by relatively weak initiators using advantage of shock waves focusing and energy cumulation.

2 Mathematical model

The mathematical model for simulations of multi-component gas dynamics with chemical reactions including transport phenomena effects and turbulence was described in details in [11]. It contains the species mass, momentum and energy variation equations, which account for turbulent fluxes based on two-equation turbulence model of Wilcox k-omega [12].

$$\frac{\partial \rho_k}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho_k u_j - J_{kj}\right) = \dot{\omega}_k \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} \quad (2)$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}\left((E + p)u_j - J_{Q,j}\right) = \frac{\partial u_i \tau_{ij}}{\partial x_j} \quad (3)$$

In equations Eq.(1) – (3), index k takes values 1 … N_C (number of components), and indices i,j – values 1, 2, 3 (number of dimensions); repeated indices presume summation. In total, there are N_C +4 differential equations in the set. There is summation upon the repeating indices in Eq. (1) – (3).

Differential equations (1) – (3) are complemented with algebraic relations and algebraic representations for chemical and mass and energy sources [12].

Explicit second-order in space and time method based on the MUSCL-interpolation of variables on a face at a convective flux calculation. Interpolation direction choice and pressure interpolation were performed by means of AUSMP method. The method was implemented on a regular grid containing equal elements (rectangular parallelepipeds) connected generally in arbitrary topology. The source code was written in C. Parallel execution support was implemented using OpenMP library.

3 Results of numerical simulations

The problem simulating processes in the final section of the cylindrical shock tube was regarded. The geometry and size of computational domain coincides with that in the shock tube used in experiments. The shock tube diameter was 2R=76 mm, length – L=720 mm. (Fig. 1).

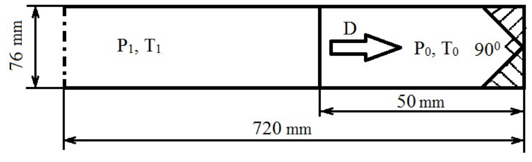

Fig. 1. Scheme of computational domain, initial and boundary conditions.

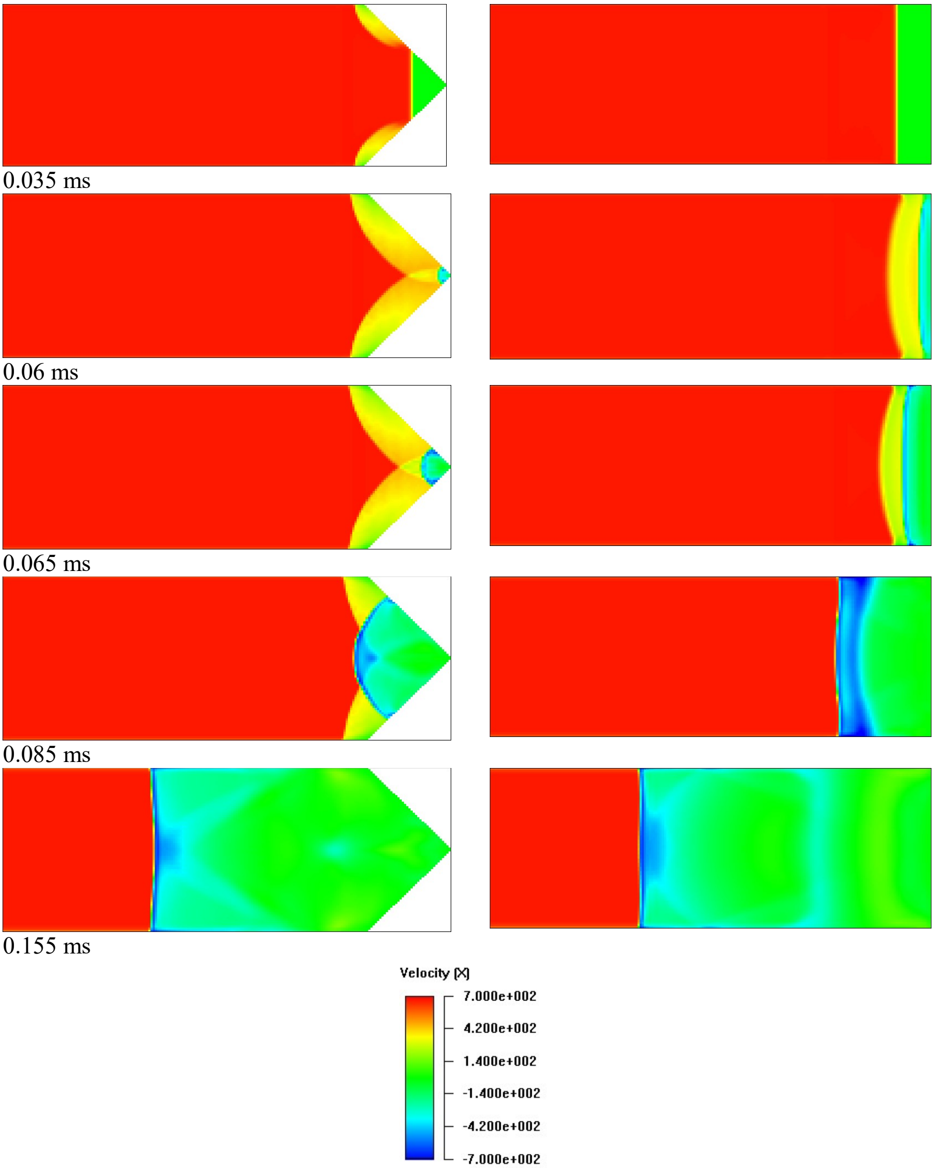

Fig. 2. Axial velocity fields in (m/s) on focusing of a strong shock wave and detonation onset in reflection from a wedge surface. Meridian cross-sections Oxy (left) and Oxz (right).

At time 0.065 ms onset of detonation is observed in the tip of the wedge. Then detonation wave propagates outside the wedge. Temperature maps in Oxy and Oxz planes testify that the burnt gas has temperature 1600 – 2000 K. For smaller intensity of incident shock wave its focusing in reflection from a wedge does not bring to immediate formation of detonation wave but it could cause mixture ignition and flame propagation. A transient regime is possible, characterized by formation of a leading reflected shock wave and flame zone lagging behind it. Then acceleration of the flame could bring to onset of detonation.

Fig. 3 illustrates successive stages of the process of deflagration to detonation transition after reflecting of shock wave from a wedge

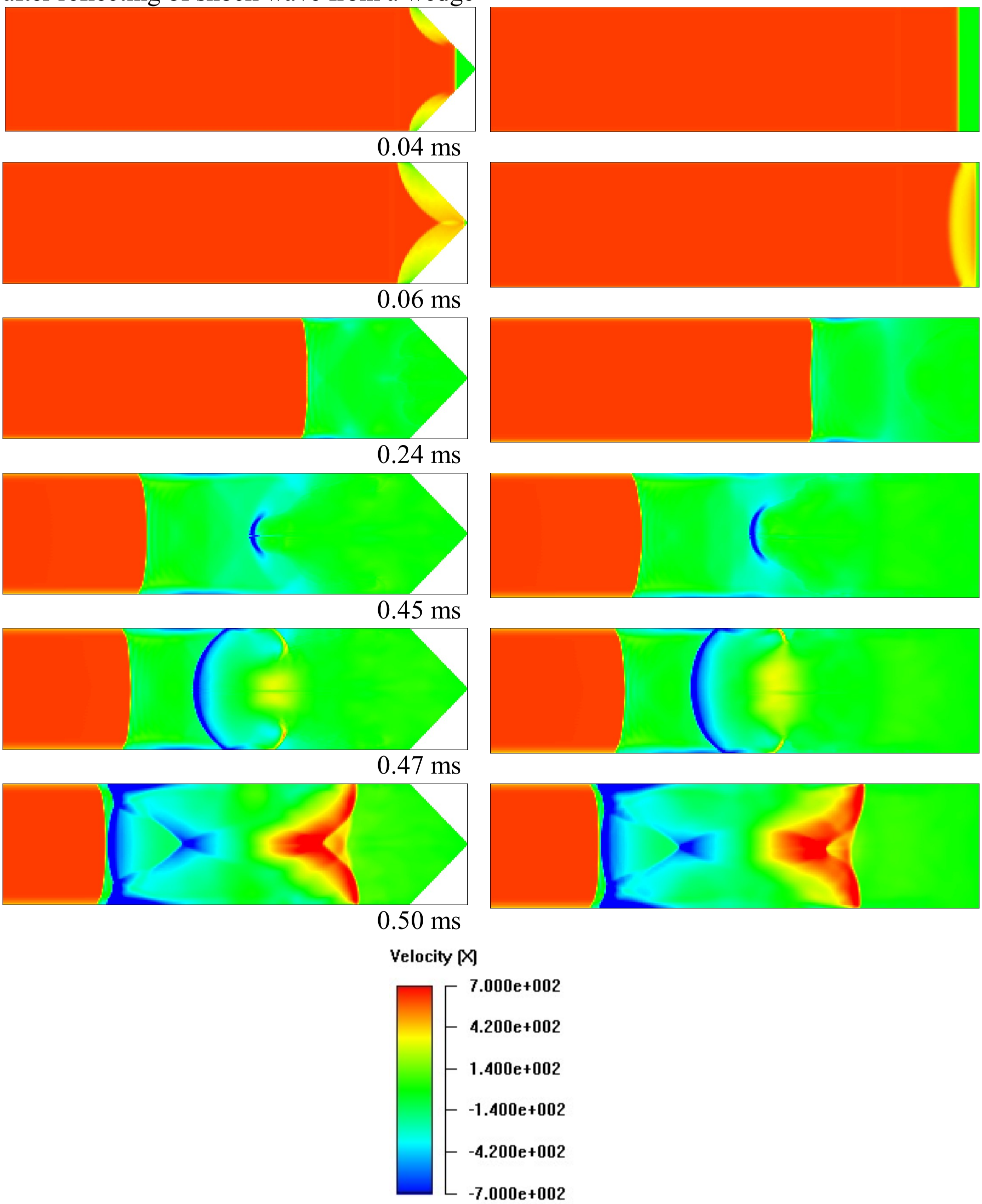

Fig. 3. Axial velocity fields in (m/s) on focusing of a weak shock wave and deflagration to detonation transition in reflection from a wedge surface. Meridian cross-sections Oxy (left) and Oxz (right).

Velocity field in the Fig. 3 testifies that on reflection of shock wave from the wedge surface cumulative effect is not strong enough for the onset of detonation wave. Shock wave is reflected. Ignition of mixture in the tip takes place later, and accelerated flame moving in pre-compressed and non-uniformly heated gas in the long run gives birth to local explosion and formation of detonation and retonation waves. Velocity field makes it possible distinguishing between detonation and retonation waves due to positive and negative velocities being depicted in different colours.

4 Conclusions

It was demonstrated that onset of detonation due to focusing of a strong shock wave takes place via an overdriven detonation mode. Then detonation wave slows down to a self-sustaining mode.

The transient regime has the following characteristic stages. First, at the tip of the wedge in the center a hot spot appears, which later increases rapidly in all directions, nevertheless lagging behind the reflected shock wave. Combustion wave is thus formed. Second, the combustion zone grows the leading front being unstable. Wrinkles are formed on the leading front, which is noticeable especially in the plane orthogonal to wedge. Third, velocity of combustion wave drastically increases, especially in the wrinkled zone, the wrinkles become deeper. Forth, the zone grows near the axis, which testifies formation "explosion in the explosion" and onset of detonation wave. The detonation wave begins reflecting from side walls of the cylinder and further propagate as detonation and retonation waves in all directions.

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