Detailed Study on the Structure near Hot Spots in Hydrogen-Air Detonation

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Abstract

The structure of the gaseous detonation is measured experimentally and its characteristics have been calculated from the development of computational fluid dynamics. The governing equations are two-dimensional Euler equations including the conservation of mass with 9 species. A model for nineteen forward- and backward- elementary reactions is used to explain the detail structure of hydrogen-air detonation for both the reliability evaluation of numerical analysis and review of the experimental results. A detonation tube with a square section is used. It is shown in the numerical analysis that the irregularity of cell structure appears due to a long induction length behind the incident shock. This long induction length comes out because the reaction region interacts with the shock front. As for this interaction, the rapid local explosion of unreacted gas pokets creates the jet flow,which influences the propagation mechanism of detonation.

Introduction

There have been many numerical and experimental studies related with the detailed structure of the detonation . As for the experiment, the understanding of the detonation wave structure has been extensively studied for more than thirty years by Oppenheim and Soloukhin[1] , Lee [2] etc, while in the numerical analysis, the detailed structure of detonation wave has been calculated recently by Taki and Fujiwara[3],Oran et al.[4] [5] . A process to be an irreglar structure in the detonation wave front is also confirmed numerically by Jones et al. [6] [7] and Bourlioux and Majda [8] ,etc. Hydrogen-air detonations with the irregular cell structure have been observed in details in our and other experiments.

In the present study, unsteady two-dimenstional numerical simulation of detonation using a detailed chemical reaction model is performed together with the basic experiment of hydrogen-air detonation. Both results are compared based on the fundamental characteristics of detonation. The detailed structure around the hot spots near the triple points collision is examined thoroughly.

Experiment

The detonation tube is about 3.5 m in length with a rectangular section of 40 mm× 40 mm. Four pressure sensors are installed on the tube wall to measure pressure and propagating speed . A soot pattern is obtained on the separatable wall where methacrylic resins (PMMA) are burned for coating.

Experiments are carried out at the equivalence ratios of 0.7-1.5 for the premixed hydrogen-air mixture, the atmospheric pressure and the room temperature. An experimental apparatus is shown in Fig.1.

Numerical Simulation

To derive the governing equations, the following assumptions are made to simplify the problem: 1) The species considered here are H_2 , O_2 , O , H , OH , HO_2 , H_2O_2 , H_2O as reacting species and N_2 as a diluent; 2) The specific heat of each species is a polynomial of temperature and the equation of state for ideal gas is used. 3) Bulk viscosity, Soret effect, Dufour effect and diffusion due to the pressure gradient are neglected and also viscosity is neglected.

On the basis of these assumptions, we derive the two-dimensional non-steady and compressible Euler equations as the governing equations which includes the conservation of mass of each species.

A nineteen elementary forward- and backward- reactions developed by Hishida[9] is adopted. The forward reaction rates are given by the modified Arrhenius form and backward reaction rates constants are calculated using the forward reaction rates and the equilibrium constants from the JANAF table[10].

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}=S$$

U : Conservative vector F , G : Convective terms S : Source term

Numerical method

The governing equations are solved semi-implicitly using the second-order Harten-Yee non-MUSCL modified-flux type TVD-upwind scheme for the convective terms and the Crank-Nicholson type implicit scheme for the source terms.

The present simulation deals with the finite difference method on a Cartesian grid system of 200(dx=0.01 mm) × 100(dy=0.03 mm) grid points. Therefore the size of the computational area is 2 mm× 3 mm. In order to simulate a detonation wave front, a moving grid coordinate system is applied for the numerical system. In order to obtain a numerical smoked foil record, a fixed coordinate system of 1200 points in the propagating direction (dx=0.01 mm) is used to calculate the maximum pressure for scratching the smoked foil on each grid point.

The boundary conditions are : 1) adiabatic, slip, and non-catalytic on the wall , 2) an inflow unburned mixture, and 3) an outflow burned mixture.

To obtain an initial 2D-detonation profile including cellular structures, we first calculate the one-dimensional detonation for the same system of equations as the 2-D one and the 1D-detonation profile is verlaid onto the 2D-grids, The 2D self-sustaining detonation with cellular structures is obtained by giving the artificial disturbances on the detonation front. The schematic figure for the start of 2D calculation is shown in Fig.2.

Results and discussions

The experimental result of smoked foil record(.=1.0) is shown in Fig.3, where the strong and weak traces are seen in the course of the triple points and the straight jet-like traces are observed in the propagating direction from the position of triple point collision.

Figure 4 is a smoked foil record in the present two-dimensional simulation, where the dark region is at the pressure of below 2.6 MPa. The trace made by the jet due to an explosion near the triple point collision is also confirmed in the numerical result. Fig 5 is a maximum pressure history of detonation front in the numerical results. The figure is rewritten for the pressure history from Fig.4. Pressures near the triple point collisions are very high when the jets appear in the propagating direction.

A time sequence of detonation front propagation is shown in Fig.6. Unreacted gas pockets are trapped behind the incident shock just before the triple point collision occurs during the period between t=0 and 0.18.s and cause a local explosion during the period between t=0.18 and t=0.27.s. Due to this explosion, the pressure waves propagate spherically to a region between the pressure wave and mach stem. Then, the spherical propagetion of mach stem is seen. In the velocity vector, the jet flows to both the propagating and the oppsite direction by a local explosion are seen at the central part of unreacted gas pockets. Due to the jet flow, a pair of the vortex is formed behind the mach stem. Therefore, the central part of the mach stem is pushed out further. As a result, the incident shocks on the both sides of the mach stem is bent; temperature behind the incident shock decreases, and its induction region becomes longer. The unreacted gas pockets which appear again are trapped and cause another local explosion. When the unreacted gas pockets behind incident shock are large, a strong explosion occurs and the mach stem propagetes straight at a faster speed.(0.27-0.36.s) Then, a triple point collides quickly to form an incident shock again. However,since small unreacted gas pockets appear at this time, the next explosion becomes weaker.(0.48.s) Then, the following mach stem propagates relatively slow with its curved shape and large unreacted gas pockets are formed again. Then, the next explosion becomes stronger. By repeating this process, a high pressure and low pressure region through triple point collisions come out alternatively. This is one of the explanations for the irregularity of the detonation cell structure.

Figures 7 and 8 are the enlargement of Figs.3 and 5. The strong traces are confirmed in the first half part of the cell structure formed due to the propagation of the mach stem. Furthermore, the low pressure region exists in the central section. This is because the jet flow occurs from the formation of the vortex around the central section behind the mach stem due to the interaction of the reflected shock with the explosion of the unreacted gas pockets.

Conclusion

The following becomes clear as a result of experiments and numerical simulations on the irregular cell structure of hydrogen-air detonation.

- The unreacted gas pockets formed behind the incident shock are trapped in the hot region to cause local explosions.
- Vortices are formed behind the mach stem due to the interaction between the pressure wave from the explosion and the reflected shock, then the mach stem propagetes spherically.
- The propageting patern of the mach stem depends on the size in the explosion of the unreacted gas pockets, which causes the irregularity of the cell structure.
- The straight jet in the cell patern influences the interaction between the preceding shock front and its hot region to produce vortices.

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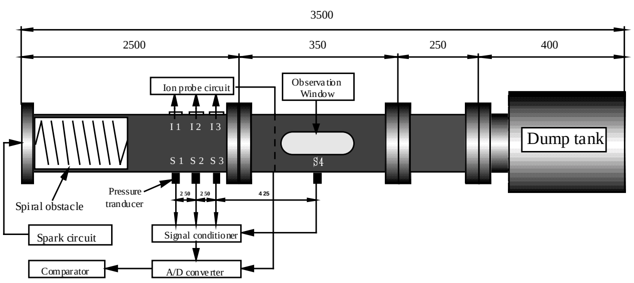

Fig.1 Experimental set-up

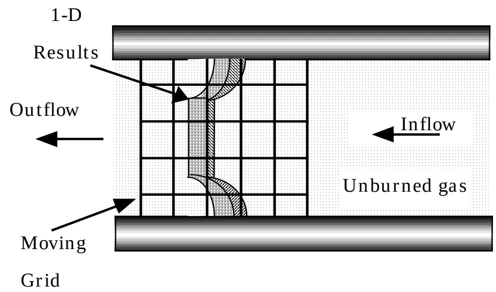

Fig.2 Schematic of the two-dimensional grid image used in the detonation simulation.

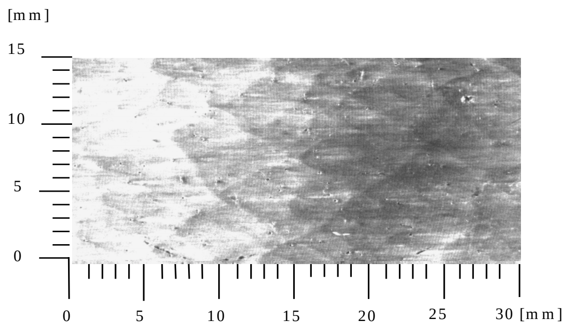

Fig.3 Smoked foil resords in the experimental result at the hydrogen-air mixture, . of 1.0 , initial pressure,P_0 of 1atm, initial temperature,T_0 of 298 K.

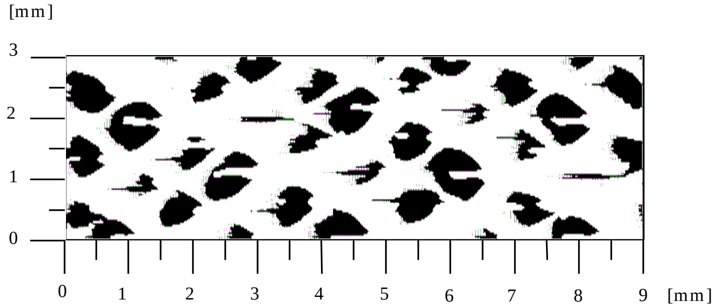

Fig.4 Smoked foil records in numerical result at the hydrogen-air mixture, . of 1.0, initial pressure,P_0 of 1atm, initial temperature,T_0 of 298.15 K, and minimum pressure,P_{min} of 2.6 MPa.

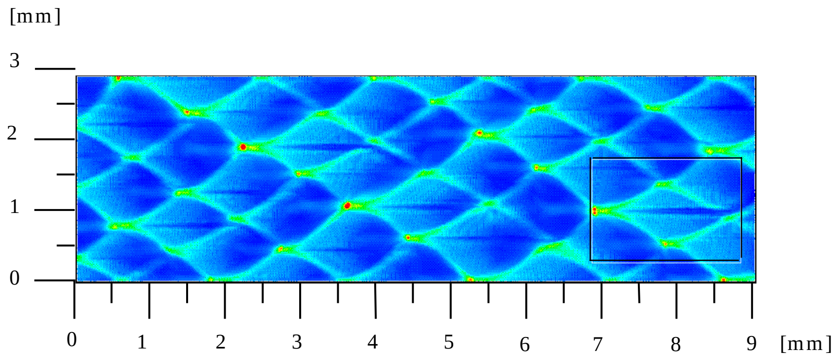

Fig.5 Maximum pressure history in numerical result at the hydrogen-air mixture, . of 1.0, initial pressure,P_0 of 1atm , initial temperature,T_0 of 298.15 K

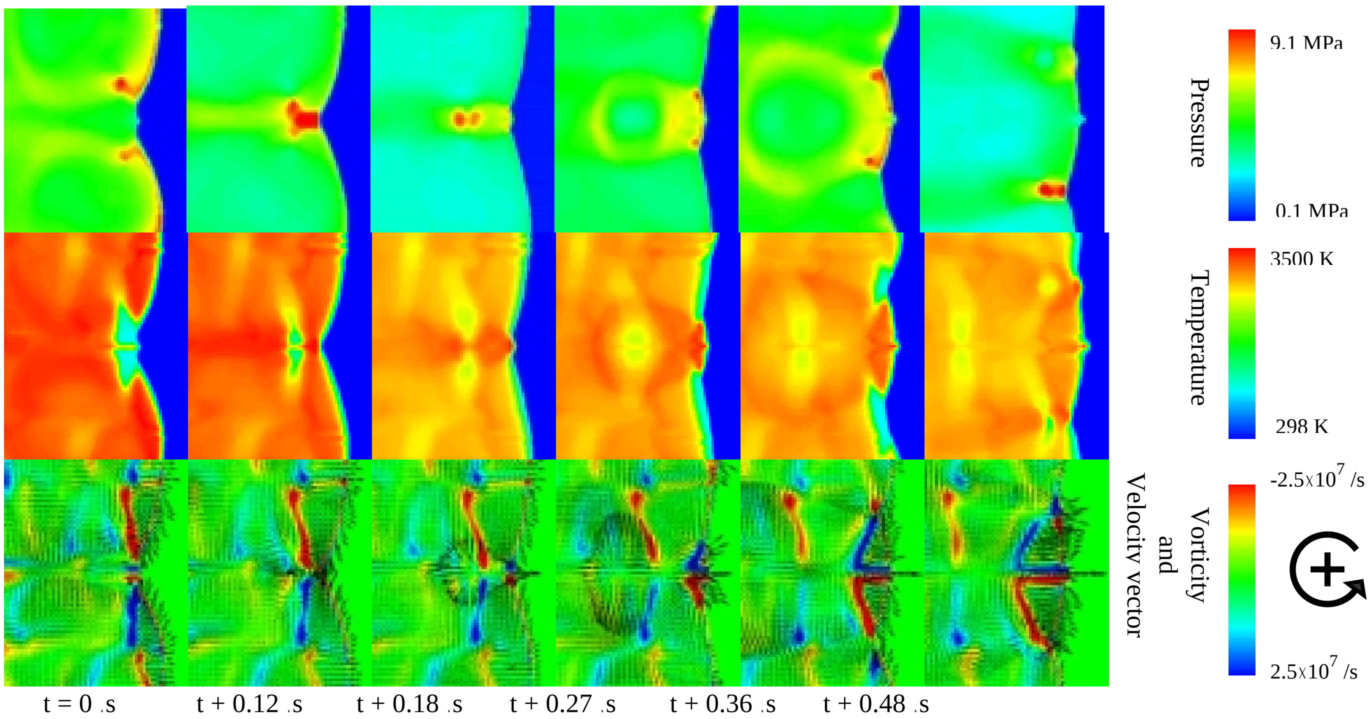

Fig.6 Time sequence of enlarged contours of the detonation wave through an half cell cycle

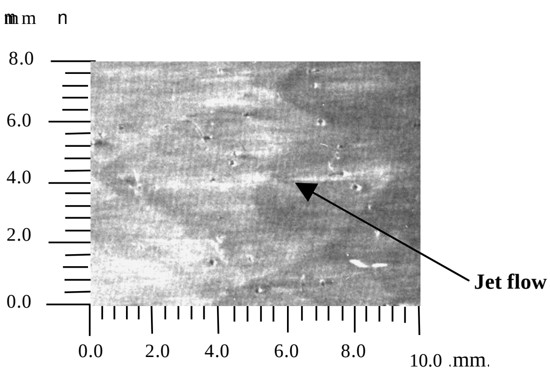

Fig.7 Enlargement of smoked foil records in the experimental result

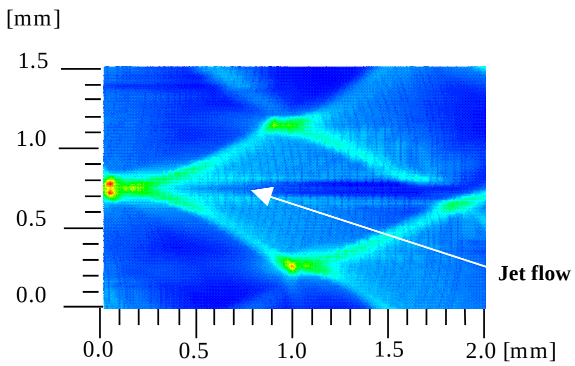

Fig.8 Enlargement of the maximum pressure