Effect of wall conditions on DDT in Hydrogen-Oxygen mixture

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1 Introduction

Detonation has enormous danger causing of a large accident, in another hand its practical applications to next generation type aerospace thrust system are expected. Over 130 years have passed since the research on detonation was started, various experiments and numerical analyses have performed to elucidate detonation. As far as the beginning of the numerical work, Taki and Fujiwara[1] were succeeded in 2-D numerical simulation of detonation in 1980.

Deflagration to detonation transition (DDT) is one of the major unknown problems related to detonation. Urtiew and Oppenheim [2] have performed a visualization of DDT by using a high speed Schlieren system. They observed the phenomena of an *explosion within the explosion* saying that *there are various ways in which the genesis of detonation waves can take place*. These days a number of approaches to understand DDT numerically have done. Liberman [3] et al. did the similar work on DDT recently as we did [4] in a different way numerically. Kagan and Sivashinsky [5] performed a 2-D numerical simulation of DDT under the adiabatic and isothermal wall conditions with one-step Arrhenius type reaction model, but they did not have enough resolution to explain their DDT sequences. However they showed the difference in flame shape between the adiabatic and isothermal wall conditions. It is thought that the heat loss does not affect the transition to detonation due to the high speed of propagating flame, but actually it does..

The objective of the present study is to reveal the effect of the adiabatic and isothermal wall conditions on DDT mechanism with a detailed chemical reaction model considering pressure dependency of reaction rate constants.

2 Numerical method

The governing equations are Navier-Stokes equations with 8 species (H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O) and 18 elementary reactions, which are explicitly integrated by the strange type fractional method. The chemical reaction source terms are treated in a linearly point-implicit manner. A second-order Harten-Yee non-MUSCL type TVD scheme is used for the numerical flux in the convective terms. The Petersen and Hanson model is used for chemical kinetics to solve detonation problems. This model contains 9 species and 18 reactions, and it is based on the H_2/O_2 sub-mechanism of the RAMEC/Gas Research Institute GRI-Mech 1.2 methane-oxidation mechanism. The significance of this model is the pressure dependence on a forward reaction coefficient included in the collision reaction with a third body: HO_2 and H_2O_2 chemistries near the second and third explosion limits, which are necessary for ignition at extremely high pressure, are considered while lacking in certain finite rate chemical models currently in use.

The computational grid has a rectangular mechanism with 8752×400 points. The x-direction is equally spaced intervals 6.8μm and the y-direction is unequally-spaced intervals which has the minimum size 1μm and the maximum size 6.8 μm. The boundary conditions are as follows: the left side, top, and bottom are wall, and the right side is free stream; the upstream conditions are at the pressure of 0.073 MPa and temperature of 298.15 K, and the upstream gas is stoichiometric mixture $H_2/O_{2;}$ and the downstream conditions are composed of ignition region and in front of it the shock region is formed which is calculated based on the Rankine -Hugoniot relations.

3 Results and discussion

Figure 1 shows the series of process of the transition to detonation. Fig.1-(a) and Fig.1-(b) are the adiabatic case and the isothermal case, respectively. In the adiabatic case a local explosion occurred in the boundary layer near the tube wall, but in the isothermal case a local explosion occurred at the flame tips. In the former case due to no heat loss effect, the wall temperature continues to increase gradually as shown in Fig.3-(a), which gives an ignition in the boundary layer to form a flame in the boundary layer (Fig.1-(a): t=14.594 μs). Generally to say the viscosity tends to increase proportional to the square root of temperature in gas. Eventually the bow shock waves form just ahead of the flame front by so-called a piston effect as shown in figure 2, then this bow shock waves interact with the boundary layer to cause an increase of the boundary layer temperature due to the adiabatic condition, then to enhance the chemical reactions in the boundary layer there. Thus this positive feedback cycle between the bow shock heating and the chemical reaction heating in the boundary layer drives a local explosion in the vicinity of the wall. In the latter case due to the heat loss at the wall the ignition and explosion do not occur in the boundary layer, instead the explosion occur between the bow shock wave, which came out in front of the fast propagating flame, and the flame front in the tube. These phenomena are described in Fig. 4-(a) and –(b) which show the pressure profiles for the adiabatic and isothermal case just before local explosion happens, respectively. As one can see in the latter case the stronger shock wave forms in front of the flame and the distance between the flame and the precursor shock becomes shorter than the former case. It is expected that a bigger piston effect acted as seen in Fig.4-(b).

4 Conclusions

- In the isothermal condition case detonation tends to occur at the flame tip. It is related to the formation of pressure waves and it is supporsed that the heat loss is affected by th wall temperature.
- It is important that much further analysis is performed with a larger width tube because it is expected that the tube width might affect the activety of reaction near the tube wall and if in the smaller tube that the effect of the reaction near the tube wall becomes more dominantly.

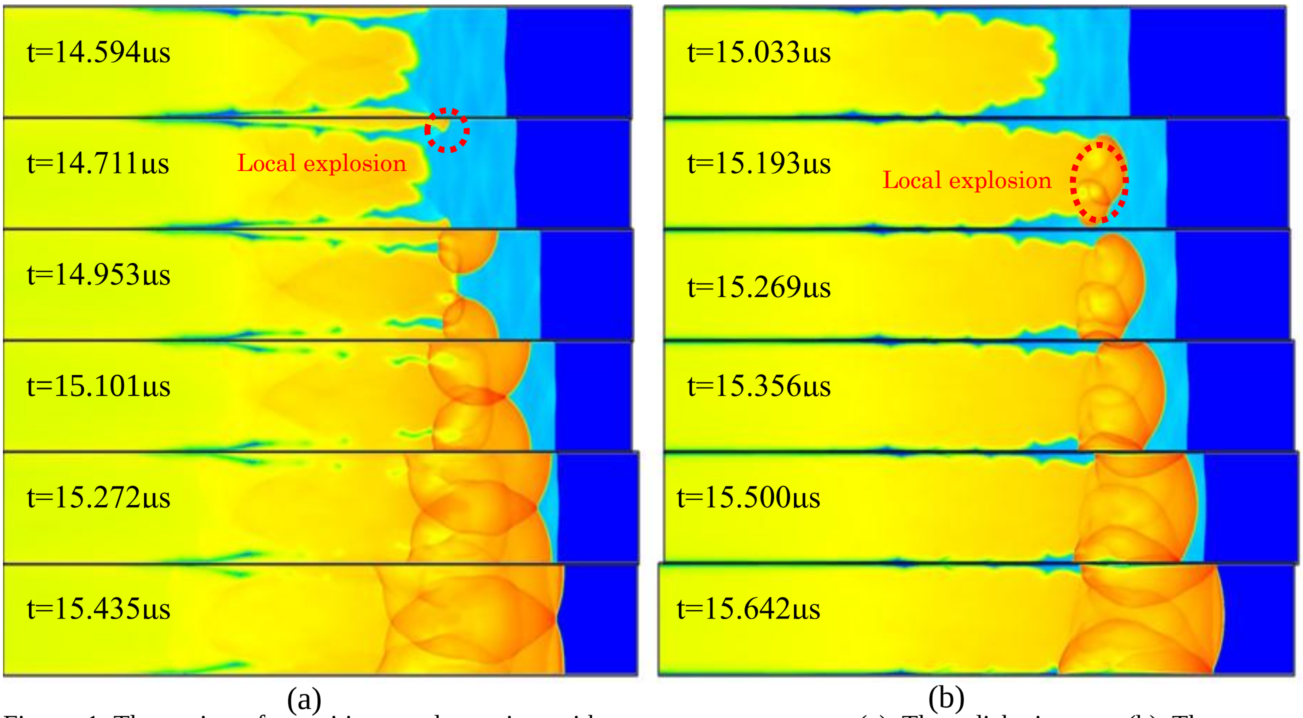

Figure 1 The series of transition to detonation with temperature contour: (a) The adiabatic case (b) The isothermal case

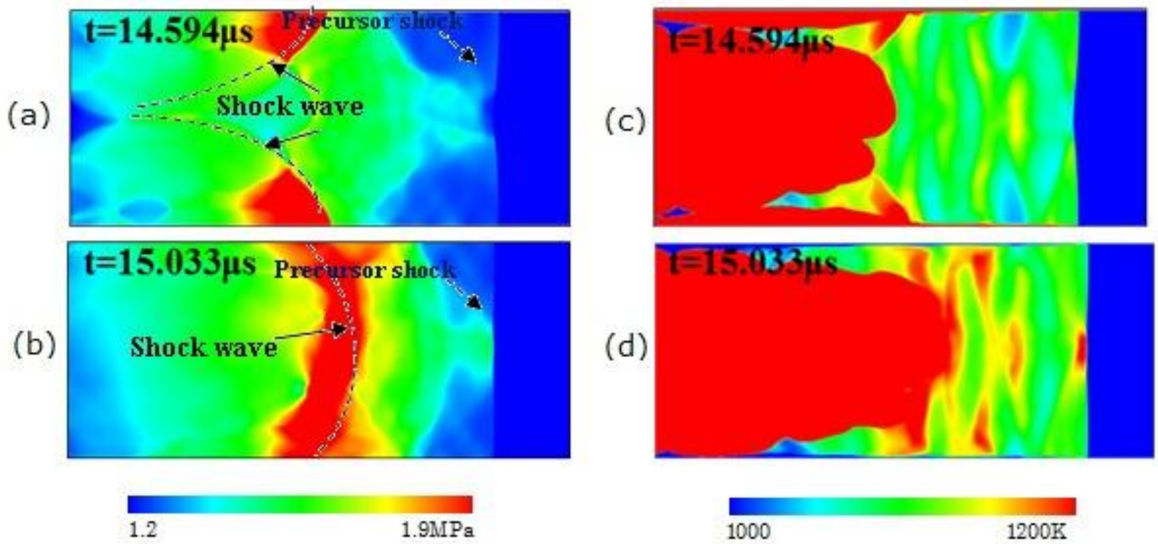

Figure 2 Pressure (a), (b) and the temperature (c), (d) profiles before transit to detonation; top is adiabatic case and bottom is isothermal case respectively.

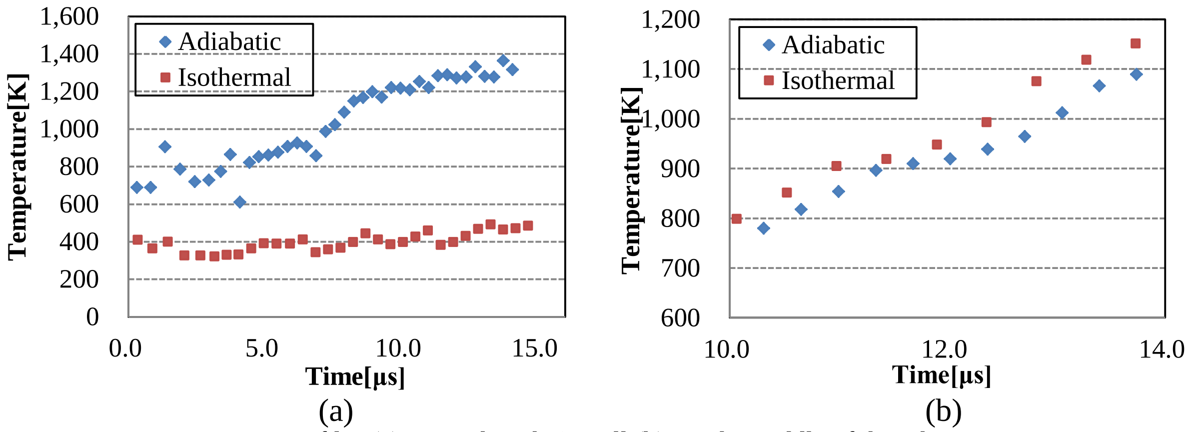

Figure 3 Temperature profiles (a): Near the tube's wall (b): At the middle of the tube

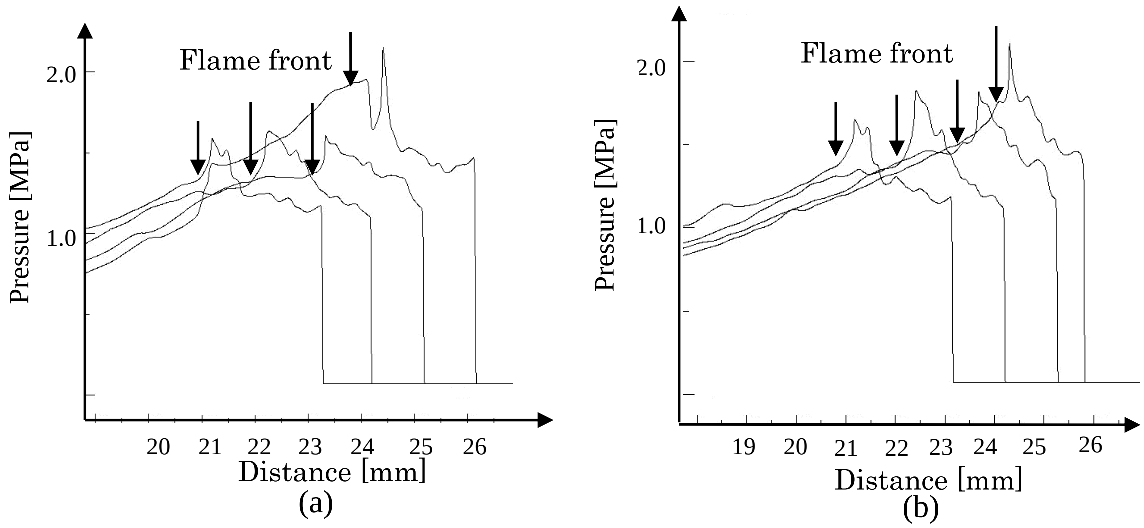

Figure 4 Pressure profiles for (a) Adiabatic and (b) Isothermal case just before the local explosion happens

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