Argon or Nitrogen Diluted Hydrogen/Oxygen Detonation in Tube with Obstacles

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Introduction

Numerical simulation on detonation has been extensively performed these decades in detail, but many of them are the simulation using single-step or two-step reaction mechanism. There may be not much difference in detonation simulations in a simple tube using a single-, two-step mechanism or a detailed mechanism, but when detonation propagates through a tube with obstacles, their difference in simulation may appear especially in the case of using Euler equations which do not calculate turbulent mixing and do calculate shock wave-based ignition. When the reaction mechanism has a high activation energy, detonation may be quenched at the collision to obstacles by using Euler equations, but may not be so with the detailed mechanism.

Authors have studied the detonation propagation structure in obstacled tubes and shown the numerical results simulating well the experimental ones for several types of obstacle configurations [1-3]. Teodorczyk et al. [4,5] have also studied extensively around 1990 to present quasi-detonation and fast deflagration propagation mechanism in tubes with obstacles.

The present study performs numerical simulation of detonation propagating in a tube with obstacles and with argon or nitrogen diluted H_2/air mixtures. The argon diluted mixture may be the mixture with high activation energy and nitrogen diluted mixture may be low activation energy. The simulations with a single-step and two-step reaction mechanisms will also be performed to compare with the case of a detailed reaction mechanism.

Experimental Methods

Detonation tube has a 40 x 40 mm section and a 4 m length. The first observation section locates at 3 m from the ignition point with a commercial spark plug and the second observation section locates next to the first one, which provides information of detonation re-ignition. Two ICCD cameras are set in front of each observation section to catch self-emissions from combustion waves. A 0.5 m Shchelkin wire is installed from the point of ignition to downstream. A staggered type obstacle (interval: 60 mm, width: 4 mm, height: 8 mm) is set at the first observation section to see a possibility of detonation quenching.

Detonation velocities at several points are measured by eight PCB pressure transducers.

Numerical Methods

For nitrogen and argon dilution cases numerical simulation is performed using 2D compressible Euler equations with Petersen and Hanson detailed $H_2/O_2/N_2/Ar$ reaction model which has 9 species and 18 elementary reactions. The third body collision frequencies are different between argon and nitrogen, which will give the different activation energy. Both cases will be calculated in the presentation, but the nitrogen case is shown in this abstract. Production terms are treated implicitly and other terms are done explicitly (semi-implicit method), where the convective term is integrated by a Harten-Yee-developed non-MUSCL modified flux type TVD scheme. The second order Strang type fractional step method is used for time integration. The accuracy of computation is kept to be the second order. The initial conditions for 2D calculation are constructed from 1D result with the atmospheric pressure, temperature of 298 K, and stoichiometric condition. The boundary conditions are that the wall is adiabatic, non-slip, and non-catalytic.

For the numerical comparison among a single-step, two-step, and full step mechanism, 2D Euler equations are also used for a tube with 2mm diameter. In this case the grid size is kept for 5μm. Other conditions are the same as nitrogen and argon dilution cases.

The NEC SX-6 1 node (8CPU) of ISAS/JAXA is used for the present calculation.

Results and Discussion

Experiments are performed for mixtures diluted by argon and nitrogen at equivalence ratios of 3.76 and 5.0. In the case without obstacles detonation velocities are stable along the tube for all mixtures (Fig. 1), but the detonation velocities in the nitrogen diluted mixture get influence from obstacles (Fig. 2). All cases recovered their detonation velocity at the second observation section. From these results the mixture of $H_2/O_2/3.76N_2$ gives the fastest detonation velocity, but the mixture of $H_2/O_2/5.0N_2$ provides the deflagration; detonation in the nitrogen diluted mixture is affected by obstacles more than that in the argon diluted mixture; and the extinction effect by obstacles is less effective than the collision effect by argon, then the detonation extinction is not observed in the present location. In nitrogen diluted case detonation energy is calculated by the smaller specific heat ratio than the argon case.

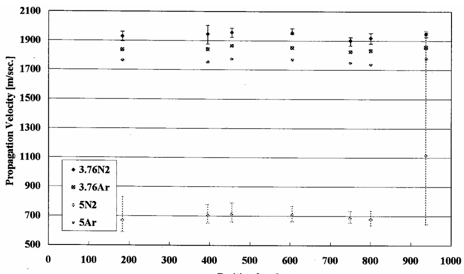


Fig.1 Propagation velocity along the tube without obstacles for stoichiometric H_2/O_2 diluted with N_2 and Ar

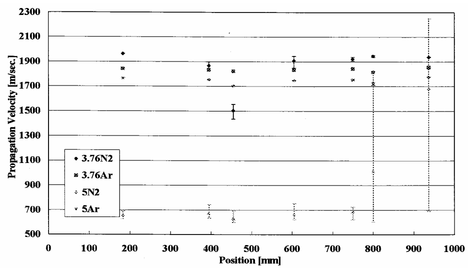


Fig.2 Propagation velocity along the tube with staggered array obstacles at the brockage ratio of 0.20 for stoichiometric H_2/O_2 mixture diluted with N_2 and Ar

Numerical simulation for dilution cases is performed only for the nitrogen diluted mixture ($2H_2+O_2+3.76N_2$), but the present numerical results are compared with experimental ones. The real size of computational space is 2 x 17.2 mm with the grid size of 5 x 5 μm. Figure 3-(a)~-(h) shows the temperature profiles of detonation propagation in the nitrogen diluted mixture through staggered obstacle array. The blue color is 300 K and red one is 3700 K. The areas behind and between obstacles becomes in high temperature.

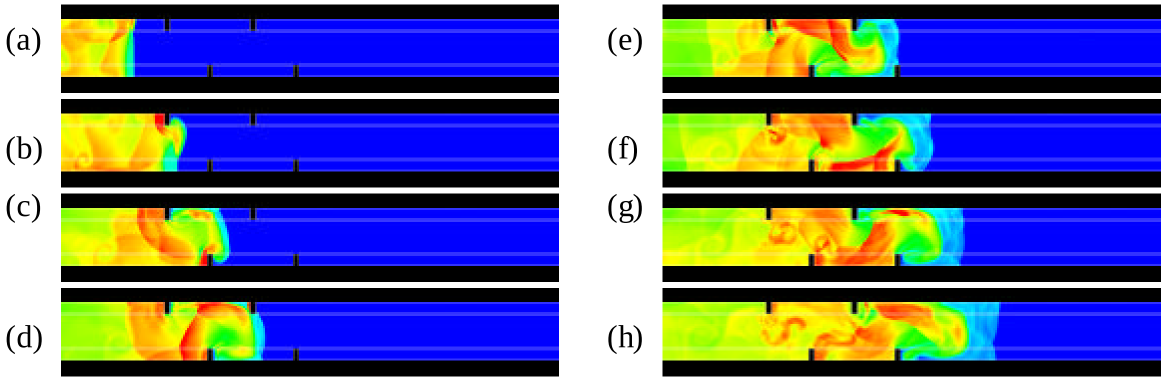
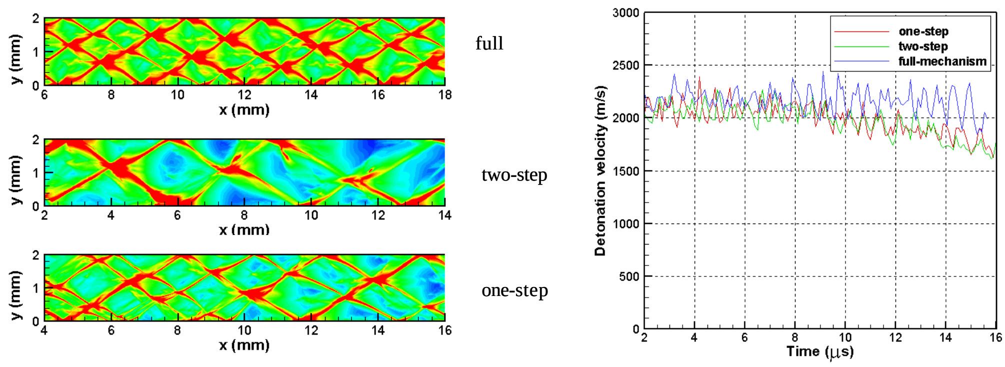


Fig.3 Numerical temperature profiles of detonation propagation through a staggered obstacle system in a hydrogen/oxygen mixture diluted with nitrogen.

The results in Fig. 3 show that there is some low temperature area between the wave front and the high temperature region near the front after the combustion wave passes the obstacle section and this low temperature region becomes bigger as the wave proceeds. It looks that the detonation re-ignition may not occur, which is not the experimental results. This is because the numerical detonation has only one triple point, while the experimental one has more triple points. It implies that the experimental detonation is stronger than the numerical one. We will get the similar experimental condition with the numerical one by keeping the number of triple point; the reduction of initial pressure may provide such condition.

Figure 4 shows the detonation propagation through a smooth wall for a single-step, two-step, and full step chemical reaction mechanism cases. The case with a full-step react-



(a) (b)

Fig.4 A comparison of (a) detonation cell sizes and (b) detonation velocity through a smooth wall using a One-step, two-step, or full-step H_2/air reaction mechanism.

ion mechanism provides a steady detonation propagation. When the grid size becomes wider, the cases of one-step and two-step mechanism become better due to their reaction structure. We will extend our calculation for obstacles cases and will discuss the results in details at the presentation.

Conclusion

Detonation propagating in the argon or nitrogen diluted mixture through obstacles is studied experimentally and numerically to clarify the specific heat effect on detonation quench. Especially it is an objective to investigate whether the use of Euler equations together with a single-step reaction mechanism causes detonation quenching or not. This objective is not attained at this moment, but will be obtained by the conference. And comparison of numerical results on detonation propagation through a smooth wall using a single-step, two-step, or full-step mechanism are performed to see the full-step mechanism case can use the small grid size, but the one-step and two-step mechanism cases can not get a steady propagation of detonation for 5μm grid size case. A further numerical simulations of argon diluted case and comparisons using three different reaction mechanisms are planned to clarify such activation energy and specific heat ratio effect on detonation calculation by Euler code.

References

1. A.K. Hayashi, K. Asami, S. Shiokawa, H. Sato, and J.H.S. Lee, *19th ICDERS*, Th3-2-2, 2003.
2. K. Asami, S. Kato, H. Sato, and A.K. Hayashi, *H14 Shock Wave Symp. (Japanese)*, A15-2-4, 2003.
3. S. Shiokawa, K. Eto, J. Misawa, H. Jotaki, H. Sato, and A.K. Hayashi, *41st Combustion Symp. (Japanese)*, E222, 2003.
4. A. Teodorczyk, J.H.S. Lee and R. Knystautas, *Proc. 22nd Symp. (Int.) on Combustion*, The Combustion Institute, pp.1723-1731, 1988.
5. A. Teodorczyk, J.H.S. Lee and R. Knystautas, Proc. 23rd Symp. (Int.) on Combustion, The Combustion Institute, pp.735-741, 1990.