Velocity Deficits of Ar and He diluted H_2-O_2 System in Small Diameter Tubes

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1 Introduction

Detonation is a self-sustained shock-induced supersonic combustion wave propagating in reactive media. From a safety engineering point of view or a fundamental study of gaseous detonation, gaseous detonation has been extensively studied. Classical theory of detonation [1] is often highly successful theory for predicting the detonation velocities and many of other parameters. This theory considers one dimensional supersonic wave in a reactive media which is capable of exothermic reactions. This theory also assumes that the experimentally observed detonation wave corresponds to the one-dimensional wave having the lowest velocity which attains the chemical equilibrium in a steady flow. This hypothesis is the well-known Chapman-Jouguet (C-J) theory which leads to the Zeldovich-Döring-von Neumann (ZND) theory of one-dimensional detonations. Zeldovich [2] showed that the balance of the energy loss and exothermic reaction determines detonability limits using one dimensional model which include both heat and momentum loss.

When we consider detonation near extinction limit, transverse (spinning) waves[3], turbulence[4], viscous drag force which leads to the boundary layer theory of Fay[5] are very important. Experimentally, Berets [6] performed detonation velocity measurements which were affected by boundary layer for various tube diameters. The rate of chemical reactions was also important factor for determining the detonation limit [7]. On the basis of experimental results of Moen [8] and Lamberge [9], velocity deficit is not consistent with the model of Fay-Dabora [5] in some case. On the other hand Strehlow [4] discussed about the strength of transverse wave in propagating detonation. Moreover effect of surface roughness was investigated by M. I. Radulescu [10].

Concerning about chemical kinetics, Agafonov [11] demonstrated computation of detonation limits with detailed chemical kinetics using ZND model including energy losses. Recently Camargo [14] showed curvature effect [14] of shock front might be important as well as boundary layer theory [5].

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Of course Fay's turbulent boundary layer model might be replaced to a model which includes laminar to turbulent transition in the boundary layer when we consider one dimensional flow. Real condition near detonation limits should include momentum and heat loss, curvature effect of shock front, boundary layer theory and effects of three dimensional detonation structures.

In recent years numerical simulations can simulate detailed structure of detonation front with two or three dimensional code [16-18]. Although they described the remarkable insight of detonation structure, once, these computer fluid dynamics simulations are coupled with detailed chemical kinetics model, huge amount of computational resources [17-18] are required to simulate. Those recent models which predict detonation velocities with three dimensional structures are not still quantitative.

For practical purposes in safety engineering, detonation propagation limit is very important. Although one dimensional model [3][10][11] is still convenient and attractive, its validity is still uncertain, many uncertainties of detailed reaction models and many three dimensional effects of real detonation also deviate the model prediction from experimental results. In the present study, velocities of detonation in Ar and He diluted H_2-O_2 mixtures ($2H_2+O_2+\beta Ar(He)$, β=0, 1, 2, 3.76) were precisely measured near propagation-limit conditions. The results are compared with modified one-dimensional ZND model to reveal the difference between ideal one dimensional flow and three dimensional flows in real detonation. Many detailed chemical kinetic models were also compared to declare uncertainties of detailed reaction kinetic model in recent years at high temperature detonation conditions.

2 Experimental

Schematic diagram of our present study is shown in Fig. 1. The detonation tube was nearly 5 m in length and 3.1, 6.0, 8.8 mm in inner diameter. The tube was made of quartz glass which was manufactured by Tosoh Quartz Corporation. Premixed sample gas was prepared in a stainless mixing tank. After evacuating the tank by a rotary pump, H_2, O_2 and Ar or He gases were introduced into the tank up to 1000 Torr and was kept about 1day to attain complete mixing. The pressure of the gas line was monitored by a capacitance manometer (MKS Baratron). Before ignition, quarts tube was evacuated more than 15 min to obtain high vacuum for high voltage discharge. Next Pre-mixed gas was introduced to the quartz tube from the mixing tank ranging from 80 to 400 Torr. High voltage (Matsusada Precision Inc.), typically 3 kV was applied to the needle to ignite. Triggering signal was transferred by coaxial cable (RG-58 A/U) to digital oscilloscope. After ignition, flame was accelerated in the quarts tube to obtain detonation. Self-luminescence of detonation front was captured by optical fibers (OFS Specially Photonics Division; All Silica 365, core clad of 400 μm with numerical aperture of 0.22), which were placed along the quartz tube with 10 cm interval. Total of 45 fibers were placed. Luminescence light of detonation was guided to photoelectric surface of two photo-multipliers (PMT: HAMAMATSU R1527). After deflagration to detonation transition (DDT) was occurred, overdriven detonation was observed. Overdriven detonation immediately converged to steady speed. For precise measurements, 22 sections of speed were averaged. When only deflagration occurred, self-luminescence peaks were not observed because of low luminescence intensity of deflagration flame. Finally PMT signals were recorded in the digital oscilloscope.

Initial pressures in the present study are 80-400 Torr (1 Torr = 133.3 Pa) and the equivalence ratios of 1.0.The mixtures were diluted to a certain dilution ratio β of 0, 1, 2 or 3.76 ($2H_2+O_2+\beta Ar$(or He)).

3 Experimental results

A typical profile of detonation velocities are shown in Fig. 2. In usual conditions, Flame was already accelerated over C-J velocity of detonation at the first section. The first fiber was settled within 5 cm from the quartz tube inlet. Overdriven detonation speed was about 20 % higher than the steady speed section. Within 2 m distance from the first fiber, detonations were immediately converged to steady speed around 2500 m/s. In some case, velocity at steady speed section seems to be fluctuating. Because of the long interval (10 cm) of glass fibers, details are not clear. In our present study, we concentrated on the averaged value of detonation velocities obtained from 22 measurement sections along the quartz tube. We could reproduce very precise detonation velocities typically within 10 m/s error for 2500 m/s detonation velocity.

Detonation velocities of Ar and He gas diluted H_2-O_2 system were systematically measured by changing dilution ratio (0, 1.0, 2.0, 3.76). As shown in Fig. 3, detonation velocities decreased as the initial pressure decrease. Propagating mode was also changed from multi-headed mode to single spinning mode which was confirmed by soot patterns using Mylar® film. At the transition of those two modes, velocity deficit did not increased monotonically. In the single spinning mode, one transverse wave revolves inside the tube wall. Namely flow around detonation wave cannot be approximated to one dimensional flow. As a result actual line of flow increased and the distance from shock front to C-J plane shortened. That leads to lower velocity deficits in the single spinning mode compared to one dimensional model prediction.

By diluting the H_2-O_2 system, we also obtained dilution effects on velocity deficits as shown in Fig. 5. Dip at the mode transition point seems to be weak in the Ar diluted conditions. An example of Ar gas dilution (β=1.0), is shown in Fig. 4. As the dilution ratio increased, the ratio of velocity deficit to C-J velocity increased except for the case of non diluted condition. In the case of He gas dilution conditions in Fig. 5, because of the small molecular weight of He, absolute detonation velocity increased as the C-J value increased. However the ratios of velocity deficit to C-J value were monotonically increased. Those results shows that Ar dilution affect on the irregularity of three dimensional structure in detonation compared to the case of He. Fluctuations of velocities in the single spinning mode was larger in the case of He diluted conditions, which indicates the transverse wave seems to be stable in the case of Ar diluted conditions.

4 One dimensional model and reaction mechanisms of H_2-O_2 system

As a next step of Zeldovich[2] and Agafonov[11], Kitano[3] applied one dimensional ZND theory with detailed chemical kinetics model for H_2-O_2 system. Their one dimensional model was based on Zeldovich[2], which assumed fully developed flow. Dove[7] also applied one dimensional model with turbulent boundary layer theory which was firstly used for detonation by Fay[5]. In recent years, Camargo[12], Chao[23] compared their results of $C_2H_2/O_2/Ar$ and $CH_4/O_2/Ar$ mixtures with one dimensional model which includes turbulent boundary layer. In the present study, we used modified one dimensional model with energy losses based on Kitano et. al [3]. The present one dimensional model also includes viscosity calculation as reactions proceeds behind the shock front. Turbulent boundary layer (Fay[5]), laminar boundary layer and fully developed flow (Zeldovich[2]) also included. However, in the present study, turbulent boundary layer calculations are mainly performed. The conservation of laws for one dimensional steady detonation are written as follows.

$$\frac{d}{dx}(\rho u A) = \left\{ \rho \frac{du_s}{dx} + u_s \frac{d\rho}{dx} \right\} A = 0 \quad \cdots(1)$$

$$\frac{dp}{dx} + \rho u_s \frac{du_s}{dx} = \frac{4\sigma}{d} \equiv f \quad \cdots(2)$$

$$\rho u_s \frac{d}{dx}\left(h + \frac{u_s^{\,2}}{2} \right) = \frac{4\sigma}{d} D - \frac{4\theta}{d} \equiv g \quad \cdots(3)$$

Here ρ, u_s, p, σ, d, D, h and θ are the density, particle velocity, pressure, friction loss, tube inner diameter, detonation velocity, enthalpy and heat loss respectively. Friction and heat losses are written in a coordinate system fixed to the propagating detonation front [11]. Friction loss σ and heat loss θ are assumed as bellows using Reynolds analogy of viscosity and thermal conductivity with a factor of unity.

$$\sigma = \frac{1}{2}\xi \rho u_s^{\,2} = \frac{1}{2}\xi \rho (D-u)^2 \quad \cdots(4)$$

$$\theta = \frac{1}{2}\xi \rho (D-u_s)\left[C_P (T-T_0) + \frac{1}{2}(D-u_s)^2 \right] \quad \cdots(5)$$

$$\xi = 0.3164\,\mathrm{Re}^{-0.25} \quad \cdots(6)$$

$$\frac{1}{\sqrt{\xi}} = 2.0 \log_{10}\left(\mathrm{Re}\sqrt{\xi} \right) - 0.8 \quad \cdots(7)$$

$$\frac{A}{A_0}-1=\frac{\pi d\delta}{\pi d^2/4}=4\frac{\delta}{d} \quad \cdots(8)$$

$$\delta^*=0.22x^{0.8}\left(\frac{\eta}{\rho_1 D}\right)^{0.2} \quad \cdots(9)$$

$$\delta^*=1.721\sqrt{\frac{x\eta}{u\rho}} \quad \cdots(10)$$

Here ξ , Cp, T, is friction factor. ξ is estimated by Blasius formula[3] and also Plantle formula in the present study. Turbulent flow was assumed for both friction factor. In the case of turbulent boundary layer, equation (8) and (9) based on P. B. Gooderum[14] are applied without term f and g. Here δ, A, η are displacement factor, and cross section of flow and viscosity. In the case of laminar boundary layer, Blasius's analytic solution (equation (10)) was also applied without term f and g in equation (2) and (3). Time derivatives of pressure were also concerned with those equation listed above. When we estimate time derivatives of pressure, we need heat release rate of our system which was estimated by detailed chemical kinetics model of H_2-O_2 system [20] [21]. The time derivatives of each species were calculated by CHEMKIN-II package code [13].

The detailed reaction mechanisms are responsible for the time profiles of heat release rate. Heat release rate also related to the distance from shock front to C-J plane and total energy loss. In the present study, recent reaction mechanisms K. Shimizu [15], M. Burke [16] and M. Conaire [17] were applied. Old mechanism of M. Hishida [18] was also applied for a comparison. All the thermochemical data and reaction mechanisms were based on the original electric files. Transport properties, which were used for calculating viscosities, were adopted from L-J parameters in CHEMKIN input files.

As indicated in Fig. 5, in the Ar and He diluted condition (β=1.0), Conaire (2004) and Shimizu (2012) seems to be well suited for predicting the multi-headed region of experimental data. Turbulent boundary layer model were applied in this calculation. Burke (2012) overestimates velocity deficit. On the other hand, Hishida (1992) underestimate velocity deficits. However in the case of non diluted condition (β=0), Burke (2012) was suitable for predicting experimental data and Conaire (2004) underestimates velocity deficit. As the range of temperature in detonation is very wide (typically 1500-3300 K in the present study), these results show the range of errors included in reaction mechanisms in recent years. These reaction mechanisms are not validated such wide range of temperatures. The discrepancy between the case of Ar diluted and non diluted condition can also be ascribed to a difference of 3 dimensional flows in those conditions such as irregularities of flows, strength of transverse wave and so on. In the Ar diluted conditions, the model results overestimate the experimental results as β increased. Those Ar dilution effects indicate that error in our model increases as β increased. Laminar boundary layer to turbulent boundary layer transition is not considered in our model. Those effects might be a candidate for a cause of error in our model.

5 Conclusions

Detonation velocities of $2H_2+O_2+\beta Ar$ (βHe) in 6 mm diameter tube were precisely measured using the self-luminescence of detonation wave. As dilution ratio β was increased, velocity deficits increased for both case of Ar and He dilution. The results of Ar diluted conditions suggested that the irregularities of cell structure of detonation were changed as the β increased. More stable transverse waves in the three dimensional structure in real detonation were suggested in the case of Ar dilution. In the single spinning mode, detonation flow cannot be approximated to one dimensional flow as the profiles of experimental detonation velocities cannot be reproduced by one dimensional model calculations. One dimensional model with detailed chemical kinetic model also indicated errors including in recent kinetic models when they are used in one dimensional model calculations of detonation. The main cause of such errors might be the wide temperature range of detonation. As mentioned above, precise velocity measurement reveals that the velocity deficits are affected by irregularities of three dimensional flows and the stabilities of transverse waves especially in a single

spinning mode. Those effects will cause errors when we predict detonation limit using those one dimensional models.

6 Acknowledgements

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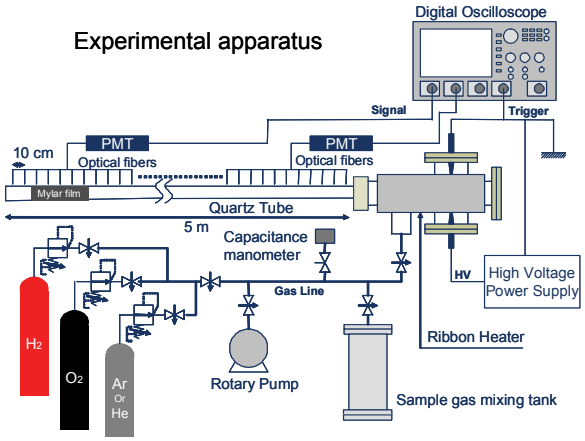

Figure 1. Schematic diagram of experimental appratus.

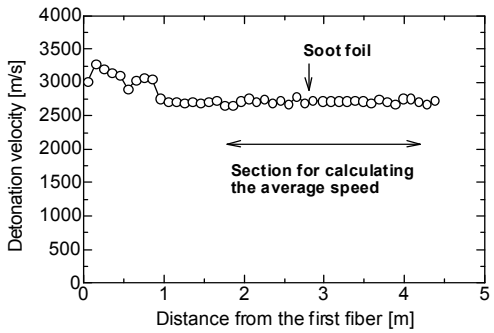

Figure 2 Typical detonation velocity profile.

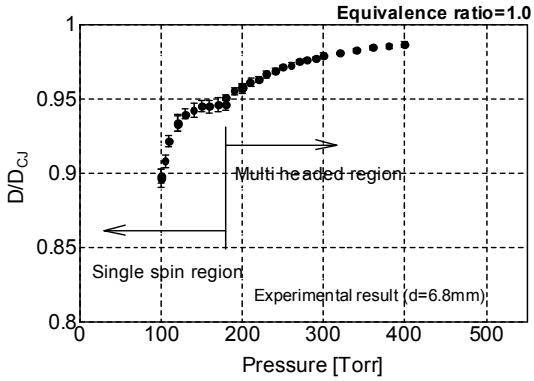

Figure 3 Detonation velocities and propagating mode near extinction limit at non diluted condition.

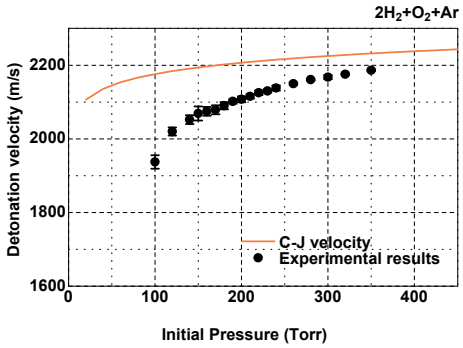

Figure 4 Detonation velocities at Ar diluted conditions

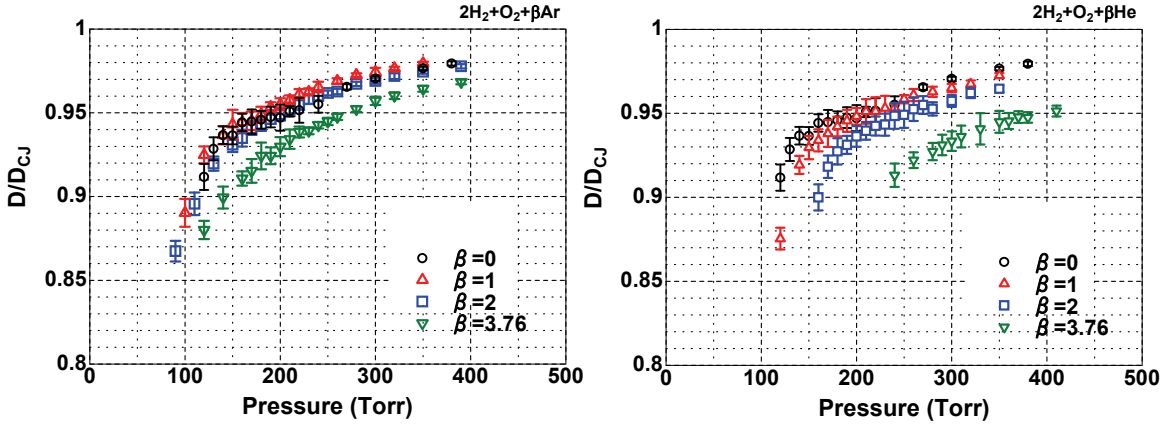

Figure 5 Measured detonation velocities of Ar and He diluted conditions (β =0, 1, 2, 3.76).

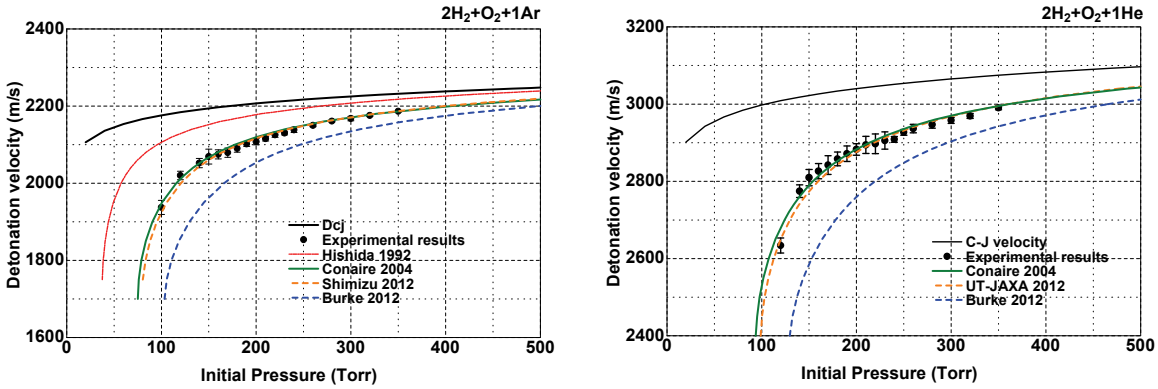

Figure 6 Detonation velocities at Ar and He dilution conditions compared with 1D model with detailed reaction models.