Pressure Limits of Gas Detonation

Takayuki Tomizuka¹, Masashi Fukao¹, Akio Susa¹, Masayasu Mohri², Masatake Yoshida³, Sukumar Chakravarthy⁴, Mitsuo Koshi¹

¹The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, Japan
 ²Delight Co.,Ltd., Manpukuji 1-2-3, Asao-Ku,Kawasaki-shi, Kanagawa-ken, Japan
 ³Explosion Research Institute Inc., 5-18-2 Chuo, Ushiku-shi, Ibaraki-ken, Japan
 ⁴Metacomp Tech Inc., 28632-B Roadside Drive, Suite 255Agoura Hills, CA 91301, USA

1 Introduction

Prediction of the limits of gas detonation is very important for the safety of various chemical plants, and there have been many studies on the detonation limits. In the one-dimensional theory, the actual wave structure was replaced by an averaged flow with the friction and the heat exchange behind the detonation wave on the reactor wall. These frictions and heat exchanges lead to losses in momentum and energy in the reaction zone of detonation wave. As the diameter of the detonation tube decreases, the relative losses become greater. At some diameter, a steady solution of the detonation wave propagation problem vanishes, and the limiting diameter is defined at this point. It has been shown that the one dimensional model with the corrected friction and heat transfer coefficients provides a satisfactory prediction of the detonation limits. Agafonov et al.[1] estimated the limiting diameter for the H_2 -air and H_2 - O_2 detonation by including full chemical kinetics.

In these one-dimensional theories, the detonation limit is determined by the balance between the rate of heat production and the rate of energy and momentum losses to the wall. Reduction of the diameter of the detonation tube will increase the rate of energy and momentum losses. Similarly, lower initial pressure will cause lower rate of energy production and faster rate of energy and momentum losses. Therefore, there should be limiting pressure for the gas detonation. The limiting pressures of the detonation of some fuels were measured in the present study to compare the theoretical prediction.

In the present study, the detonation limits for hydrocarbon fuels were predicted on the basis of the onedimensional theory with full chemical kinetics.

It is well known that the detonation wave structure is not one dimensional and the structure changes from the multi-front configuration to the spinning single head configuration at near the detonation limit. The derivation of a multi-dimensional theory of the detonation limits is extremely difficult since it is necessary to include the transverse wave interaction with the near-wall boundary layer and the other accompanying effects such as boundary layer separation, non-uniform turbulence. In order to understand the effects of the multi-dimensional structure on the detonation limit, multi-dimensional numerical simulations for H_2 - O_2 mixtures were also tried with the full chemical kinetics and with loss terms.

2 Experimental section

A schematic diagram of the present experimental apparatus is shown in Fig. 1. The detonation tube is a pyrex glass tube of 3m in length and 6 mm in inner diameter. A sample gas in the detonation tube is ignited by the pulsed discharge. Pre-mixtures of hydrogen-oxygen were filled up into the tube from a gas tank. UV emission from the detonation front was monitored by using the optical fiber, which were placed beside the glass tube at

10cm interval. Total of 27 fibers are placed and the output of these fibers were introduced to one photomultiplier tube. A band pass filter centered at 308nm is used to isolate the UV emission. An example of the time profile of those emission is shown in Fig. 2. Very sharp emission pulses were observed, and the detonation velocities were calculated from the time intervals of these pulse emission.







As can be seen in Fig.2, the detonation velocities along the detonation tube is almost constant at the end of the detonation tube. Detonation seems to be steady at this length (3m) of the detonation tube in this condition. Those steady detonation velocities are plotted in Fig.3 as a function of initial pressure. The measured velocities are always lower than the CJ detonation velocities and the difference is increasing as the initial pressures are decreasing. No sharp emission pulse was observed at the initial pressure lower than 120 Torr for the equivalence ratio ϕ =1.5, 170 Torr for ϕ =1.0, and 90 Torr for ϕ =0.5.



Fig.3 The detonation velocity as a function of initial pressure

3 One-dimensional simulation(the ZND model)

The one-dimensional simulations under the same physical condition with the experiments were carried out. It is based on the ZND theory[1] and the governing equations are as follows.

$$\frac{d(\sigma u)}{dz} = 0 \tag{1}$$

$$\frac{d}{dz}(p^2 + \sigma u^2) = \frac{4\sigma}{d} \equiv f$$
⁽²⁾

$$\sigma u \frac{d}{dz} \left(h + \frac{u^2}{2} \right) = \frac{4\sigma}{d} D - \frac{4\theta}{d} \equiv g$$
(3)

Here D,u,h, ρ ,p,and d are detonation velocity, particle velocity, enthalpy, density pressure and tube diameter. In this model, friction and heat loss due to the tube wall are considered. The friction loss σ and heat loss θ at the tube wall are approximated as follows[1].

$$\sigma = \xi \sigma (D-u)^2 / 2 \tag{4}$$

$$\theta = \frac{1}{2}\xi\sigma(D-u)\left[c_p(T-T_0) + \frac{(D-u)^2}{2}\right]$$
(5)

$$\xi = k\xi' = k(0.3164 \,\mathrm{Re}^{-0.25}) \tag{6}$$

 ξ' is the Blasius friction-factor. We introduce the factor k as an adjustable parameter. By combining those equations, the equation for the pressure variation can be obtained.

$$\frac{dp}{dt} = \left(\frac{dQ/dt + u(1 + 1/(\gamma - 1)M^2 f - g)}{(1 - M^2)/((\gamma - 1)M^2)}\right)$$
(7)
$$\frac{dQ}{dt} = \sum_k h_k w_k \frac{d[X_k]}{dt}$$
(8)

Here, Q is the heat generated by the chemical reactions, and M is the local Mach number. It is noted that if f=g=0 (no loss term), the eq.(7) gives the C-J condition. If there is loss term (f or g is not zero), the condition for steady propagation of detonation wave is not given by the chemical equilibrium, where dQ/dt=0. By solving the full detailed chmical rate equations, the value of eq.(8) can be obtained. In the present work, the kinetic mechanism consist of 8 species and 27 reactions is used.

Simulation results are compared in Fig.3. 1-D similation are well-fitted with a value of k=1.3 for ϕ =1.5, k=2.0

for $\phi = 1.0$, and k=1 for $\phi = 0.5$.

4 Three-dimensional simulation

The three-dimensional simulations were performed with the CFD++ software package. The grid domain was cylindrical with a diameter of 6.5 mm and length of 200 mm, and it consisted of about 1 million computational cells. The height of the first cells adjacent to the wall was 1.26E-2 mm. This height was sufficient to resolve the



Fig. 4. Mesh views on x=0.0 (left) and z=0.0 (right) cut-planes

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viscous boundary layer and heat flux through the wall while allowing an acceptably large global time step. Figure 4 shows mesh views on the x=0.0 end-wall and z=0.0 symmetry plane.

The bulk of the domain was prescribed a pressure of 53 kPa (400 Torr) and temperature of 298 K. A small region at one end of the tube was given a pressure of 799 kPa and temperature of 2000 K (sufficient to ignite the mixture and propel the shock down the tube). The entire system was initially at rest with a stoichiometric composition of H_2 and O_2 .

All boundaries of the tube were modeled as viscous, isothermal walls. A constant atmospheric temperature of 298 K was prescribed at the walls, thus, allowing heat loss from the tube.

The 18-reaction mechanism was used to solve the species equations. 8 species equations were solved, in addition to the global continuity equation. The species included H_2 , O_2 , OH, H, O, H_2O , HO_2 , H_2O_2 , and N_2 . Though there is no N_2 in the mixture, it was included as the final, "hidden" species so that any round-off error would not corrupt the solutions of free radicals with small concentrations.

Figure 5 shows the pressure and temperature profiles at the centerline of the tube at t=4.0e-5 seconds. The nearly coincident peak in both quantities indicates that the detonation is being resolved as a reacting shock. The time-dependent incrementally-averaged speed and position of the shock are shown in Figure 6. The shock speed continues to increase at a progressively lower rate, asymptotically approaching the Chapman-Jouguet (CJ) velocity, or a value close to it. The approximate CJ speed of 2810 m/s is for a detonation wave at 0.526 atm (400 Torr) with stoichiometric hydrogen-oxygen composition and was determined by interpolating between corresponding CJ speeds at 0.5 and 1.0 atm. The actual value to which the shock speed is converging may be limited by the viscous effects of the narrow tube and heat loss through the walls. The speed is nearly stabilized before the shock reaches the end-wall, as the difference in average speeds between the last two increments is only 0.37%. The average speed over the final increment is 2681 m/s.

This numerical results suggest that the detonation wave near the CJ speed has an effect of vicosity. Therefore, the relation between 3-D structures of detonation wave and the viscous effects at boundary layer must be revealed in order to understand the mechanism of detonation limit.



Fig.5 Centerline pressure and temperature at t=4.0E-5 seconds

Fig.6 Detonation wave position and speed before first reflection

References

[1] Agafonov, G.L, and Frolov, S.M., Combustion, Explosion, and Shock Waves 30 pp.91-100 (1994)