Two-Dimensional Detailed Numerical Simulation on Ammonia/Hydrogen/Air Detonation

-Stability of Cell Structure-

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1   Introduction

Detonation is the premixed and self-sustained phenomenon with supersonic propagation speed. If detonation occurs, it may lead to a major accident due to such characteristics. In fact, explosion accidents related to detonation have been recorded [1]. Therefore, it is important to study the detonation characteristics.

Ammonia fuel, which does not produce CO_2, is one of the most promising fuels for global warming and has become a growing concern around the world in recent years. Ammonia also has the advantages of easy transportation and storage, and industrial production methods have been established. Therefore, the use of ammonia is expected to increase in the future. On the other hand, ammonia is relatively difficult to burn and is known to be a fuel less likely to cause a stable detonation. [2]. Here, attempts have been made to improve the combustion properties of ammonia. For example, there are reports that hydrogen addition has improved the combustion properties of ammonia[3]. On the other hand, there are few examples of detailed evaluation of the propagation mechanism of detonation with ammonia fuel. Two-dimensional analysis of ammonia combution can be used to analyze the formation process of cellular structure and detonation propagation in detail. It is also known that detonation cell structure is an important property of detonation waves. Therefore, it is important to understand the cell structure in order to use ammonia as a detonation fuel in the future. In this study, we attempted to improve the combustion characteristics of ammonia fuel by adding highly reactive hydrogen and evaluated the characteristics of its cell structure.

2   Numerical Method

The governing equations are the two-dimensional compressible Euler equations with species conservation equations. The numerical flux for the convective term uses the hybrid method combining the Harten-Lax-van-Leer-contact (HLLC) [4] and the local Lax-Friedrich (LLF) scheme. Its accuracy is increased using the fifth-order weighted compact nonlinear scheme (WCNS) [5-12]. The fourth-order

TVD Runge-Kutta method [13] is used for the time integration method to increase numerical robustness. The chemical reaction source term is integrated by the extended robustness-enhanced numerical algorithm (ERENA) [14]. The chemical reaction model adopts the UT-LCS model [15]. The model has 32 species and 213 elementary reactions. The Cantera library[16] is used to solve this chemical reaction because the Cantera supports the PLOG function in this reaction model.

Figure.1 shows the numerical domain of the study. In this study, the shock wave coordinate system is used to reduce the calculation cost. The boundary conditions of the top and bottom walls are slip and adiabatic wall conditions. Outlet condition at the left-side boundary is decided by referring to the conditions of Gamezo et al [17]. Y_b, Y_1, and Y_e in Fig.1 refer to every boundary value, the current position in the first cell near the boundary, and the extrapolation limit, respectively. The unburned gas is composed of NH₃/H₂/air-premixed gas at 1 atm and 300 K. A small amount of burnt gas is placed behind the shock wave to create a small disturbance to start the detonation. The unburned gas enters with a Chapman-Jouguet (C-J) detonation velocity from the inlet side at the right boundary. The one-dimensional numerical results are also used to start the two-dimensional detonation.
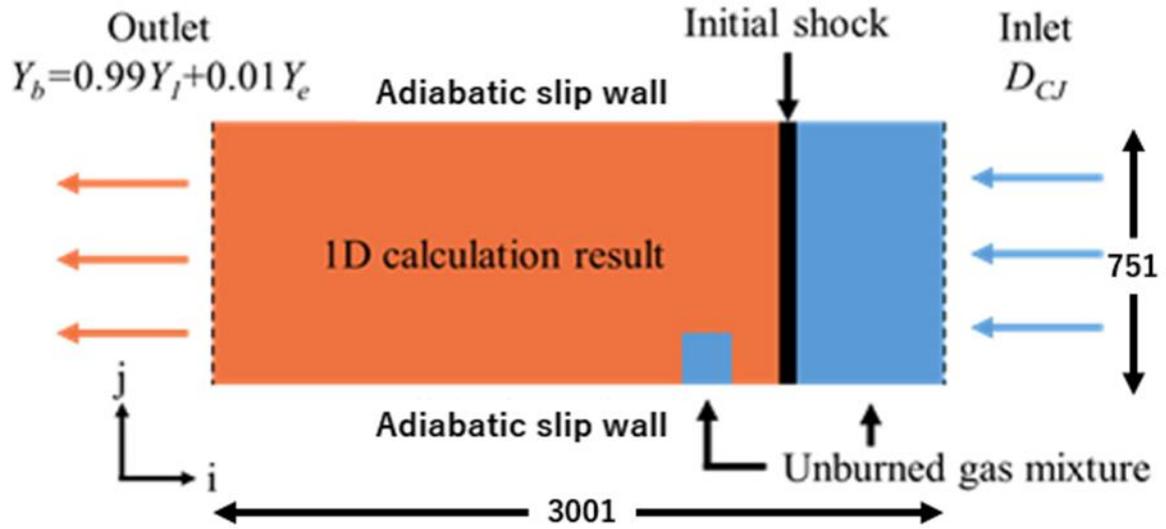

Figure 1: Present calculation domain and boundary conditions.

Table 1 shows the cases of the present study, where the ammonia/hydrogen mixing ratio was varied by changing α in Eq. (2.1).
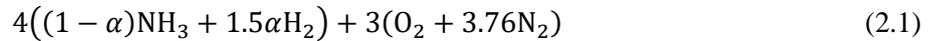
$$4\big((1-\alpha)\mathrm{NH}_3 + 1.5\alpha\mathrm{H}_2\big) + 3(\mathrm{O}_2 + 3.76\mathrm{N}_2) \tag{2.1}$$

Table 1: Simulation conditions for various α

Case	1	2	3	4
α	0.3	0.5	0.8	1.0
C-J velocity [m/s]	1888.5	1911.7	1945.9	1968.4
Grid Width [μm]	60.7	22.8	6.42	4.22
Channel Width [mm]	45.6	17.1	4.81	3.17
Channel length [mm]	151.1	57.1	16.1	10.5

At ammonia/air gas mixture(α=0), because the detonation does not start in the one-dimensional calculation, we do not calculate this case. The grid width for each case is determined to give the induction length of 50 grid points. The channel width should be determined according to the cell size of the experiment. We first decided to set the channel width of the hydrogen/air gas mixture on the experimental data from Chen et al.[17]. As a reference, the detonation cell size of the hydrogen/air mixed gas is set to about 10 [mm], and the channel width is set to about 0.3 times of the detonation limit based on Chen et al. experimental data [18]. The number of grid points (751 x 3001) has been determined because the channel width and grid size in hydrogen/air have been determined so far. Other ammonia/hydrogen/air mixtures are also calculated with the same number of grid points as hydrogen/air. The initial pressure and temperature are set to 1[atm] and 300[K].

3   Results

In all cases, detonation propagation is confirmed by two-dimensional analysis. Also, in all cases, a small cell structure is formed in the initial stage of the calculation, but a large cell structure become formed as the calculation continues.

3.1 Maximum pressure history

The cellular structure of detonation is a key characteristic of a detonation wave. Figure 2 shows the maximum pressure histories for each case. Comparing these case, it can be seen that the cell shape is irregular for case 1 and case 2. We can identify cell structures of various sizes in Case 1. In contrast, Cases 3 and 4 have a regular cell shape. Therefore, the larger the ratio of ammonia, the more irregular the cellular structure.
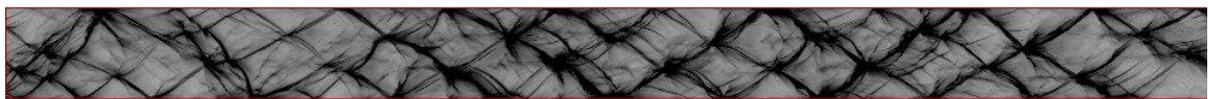
Case 1
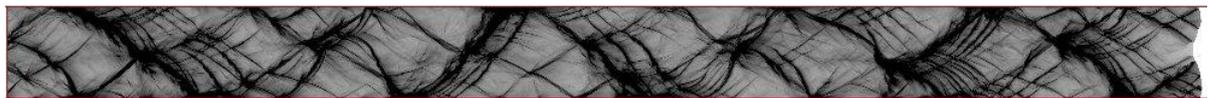
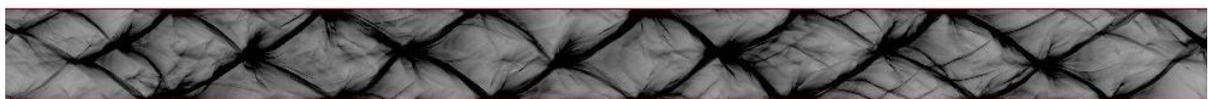2452   3065[mm]

Case 2

912   1140[mm]

Case 3

244   306[mm]

Case 4

160   200[mm]

1   Pressure[atm]   60
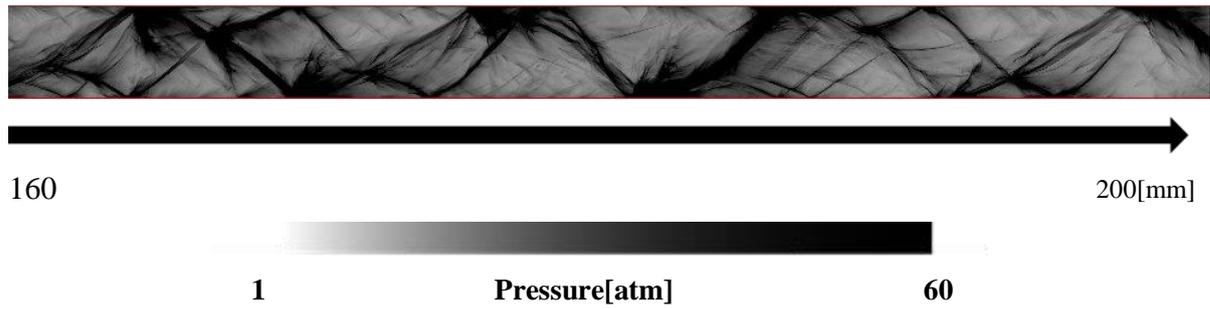
Fig.2: Maximum pressure histories for various α.

3.2 Generation of new triple points

The pressure and temperature distributions around a part of Case 2 are shown in Fig.3. The figure resolves triple points of the substructures that follow the transverse detonation (TD). The number of the triple points is higher with increasing the percentage of ammonia. The triple points are inferred to make the cellular structure show in Fig.3. Figure 4 shows the triple points process in Fig.3. Asahara showed that the sub-transverse wave behind the transverse detonation propagates to the Mach stem (MS) [19]. As shown in Fig. 4, sub-transverse waves are confirmed behind the transverse detonation in this study as well. These sub-transverse waves become a triple point while propagating as indicated by the orange arrows in Fig.4. These triple points are thought to form small cell structures.

On the other hand, Asahara showed that the sub-transverse wave is caused by the micro-explosion that occurs at the junction of the reaction front and the transverse detonation. However, this explosion could not be confirmed in this study. Therefore, calculations with smaller grids are necessary for the future.
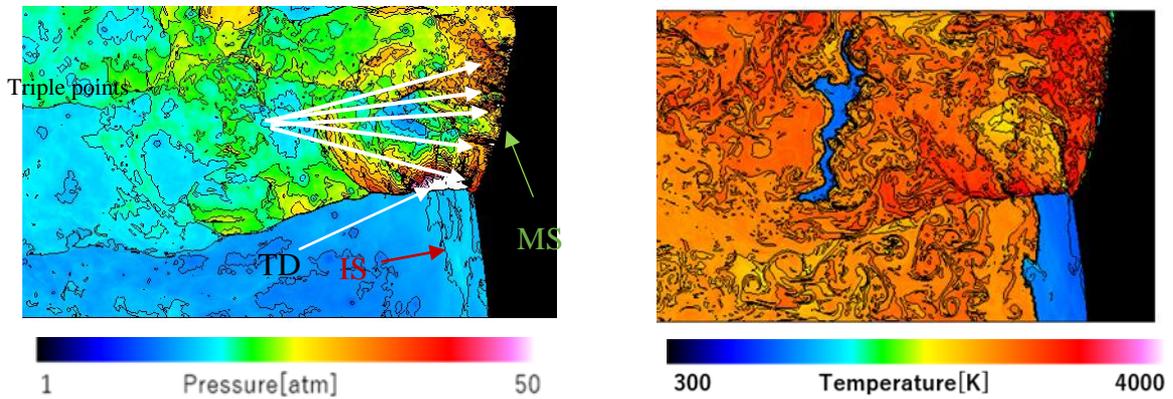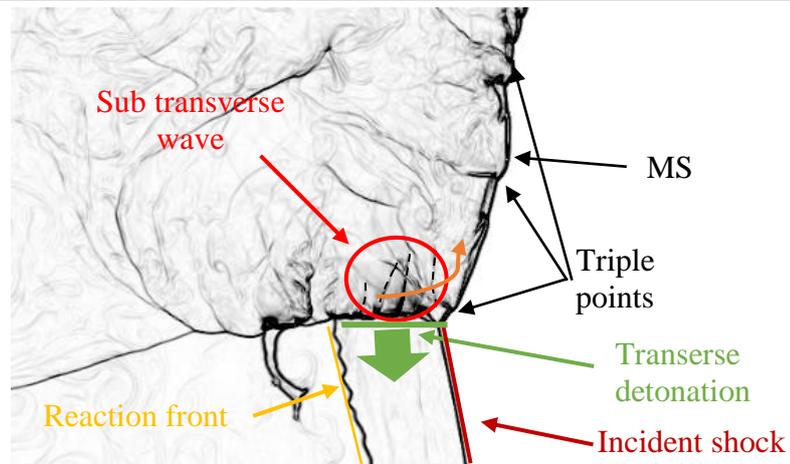

Fig.3 Irregular Cellular structure

Fig.4 Generation triple points (density gradient)

4   Conclusions

Two-dimensional detailed numerical simulations of NH$_3$/H$_2$/air detonation are performed and the results are summarized as follows:

(1) Hydrogen to ammonia fuel improves detonation stability of cellular structure by Improved reactivity.

(2) When the ratio of ammonia is large, the transverse shock wave has many triple points.

(3) New triplets are formed by the sub-transverse waves generated when transverse detonation occurs.

Acknowledgments

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