3D Numerical Simulation on Shock Front Structure of Hydrogen/Air Spinning Detonation

-Effect of Higher-order Scheme-

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1   Introduction

The wavefront structure of detonation is a phenomenon in which a shock wave heats combustible gas, and the combustion wave induced by the shock wave supports the shock wave front and propagates continuously. Since detonation propagates at supersonic speed and high pressure, its unintentional occurrence can lead directly to a major accident. Therefore, research continues from a safety perspective, but there are also attempts to apply detonation to engineering, focusing on its high thermal efficiency. Research on detonation has been conducted for about 150 years and can be divided into two main directions. One is research on the fundamental phenomena of detonation. The first is to find the fundamental phenomena of detonation, including the detailed propagation mechanism of self-sustained detonation, deflagration-to-detonation transition (DDT), and detonation cellular structure. The other is an application such as the pulse detonation engine (PDE) or the rotating detonation (RDE) using detonation as a propulsion source. In this study, the unsteady three-dimensional front structure on hydrogen-air spinning detonation in a square tube is simulated in the former research direction.

The numerical simulation on hydrogen/air detonation has been studied by various researchers with the development of computers because hydrogen is the simplest and carbon-free combustible fuel. Two-dimensional numerical simulations have been studied for various fuels such as hydrogen, hydrocarbon, and ammonia, however, three-dimensional structures are compared with experimental data for only hydrogen fuel because of the simulation cost and stiffness problems.

Tsuboi [1, 2] et al. performed three-dimensional detonation analysis in circular and rectangular tubes using a detailed chemical reaction model and clarified the propagation structures of spin, rectangular, and diagonal modes. Jackson Crane [3] et al. performed 3D numerical analyses of square and circular tubes and compared them with 2D analytical results under the same conditions and compared them with experimental results for circular tubes. The regularity of the propagation structure differs depending on the tube cross-section, the existence of a three-dimensional detonation structure, and the regularity of

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the maximum pressure history indicates that the phenomenon is fundamentally different from that of two-dimensional detonation.

Vianney Monnier [4] et al. conducted an experimental study of detonation cell widths in different cross-sectional shapes with the same cross-sectional area and initial pressure, and they investigated the maximum pressure history in the direction of detonation and the frontal plane. The results showed that there was a difference in the structure of the detonation cell between the side and the cross section depending on the initial pressure. This indicates that it is insufficient to characterize detonation from the pressure history of one side, and that information that cannot be obtained from a two-dimensional calculation can be obtained from a three-dimensional calculation. It is also clear that as the initial pressure becomes 1 atm (≈100 kPa), cell size does not depend on the cross-sectional shape of the tube.

Based on the above research, this study aims to find the influence of the higher-order numerical accuracy on the detonation front, including the ignition near the wall by using the three-dimensional simulation on hydrogen/air spinning detonation in a square tube.

2   Numerical Method

In this analysis, an in-house code is used, and the governing equations are the three-dimensional compressible Navier-Stokes equations. A comparison is made between the second-order accurate MUSCL and the fifth-order accurate Weighted Compact Nonlinear Scheme (WCNS)-Z+M method [5] for the convection term. The numerical inviscid flux uses the HLLC/LLF hybrid for MUSCL and the HLLC-LM [6] for WCNS. The detailed chemical reaction model used is the UT-JAXA model with nine chemical species and 21 elementary reactions [7], which predicts the experimental ignition delay data under high-pressure conditions. The time integration method is a ten-stage robust TVD Runge-Kutta method [8]. To reduce the computational cost, calculations are performed using the shock wave coordinate system, and the boundary condition of the inner wall of the tube was an adiabatic and slip wall. The initial pressure and temperature are 1 atm and 300 [K], respectively. The induction length in these conditions for stoichiometric hydrogen/air gas mixture is calculated by ZND to be 2.6×10^{-4} [m]. The present computational grid width uses 5 [μm] and this value is approximately 1/50 of the induction length.

Table 1: Comparison cases

	Case 1	Case 2
Grid point	601x201x201	601x201x201
Higher-order accuracy	2nd-order MUSCL	5th-order WCNS-Z+M
Detailed chemical reaction models	UT-JAXA model 9 chemical species and 21 elementary reactions	
Time integration method	Ten-stage TVD Runge-Kutta method	
Combustion gas	H_2/Air	
Equivalent ratio	1	
Initial pressure [atm]	1	
Initial temperature [K]	300	
Grid width [μm]	5	

3   Results and Discussion

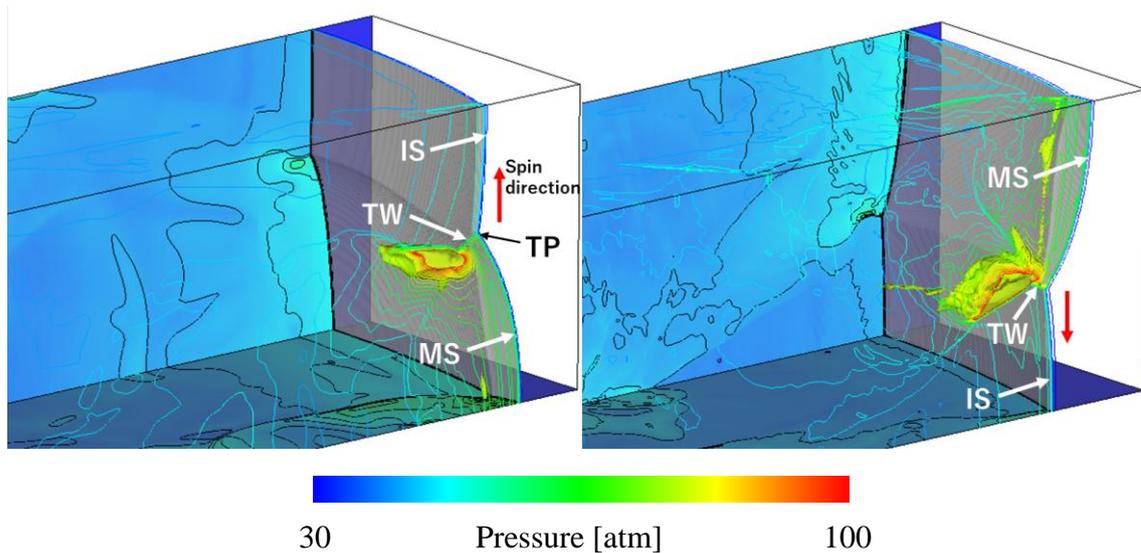### 3-1 Leading shock wave surface structure (pressure)

Fig.1 Pressure isosurface and contours behind detonation front (Cases 1 and 2).

Fig. 1 compares the leading shock wavefronts in Cases 1 and 2, viewed from obliquely behind the direction of propagation. The direction of rotation is different in both cases. Steady propagating spin detonation was observed, indicating that the initial condition was near the detonation propagation limit. Focusing on the vicinity of the shock wave surface, three types of waves, called Mach shock waves (MS), incident shock waves (IS), and transverse waves (TW), are observed to interfere with each other at the triple point (TP). Behind the triple point, there is a high-pressure area indicated in red, which has a rhombic shape in Case 1 but a triangular shape in Case 2, indicating that the structure behind the wavefront is different.

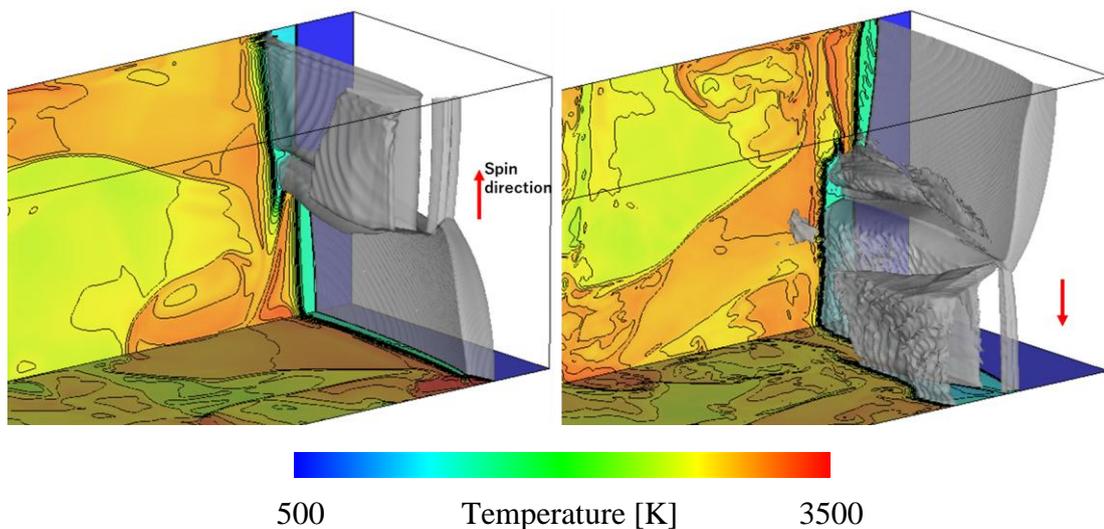### 3-2 Leading shock wave surface structure (temperature)

Fig.2 Temperature isosurface and contours behind detonation front (Cases 1 and 2).

Fig. 2 shows a temperature comparison at the same time as Fig. 1. 1400 degree isosurface is shown in gray, and the temperature distribution behind the wavefront is very different, but this is due to the different spin directions. The parallel surface behind the incident shock wave shows a rippled pattern in Case 1, but a disordered pattern in Case 2. This is thought to be due to the fact that the effect of the expansion wave caused by combustion after the shock wave passes is more dominant than the effect of the reflected shock wave from the wall due to the improved accuracy of the convection term that governs the momentum of the fluid.

3-3 OH contours

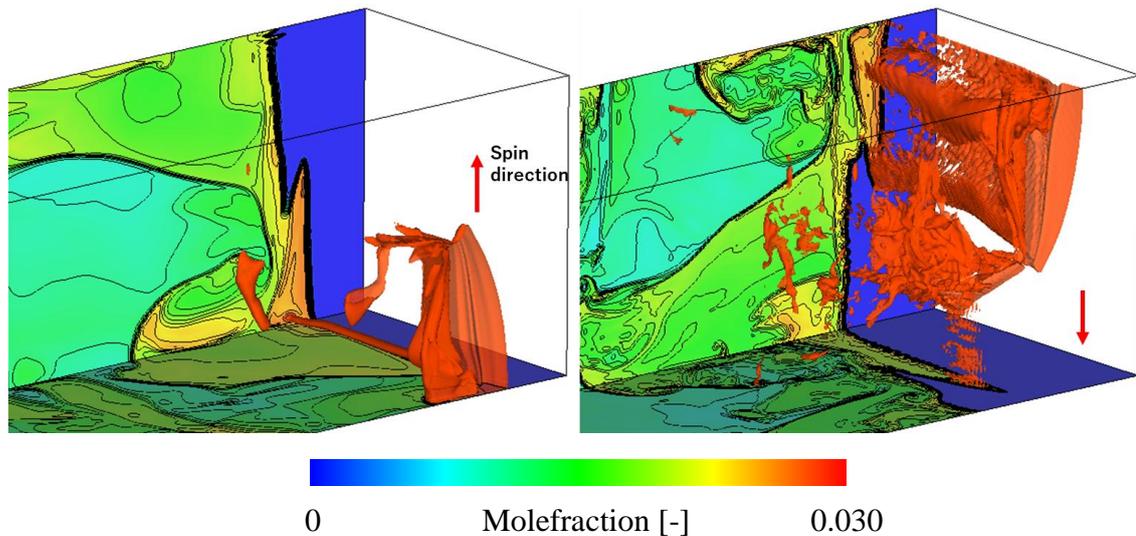0   Molefraction [-]   0.030

Fig.3 OH isosurface and contours (Cases 1 and 2)

Fig. 3 shows the distribution of OH in a composition similar to Fig. 2. Comparing the two cases, the area of dense OH distribution indicated in red is larger in Case 1 with higher accuracy, and the reaction occurs behind the triple point in Case 1, while it extends behind the Mach shock wave as well as behind the triple point in Case 2. In Case 2, the distribution of OH is also observed behind the transverse wave. It is considered that transverse detonation occurs, in which the transverse wave becomes a detonation wave and burns unburned gas.

3-4 Density gradient contours on wall
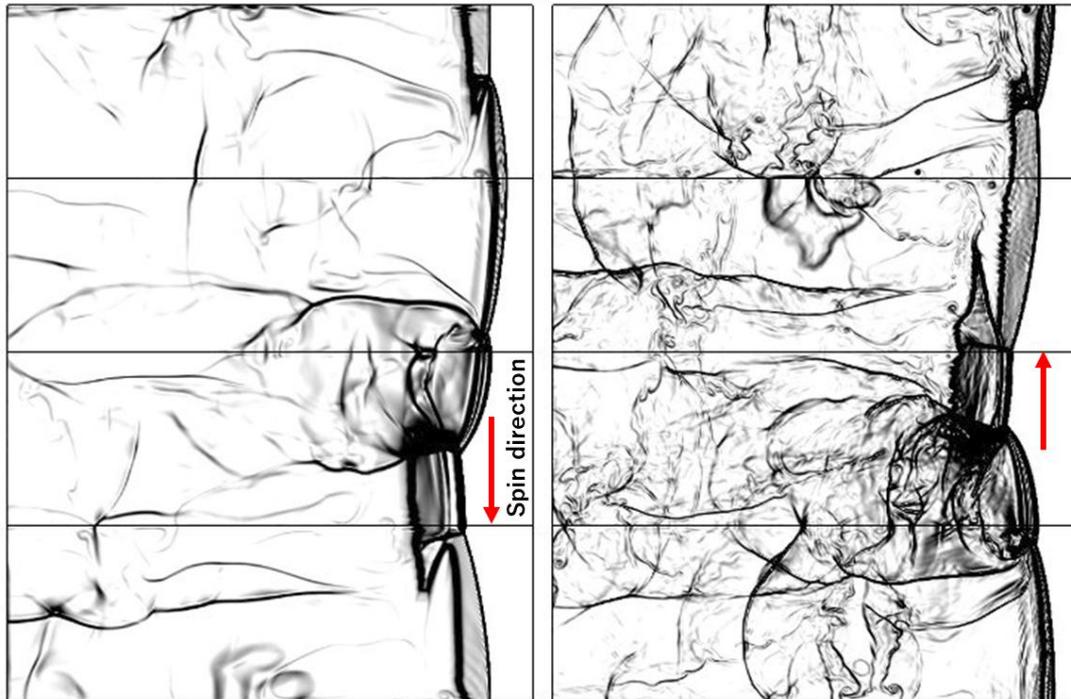
Schelen [-]

Fig.4 Density contours on wall (Cases 1 and 2)

Fig. 4 shows the density gradient of the four walls of the square tube at the same time as Figs. 1~3. In this figure, Case 1 propagates from top to bottom and Case 2 from bottom to top due to the difference in spin direction as described in 3-1. No difference in the shape of the incident and reflected shock waves was observed in the vicinity of the shock wave surface. However, behind the Mach shock wave and the transverse wave, a more complex and detailed pattern appears in Case 2, and a density gradient of the combustion gas can be observed. This may be due to the effect of the expansion wave caused by the small explosion in Case 2 of 3-3, which is caused by transverse detonation. In summary, the density gradient is not caused by the increased accuracy, but rather the increased accuracy causes transverse detonation, which in turn causes the density gradient to become more pronounced.

These results indicate that the effect of higher-order accuracy in this analysis does not appear near the leading shock wave front, but appears well behind it. The analysis of the propagation structure formed by the regular intersection of longitudinal and transverse waves could not be performed this time because of the spin. In the future, it is necessary to change the initial conditions to move away from the propagation limit, select a propagation mode other than spin, and confirm that structural changes behind the wavefront appear as in the present study by using higher-order accuracy, and to conduct quantitative analysis. We would also like to analyze what parts in the vicinity of the wavefront are affected by the higher-order accuracy and what causes transverse detonation.

4 Conclusions

A three-dimensional analysis of hydrogen/air detonation was performed, and the following conclusions were drawn about the wavefront structure and the effect of higher-order accuracy.

(1) In the numerical analysis of hydrogen/air detonation, the structure of the leading shock wave shows little difference depending on the calculation accuracy of the convection term.

(2) The structure behind the leading shock wave surface is affected by the calculation accuracy, and the transverse detonation phenomenon is confirmed from the OH distribution behind the transverse wave at high accuracy.

(3) The influence of the convective term is not significant. The influence of the higher accuracy of the convection term is also shown in the density gradient away from the wavefront, which affects the structure near the upstream wavefront.

Acknowledgments

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