Numerical Simulation on Two-Dimensional Detonation with Boundary Layer

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Two-dimensional full Navier-Stokes simulations on the detonations are presented in order to estimate the boundary layer development behind the front. The multi-zone grid system is applied to simulate the detonation front and the boundary layer. The results show that the boundary layer thickness behind the front is approximately 10% of the channel width for the adiabatic wall and 20% for the isothermal wall. The detonation velocities are also affected by the wall boundary due to the boundary layer thickness.

1 Introduction

Detonation is a shock-induced combustion wave propagating through a reactive mixture or pure exothermic compound, and has been studied from the safety engineering point of view such as for coal mine explosions or from the scientific point of view of astrophysics as in star explosions. Numerical simulations on the detonations usually neglect viscous and thermal losses because its propagation speed is supersonic and the pressure at Chapman-Jouget state is approximately 20 times the initial pressure. However, the DDT (Deflagration to Detonation Transition) phenomena are generated by the strong turbulent and viscous effects near the wall so that the numerical simulations on DDT must include the viscous and thermal effects in the governing equations[1].

The propagations near the detonation limit are also affected by the viscous and thermal losses. The single spinning detonation appears near the detonation limit and the experimental and numerical researches show that the spinning detonation stably propagates in the tube[2, 3]. The detonation velocity of the spinning detonation is approximately 80∼90% of D_{CJ} and this reason is thought to be the viscous effects.

These detonation velocity deficit can be simulated by using the ZND simulations including the laminar viscous and thermal losses[2, 4]. One parameter in these simulations, which changes the amount of friction loss and heat loss, control the effects of their losses as the numerical results agree with the experimental results. Fay[5] found that the magnitude of the velocity deficit was consistent with the existence of the boundary layer by using analysis. However, the release energy near the spin head also decreases near the detonation limit with decreasing the initial pressure. This means that the transverse detonation in the spin head also becomes weak to decrease the propagating velocity. The dependency of the initial pressure on the release energy is also included in the CJ state, however, the multi-dimensional effects are not included. Therefore the effects of the release energy cannot be cleared on the two-dimensional and three-dimensional detonations. Furthermore, it should be evaluated whether the viscous losses or the reduction of the release energy dominate on the detonation velocity deficit under the low pressure conditions.

In this paper, the results of the two-dimensional full Navier-Stokes simulations for the detonations are presented. Final goal is to estimate the viscous losses and the reduction of the release energy on the three-dimensional spinning detonation. At first, the present paper discusses the boundary layer development near the wall behind the detonation front by using some fine grids near the detonation front and the wall.

2 Numerical Method

The governing equations are the full Navier-Stokes(NS) equations with 9 species ($H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O$, and N_2) and 18 elementary reactions and they are explicitly integrated by the Strang type fractional step method. The chemical reaction source term is treated in a linearly point-implicit manner. A Harten-Yee non-MUSCL type TVD scheme is used for the numerical flux [6]. The Petersen and Hanson model[7], which is a detailed chemical reaction model, is used for chemical kinetics to solve detonation problems.

The computational meshes are shown in Fig. 1. The present grids consist of three grids. Zone 1 (grid points are 401x401) is produced near the detonation front and its resolution is 2.5 μm. Zone 3 (201x101) is for the reward domain with 10 μm or coarser resolution. Zone 2 (101 x 201) connects between zone 1 and zone 3. All grids have minimum grid width of 2.5 μm near the walls. 2.5 micrometer corresponds to a resolution of 64 grid points in the theoretical half reaction length which equals 1.6×10^{-4}m for H_2 at atmospheric pressure. The length of the computational domain is seven times the channel width. The channel width is 1 mm.

The boundary conditions are as follows: the upstream conditions are at pressure of 0.1 MPa and temperature of 300K, and the upstream gas is stoichiometric H_2/air gas mixture; the wall boundary conditions are non-slip, and non-catalytic. The wall condition selects the adiabatic wall or the isothermal wall with 300 K, respectively. The downstream condition is the non-reflected boundary proposed by Gamezo et al.[8]. The present simulations adopt the moving grid system instead of the wave coordinate system because a carbuncle at the detonation front appears near the wall. This means that the computational grid moves with CJ velocity. The time-dependent metrics are included in the present numerical schemes.

The initial conditions for the one-dimensional simulations are given in two computational domains with high pressure in the vicinity of a closed end wall and low pressure. These results are used to start the two-dimensional simulations.

3 Results and Discussions

Figure 1(right) shows the comparison of maximum pressure histories between the results of the Euler, NS+slip, NS+non-slip adiabatic wall, and NS+non-slip isothermal wall, respectively. The results for inviscid simulation do not use the moving grid system but the wave coordinate system. These results show that the lengths of the cells are not affected by the viscous effects. These lengths of the cells also are not affected by the moving grid system. Therefore the present method can simulate adequately.

The instantaneous contours near the detonation front are shown in Fig.2(left). The present resolution near the front increases more than the previous authors' simulations. The shock waves near the front can be observed clearly and the viscous effects appear near the upper and lower walls. The ignition delays in the temperature and H_2 mass fraction contours are observed near both walls as shown in Fig.2(left). These features should be carefully estimated by using finer grid resolution than the present

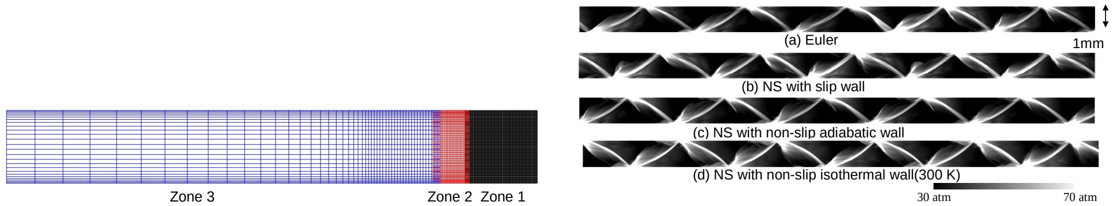

Figure 1: Present grid system and maximum pressure histories. Left: Computational grid in present simulation. A grid point for every four points is plotted. Right: Maximum pressure histories in 2D simulations.

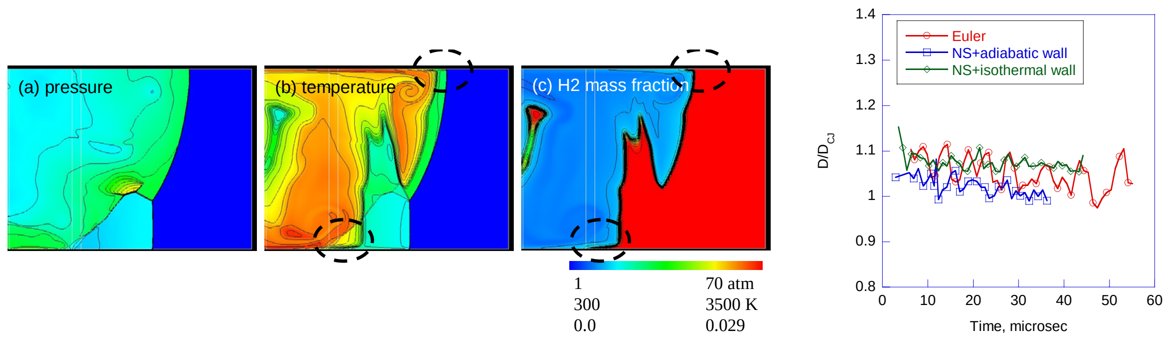

Figure 2: Instantaneous results and detonation velocities. Left: Instantaneous contours for NS+non-slip(adiabatic wall). Right: Average detonation velocities during one cycle.

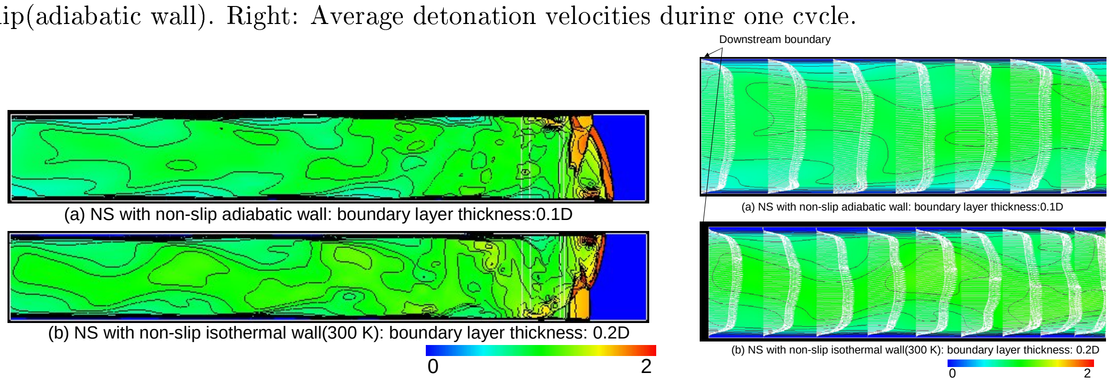

Figure 3: Instantaneous Mach number contours and velocity vectors for NS+non-slip. Left: Whole domain. Right: Close-up view near downstream boundary. D is the channel width.

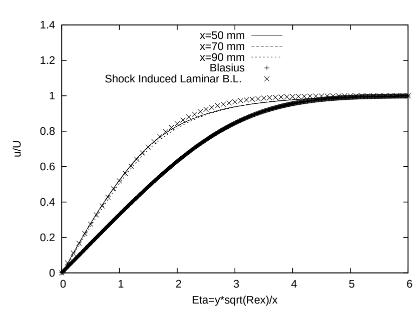

Figure 4: Comparison between calculated shock induced boundary layer profiles and theories.

simulations.

Figure 3 shows the Mach contours and velocity vectors in the whole domain and near the downstream boundary. These results present the effects of the wall boundary conditions. The detonation propagates so fast that the isothermal wall is thought to be more realistic wall boundary condition. These results show that a thick boundary layer develops from the detonation front for both cases. The thickness of the boundary layer at the downstream boundary is approximately 10% of D for the adiabatic wall and 20% of D for the isothermal wall, respectively, where D is the channel width. The boundary layer cannot develop thicker than the present results because the pressure fluctuation due to the detonation front impacts on the boundary layer. These results should be estimated carefully by comparing with the results of the boundary layer development behind the moving shock wave[9].

Figure 2(right) shows the averaged detonation velocities during one cycle. Though the simulations should be continued more than the present results, the detonation velocities for the adiabatic wall are lower than those for the isothermal wall. This reason would be the displacement effects of the boundary layer. As the boundary layer thickness for the isothermal wall is twice that for the adiabatic wall, the pressure behind the detonation front increases to generate a piston effects on the detonation. These features are also estimated by using the longer computational domain, finer grid near the wall, longer simulation time, and comparing with simple analytical methods.

Finally, the moving shock simulation without combustion also estimated by using the present simulation code. The shock Mach number is 1.9, $Re = 50 \times 10^6$/m, upstream gas is air, initial pressure is 0.1 MPa, and initial temperature is 300 K. The channel width is 3 mm and minimum grid size near the bottom wall is 0.5 μm. The wall is adiabatic boundary condition. The laminar flow is assumed. The results and the comparison with the theories are shown in Fig.4. The velocity profiles in the boundary layer agree well with the shock induced laminar boundary layer theory proposed by Sturtevant et al[10]. The velocity gradient in the boundary layer behind the moving shock wave is 60% larger than the Blasius theory.

4 Conclusions

Two-dimensional full Navier-Stokes simulations on the detonations are presented in order to estimate the boundary layer development behind the front. The multi-zone grid system is applied to resolve the detonation front and the boundary layer behind the front. The present results show that the boundary layer thickness behind the front is approximately 10% of the channel width for the adiabatic wall and 20% for the isothermal wall. The detonation velocities are also affected by the wall boundary due to the boundary layer thickness.

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