Three-Dimensional Simulation on Deflagration to Detonation Transition with a Detailed Chemical Reaction Model

T. Machida[1], M. Fukuda[1], M. Asahara[1], E. Yamada[1], A. K. Hayashi[1], and N. Tsuboi[2]

[1]Department of Mechanical Engineering, Aoyama Gakuin University,
Sagamihara, Kanagawa, Japan
[2]Department of Mechanical and Control Engineering, Faculty of Engineering, Kyushu Institute of Technology,
Kitakyushu, Fukuoka, Japan

1 Introduction

Various experimental or computational studies on detonation have been performed since the study on detonation was started over 130 years ago. On computational study, Taki and Fujiwara [1] performed in 1978 two dimensional simulation of detonation for the first time. While detonation involves risk or danger which could lead to serious accidents because of its explosive reactivity, a lot of research is performed in terms of the applications for the next-generation propulsion systems of aerospace plane.
On deflagration to detonation transition (DDT), many studies are performed fundamentally and applied to the next-generation propulsion system. Urtiew and Oppenheim [2] visualized DDT using the Laser Schlieren photography. Though the overview of DDT is revealed by such experiments, the details are not clarified yet. Therefore the details of DDT are the problem which hoped to solve. Hence, it is hoped that the DDT phenomenon is made clear by numerical simulation because the process of DDT is highly complex phenomena. Nevertheless numerical simulation on DDT did not progress much because DDT includes not only detonation but also deflagration which propagates slowly compared to the detonation. Thus the simulation of the DDT calculation is taken time much more than the detonation's one. As a recent study on DDT, Liberman et al. [3] performed two-dimensional simulation with a simple chemical reaction mechanism which has very large area of 10 mm x 1200 mm. Generally, the pressure is elevated very high in detonation. Then the chemical reaction model which includes pressure dependence should be used in the numerical simulations on DDT.
Detonation wave is treated adiabatically on the wall because it is supersonic phenomenon, but the heat loss on the wall should be considered in DDT because the DDT initiation involves deflagration stage. Therefore, in the present study, three-dimensional simulations are performed under the boundary conditions of isothermal wall.
On the other hand, DDT is discussed whether its flow field is turbulence or not. Kuznetov et al. [4] performed experiments with smooth tubes for DDT and showed that DDT and flame acceleration are influenced on turbulent boundary layer. Wu et al. [5] performed the experiment with small tubes using ethylene and reported the flow field of DDT and flame are turbulence flow in terms of the Reynolds

Correspondence to: c5612103@aoyama.jp

number. Thus, it is necessary that the numerical simulation on DDT includes turbulence influence. In this study, Baldwin-Lomax model [6] is applied as a turbulence model because of its simplicity and computational cost. Numerical results obtained are compared to numerical study by Fukuda et al. [7]. Three-dimensional simulation is performed using the code which is converted from the conventional two-dimensional code used in a past study.

2 Numerical simulation setup

In this simulation, the compressible Navier-Stokes equations and mass conservation equation for each species (H_2, O_2, H, O, OH, HO_2, H_2O_2, and H_2O) are used. As the numerical method for each term of the equations, Harten-Yee's non-MUSCL modified-flux type TVD scheme is used for the convection term, point implicit method is used for source term, and fractional time step method by Strang is used for unsteady term. Moreover, the detailed chemical reaction model by Petersen et al. [8] including pressure dependence is used.

In 3D simulation, a rectangular tube is used which has the source region (I) which is semi-sphere of 0.5 mm in diameter, high pressure and temperature region (II), and ambient region (III) are shown in Figure 1. Grid points are set at even intervals in 8.0 μm for x-direction, and set as finer near the wall than other area in 1.0 – 8.0 μm for y-direction and z-direction to solve the boundary layer. As for boundary conditions, opposite side of boundary which is set source region is set to free outlet boundary and the others are set to isothermal and non-slip wall boundary. The mixture gas of stoichiometric H_2-O_2 is filled in each area. Also the total grid points for 3D calculating area is about 66 million points; x, y, and z are 1875, 188, and 188 points, respectively. Physical size of the numerical domain is 15 mm, 1 mm, and 1 mm for x, y, and z direction respectively. This grid system is made using Gridgen, by setting physical size of the domain and then the number of grid point. Shock conditions are not set in the initial condition, but the pressure and temperature difference between region (II) and (III) are set, thus when the calculation is started, the precursor shock propagates to the region (III) from the region (II).

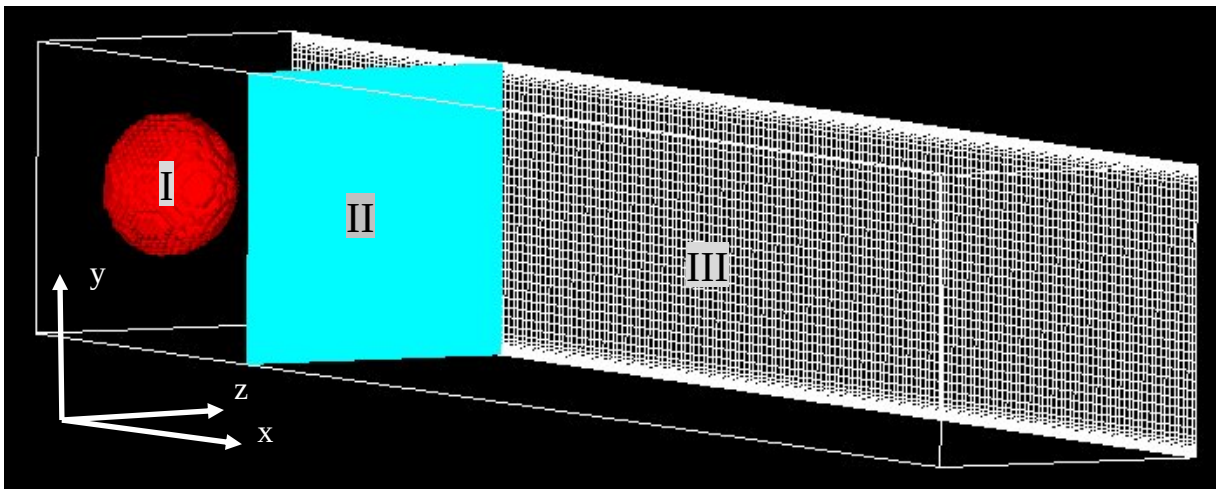

Figure 1. Schematic drawing of calculating area for 3D simulation ; Ⅰ: source region, Ⅱ: high pressure and temperature region, Ⅲ: ambient region.

The initial conditions of this simulation are shown in Table 1.

Table 1: Initial conditions for each region.

	P_I [MPa]	T_I [K]	P_{II} [MPa]	T_{II} [K]	P_{III} [MPa]	T_{III} [K]
	2.5	2000	1.52	705	0.073	300
Grid	1875×188×188					

To decide the coefficient of eddy viscosity μ_t , in this simulation, Baldwin-Lomax [6] model is used. The boundary layer is considered separately in inner and outer layer in this model. The coefficient μ_t in inner layer is expressed by the formulation of Prandtl-Van Driest and the coefficient in outer layer is expressed by the modified formulation of Clauser. The influence of the turbulence is estimated for the term of coefficient μ_t and the viscosity coefficient is taken place to the coefficient of eddy viscosity μ_t which is expressed in following equation:

$$\mu_t = \begin{cases} \mu_{t,inner}; y_n \le y_{crossover} \\ \mu_{t,outer}; y_n > y_{crossover} \end{cases}$$

where y_n is the distance from the wall in vertical and $y_{crossover}$ is the smallest distance from the wall where $\mu_{t,inner}$ is equal to $\mu_{t,outer}$. Finally, the coefficient of eddy viscosity is determined by following equations:

$$\begin{cases} \mu_{t,inner} = \rho l^2 |\omega| \\ \mu_{t,outer} = \rho K C_{CP} F_{WAKE} F_{KLEB}(y_n) \end{cases}$$

where, ρ is the density, l is the mixing length , ω is the vorticity, K is the Karman constant, C_{CP} is the correction factor, and F_{KELB} is the intermittency factor respectively.
This model is the 0 th order turbulence model. In the simulation, present model is picked up bucause of its simplicity. Nevertheless it is not clear that the model estimates the eddy viscousity correctly or not.

3 3D effects on propagating construction of DDT

Figure 2 shows the comparison between 2D and 3D simulation on the sequence of temperature profiles under the isothermal wall boundary condition. 2D result in Figure 2(a) is shown by Fukuda et al [7].

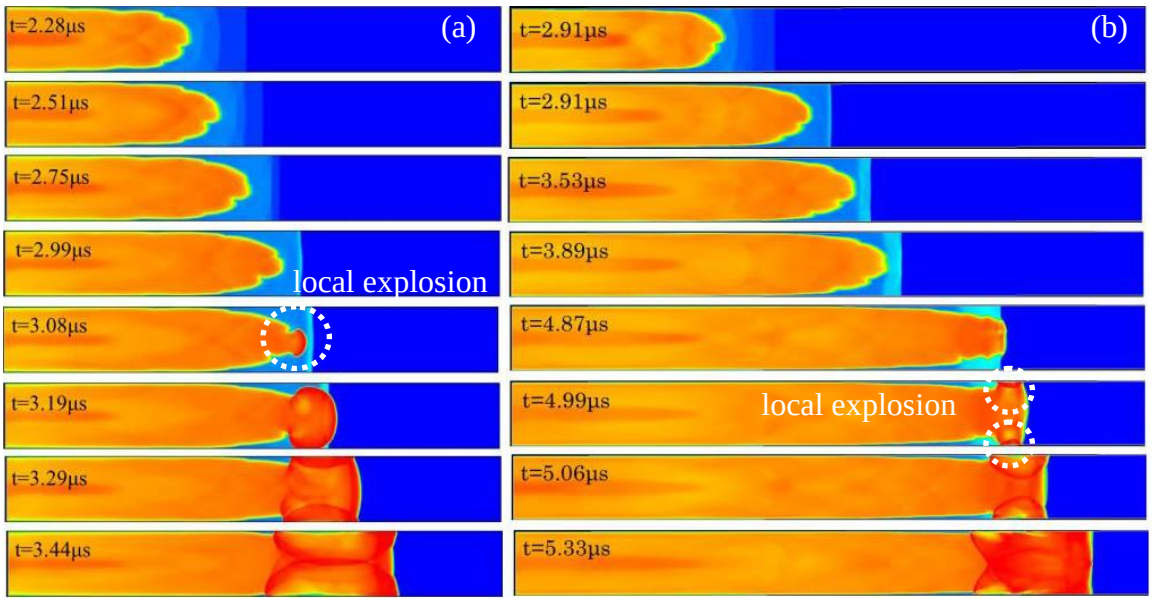

Figure 2. Comparison between 2D and 3D simulation on sequence of temperature profiles under the isothermal wall boundary condition; (a): 2D and (b): 3D in x-y plane near the center of z-direction.

As shown in Figure 2, while time of transition of deflagration to detonation is different between 2D and 3D simulation, the qualitative phenomena such as flame configuration or local explosion in 2D result are similar to 3D result. 2D-DDT could be reproduced in 3D simulation because the similar things occur in 2D and 3D simulation. Nevertheless, this phenomenon is in detail, quite different between 2D and 3D. In 2D simulation, the flame accelerates while generating shock ahead and local explosion occur near the center of y-direction just behind the shock wave because the reaction is highly promoted by high temperature behind the shock wave. As a result, DDT occurs in short time because of this local explosion in 2D simulation. While in 3D simulation, the flame overtakes the shock wave without the local explosion and then the flame propagates toward both walls. The local explosions occur near the upper and bottom walls. As a result, DDT also occurs because of these local explosions in 3D simulation. The reason why the flame overtakes the shock wave is high pressure and temperature behind of the shock wave which is coupling of the precursor shock generated by pressure difference between region (II) and (III) and the compression waves produced by the flame. In 2D simulation on isothermal wall boundary condition, the local explosion occurs near the center in the channel, but on adiabatic wall boundary condition, it occurs near the wall. Therefore the results are caused by particular condition like a shooting problem and another initial condition might bring the another results.

The difference of initial source energy between 2D and 3D could be considered as the one of reason about this different result. Initial pressure in source region is 1.8 MPa in 2D simulation and is 2.5 MPa in 3D simulation. Moreover, Initial pressure in shock wave region is 1.048 MPa in 2D simulation and is 1.52 MPa in 3D simulation. If the amount of energy, which provided for the source region as initial condition, is defined by the internal energy, it is expressed with ratio of specific heat, pressure, and volume, and the volume is taken placed in the area for 2D simulation. Therefore in case of the comparison between 2D and 3D, non-dimensional source energy by the area or volume should be used. The sequence of DDT in 3D simulation is shown in Figure 3.

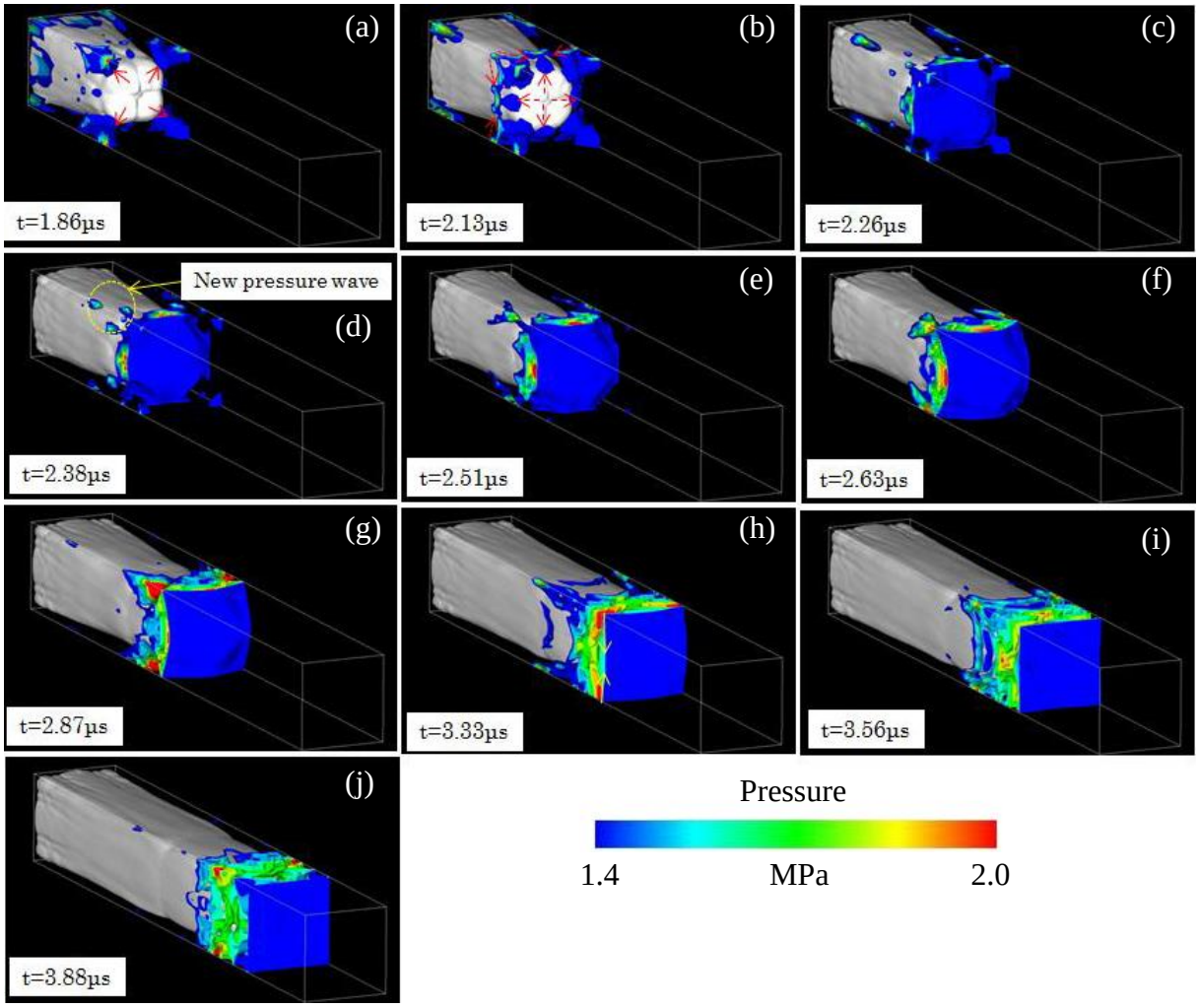

Figure 3. Sequence of pressure profiles (color scale) and temperature profiles (gray scale) under the isothermal wall boundary condition when the pressure of initial source region is 2.5 MPa.

As shown in Figure 3 (a), the pressure waves are generated toward each four corners (indicated in red allows) and as shown in Figure 3 (b), the pressure waves are generated toward each four walls (indicated in dashed red allows). Moreover, the pressure wave surface appears in front of the flame because of the combination of each pressure wave as shown in Figure 3 (c). Then, the new pressure waves are generated and propagate at the corner as shown in Figure 3 (d). Furthermore, after the generation of the high pressure spots at the corner, the pre-heated zone is generated behind the shock wave and the flow field becomes turbulent. In the 2D simulation, the high pressure zone which propagating at the corner is not generated because 2D simulation has not z-direction. The pre-heated zone is formed by the pressure wave which propagating toward the propagation direction from the flame front in 2D simulation, however, it is formed by the pressure wave which propagating toward the walls from the center of the tube in 3D simulation. It is considered that this phenomenon is the difference between 2D and 3D as for the location of local explosion. Finally, the temperature and pressure distribution at t = 3.77 μs are shown in Figure 4. It is confirmed that the Shock wave generated by the piston effect of the flame which is confirmed in 2D simulation is also represented in 3D simulation.

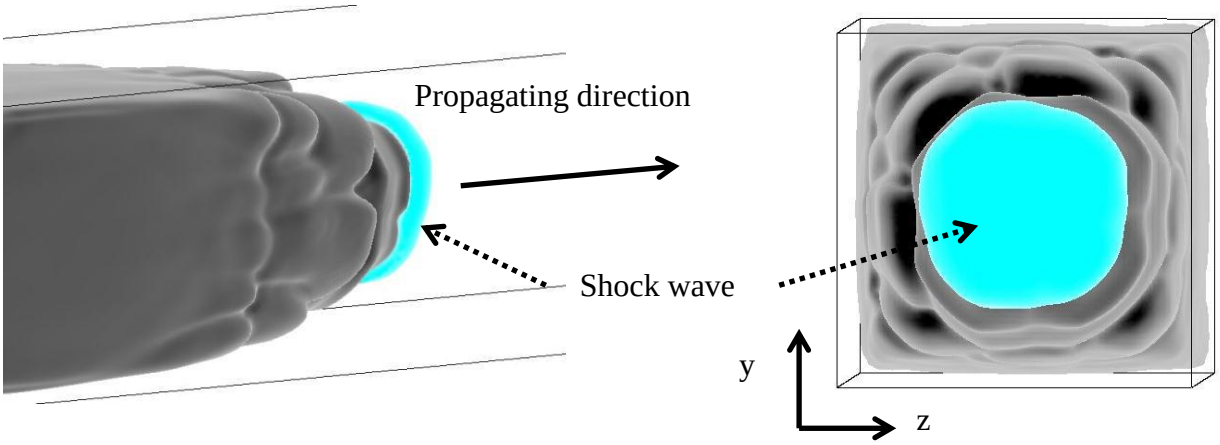

Figure 4. The temperature (as shown in gray scale) and pressure (as shown in light blue) profiles at t = 3.77 μs. The pressure profiles are shown as the isosurface in 25.0 MPa.

4 Conclusions

In this study, the three-dimensional simulation on DDT of stoichiometric H_2-O_2 mixture with a detailed chemical reaction model is performed. It is revealed that 3D effects exist for propagating mechanism of DDT in high pressure zone by compared with the two-dimensional simulation on DDT by Fukuda et al [7]. In the 2D simulation, the pre-heated zone is generated by the pressure wave which is propagating from the flame front, however in 3D simulation, it is generated by the pressure wave which is propagating to wall from the center of the tube. It is confirmed that the Shock wave generated by the piston effect of the flame is represented in 3D simulation.

References

[1] Taki S and Fujiwara T. (1978). Numerical analysis of two-dimensional non-steady detonations. AIAA Journal. 16: 73.

[2] Urtiew PA and Oppenheim AK. (1966). Experimental Observations of the Transition to Detonation in an Explosive Gas. Proceedings of the Royal Society. 295: 13.

[3] Liberman MA, Ivanov MF, Kiverin AD, Kuznetsov MS, Chukalovsky AA, and Rakhimova TV. (2010). Deflagration-to-detonation transition in highly reactive combustible mixtures. Acta. Astronautica. 67: 688.

[4] Kuznetsov M, Alekseev V, Matsukov I, and Dorofeev S. (2005). DDT in a smooth tube filled with a hydrogen-oxygen mixture. Shock Waves. 14: 205.

[5] Wu M, Burke MP, Son SF, and Yetter RA. (2007). Flame acceleration and the transition to detonation of stoichiometric ethylene/oxygen in microscale tubes. Proceedings of the combustion institute. 31 : 2429.

[6] Baldwin BS and Lomax H, Thin-layer approximation and algebraic model for separated turbulent flows. (1978). AIAA Paper. 78-257.

[7] Fukuda M, Dzieminska E, Hayashi AK, Yamada E, and Tsuboi N. (2011). 23rd International Colloquium on the Dynamics of Explosions and Reactive Systems. Paper number: 207.

[8] Petersen EL, Davidson DF, and Hanson RK. (1999). Reduced Kinetics Mechanisms for RAM Accelerator Combustion. Journal of Propulsion and Power. 15: 591.