Multidimensional Wave Propagation of Direct Initiation on Detonation

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1 Introduction

Detonation is a supersonic combustion wave propagating with a leading shock wave. It is confirmed that detonation has an unsteady property and a complicated propagating structure, and it propagates lengthwise and crosswise with transverse waves. Direct initiation is known as the method to initiate detonation. It is the method in which the reaction starts by self-ignition behing the leading shock wave generated from the high-energy source, and detonation occurs. In the previous experimental investigations [1,2], it was specified that there was the critical energy for initiating detonation. The numerical study on direct initiation by Eckett et al. [3] demonstrated that the unsteadiness of the induction zone was dominant in the failure of spherical detonation, numerically comparing the magnitude of the term of the curvature, heat release and unsteadiness by the reaction-zone structure equation. Watt and Sharpe [4] carried out the two-dimensional simulation in order to determine the cellular stability. They clarified the cell length and the evolution strongly depended on the grid resolution and the cells were more irregular at the higher grid resolution.

In this paper, initiation process of spherical detonation by direct initiation with various initial energy is numerically investigated in two-dimensional simulations. In addition, the propagating wave front structure of spherical detonation is discussed.

2 Numerical Setup

The governing equations are one-dimensional compressible Euler equations for spherical symmetry and two-dimensional compressible Euler equations for axis symmetry with one-step reaction model of Arrhenius' form. For convective term, numerical scheme is Yee's non-MUSCL type 2^{nd}-order upwind scheme. Point-implicit method that treats only source term implicitly is used for time integration. Physical values in the governing equations are normalized by standard values and half-reaction length $L_{1/2}$. Half-reaction length is the distance required for mass fraction of reactant reducing to 0.5 in one-dimensional steady analysis for CJ detonation and it is used as unit length. Grid resolution is definded by grid points in half-reaction length. Chemical parameters in the reaction model are activation energy E_a, heat released parameter Q and specific heat ratio γ. These values are identical to Ref. 3 as E_a=17.0, Q=22.5 and γ=1.2. Initial condition consists of two regions; high-energy region with burned gas and ambient region with premixed gas. In the former region, the radius of the region is fixed to 19.0 $L_{1/2}$ and only total energy E normalized by standard pressure and half-reaction length cubed is changed. According to the Ecketts' report, non-dimensional critical energy is 166×10^6 under their condition. Temperature and density are obtained from equation of isentropic relation. The latter condition is standard state. Since flowfield has symmetric property, mirror condition is used on the symmetric plane as the boundary condition. Circular and orthogonal grids are used in two-dimensional simulation. The computational region is long enough to avoid the influences of detonation reaching the calculating boundary. The domain where a leading shock wave arrived is calculated because of reducing computational time.

3 Results and Discussions

One-dimensional simulations were carried out to clarify the influences of the initial total energy and grid resolution on the propagating direction. Figure 1 shows the shock pressure histories of E=50x10^6, 100x10^6, 166x10^6 and 169x10^6. 20 points per half-reaction length are set as the grid resolution. The dashed line in Fig. 1 denotes the value of von Neumann spike for CJ detonation (P_{vN}=20.03). The result indicates that detonation did not occur in the cases of less than 169x10^6. In the successful case of 169x10^6, after the pressure of the shock wave kept decaying like the failed cases, it drastically increased at t=100. The time of the maximum pressure denotes the moment of detonation initiation and detonation became the overdriven state instantaneously then. Figures 2 (a) and (b) respectively show the pressure histories of E=166x10^6 and 169x10^6, changing grid points in half-reaction length to 5, 10, 20, 50 and 100. The results in Fig. 2 indicate that the energy required for the initiation did not depend on the grid resolution. In the initiated case of Fig.2 (b), as the grid resolution was higher, the time when detonation occurred converged to t=95 and the maximum pressure value increased. From the above, it was demonstrated that the total energy required for initiating detonation was at least 169x10^6, regardless of the grid resolution. That corresponded to the Ecketts' report [3].

Figure 3 (a) shows the shock pressure histories on the line of X=Y in E=50x10^6, 100x10^6, 166x10^6 and 169x10^6. Figures 3 (b)-(d) respectively show the temperature distributions of E=50x10^6, 166x10^6 and 169x10^6 at t=110 in two-dimensional simulation with circular grid. As the grid resolution, 20 points and 1 point are set in the radial and the circumferential directions respectively. The results in Fig. 3 (a) were good agreement with the results in Fig. 1. The reaction zone separated from the shock wave and the distance between them spread widely in the failed cases of Figs. 3 (b) and (c). Especially, that was clarified in Fig. 3 (b). The shock wave deaccelerated due to the separation. On the other hand, the shock wave and the reaction zone coupled, propagating as detonation in Fig. 3 (d). Comparing the flowfields of 166x10^6 and 169x10^6, the positions of the shock wave were almost equal, however temperature behind the shock wave was different mainly. This is the difference between detonation and shock wave. It was found that the results of two-dimensional simulation with the circular grid were good agreement in those of the one-dimensional simulation. As the reason, since the computational grid was formed perpendicularly for the propagating direction, the shock wave and the reaction zone propagated one-dimensionally.

Figure 4 (a) shows the shock pressure histories on the line of X=Y in E=50x10^6, 100x10^6, 166x10^6 and 169x10^6. Figures 4 (b)-(d) respectively show the temperature distributions of E=50x10^6, 100x10^6 and 169x10^6 at t=65 in two-dimensional simulation with orthogonal grid. 10 points per unit length are set in the X and Y directions as the grid resolution. In Fig. 4 (a), detonation occurred and the irregular pressure jumps appeared, excepting the case of 50x10^6. In the successful cases, the periods of pressure jump were different and the case of 100x10^6 had longer period than those of 166x10^6 and 169x10^6. The result of 166x10^6 was quantitatively good agreement in that of 169x10^6. In the failed case of Fig. 4 (b), the reaction zone separated from the shock wave. On the other hand, the shock wave propagated with the reaction zone and the transverse waves were generated at the detonation front in Figs. 4 (c) and (d). The pressure jumps in Fig.4 (a) indicate the collisions of the transverse waves. The collisions make up for pressure decaying and the detonation propagation is carried on. The results of Figs. 3 and 4 imply that the propagating mechanism and the energy required for the initiation were different. The cause was due to the increase of the numerical disturbance. Since the orthogonal grid was not formed perpendicularly for the propagating direction, the disturbance increased further in the comparison with that of the circular grid. The increase of the disturbance made the detonation front unstable and the transverse waves were generated at the front. As shown in Figs. 4 (b)-(d), the influence of the disturbance also appears at the interface and the vortexes are generated there.

Figure 5 (a) shows the plots of the averaged non-dimensional cell width $\lambda_{ave}/L_{1/2}$ and the cell number every t=5 in the cases of E=100x10^6, 169x10^6 and 250x10^6. The cell patterns by the maximum pressure distributions are shown in Figs. 5 (b)–(d). In Fig. 5 (a), the cell width lengthened and the cell number did not change with the detonation expanding. In the results of 169x10^6 and 250x10^6, the cell length and the number were almost equal.

In Fig. 5 (b), the cells propagated less regularly and the cells having the different width were appeared. On the other hand, the cells propagated regularly and the cell width was longer with the propagation in Figs. 5 (c) and (d). The frequency of the pressure jump in Fig. 4 (a) depended on the cell number and the width.

Grid resolution was changed to clarify the effect of the numerical disturbance of $100\mathrm{x}10^6$ with orthogonal grid. Figure 6 shows the temperature distributions in two-dimensional simulation at t=16 for the number of grid points per unit length of (a) 2, (b) 10, (c) 20 and (d) 50. The propagating velocities of the shock wave were almost equal. As the grid points were increased, the interface became the finer structure. At the lowest resolution of Fig. 6 (a), the shock wave propagated spherically like the results of the circular grid in Fig. 3. In generally, at least 50 points in half-reaction length are required for the numerical simulation on detonation. The multidimensional detonation wave structure appeared in the cases of setting more than 10 points in half-reaction length.

4 Conclusions

Spherical detonation by direct initiation was investigated in two-dimensional simulations. The results with the circular grid were quantitatively good agreement in those of one-dimensional simulations. However when the orthogonal grid was used, detonation was initiated in the case of less than the critical energy obtained from the simulation with the circular grid and the multidimensional wave structure such as the transverse waves and the triple points was appeared at the detonation front. In addition, as the detonation expanded, the cell length became longer without the number of the cells almost changing. Finally the unsteady detonation wave structure was generated in the cases of setting more than 10 points in half-reaction length, using the orthogonal grid with the various grid resolution.

References

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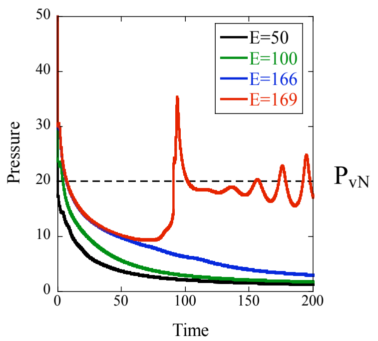

Fig.1 Shock pressure histories in 1D. (P_{vN}=20.03, 20 points in $L_{1/2}$)

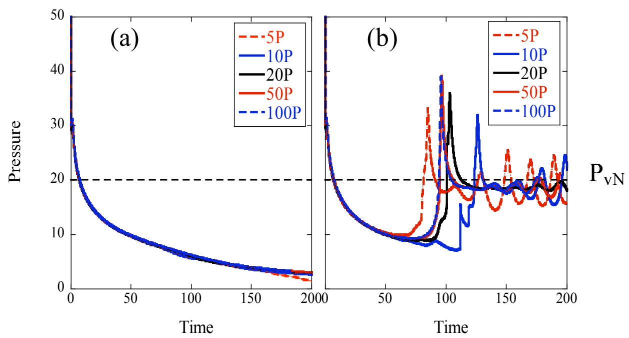

Fig.2 Shock pressure histories in 1D. (a) $166\mathrm{x}10^6$ and (b) $169\mathrm{x}10^6$ (P_{vN}=20.03)

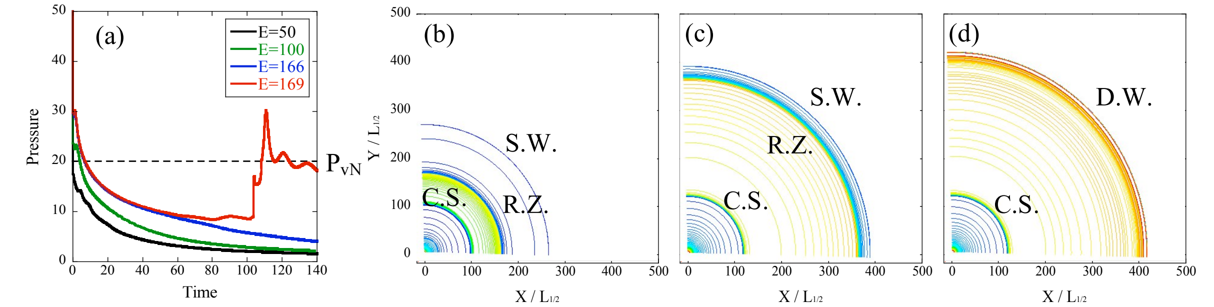

Fig.3 (a) shock pressure histories on the line of X=Y (P_{vN}=20.03). Temperature distributions of (b) E=50x10^6, (c) E=166x10^6 and (d) E=169x10^6 at t=110 with circular grid. 20 points/$L_{1/2}$ and 1 point/deg. are set. (D.W. : Detonation Wave, S.W. : Shock wave, R.Z. :Reaction Zone, C.S. : Contact Surface)

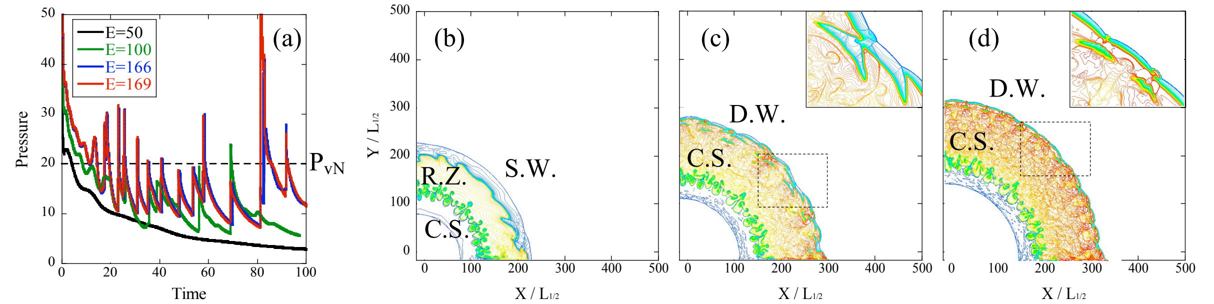

Fig.4 (a) shock pressure histories on the line of X=Y (P_{vN}=20.03). Temperature distributions of (b) E=50x10^6, (c) E=100x10^6 and (d) E=169x10^6 at t=65 with otrhogonal grid. 10 points/$L_{1/2}$ are set in X and Y directions. (D.W. : Detonation Wave, S.W. : Shock wave, R.Z. :Reaction Zone, C.S. : Contact Surface)

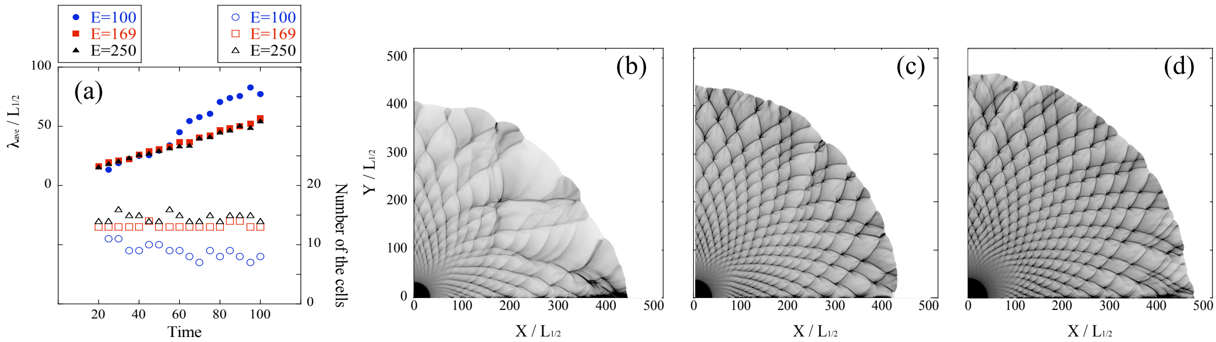

Fig.5 (a) Evolution of the averaged cell width and the cell number. The maximum pressure distributions of (b) E=100x10^6, (c) E=169x10^6 and (d) E=250x10^6. 10 points/$L_{1/2}$ are set in X and Y directions.

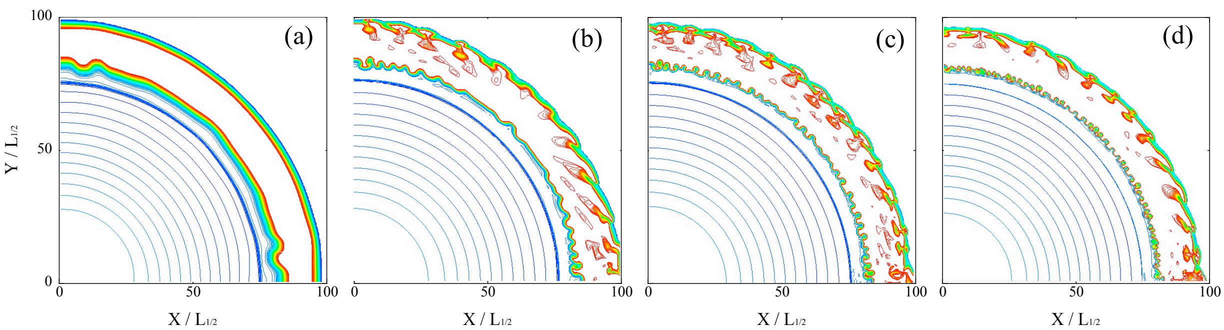

Fig.6 Temperature distributions of E=100x10^6 at t=16 in 2D with orthogonal grid for the number of grid points in $L_{1/2}$ of (a) 2, (b) 10, (c) 20 and (d) 50 points.