Study of Cell Width and Shock Pressure in Directly Initiated Spherical Detonation

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1 Introduction

Detonation is a supersonic combustion wave propagating with shock waves such as transverse wave, incident shock wave, and Mach stem, and with triple points consisting of them, so that it has complicated and unsteady structures. Direct initiation is one of methods for the onset of detonation, where it is immediately formed without the predetonation stage of flame acceleration. The magnitude of the initiation energy mainly determines whether it is successfully initiated or not. Several studies have been made on detonability limit or failure mechanism. Lee [1] reported that, in the case of successful directly initiation, its energy must be above a certain magnitude, known as the critical energy or the minimum initiation energy. In addition, for diverging detonation, the total number of detonation cells, shapes drawn by the traces of triple points, has to multiply to keep the average cell width constant for self-sustained detonation. However, the detailed mechanism for onset of direct initiation is difficult to observe in the experiments. The numerical simulations are supposed to be one of the efficient tools to reveal such underlying physics. However, the two-dimensional simulations on directly initiated cylindrical detonation by Watt and Sharpe [2] showed that grid resolution affected the formation of cellular structure. The purpose of this paper is to numerically clarify the mechanism of the change in cell width of directly initiated spherical detonation with the two-dimensional simulations under axis symmetric assumption.

2 Numerical Setup

The governing equations are two-dimensional compressible and reactive Euler equations under axis symmetry assumption. The chemical kinetics is assumed to be governed by a one-step Arrhenius law. For the discretization of convective term and the method of time integration, Yee's non-MUSCL type second-order upwind TVD scheme and point-implicit method treating only source term implicitly are used, respectively. Grid resolution is defined by grid points per half-reaction length $L_{1/2}$ (points/$L_{1/2}$ represented simply as pts). $L_{1/2}$ is the distance required to reduce the mass fraction of reactant from 1.0 to 0.5 in one-dimensional steady analysis for CJ detonation. In this report, grid resolution is changed from 2 to 50 pts. Also, the grid is uniformly spaced. Chemical and fluid parameters are fixed as follows; activation energy Ea = 17.0, heat release of reaction Q = 22.5, and specific heat ratio $\gamma = 1.2$ [3]. Initial condition consists of two regions: the high-energy region with burned gas of initiation energy $E = 250 \times 10^6$, and the ambient region with uniformly premixed unburned gas. Here, the dimensional variables in the governing equations are normalized by the ambient condition and half-reaction length. As well, initiation energy is nondimensionalized by the ambient pressure and cubed half-reaction length. For the lower and left boundary conditions, mirror condition is used as symmetric plane.

3 Results and Discussions

3.1 Appropriate Grid Resolution

The first point that we should discuss is appropriate grid resolution. Let us consider it from three perspectives; that is, the formation of cellular structure, the history of pressure, and the total number and width of detonation cell.

Firstly, considering the effect of grid resolution on the formation of cellular structure at the early stage, the maximum pressure distributions emulating the smoked foil image are illustrated in Fig. 1(*a*)-(*f*). The cellular patterns in Figs. 1(*a*) and (*b*) are not clear and are different from the others in Fig. 1. Figure 1(*c*) shows the regular cellular pattern keeping the number of cell, which means the cell width is getting larger during the propagation of spherical detonation. The increase of grid resolution slightly introduces irregular factors in the cellular pattern, as observed in Figs. 1(*c*)-(*f*). Figure 1(*g*) shows the fully developed cellular structure in the case of 20 pts. The detailed observation on development of each cell tells us that the width of cell becomes smaller after the maximum width around $400L_{1/2}$. It means that the number of cells increases after $400L_{1/2}$.

Secondly, the effects of grid resolution on shock pressure histories are shown in Fig. 2. Figure 2 shows the shock pressure histories of y-axis with various grid resolutions. The shock pressure histories of 2 and 4 pts do not have the pressure peaks, but the histories of higher resolution (10-50 pts) have strong peaks after $100L_{1/2}$.

Finally, the characteristics of spherical detonation such as the number and width of detonation cells versus distance from the initiation point are calculated from the simulated cellular pattern in Fig. 1. Figure 3 shows (*a*) number and (*b*) width of detonation cells in the cases of grid resolution 2-50 pts. All the simulated results in Fig. 3(*a*) say that the behavior of number of cells is divided into two regimes, one is $R/L_{1/2}<400$, where the number does not change very much, and the other is $R/L_{1/2}>400$, where the number linearly increases versus the distance. See the width of cell in Fig. 3(*b*), the width linearly increases in $R/L_{1/2}<400$, and arrives at the maximum value around $400L_{1/2}$. After that, the width tends to converge on the constant. These specific behaviors do not depend on the grid resolution although the quantitative value of number or width depends on it. As for the effects of grid resolution, the number and width at $R/L_{1/2}<400$ in the cases of 2 and 4 pts are smaller and larger than that in the

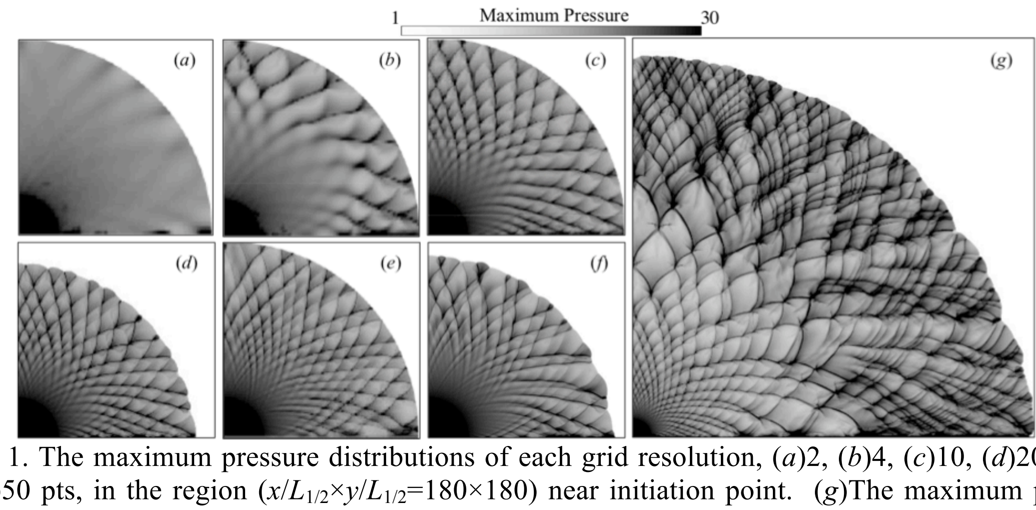

Figure 1. The maximum pressure distributions of each grid resolution, (*a*)2, (*b*)4, (*c*)10, (*d*)20, (*e*)30, and (*f*)50 pts, in the region ($x/L_{1/2}\times y/L_{1/2}$=180×180) near initiation point. (*g*)The maximum pressure distribution of 20 pts in the region (800×800).

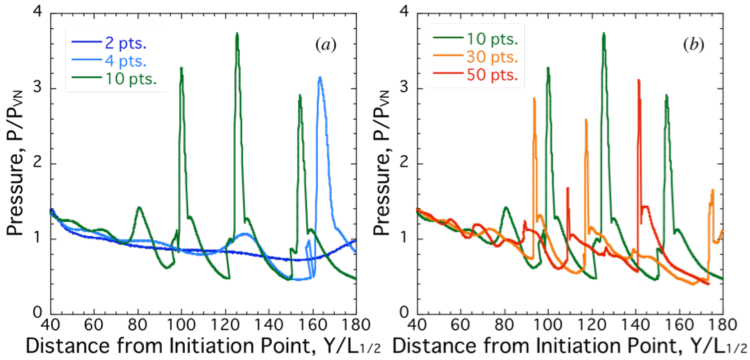

Figure 2. Shock wave pressure histories of (*a*)2, 4, and 10 pts and (*b*)10, 30, and 50 pts on the line of *y*-axis (P_{VN}=20.03 denotes the value of von Neumann spike for CJ detonation).

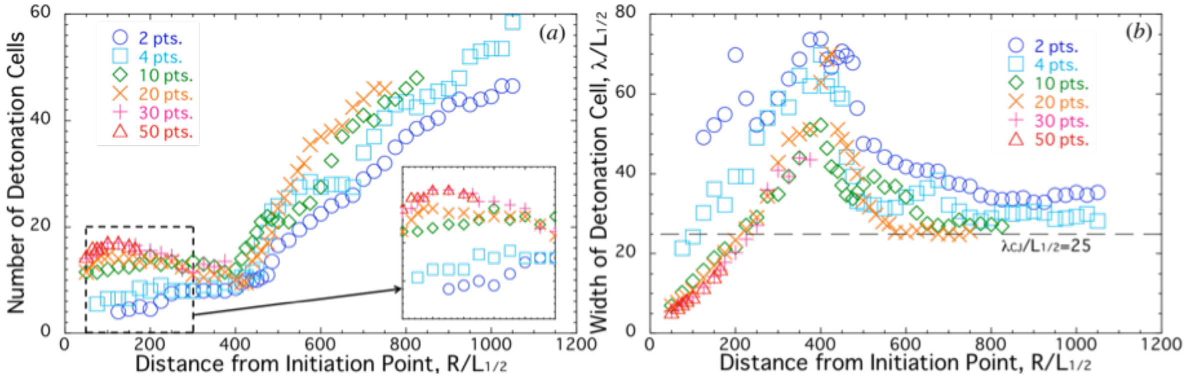

Figure 3. The (*a*)number and (*b*)width of detonation cells versus distance from the initiation point in the case of each grid resolution (the figure surrounded by broken lines is its enlargement).

others, respectively. Therefore, we need at least 10 pts resolution for the quantitative discussion. Actually, this comes from the resolution near the initiation points in Fig. 1, which affects the behavior of cell development in the spherical detonation.

3.2 Mechanism of Change in Detonation Cell Width According to Shocks

Let us focus on the mechanism of the change in cell width. Figure 4 shows the simulated results in the case of grid resolution of 20 pts. There are two symbols, one is the cell width and the other is cell width of the transverse-wave strength near y-axis in 20 pts, and one line, which is the history of the averaged maximum pressure on the same radius from the initiation point of the maximum pressure distribution in Fig. 1. From the initiation to 300$L_{1/2}$ with the propagation of detonation, the averaged pressure decays, the cell width becomes larger, and the transverse-wave strength becomes stronger. Between 300$L_{1/2}$ and 360$L_{1/2}$, the averaged pressure remains the lowest level in the history, and the strongest transverse-wave appears near the y-axis. Such lower averaged pressure makes the cell width bigger and transverse-wave strength stronger. The largest cell width is observed around 420$L_{1/2}$, which is not in the lowest pressure region. This contradiction comes from the significantly large cell length, about 136$L_{1/2}$, generated at the lowest pressure region. Therefore, the history of the cell width always has a delay of one cell behind the averaged maximum pressure history. Figure 3 indicates that the cell width of CJ state, λ_{CJ}, is 25$L_{1/2}$. The overdrive degree of the lowest pressure region shown in Fig. 4 is 0.70(=*f*), and gives the half-reaction length equal to 2.8$L_{1/2}$ (=$L_{1/2,f=0.70}$). Then assuming a proportional expression of $\lambda_{f=0.70}$=$AL_{1/2,f=0.70}$(A=$\lambda_{CJ}/L_{1/2}$=25), the cell width, $\lambda_{f=0.70}$, is estimated at 70$L_{1/2}$. This value is very close to the maximum of cell width shown in Fig. 4.

Figure 5 shows the histories of the averaged maximum pressure and cell width in the case of grid resolution 4 pts. It indicates that the increase of initiation energy causes the local minimum of the

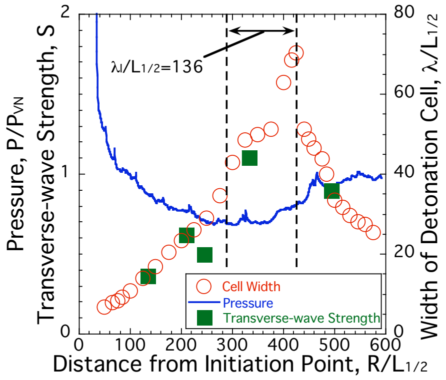

Figure 4. The averaged maximum pressure history, the width of detonation cells and transverse-wave strength near *y*-axis versus distance from the initiation point in the case of 20 pts ($\lambda_l/L_{1/2}$=136 is the averaged cell length at $420L_{1/2}$).

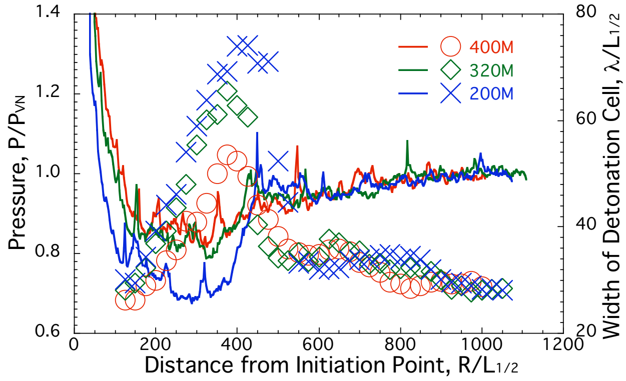

Figure 5. The averaged maximum pressure histories of 4 pts in initiation energy, E=200M (200×10^6), 320M, 400M (lines: maximum pressure, marks: cell width).

pressure to rise, so that the local maximum of cell width decreases. As the result, the delay of minimum and maximum gets smaller with increase of the initiation energy.

4 Conclusions

Two-dimensional numerical simulations under axis-symmetric assumption with one-step chemical reaction were carried out to clarify the mechanism on the change of cell width in directly initiated spherical detonation. The grid refinement study was done with the grid resolution of 2, 4, 10, 30 and 50 pts in the half-reaction length. The smoke foil images by the maximum pressure distribution were used to confirm the simulated cellular structure. The grid resolution more than 10 pts well created the cellular pattern, and the results of the higher resolution included some irregularity in the pattern. The shock pressure histories on the y-axis also showed the same tendency. The number and width of detonation cell versus the distance from the initiation point were derived from the simulated results. In all simulated results, the number of cells was almost constant for each grid resolution before $400L_{1/2}$, and linearly increased after that. Therefore, the width of cell linearly increased before $400L_{1/2}$ and converged on the constant width after that. As for quantitative consideration, the resolution more than 10 pts would be required for the scientific discussion. Furthermore, the simulated results revealed that the time lag between the lowest pressure region and location of the maximum width of detonation cell came from the one cell-length around the lowest pressure region. The effects of the initiation energy were also examined, and the relation between the averaged maximum pressure history and the maximum width of detonation cell were clarified.

References

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