Three-Dimensional Cellular Structure and Propagation Process of Spherical Detonation

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Introduction

Study on propagation of detonation has been performed by many researchers from the past up to now and the Chapman[1] and Jouget[2] (CJ) theory for steady one-dimensional detonation and the Zel'dovich[3]-von Neumann[4]-Döring[5] (ZND) theory can provide us approximate detonation propagation properties such as propagation velocity, wave front pressure, and wave front temperature. However the real detonation structure is three-dimensional and the so-called transverse wave (TW) has a key motion, propagates in the perpendicular direction toward detonation front, and depicts detonation cells. Detonation cell width depends on the initial conditions of reactive premixed mixture such as initial pressure, initial temperature, and initial concentrations of mixture. Detonation is also classified by diverging detonation in an open space: cylindrical detonation and spherical detonation. Diverging detonation in open space must have cell bifurcation phenomena which sustain detonation propagation. However the conditions of transverse wave formation have not been clarified.

Diverging detonation propagates cylindrically or spherically with a curvature. Two-dimensionally propagating detonation is cylindrical detonation and three-dimensionally propagating detonation is spherical detonation. In 1950s Taylor[6] estimates an existence of diverging detonation by assuming a perfect gas with infinite reaction rate. Zel'dovich et al.[7] prove the diverging detonation experimentally. Since late 1960s, Lee et al.[8] obtained a spherical detonation experimentally with a detail of cell structure using a Schlieren photographic system. In 1970 Bach et al.[9] predicted "supercritical regime" for diverging detonation, "critical regime" for transition from reactive blast wave to diverging detonation, and "subcritical regime" for reactive blast wave experimentally using point ignition. In 1983 Murray and Lee[10] showed micro cells of diverging detonation propagating radially from the ignition source. However they performed experiments to study direct initiation condition for diverging detonation and a very few data are obtained for the propagation mechanism of diverging detonation.

Recently two-dimensional cylindrical detonation has been studied by Watt and Sharpe[11], Nirasawa and Matsuo[12], and Asahara et al.[13]. Watt and Sharpe showed the grid resolution affects detonation cell structure. Nirasawa and Matsuo reported the grid configuration (cylindrical grids and rectangular grids) affects the detonation propagation and their cell propagation properties. Asahara et al. performed the detailed two-dimensional numerical analysis to show the growth of “sub-transverse wave (STW)” which provides micro disturbances to Mach stem to yield new TW. The STW is formed by the micro explosion from unreacted gas pocket.

The present paper clarifies three-dimensional spherical detonation structure, especially the spherical detonation front curvature and its front propagation behavior.

Governing Equations

Numerical analysis of diverging detonation requires several important physics: detailed chemical reaction system, diffusion effect, thermal conductivity effect, Kelvin-Helmhotz instability, and Richtmyer-Meshkov instability. Based on these physics, the three-dimensional compressible Navier-Stokes equations are applied for the present problem.

Numerical Methods

The generalized coordinated Navier-Stokes equations are arranged and discretized by the trapezoidal rule and are integrated by the total variation diminishing (TVD) Runge-Kutta method for unsteady terms where special and reactive time integrations are treated independently, the advection upstream splitting methods with a diminishing variation scheme (AUSMDV) for convection terms where higher order interpolation for conservative values of the 5th order robust weighted compact nonlinear scheme (RWCNS) is used, and a point implicit method for source terms with a matrix inverse by the Gauss-Jordan elimination.

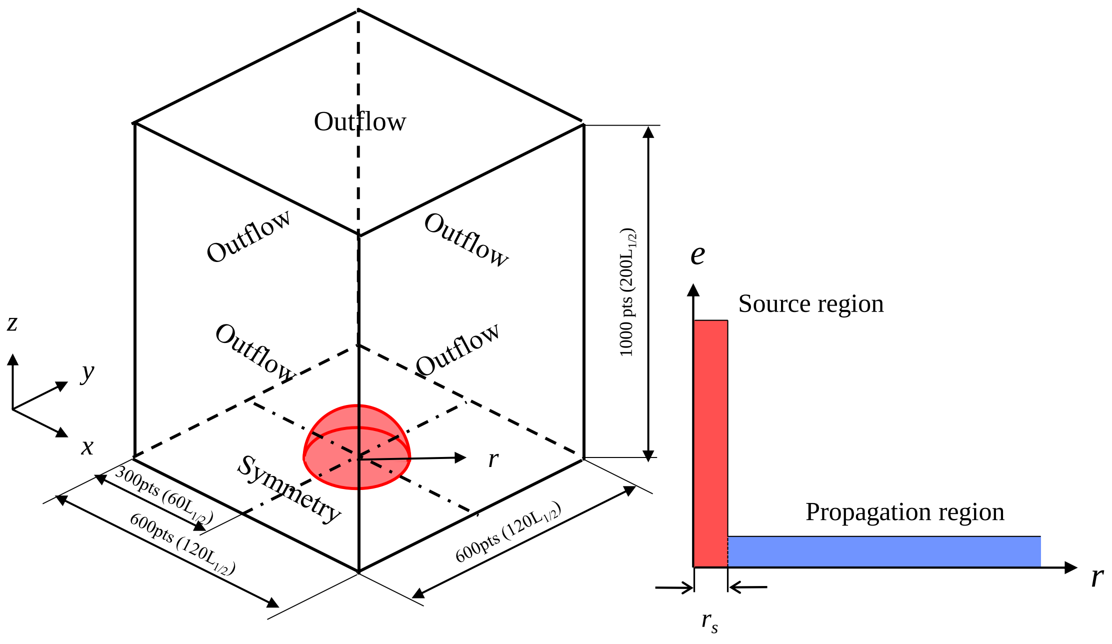
Results and Discussion of 3D Spherical Detonation Calculation

Three-dimensional spherical detonation is numerically simulated using the Navier-Stokes equations for the Cartesian coordinate using the 5th-order RWCNS for their integration.

Numerical conditions

The numerical regions for the present calculation are shown in Fig. 1 where the equal interval rectangular grid system of 601x601x601 (totally about 217 million points). The grid size is kept as 5 μ for x, y, z directions, which correspond to the size of 10 points in a half-reaction length. The symmetry condition is given to the side at x=0 which hold the origin and the outflow condition is given to other five sides of the cube. By this way the source region is given at the side of x=0 in order to get detonation propagation in x-direction (Fig. 1-a).

The initial condition is that a stationary stoichiometric oxyhydrogen mixture is set in the propagation region at the pressure of 0.1 MPa and the temperature of 300 K and a stationary stoichiometric oxyhydrogen mixture is set in the source region of 1 mm in radius at the pressure of 10.1 MPa and the temperature of 3000 K as shown in Fig. 1-b.



(a) (b)

Figure 1 Calculation condition. (a) Computational domain in this study for three dimensional simulation of spherical detonation. (b) Initial condition in the present simulation. The red and blue zones are the source region and ambient region.

Validation for the Present Numerical System

First of all it is necessary to use and keep the minimum grid size which does not affect chemical reaction calculation. The grid size of 5 μm is used in the present numerical calculation because Powers et al.[14] reported the least minimum size of the grid for the use of detailed chemical reaction model is 10 µm. Besides Shimizu et al.[15] presented the validity of detailed oxyhydrogen reaction mechanism is shown by 5 µm grid size at the pressure of 3.33 MPa. This value of 3.33 MPa is the pressure of von-Neumann for detonation at the present condition. Hence we choose 5 µm of grid size for the present calculation.

Detonation front velocity normalized by CJ detonation velocity vs. normalized cell width is compared with the experiments by Strehlow and Crooker[16] in Fig. 2. As seen in the figure, the detonation front velocity near x/ℓ=0 becomes 1.8 D_{CJ} because of two transverse waves collision. After this collision, the detonation front diverges and decelerates its velocity to 0.6D_{CJ} until the next collision. The property of detonation front velocity agrees well with the experiments by Strehlow and Crooker to say that the present numerical system is valid to calculate diverging detonation problem.

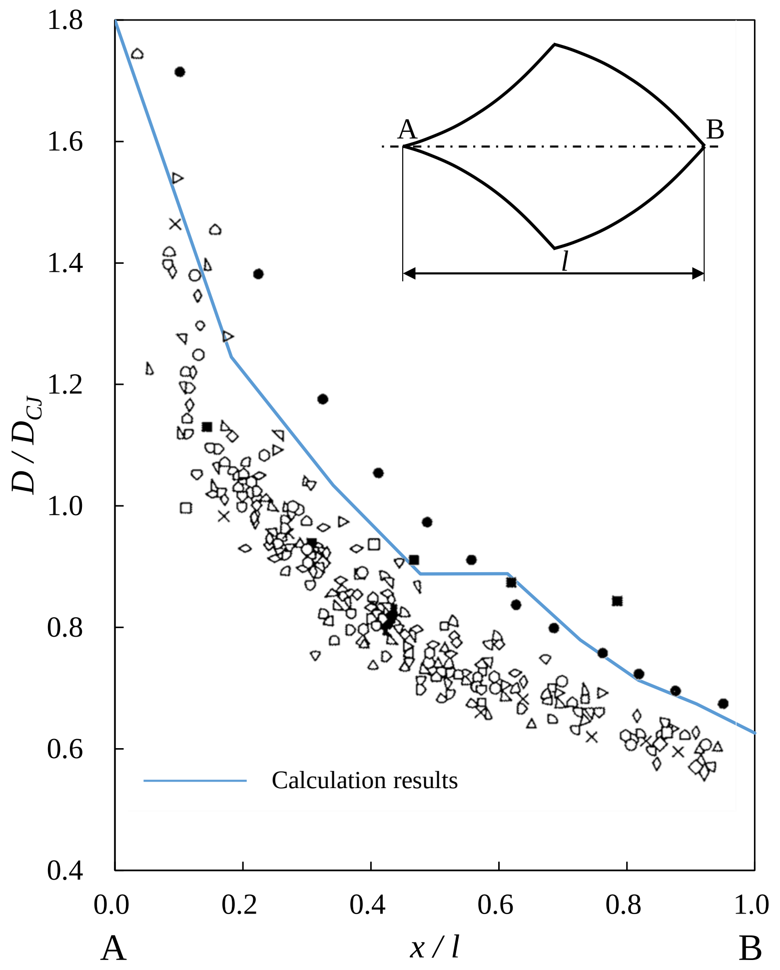


Figure 2 Velocity profile on cell. All plots are experimental data by Strehlow and Crooker[?].

Three-dimensional spherical detonation cell structure

It is difficult to describe three-dimensional configuration of spherical detonation cell, but Fig. 3 shows the maximum pressure (von Neumann pressure) iso-surfaces based on a sketch of 3D cell structure. The spherical detonation front propagates to the arrow direction in the sketch of cell structure. At the point of x=2.30 from the initiation ignition point of x=0 the TW shape is rather circle due to the ignition disturbance effect left. But later TWs collide each other to create the line of maximum pressure of 3D cell structure which is shown in the sketch at the center of Fig. 3. As seen in the sketch, the line of the maximum pressure has a negative curvature in the first half of the cell

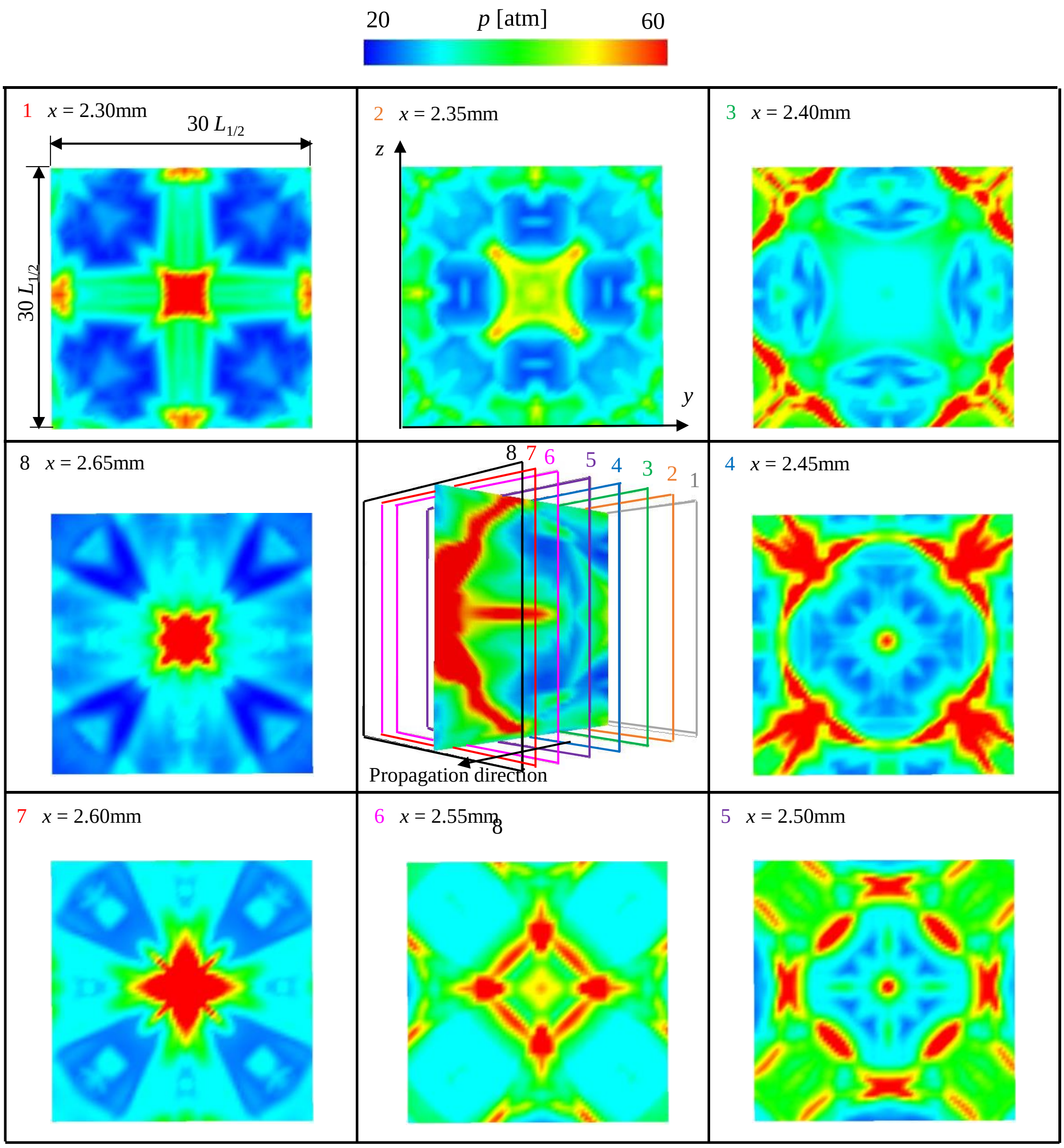


Figure 3 Three dimensional cellular structure on spherical detonation.

when TW collides with the other and has a positive curvature in the second half of the cell when TW collides with the other TW again.

Conclusion

Three-dimensional numerical simulation is performed to figure out spherical detonation cell structure and its propagation process. The numerical system as well as the chemical reaction model is validated by comparing with the experimental results. The spherical detonation cell structure is found numerically and is similar to that found experimentally a long time ago. It is also found that the cell structure is sometimes curved probably due to spherical expansion behavior. The curved cell structure will be presented at the conference.

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