# Numerical Study of Three-dimensional Detonation Wave Dynamics in a Circular Tube

D.-R Cho<sup>1</sup>, Su-Hee Won<sup>2</sup>, Edward Jae-Ryul Shin<sup>1</sup>, Jeong-Yeol Choi<sup>1</sup>,

<sup>1</sup>Department of Aerospace Engineering Pusan National University, Busan 609-735, Republic of Korea <sup>2</sup>School of Mechanical and Aerospace Engineering Seoul National Univiversity, Seoul 151-742, Republic of Korea

# **1** Introduction

Three-dimensional structures of detonation wave propagating in circular tube was investigated using a parallel computational code developed previously. A series of parametric study for a circular tube of a fixed diameter gave the formation mechanism of the detonation cell structures depending on preexponential factor, k. The unsteady results in three-dimension showed the mechanisms of the multicell mode of detonation wave front structures same as the two, three, four and six cell mode. The detonation cell number was increased but cell width and length were decreased with increased preexponential factor k. In the all multi-cell mode, the detonation wave structure and smoked-foil records on the wall are made by the moving of transverse waves. The detonation wave front structures have the regular polygon and windmill shapes periodically.

## 2 Numerical Approach

The Euler equation of compressible inviscid flow with the conservation equation of reaction progress variable can be summarized the following vector form in a three dimensional coordinate.

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial F}{\partial z} = H \tag{1}$$

The pressure is defined as:

$$p = (\gamma - 1)\rho \left[ e - \frac{1}{2} \left( u^2 + v^2 + w^2 \right) + Zq \right]$$
(2)

The specific heat ration has more complex form as Eq. (3) to satisfy the conservation law and ideal gas assumption.

$$\gamma(Z) = \frac{\gamma_U(\gamma_B - 1)(1 - Z) + \gamma_B(\gamma_U - 1)Z}{(\gamma_B - 1)(1 - Z) + (\gamma_U - 1)Z}$$
(3)

As a combustion mechanism, one-step Arrhenius reaction model are used to simulate the various regimes of detonation phenomena without the complexity and large computing time for dealing with

Correspondence to: aerochoi@pusan.ac.kr

#### Jeong-Yeol Choi

many reaction step and detailed properties of reaction species. Since the purpose of present study to understand the fundamental and characterize of the 3D detonation structure in circular tube, the computational cases was restricted to weakly unstable detonation. The thermo-chemical parameters were for the simulation was selected from Austine et al. [6]. The incoming boundary condition was used with C-J detonation speed, that corresponds to the overdrive factor,  $f = (U_{\infty}/U_{C-J})^2 = 1.0$ . The wall is assumed be slip wall and adiabatic. The exit boundary condition was used base on the characteristic boundary condition using C-J condition as a far-field condition.

# **3** Result and Discussion

The Figure 1 is shows the numerical and experimental smoked foil record and the time-evolution of the detonation front wave structures at k=1,000. Here, "t" is non-dimensional calculation time. The wave structure' oscillations of two-cell mode are observed from this result. The wave front structure is simulated well the front-end experimental soot imprint films. In the two-cell mode, the detonation wave structure has the four transverse waves moving along the circumference and two transverse waves moving along the radius direction, respectively. By the moving of four transverse waves, it means that the moving of four triple point, the two-cell mode's smoked-foil record pattern is recorded on the wall. And by two transverse waves, these can be regarded as two triple-lines, and four transverse waves, the soot imprint films of two-cell mode are made on the front-end in the round tube. Specially, the characteristic wave front structures of two-cell mode are generated by two transverse waves in radius direction. The numerical smoked-foil record is the result by moving of the four transverse waves with  $326 \times 41 \times 164$  gird and k=1,000. The smoked-foil is shows that cell structure is stabilized to a regular pattern after some period of advancement. This numerical smoked-foil record is simulated very well the experimental result.



Figure 1. The Numerical and Experimental smoked-foil record (left) and the evolutions of detonation wave oscillation on regular zone (right) in the two-cell detonation mode.

Figure 2 shows the numerical and experimental smoked foil record and the time-evolution of the detonation front wave structures. Here, the pre-exponential value is increased to k=1,500. The wave oscillations of the three-cell mode are observed from this result. It is shows that detonation wave structure has six transverse waves along the circumference and three transverse waves along the radius direction, respectively. In the three-cell mode, the detonation wave structures are made that the six transverse waves move in the circumference direction and the three transverse waves move in radius direction, respectively. The numerical smoked-foil record is result with  $326 \times 41 \times 82$  gird at k=1,500. The numerical smoked-foil is shows that cell structure is stabilized to a regular pattern after some period of advancement. In the figure 2, we can find that the transverse waves, i.e. the six triple points and the three triple lines, are arranged repeatedly to the regular triangle shape and the windmill shape with the jointed three triple lines in the center of circle at the regeneration point of cell. At this

#### Jeong-Yeol Choi

#### 3 -D Detonation Wave Dynamics a Circular Tube

point the triple points are reduced to three and the internal angle of triangle meets the each other at 60 degrees. So from the one triple point to the others, the differential of phase angle or an included angle of the triple lines in the windmill shape case is 120 degrees. In the two-cell mode, the triple point is in position on the opposite side of the each other, i.e. the differential of phase angle is 180 degrees. And it is reduced to 90 degrees in the four cell mode.



Figure 2. The Numerical and Experimental smoked-foil record (left) and the evolutions of detonation wave oscillation on regular zone (right) in the three-cell detonation mode.

Figure 3 is shown the numerical smoked foil record the time-evolution of the detonation front wave structures at k=2,000. The wave oscillations of the four-cell mode are observed from this result. It shows that detonation wave structure has eight transverse waves along the circumference and four transverse waves along the radial direction, respectively. The wave structures are arranged repeatedly to the regular rectangular shape and the windmill shape of the jointed triple lines in the center of circle at the regeneration point of cell. At this time, an included angle of jointed triple lines is 90 degrees. The smoked-foil record is result with  $326 \times 41 \times 82$  gird and k=2,000. The smoked-foil is shows that cell structure was stabilized to a regular pattern after some period of advancement as the two- and three-cell mode.



Figure 3. The Numerical smoked-foil record (left) and the evolutions of detonation wave oscillation on regular zone (right) in the four-cell detonation mode.

In the Fig. 4, the grid system was used  $322 \times 102 \times 634$  grid points and pre-exponential factor, k=2,500 was used. So, the cell resolution is higher than the two-cell mode result. The Figures 4 is shown the detonation wave structure and numerical smoked-foil record of the six-cell mode. The six cell mode is shown the transverse wave's moving in the six-cell mode same as other multi-cell mode's result. The numbers of transverse wave are twelve and six in the circumference and radius direction, respectively. Here, the six transverse waves moving along the radius direction were existed in pairs. One wave is the moving the wall and the other is the moving the center. After the moving was arrived the wall and center, the moving was reversed. As the previous result, the wave structures are arranged repeatedly to

#### Jeong-Yeol Choi

#### 3 -D Detonation Wave Dynamics a Circular Tube

the hexagonal and the windmill shape of the jointed triple lines in the center of circle at the regeneration point of cell. The smoked-foil is shows that cell structure is stabilized to a regular pattern after some period of advancement as other multi-cell mode. In the smoked foil record, the right part is the result at the latter half. The cell pattern shows slightly regular but yet has the irregular pattern. Left part is the result at near end calculation time. Here, cell is regular and was made six cells.



Figure 4. The Numerical smoked-foil record (left) and the evolutions of detonation wave oscillation on regular zone (right) in the six-cell detonation mode.

### 4 Conclusion

Unsteady three-dimensional simulations were performed in a circular tube and multi-cell detonation was simulated. The unsteady results in three-dimension showed the mechanisms of two, three and four cell mode of detonation wave. A two-, three-, four- and six-cell detonation mode has four, six, eight, twelve transverse wave along circumference and two, three, four, six transverse wave along the radius, respectively. The transverse waves moving along the radius direction were existed in pairs. One wave is the moving the wall and the other is the moving the center. After the moving was arrived the wall and center, the moving was reversed. This characteristic was observed very well in the six-cell mode result. In the all detonation mode, we investigated that the detonation wave structures and smoked-foil records on the wall are made by the moving of transverse waves. And we can find that the detonation wave front was constructed the regular polygon shape and windmill shape with multi-vanes. Also it came to conclusion that the multi-cell mode of detonation wave is characterized by pre-exponential factor k in a circular tube. It was confirmed that the cell number was increased but cell width and length were decreased with increased pre-exponential factor or the number of cell mode.

## References

[1] Fickett W, Davis WC. (2000). Detonation Theory and Experiment. Dover Publications. New York.

[2] Tsuboi N, Hayashi, AK. (2007). Numerical study on spinning detonations. Proc. Combust. Inst. 31(2): 2389.

[3] Tsuboi N, Eto K, Hayshi AK. (2007). Detailed structure of spinning detonation in a circular tube. Comb. Flame. 149: 144.

[4] Achasov OV, Penyazkov OG. (2002). Dynamics study of detonation-wave cellular structure 1.Statistical properties of detonation wave front. Shock Waves. 11: 297.

[5] Penyazkov OG, Sevrouk K L. (2007). On critical conditions of the flow within the cellular detonation structure. 21st ICDERS.

[6] Austin JM, Pintgen F, Shepherd JE. (2005) Reaction Zones in Highly Unstable detonations, Proc. Comb. Inst. 30(2):1849.