THE EFFECT OF OBSTACLES ON PROPAGATION MECHANISM OF 3D DETONATION WAVE

Cheng Wang[*][a)], Wenhu Han[*], Jianguo Ning[*], Xiangxiong Zhang[**]

[*] *State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100871, China*

[**] *Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*

Summary In this paper, based on positivity-preserving 5-th order finite difference WENO scheme, a 3D parallel code for gas detonation is developed to investigate the effect of obstacles on the detonation wave in duct. The numerical results show that positivity-preserving method can preserve positive density and pressure when detonation diffracts through obstacles, detonation wave can be inhibited by increasing the number of obstacles, and with the height of obstacles increasing, detonation wave become weaker and weaker after passing two obstacles.

INTRODUCTION

Some experiments have been performed to analyze detonation wave resulting from the gas explosion in a pipe or duct with built-in obstacles [1]. The results shown that the obstacles would effect the shape of the detonation wave and characteristics. The numerical simulation [2] demonstrated that the obstacles have a great influence on acceleration rate for detonation wave in 2D simulations. However, detail mechanisms of interaction of detonation wave and obstacles in the three-dimensional ducts remain unclear. In addition, as detonation wave diffracts through obstacles, negative density and pressure often emerge in numerical simulation [3], and this will result in blow-ups of the numerical algorithm. In this paper, based on the positivity-preserving [4], we develop a parallel code of 3D gas detonation, and simulate the interaction of detonation wave and obstacles.

GOVERNING EQUATIONS AND NUMERICAL METHODS

The governing equations are described by the three-dimensional Euler equations with a source term that represents chemical reactions.

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}+\frac{\partial G(U)}{\partial y}+\frac{\partial H(U)}{\partial z}=S$$

where the conserved variable vector U, the flux vectors F, G and H as well as the source vector S are given , respectively, by

$$U=\left(\rho,\rho u,\rho v,\rho w,\rho E,\rho Y\right)^T$$

$$F(U)=\left(\rho u,\rho u^2+p,\rho uv,\rho uw,\rho u(E+p/\rho),\rho uY\right)^T$$

$$G(U)=\left(\rho v,\rho vu,\rho v^2+p,\rho vw,\rho v(E+p/\rho),\rho vY\right)^T$$

$$H(U)=\left(\rho v,\rho wu,\rho vw,\rho w^2+p,\rho w(E+p/\rho),\rho wY\right)^T$$

$$S(U)=\left(0,0,0,0,0,\rho\omega\right)^T,\quad E=\frac{RT}{\gamma-1}+YQ+\frac{1}{2}(u^2+v^2+w^2)$$

$$\omega=-K\rho Ye^{-(Ea/RT)},\quad p=\rho RT$$

Here u, v, w is velocities in the x, y, z directions, respectively, ρ, p, E, T and Y is the density, pressure, total energy per unit volume, temperature and reactant mass fraction, respectively. Q, Ea, γ and K is the release heat of reaction, activation energy, specific heat ratio, pre-exponential factor, respectively.

Based on positivity-preserving 5-th order finite difference WENO schemes, we develop a three-dimensional detonation MPI parallel code and adopt high performance cluster in the simulation.

EFFECT OF OBSTACLES ON DETONATION WAVE

Take three-dimensional square duct as computing domain. its length and width is 40, 16, respectively. The width of obstacles is 0.6. The height of obstacles is 2.0, 4.0, 6.0, respectively. the space of obstacles is 16. Use the one-dimensional ZND analytical solution as initial value. The left of the duct is inflow boundary, and the other are rigid walls. To observe inner structure of wave system, we take a fourth part of total domain along axis line to show numerical results.

Fig.1 shows propagation of detonation wave under one obstacle. It can be seen from the Fig.1a that a very low

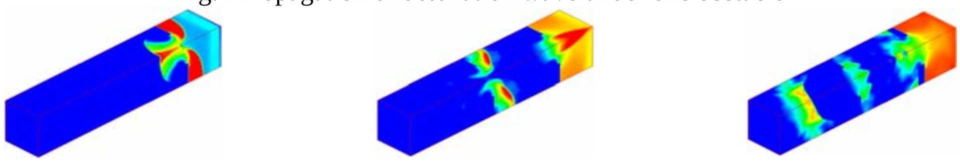
[a)] Cheng Wang. Email: wangcheng@bit.edu.cn.

pressure rarefaction zone emerges before the obstacle due to diffracting when detonation wave passes the obstacle. As shown in Fig.1b, we can know that the wave passes obstacle, with pressure on its front decreasing, then is reflected by walls. The local detonation is formed and the triple-point structure can be seen obviously.

Fig.2 shows propagation of detonation wave under three obstacles when the height is 4.0. It can be seen from Fig.2 that detonation wave attenuates intensively after passing three obstacles. Because of acceleration of obstacles on shock wave, the mixture among obstacles can not be initiated immediately. And the wave reflected by obstacles become weaker and also can not initiate the mixture. A large zone of low pressure comes into being among obstacles, as shown in Fig.2c. So, we can know that increasing the number of obstacle inhibits the propagation of detonation wave.

a)t= 1.34 b) t= 5.82

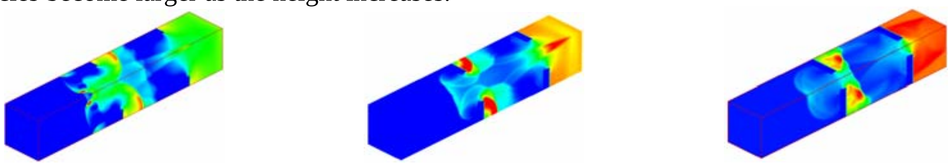
Fig.1 Propagation of detonation wave under one obstacle



a) t= 0.76 b) t= 2.62 c) t= 6.35

Fig.2 Propagation of detonation wave under three obstacles

Fig.3 shows propagation of detonation wave at different obstacles height. When obstacles height is 2.0, local reignition behaviour occurs and local detonation is formed. The triple-point structure on the front can be seen clearly. As the height of obstacles increases, detonation attenuates. When the height reach 6.0, the wave have become very weak after passing the twice obstacle, as shown in Fig.3c. It can be seen further from the Fig.3 that a very low pressure zone among obstacles become larger as the height increases.



a) t= 2.87 b) t= 2.84 c) t= 3.25

Fig.3 Propagation of detonation wave at different obstacle heights

CONCLUSIONS

A three-dimensional detonation MPI parallel code is developed to investigate the effect of obstacles on the detonation wave based on positivity-preserving 5-th order finite difference WENO schemes. By using positivity-preserving method in numerical simualtion, the numerical solutions have positive density and pressure when detonation wave diffracts through obstacles. Propagation of detonation wave can be inhibited by increasing the number of obstacles. As the height of obstacles increases, detonation wave become weaker and weaker after passing two obstacles.

References

[1] Oh K. H., Kim H., Kim, J. B., Lee S. E.: A Study on the Obstacle-induced Variation of the Gas Explosion Characteristics. *J. Loss Prevent Proc* 14: 597–602, 2001.

[2] Valiev D., Bychkov V., Akkerman V., Law C. K., Eriksson L. E.: Flame Acceleration in Channels with Obstacles in the Deflagration-to-detonation Transition. *Combust Flame* 57: 1012－1021, 2010.

[3]Wang C., Zhang X. X., Shu C. W., Ning J. G.: Robust High Order Discontinuous Galerkin Scheme for Two Dimensional Gaseous Detonations. *J. Comput Phys* 231: 653-665, 2012.

[4] Zhang X. X., Shu C. W.: Positivity-preserving High Order Finite Difference WENO Schemes for Compressible Euler Equations. *J. Comput Phys* 231: 2245-2258, 2012.