High Resolution Numerical Simulation of Multi-Phase Hybrid Detonation

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1 Introduction

Investigation on two phase hybrid detonation has a significance for the prevention and control of industrial explosion disaster. Due to the lack of investigation in experiment and theory, numerous detonation phenomena cannot be reasonably explained. Recently, with the development of computer science and numerical method, numerical simulation becomes a key method of studying two phase hybrid detonation[1-3]. Thus, more and more research of two phase hybrid detonation has been performed by numerical simulation [4,5]. In this paper, we built the fluid dynamic equations for describing the moving process of gas and solid particles, respectively. By considering the exchange modeling of mass, monentum, energy between two phase to close source term, the governing equations with chemical reaction is built for discribing the detonation wave propagaton process of gas-solid mixture. In this paper, by using high resolution WENO difference scheme, the governing equations are discreted, and a parallel code is developed. By using the code, detonation wave propagation law for aluminum powder/air and aluminum powder/ethyne/air are investigated.

2 Results and discussions

Effect of width on aluminum-air mixture detonation

The length of the computational domain is 3.6m, and the width is 0.02m, 0.5m, and 1m respectively. The mesh size is h=1 mm. The aluminum particle diameter is d_p=2 μm. The air pressure in simulation is p_g=2.5 atm, and air temperature T_g is 300 K. The aluminum particle temperature T_p is 300 K, and the particle density is $\rho_p = 0.5\text{kg/m}^3$. The upper wall and lower wall of channel are both solid, and the right side is outflow. At the left end of the channel, an ignition zone is set with the temperature of $T_g = 2576\text{K}$ and the pressure of $p_g = 8.56 p_0$. Small perturbations are imposed ahead of the zone.

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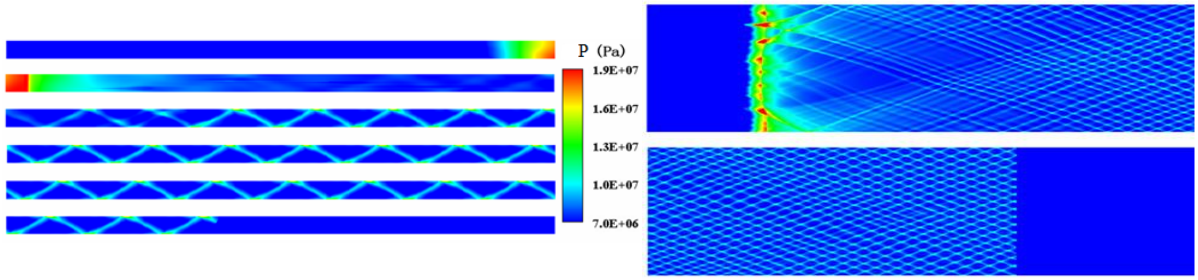
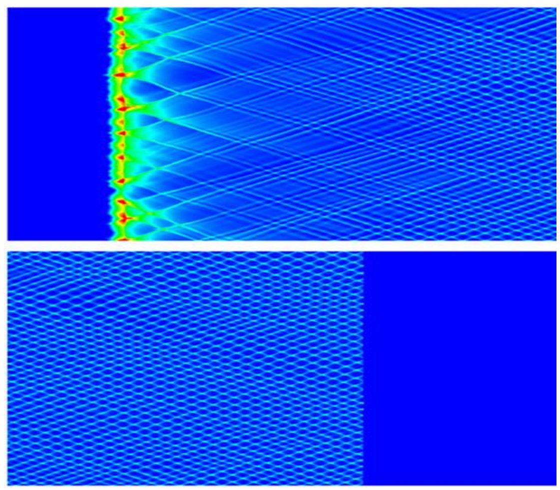


(a) W=0.02m (b) W=0.5m



(c) W=1m

Figure 1 Maximum pressure pattern

Figure 1 illustrates the maximum pressure patterns in three cases. A stable detonation wave can be formed after ignition. Due to the effect of transverse wave, the detonation front is not flat, and is composed of reflected wave Mach stems and incident waves. In the cases of width W=0.5m and W=1m, multi-head cellular structures can be seen after detonation wave propagation. In the case of width W=0.02m, the complete cell cannot be formed due to the small width of channel.

Figure 2 shows the *x* direction distribution curve of maximum pressure at *y*=W. The pressure peak value in the channel of width W=0.02 m is higher than that of W=0.5 m and W=1.0 m. While it is the same in the case of channel width W=0.5 m and W=1.0 m. Figure 3 shows a similar phenomenon of the maximum pressure pattern at the detonation wave front. When the channel width are W=0.5 m and W=1.0 m, the cell size in *x* direction is about 0.07m and in *y* direction is 0.027m. The channel width has not much effect on the cell size of detonation wave. In the case of W=0.02 m, because the channel width is smaller than the cell size in *y* direction (0.027m), cell size in *x* direction will increase due to the limitation of channel wall.

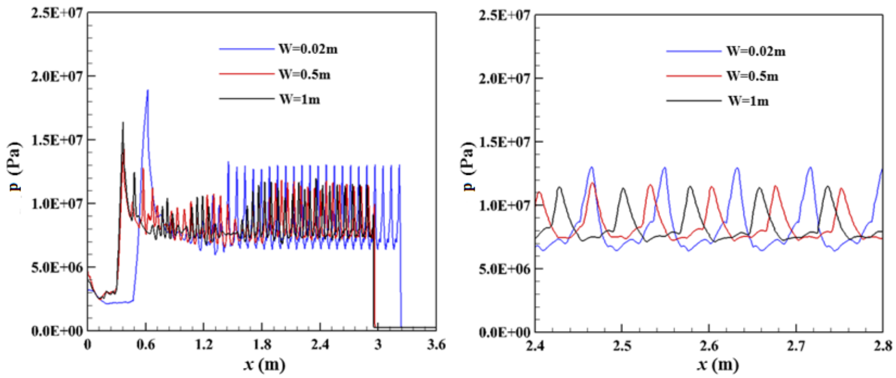


Figure 2 Maximum pressure pattern at y=W.

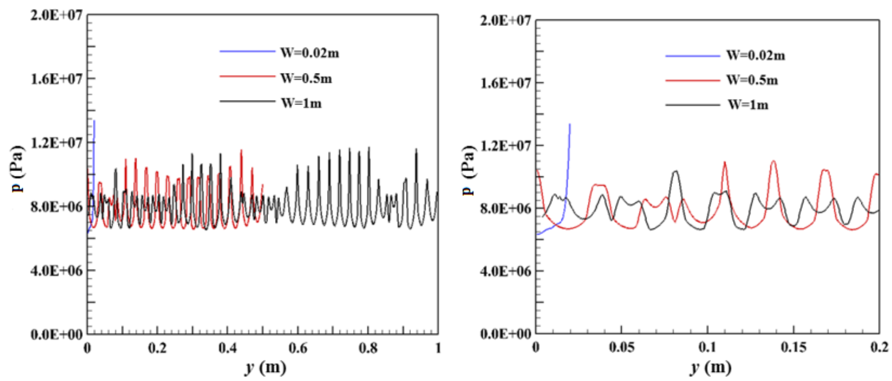


Figure 3 Maximum pressure pattern at detonation wave front.

Effect of aluminum powder density on aluminum-air mixture detonation

The length of the computational domain is 3.6m and the width is 0.5m. By using a high resolution numerical method, aluminum powder-air mixture detonation propagation process is simulated. The mesh size is $h = 1\text{mm}$. The parameters and ignition zone are the same as above. Aluminum powder density is $\rho_p = 1.25\text{kg/m}^3$. The curve of maximum pressure at *y*=W in *x* direction and at the detonation wave front are shown in Figure 4, respectively. The result in the case of aluminum powder density $\rho_p = 0.5\text{kg/m}^3$ is simulated too. Figure 4 shows that the pressure peak value in the case of $\rho_p = 0.5\text{kg/m}^3$ is lower than that of $\rho_p = 1.25\text{kg/m}^3$. It indicates that the transverse wave impact on the channel wall more intensively when the aluminum powder density is higher.

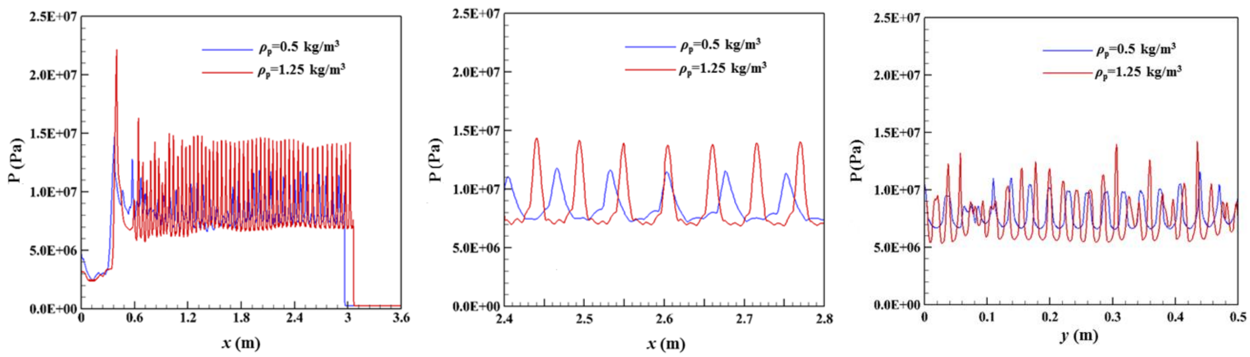


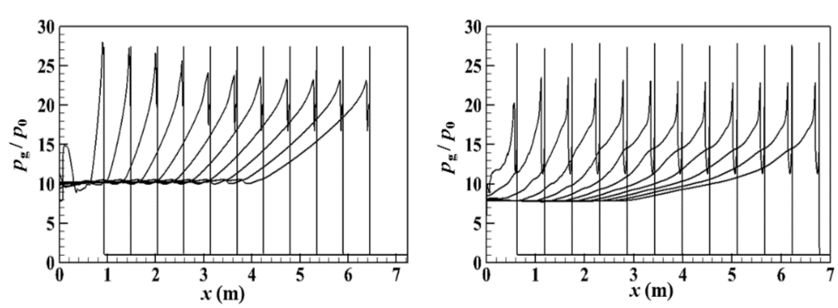
Figure 4 maximum pressure pattern at y=W, and at detonation wave front.

The average cell size of two phase detonation wave at different densities can be seen from Figure 4. When the aluminum powder density is $\rho_p = 0.5\text{kg/m}^3$, the detonation wave cell size in *x* direction is 0.07m and in *y* direction is 0.027m. When the aluminum powder density is $\rho_p = 1.25\text{kg/m}^3$, the detonation wave cell size in *x* direction is 0.055m and in *y* direction is 0.022m. The numerical result shows that aluminum powder density has a large effect on the detonation cell size. The detonation cell size decreases with the increase of aluminum powder density.

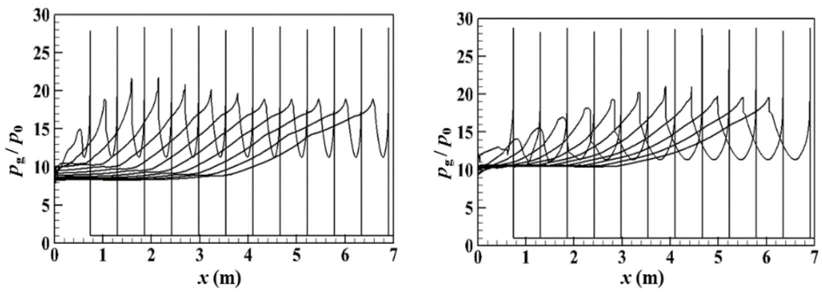
Aluminum powder/ethyne/air mixture detonation

By 1D simulation of detonation wave propagaton for aluminum powder/ethyne/air mixture, the effect of aluminum particle size on detonation wave structure can be investigated. The gas pressure is p_g=1.0 atm, and gas temperature T_g is 300 K. The aluminum particle temperature T_p is 300 K, and the particle density is $\rho_p = 0.5\text{kg/m}^3$, and equivalent proportion of ethyne is Φ=0.8. The computational domain is [0, 7m] and mesh size is h=0.025 mm· In simulation, a high-temperature and high-pressure ignition zone is set at [0, 0.01 m] with the temperature of $T_g = 2576\text{K}$ and pressure of $p_g = 8.56 p_0$ respectively. A solid boundary condition is set at the left side, and the outflow boundary condition is set at right side. Particle size of aluminum powder is $2\mu\text{m}$,$15\mu\text{m}$, $30\mu\text{m}$ and $60\mu\text{m}$,respectively.

Figure 5 presents the pruessrue curves of four particle sizes. The difference of pressure peak value for the four particle sizes is not too much. The pressure wave curve does not decrease monotonically, which has two peak values, i.e. double-front detonation structure. There are sevral types of propagations for the double-front detonation structure. In Figure 5(a,b), the detonation wave can form a stable double-front detonation structure. In Figure 5(c,d), the second detonation wave front does not have a stable propagation, it departs from the first detonation wave front, meanwhile, the peak value decreases.



（a） d_p=2μm （b） d_p=15μm



（c） d_p=30μm （d） d_p=60μm

Figure 5 pressure distribution curves.

When the particle size of aluminum powder is $d_p = 15\mu m$, the double-front detonation wave structure is further analyzed. We fix the coordinate at the first detonation wave front, and turn round the coordinate axis. Figure 6a shows the pressure and temperature curves of the fluid field after the detonation wave. When detonation wave passed, the gas temperature sharply increases due to the effect of shock wave. Under the effect of shock wave, the temperature of two phase particles keeps constant. However, the heat conduction between two phases leads to the temperature of particles rise, and the gas temperature decrease. The thermal equilibrium is achieved in the end. Figure 6b shows the velocity balance is only achieved in a local zone.

When the particle size is $d_p = 15\mu m$, we investigate the 2D mixture detonation wave structure. The computational zone is [0, 3.6 m] × [0, 0.05 m], and the mesh size is h=0.025 m. The initial condition is the same with the 1D case. The boundary condition of channel and ignition zone are also the same to the condition mentioned above. Figure 7 presents the maximum pressure distribution in the computational zone. It could be seen that under the effect of transverse wave, the plane detonation wave can evolve into stable 2D detonation wave. Numerous triple points occurs near the detonation wave front. The cellular structure of two phase hybrid detonation wave becomes more regurlar and smaller comparing the gas phase.

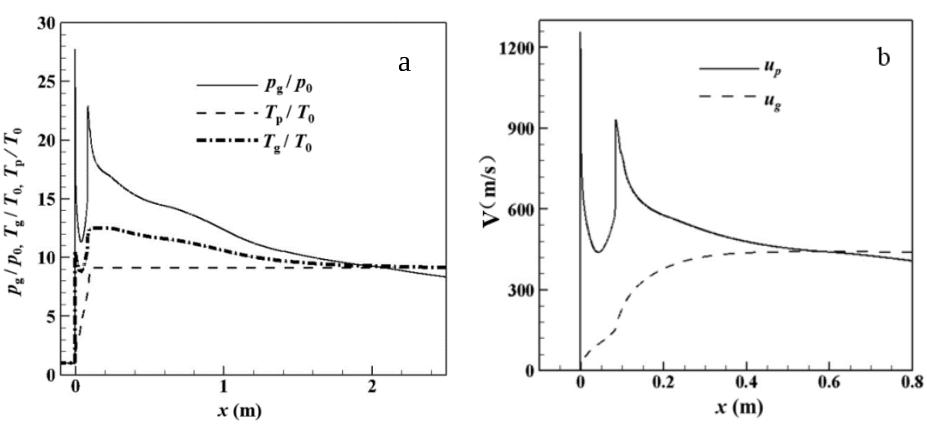
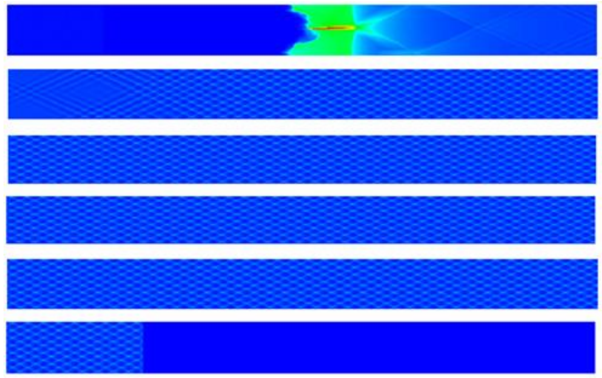


Figure 6 Temperature and pressure curves after detonation wave (a), and Speed curve after detonation wave (b).



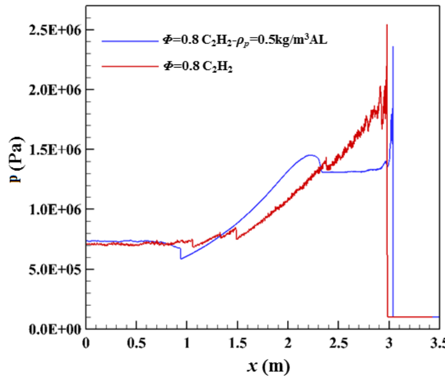


Figure 7 Maximum pressure pattern（Φ=0.8, ρ_p=0.5kg/m^3） Figure 8 pressure distribution curve.

Figure 8 shows the pressure curve at $y = 0.05\text{m}$, when the detonation wave propagates to $x = 3\text{m}$. This figure shows the gaseous detonation is different with the two phase hybrid detonation in wave pattern. The pressure regularly decreases behind the detonation wave of gaseous detonation. However, for two phase hybrid detonation, due to the heat release resulted from aluminum powder chemical action, the pressure after detonation wave can firstly decrease and then increase, forming the second pressure peak.

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