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Numerical Simulation of Detonation in Suspended Aluminum Dust

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Detonation in suspended aluminum dust is numerically simulated with two-phase flow model. The development and propagation process of detonation in suspended aluminum dust are obtained by numerical simulation with distribution of pressure, density, velocity, temperature in the flow field behind shock waves. Parameters of detonation of aluminum dust with different concentrations are calculated. Lower limit of detonation of aluminum dust is also obtained by calculation. At the same concentration, the nano aluminum dust detonation has higher pressure and faster detonation velocity compared with micro aluminum dust. Detonation of suspended aluminum dust in enclosed channel is numerically simulated. The result of numerical simulation shows distinctly that the shock front caused by initiation, and the combustion front of the aluminum particles caused by the high temperature behind the shock front, and the shock front pursued by burning front in aluminum dust and the formation of the detonation. Then the detonation wave is reflected in the wall, and the pressure and temperature increase greatly near the wall.
Key Words：Dust detonation; Aluminum dust; Parameters of dust detonation

1. Introduction

Metal dust explosion is a frequent occurrence in industry for example in polishing operation of metal, causing casualties. In August 2, 2014 in Kunshan, China, a factory for wheel grinding and polishing, happened a particularly serious aluminum dust explosion, lead to heavy casualty. It is very important to study the metal dust detonation for safety in industry.

There are some researches on numerical simulation of suspended aluminum dust. Fedorov (1999) analyzed steady detonation of suspended aluminum dust in oxygen with diameter larger than 10μm. The temperature of gas in the flow field is less than 2500K. Veyssiere (2005) numerically simulated the cellular structure in suspended aluminum dust detonation with diffusion burning rate. Briand (2010) also studied cellular structure in suspended aluminum dust detonation with two steps of burning rate including kinetics and diffusion. These numerical simulations are usually for micrometer aluminum dust.

For nanometer aluminum dust, heat transfer between aluminum particles and gas is much rapid because of larger surface area for smaller size particles per unit of mass. The research on nano aluminum dust detonation is less than that of micrometer aluminum dust. In this paper, the detonation in the suspended micro and nano aluminum dust is numerically simulated.

2. Numerical modeling

Detonation in suspended aluminum dust is numerically simulated with two-phase flow model. The model assumes that aluminum particles are uniformly distributed in air and their initial diameter is the same. Temperature in a single aluminum particle is uniform. Energy released by Chemical reaction of aluminum is only absorbed by gas phase. Gas and solid satisfy the conservation laws respectively. There are mass, momentum and energy exchange between the gas phase and solid phase.

Following is the description of conservation law of gas and particles.

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Gaseous phase

$$\frac{\partial \rho_1}{\partial t} + \nabla \cdot (\rho_1 \vec{u}_1) = m \tag{1}$$

$$\frac{\partial (\rho_1 \vec{u}_1)}{\partial t} + \nabla \cdot [(\rho_1 \vec{u}_1) \otimes \vec{u}_1] = -\nabla p + m\vec{u}_2 - \vec{f} \tag{2}$$

$$\frac{\partial (\rho_1 e_1)}{\partial t} + \nabla \cdot [(\rho_1 e_1 + p)\vec{u}_1] = m(e_2 + q_{chem}) - \vec{f} \cdot \vec{u}_2 - q \tag{3}$$

$$\frac{\partial (\rho_1 Y_j)}{\partial t} + \nabla \cdot (\rho_1 Y_j \vec{u}_1) = \omega_j \tag{4}$$

Solid phase

$$\frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 \vec{u}_2) = -m \tag{5}$$

$$\frac{\partial (\rho_2 \vec{u}_2)}{\partial t} + \nabla \cdot [(\rho_2 \vec{u}_2) \otimes \vec{u}_2] = -m\vec{u}_2 + \vec{f} \tag{6}$$

$$\frac{\partial (\rho_2 e_2)}{\partial t} + \nabla \cdot (\rho_2 e_2 \vec{u}_2) = -me_2 + \vec{f} \cdot \vec{u}_2 + q \tag{7}$$

$$\frac{\partial N}{\partial t} + \nabla \cdot (N\vec{u}_2) = 0 \tag{8}$$

Where the subscripts 1 and 2 denote the variables of the gas and particles. The ρ is the apparent density with $\rho_1=\rho_g\varphi_1$ and $\rho_2=\rho_s\varphi_2$ in which the φ is the volume fraction and yields $\varphi_1+\varphi_2=1$. In numerical simulation, ignition temperature of aluminum is in its oxide melting point 2300K because aluminum particle is coated by its oxide and it is ignited after its oxide melted. The model of Price (1984) is used to describe the reaction rate for combustion aluminum particles.

$$\frac{1}{R}\frac{dR}{dt} = -\frac{1}{k d_0^n \phi^{0.9}} \tag{9}$$

$$m = -N\rho_s 4\pi R^2 \frac{dR}{dt} \tag{10}$$

N is the number of particles in per unit volume, R is the radius of particle, d_0 is the initial diameter of aluminum particles, ϕ is the mole fraction of oxygen in air, and n equals to 1.75.

The interphase drag force is

$$\vec{f} = N \cdot \frac{\pi d_p^2}{8} \cdot C_d \cdot \rho_g \left|\vec{u}_1 - \vec{u}_2\right| (\vec{u}_1 - \vec{u}_2) \tag{11}$$

Where the d_p is the particle diameter, and the C_d is the drag coefficient given by $C_d=24(1+Re^{2/3}/6)/Re$ for $Re<1000$ and $C_d=0.44$ for other Re. The convective heat exchange is

$$q = N \cdot \pi d_p \cdot Nu \cdot \lambda_g (T_1 - T_2) \tag{12}$$

Here the Nusselt number Nu is given as $Nu=2+0.459Re^{0.55}Pr^{0.33}$. The Prandtl number is $Pr=\mu_g C_g/\lambda_g$. Where the μ_g, C_g, and λ_g are the dynamic viscosity, heat capacity and thermal conductivity of the gas.

The chemical reaction of aluminum with oxygen in gas is $4Al+3O_2=2Al_2O_3$. The production of Al_2O_3 is in liquid phase and its temperature, velocity is same as gas. There is no contribution for pressure by aluminum oxide in liquid phase. As gas temperature reaches boiling point of aluminum oxide, aluminum oxide will be decomposed to aluminum in gas so that temperature of gas phase will not higher than the boiling point of aluminum oxide with 3800K.

In simulation, two numerical schemes are used. First is MacCormack with FCT technique used to calculate the micro aluminum dust detonation and second is CESE scheme with fourth-order Runge-Kutta method to calculate the nano aluminum dust detonation.

3. Numerical simulation results

3.1 Comparison with experiment results

To validate the numerical method, the aluminum dust detonation are simulated and compared with experiment. For the aluminum dust, the concentration is 0.304kg/m^3 and the radius is 1.7μm. The ignition conditions at left are φ_1=1, ρ_1=3kg/m^3, u_1=1000m/s, T_1=3600k. Figure 1 shows the pressure profiles with interval of 0.476ms after initiation. Detonation velocity is 1.63km/s and peak pressure is 3.31MPa. In the experiment of Tulis (1982) the detonation velocity is 1.65km/s. Results of simulation of detonation velocity agree well with experiment's. Table 1 lists the parameters in CJ point of the suspended aluminum dust detonation.

Table 1 The parameters of detonation in CJ point

Scheme	Radius of particles	ρ_1(kg/m3)	u_1(m/s)	p(MPa)	T_1(K)
MacCormack+FCT	1.7μm	2.48	681	1.91	3800
CESE+Runge-Kutta	1.7μm	2.43	673	2.04	3800

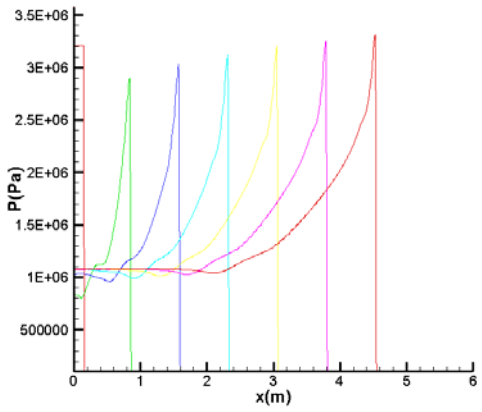

Figure 1. Pressure distribution of detonation of suspended aluminium dust at different time with radius of 1.7μm

3.2 Numerical simulation of suspended micrometer aluminum dust detonation

Parameters of suspended aluminum dust detonation with different concentration are obtained by numerical simulation. Radius of aluminum particles is 1.7μm. Table 2 lists the parameters in CJ point of the suspended aluminum dust detonation. Figure 2 is the peak pressure of leading shock front at different position of detonation with different concentration. As the concentration of aluminum particles is 45.6g/m^3, pressure of leading shock front decays rapidly, and no detonation forms. As the concentration of aluminum particles is 49g/m^3, pressure of leading shock front tends to be stable and detonation forms. So that the lower limit of detonation of suspended aluminum dust with 1.7μm radius is about 49g/m^3 from numerical simulation.

Table 2 Parameters of detonation in CJ surface

concentration(g/m^3)	ϕ	ρ_1(kg/m^3)	u_1(m/s)	T_1(K)	p	D(m/s)
304	1.0	2.56	742	3800	2.02	1722
243	0.8	2.49	764	3800	2.05	1741
182	0.6	2.38	741	3671	1.94	1718
122	0.4	2.28	686	2898	1.60	1600
61	0.2	2.15	559	1888	1.07	1349
49	0.16	2.11	516	1636	0.93	1263

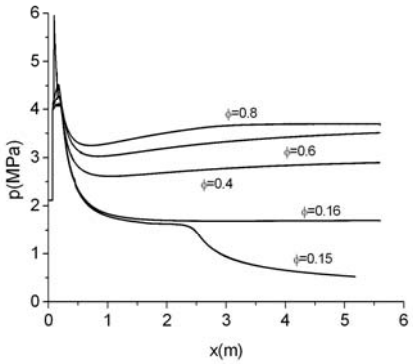

Figure 2. Peak pressure of leading shock front of detonation with different concentration

3.3 Simulation of suspended nanometer aluminum dust detonation

Suspended Nano aluminum dust detonation is numerically simulated. Radius of aluminum particles is 80nm and concentration of aluminum dust is 304g/m^3. Detonation velocity is 1855 km/s and peak pressure is 4.2MPa. This is faster and higher than that of radius aluminum particles 1.7μm. Figure 3 is the distribution of pressure, gas density, velocity and temperature in the flow field. The parameters of detonation in CJ point list in table 3. Besides the temperature, other parameters are almost same as the parameters of CJ point of aluminum dust detonation of 1.7μm. For nano aluminum particles, reaction rate is much faster than micro particles, energy release is completely within a thin area after leading shock wave, resulting in the temperature drop in the flow field compared with that of micro aluminum dust.

Table 3 The parameters of detonation in CJ point

Radius of particles	ρ_1(kg/m3)	u_1(m/s)	p(MPa)	T_1(K)
80nm	2.41	676	1.94	3461

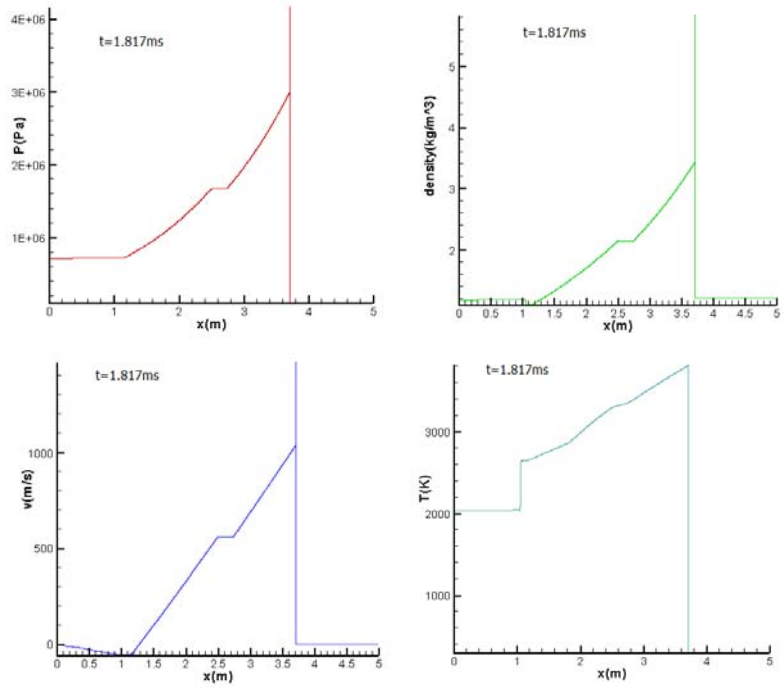

Figure 3. Pressure, density, velocity and temperature distribution of gas in the flow field of detonation of suspended aluminium dust with radius of 80nm at t=1.817ms

3.4 Simulation of aluminum dust detonation in an enclosed channel

Explosion of suspended aluminum dust usually happens in an enclosed space. Detonation of suspended aluminum dust in enclosed channel with 5m×0.3m is numerically simulated. Detonation is initiated in lower corner of left in Figure 4. Concentration of aluminum dust is 750kg/m^3, Radius of aluminum particles is 800nm. Initiation condition is high temperature and high velocity gas with ρ_1=10kg/m^3, u_1=1000m/s, v_1=1000m/s ,T_1=3000k in area 12.5cm×0.5cm.

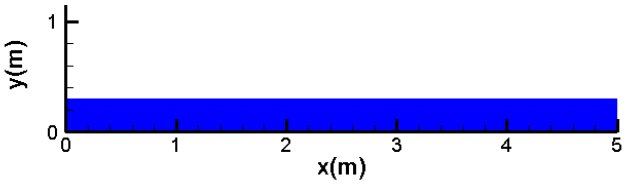

Figure 4. Sketch map of enclosed channel in calculation

Figure 5 is the pressure distribution in the flow field of suspended aluminum dust at different time. At t=0.185ms, shock wave produced by initiation propagates through the channel forward and upward. Aluminum particles are ignited by the high temperature gas flow. At t=0.326ms, it shows the separation of the leading shock front and burning front in the flow field. Also, curved shock front and burning front reflects on the upper wall of channel. At t=0.627ms, it can be seen the much higher pressure near the upper wall because of the reflection of shock front and burning front. At t=1.162ms, accelerated burning front catches up the leading shock front and detonation forms in the channel. At t=4.346ms, detonation has reflected from end wall of channel and propagates to the left. At t=5.013ms, leading shock wave attenuates.

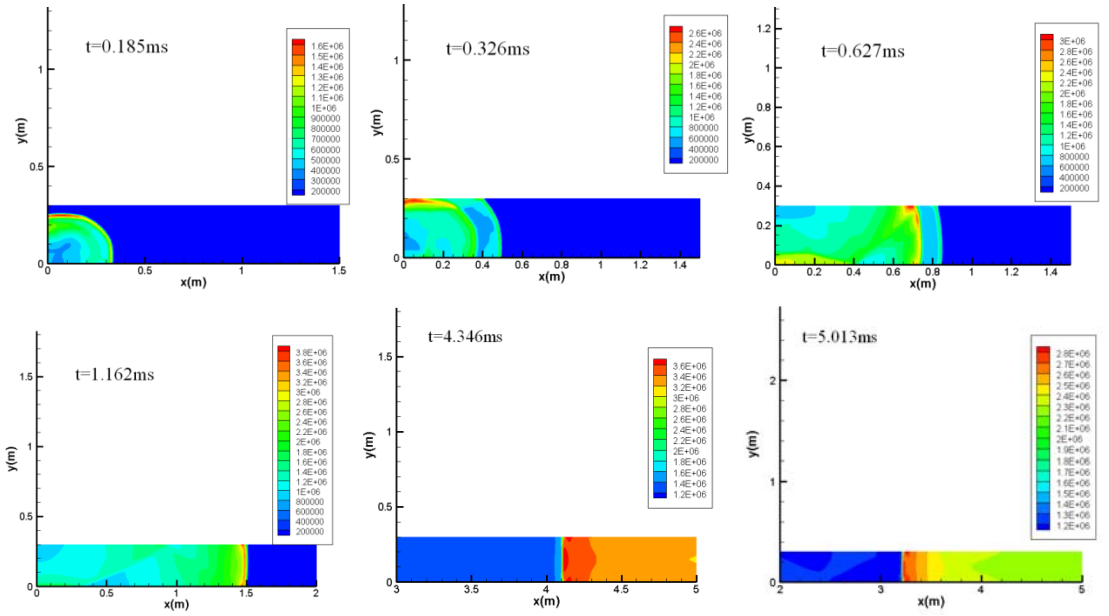

Figure 5. Pressure distribution at different time. The figures show the formation, propagation and reflection of detonation in suspended aluminum dust in channel

Figure 6 shows the reflection of the detonation on the end wall of the channel. At t=3.506ms, detonation just begins to reflect on the wall and produces about 10MPa high pressure. At t=3.561ms, highest pressure in flow field is about 8.0MPa, this is much higher than the pressure of leading shock front of pressure as the detonation forms and propagate before reflection.

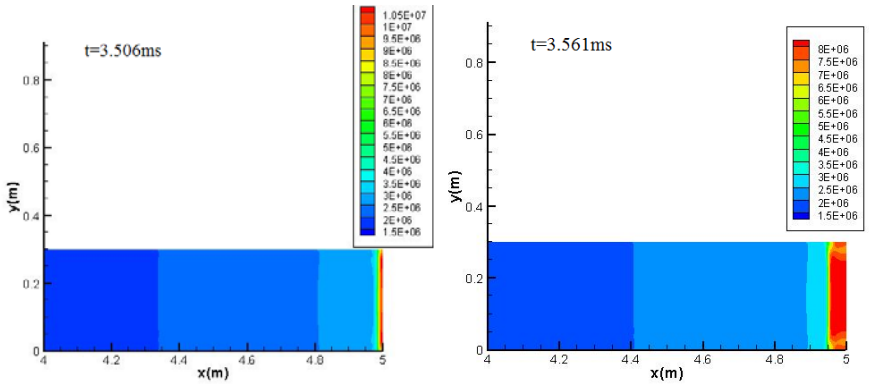

Figure 6. Detonation reflects on the wall in the end of the channel

4. Discussion

In this paper, a simplified model of reaction of aluminium with oxygen is used in numerical modelling. In order to more accurately predict the temperature of aluminum dust detonation, a more detailed description of the chemical reaction of aluminum to consider the composition of other products such as AlO, Al_2O should be included in modelling. And also, even the two dimensional calculation is not in a large space in this paper. For simulation of the aluminum dust explosion in large scale space such as in industrial plant, it needs to develop parallel computation.

Conclusion

Detonation in suspended aluminum dust is numerically simulated with two-phase flow model. Parameters of detonation with different concentration of micrometer aluminum particles and lower limit of detonation are obtained. For radius 1.7μm, lower limit of detonation is 49g/m^3. For suspended Nano aluminum dust, velocity of detonation is faster and pressure of leading shock wave is higher, but temperature in CJ point is lower than that of micrometer aluminum dust with same concentration. For detonation in an enclosed channel, reflection of detonation on wall will produce high pressure area near the wall.

References

Fedorov A V, Khmel T A , Fomin V M, 1999, Non-equilibrium model of steady detonations in Aluminum particles-oxygen suspensions[J], Shock Waves, Vol. 9, No.5:313-318

FedorovA V and KhmelT A., 2005, Numerical simulation of formation ofcellular heterogeneous detonationof aluminum particles in oxygen[J]. Combustion, Explosion, and Shock Waves, Vol. 41, No. 4, 435–448

Briand A, Veyssiere B, Khasainov B A, 2010, Modelling of detonation cellular structure in aluminium suspensions[J], Shock Waves, Vol. 20:521-529

Price E.W., 1984, Combustion of metalized propellants[A]， Progress in Astronautics and Aeronautics: Fundamenals of Solid-Propellant Combustion, AIAA, New York, Vol.90, Chapter 9:479-513

Tulis A J, Selman J R., 1982, Detonation tube studies of aluminum particles dispersed in air[A]. 19th International Symposium on Combustion[C], The Combustion Institute, 655-663