Simulation ofsuspended mixed RDX and Al dust inone dimension withtheCESE method

Zan Wentao[1,2] Hong Tao[1] Dong Hefei[1]

1 Institute of Applied Physics and Computational Mathematics, Beijing 100094, China

2 BeiJing Institute of Technology, Beijing 100081,China

.

1 Introduction

The research of dust detonation is very important both in weapons and industrial hazards. There is a lot of damage of dust detonation in the industry security. Every year many people died of the dust detonation in the world such as the coal dust and the aluminum dust explosion. The accident of wheel hub work shop happened in KunShan China August 2014was a serious dust explosive disaster. There are 75 people died and 260 people injured in the accident. The RDX is a common explosive and it's very easy ignited. The Al is light, cheap and has much energy as a metal. So it has much significance to study the mechanisms and effect of the detonation of two-phase.

The problem of two-phase detonation is very complex. There are three propagation regimes[1]: the Pseudo-Gas Detonation, the Single-Front Detonation and the Double-Front Detonation. The production of the different detonation structures is due to the difference of heat release process. For this paper, we investigate the difference of the Single-Front Detonation and the Double-Front Detonation. We use the two-phase model to simulate the detonation with CE/SE method. The detonation of RDX particles in air, aluminum particles in air and RDX and aluminum particles in air together are all simulated.

2 Model

The two-phase model is used in the simulation. And also we purpose the particles are spherical, theinitial diameters are same, the temperature of every particles is balance, the interaction of particles is ignored, theenergy of chemical reaction is absorbed by gas, the component of gas are homogeneous, the frictional force betweenparticles and the wall is ignored, the radiation between particles and gas is ignored, both the solid phase and gas phase satisfied the equation.

Gas equation:

$$\frac{\partial \rho_1 \varphi_1}{\partial t} + \frac{\partial \rho_1 \varphi_1 u_1}{\partial x} = I_{d2} + I_{d2a}$$

$$\frac{\partial \rho_1 \varphi_1 u_1}{\partial t} + \frac{\partial \left(\rho_1 \varphi_1 {u_1}^2 + P\right)}{\partial x} = I_{d2} u_2 - F_{d2} + I_{d2a} u_{2a} - F_{d2a}$$

$$\begin{aligned}\frac{\partial \rho_1 \varphi_1 (e_1 + 0.5{u_1}^2)}{\partial t} + \frac{\partial \varphi_1 u_1 \left(\rho_1 e_1 + 0.5\rho_1 {u_1}^2 + P\right)}{\partial x} &= -Q_{d2} + I_{d2}(e_2 + 0.5{u_2}^2) + I_{d2} q_2 - F_{d2} u_2 - Q_{d2a} + I_{d2a}(e_{2a} + 0.5{u_{2a}}^2) \\ &\quad + I_{d2a} q_{2a} - F_{d2a} u_{2a}\end{aligned}$$

Solids equation:

$$\frac{\partial \rho_i \varphi_i}{\partial t} + \frac{\partial \rho_i \varphi_i u_i}{\partial x} = -I_{di}$$

Correspondence to: Hong Tao E-mail: hongtao@ iapcm.ac.cn

$$\frac{\partial\rho_i\varphi_i u_i}{\partial t}+\frac{\partial\rho_i\varphi_i {u_i}^2}{\partial x}=-I_{di}u_i+F_{di}$$

$$\frac{\partial\rho_i\varphi_i(e_i+0.5{u_i}^2)}{\partial t}+\frac{\partial\rho_i\varphi_i u_i(e_i+0.5{u_i}^2)}{\partial x}=Q_{di}-I_{di}(e_i+{u_i}^2)+F_{di}u_i$$

$$\frac{\partial n_i}{\partial t}+\frac{\partial nu_i}{\partial x}=0$$

Component of gas equation:

$$\frac{\partial\rho_1\varphi_1 y_j}{\partial t}+\frac{\partial\rho_1\varphi_1 y_j u_1}{\partial x}+\frac{\partial\rho_1\varphi_1 y_j v_1}{\partial y}=w_j$$

State equation

$$P=\rho RT\sum_1^m\frac{y_j}{w_j}$$

In these equations, i=2, 2a and the subscripts 1, 2 and 2a denote the variables of gas, RDX and Al. The variables are follows: ρ the density, u the horizontal velocity , v the vertical velocity, e the internal energy, P the pressure, $\varphi(\varphi_1+\varphi_2+\varphi_{2a}=1)$ the volume fraction, I the ratio of mass of unit volume, There are seven component in gas which are O_2, N_2, CO, CO_2, H_2O,Al(g) and Al_2O_3(g). y is concentration, w is molecular weight of gram.

For the RDX, we use the model in Hong[2], as follow:

$$I_{d2}=\begin{cases}0 & T_2<T_m\\ Q_{d2}/L & T_2\geq T_m\end{cases}$$

T_m is the melting point of RDX, L is latent heat. The RDX particles move under the effect of shock wave and heat up because of the heat conduct. And it begin to be peeled after melt and break down in the high temperature.

For the Al, we use the model[3], as follow:

$$I_{d2a}=-n\rho_{2a}4\pi R^2\frac{dR}{dt}$$

$$\frac{1}{R}\frac{dR}{dt}=-\frac{1}{k{d_0}^m/\Phi^{0.9}}$$

N is the number of particles in unit volume, R is the radius of particles, d_0 is the initial diameter, Φ is the fraction of O_2， m=1.75.

F is the force that the gas to particles:

$$F_{di}=\frac{n\pi R^2C_d\rho_1\sqrt{(u_1-u_i)^2+(v_1-v_i)^2}(u_1-u_i)}{2}$$

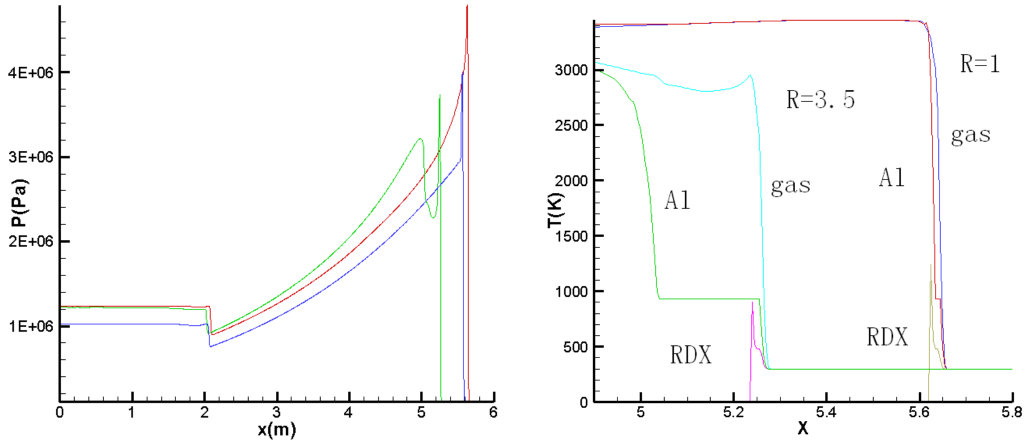
C_d is the drag force, Q is the conduct heat:

$$Q_{di}=4n\pi R^2\lambda_1 Nu(T_1-T_i)/(2R)$$

λ_1 is the heat conduct coefficient, Nu is the Nusselt number, q is the reaction power of unit mass. The metallic oxide will decompose to Al(g) and O_2 when the temperature is higher than the boiling point[4]. So the temperature will keep below the boiling point.

3 Simulation

To check the correctness of the program, we simulate the two dust separately. For the density of RDX is 0.75kg/m^3, the speed of the detonation wave is 1.899Km/s, the peak is 4.75MPa. S.Eidelman[5] achived the peak was 4.84MPa, Hong[2] got the speed was 1.802Km/s and Dong[6] got the speed was 1.916Km/s. For the density of Al is 0.304kg/m^3, we achieve the parameter of the detonation wave is $D=1.63\text{Km/s}, \rho_{CJ}=2.43\,\text{Kg/m}^3, u_{CJ}=673\,\text{m/s}, P_{CJ}=2.04\text{MPa}, T=3800\text{K}, P=3.31\text{MPa}$. The experiment of A.J.Tulis[7] achieved the speed is 1.65Km/s and result of literature[8] is $D=1.63\text{Km/s}, \rho_{CJ}=2.48\,\text{Kg/m}^3, u_{CJ}=681\,\text{m/s}, P_{CJ}=1.91\text{MPa}, T=3800\text{K}$. The simulate result correspond to other researchers' very well.



(a) (b)

Fig.1 Pressure and temperature at the same moments of different model

In the simulation, $\rho_{RDX} = 0.565\,kg/m^3$, $\rho_{Al} = 0.145\,kg/m^3$. For $r_{RDX} = 10\mu m$, Fig.1(a) is the pressure of the detonation wave and the lines from left to right are in condition that $r_{Al} = 3.5\mu m$, the RDX is only and $r_{Al} = 1\mu m$ at the same moment. Fig.1 (b) is temperature of gas, Al and RDX for $r_{Al} = 3.5\mu m$ and $r_{Al} = 1\mu m$ at the same moment. The three lines on left are temperature of gas, Al and RDX for $r_{Al} = 3.5\mu m$ and the three lines on right are temperature of gas, Al and RDX for $r_{Al} = 1\mu m$. From the picture we can see when the radius of Al is small, the power of RDX can make the Al react rapidly and the time of exothermic differ small so that the wave only has one peak. The peak of the wave is far from the wave of RDX only. When the radius of Al becomes bigger, the two dusts exothermic at the different time, the two peaks of detonation wave are observed. The first crest is the reaction of RDX. From the picture we can see the reaction time of RDX is very short. And the second crest is Al. The peak of pressure of Al is smaller than RDX and the reaction time of aluminum is longer than RDX. The speed and the pressure of the double-front detonation are both smaller than that of the single-front detonation. But the reaction region of the double-front detonation is longer.

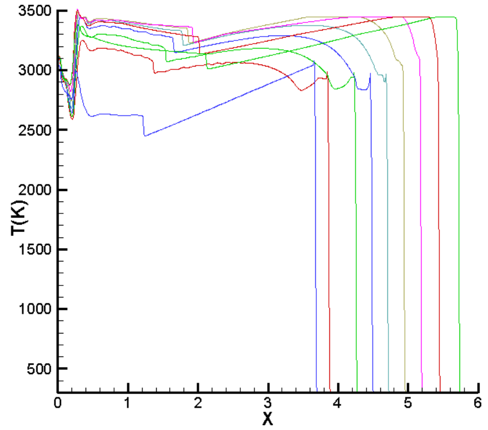


Fig.2 Temperature at different moments of different model

The curves of Fig.2 from left to right are the temperature in condition that the RDX only and the density of Al is 4.5μm, 4.0μm, 3.5μm, 3.0μm, 2.5μm, 2.0μm, 1.5μm, 1.0μm. Compared the RDX dust only, the temperature of the two dusts is obvious higher, but when the radius of Al is greater than2.0μm, the temperature will less but it will increase as the time go on.

Table 1 is the parameters of detonation wave of different radius of Al. While the radius of Al becomes larger, the wave speed will smaller, however when the radius reach the limit, the wave speed will keep const that the maximum wave speed of the Al only at the same density.The pressure of the second wave which is the peak of the second wave and the parameter of CJ point also become smaller with the radius of Al become larger. The CJ points are all behind the second wave.

Table 1 Parameters of detonation wave of different radius of AL

Radius of Al (μm)	Wave speed (Km/s)	Pressure of front wave (MPa)	Temperature of front wave (T)	Pressure of second wave(MPa)	Temperature of second wave(T)	Pressure of CJ point (MPa)	Temperature of CJ point(T)
1	1.90	4.79	3083			2.84	3411
1.5	1.85	4.62	3018			2.76	3442
2	1.86	4.41	2979			2.65	3446
2.5	1.78	4.06	2749	3.82	3103	2.48	3445
3	1.77	3.85	2717	3.58	3013	2.28	3415
3.5	1.73	3.74	2608	3.24	3000	2.07	3338
4	1.74	3.76	2579	2.94	3007	1.92	3285
4.5	1.74	3.75	2595	2.59	3016		

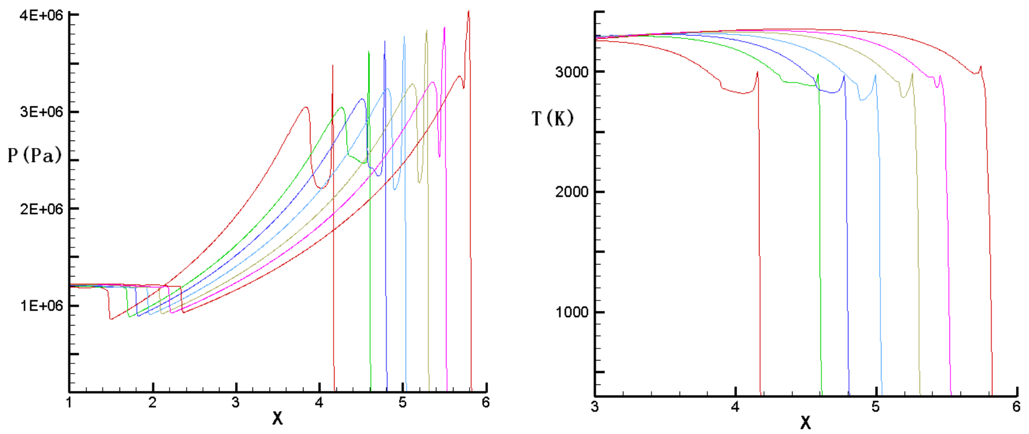


Fig.3 Detonation pressure and temperature of different moments of different radius of RDX

Table 2 Parameters of detonation wave of different radius of RDX

Radius of RDX (μm)	Wave speed (Km/s)	Pressure of front wave (MPa)	Temperature of front wave (T)	Pressure of second wave (MPa)	Temperature of second wave (T)	Pressure of CJ point (MPa)	Temperature of CJ point (T)
5	1.78	3.47	2999	3.31	3044	2.13	3358
7.5	1.75	3.65	2982	3.25	3036	2.11	3354
10	1.75	3.73	2970	3.29	3002	2.06	3353
12.5	1.72	3.78	2968	3.34	2948	2.14	3343
15	1.72	3.84	2989	3.33	2952	2.14	3341
17.5	1.72	3.87	2965	3.32	2971	2.13	3343
20	1.74	4.03	3038	3.33	2994	2.14	3340

Set the radius of Al as 3.5μm, the graphs of fig 3 are the pressure and temperature. The lines from left to right are in condition that the radius of RDX are $5\mu m, 7.5\mu m, 10\mu m, 12.5\mu m, 15\mu m, 17.5\mu m, 20\mu m$. The pressure of front wave is higher with the radius. For $r_{RDX} = 20\mu m$, the two peak of wave is not obvious. When the radius becomes smaller, the distance of the two waves become longer. The energy of RDX will warm up the Al, so the temperature of the wave will decrease. But with the Al exothermic, the temperature will trend to same.

4 Conclusion

In this letter, it simulates the detonation of RDX and aluminum particles in air alone. And the result fit the achievement of other researches very well. From the result it's found that the CE/SE method is suitable to simulate the problem of multiphase detonation. With the program the two mixed dusts detonation is studied. The research is focused on the double-front detonation wave structure. We studied the relationship of the speed and peak of pressure of detonation wave with radius of Al and the effect of radius of Al. And quite satisfactory calculation results are obtained.

References

[1]Khasainov B A, Veyssiere B. Initiation of detonation regimes in hybrid two-phase mixtures[J]. ShockWaves, 1996,6(1):9-15.

[2]Hong T, Lin W Z, Qin C S. Numerical simulation of suspended RDX dust detonation in a shock tube［J］. Chinese Journal of High Pressure Physics, 2010.24(1): 15-20.

[3] Price E.W.， Combustion of Metalized Propellants [A], Progress in Astronautics and Aeronautics: Fundamenals of Solid一Propellant Combustion， edited by K .K. Kuo， and M. Summerfield， 1984， AIAA， New York, Vol.90， ChaPterg:479-513

[4] Steinberg T.A, Wilson D.B, Benz F. The Combustion Phase of Burning Particle[J],Combustion and Flame,Vol.91,200-208,1992

[5] Eidelman S，Yang X L． Detonation wave propagation in combustible particle/air mixture with variable particle density distributions［J］． Combust Sci Tech, 1993, 89: 201-218．

[6]Dong Hefei, Hong Tao, Zhang Xiao-li, Numerical Simulation of Explosive Dust Detonation with CE / SE Method [J],Chinese Journal of Computational Physics, 2012, Vol. 29, No. 4, 495-502

[7] Tulis A J, Selman J R. Detonation Tube Studies of Aluminum Particles Dispersed in Air[A]. 19th International Symposium on Combustion[C], The Combustion Institute,655-663,1982

[8] Hong Tao, Qin Cheng-sen. Parameters of Detonation in Suspended Aluminum Dust[J], Energetic Materials, 2004, Vol.12,No.3, 129-133