Numerical Simulation of Detonations in Suspensions of RDX Particles by the CESE Method

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1 Introduction

The RDX (octahydro-1, 3, 5, 7-tetranitro-1, 3, 5, 7-tetrazocine, $C_3H_6N_6O_6$) is widely used in composite propellants of solid rocket because of its energetic and smokeless features. When RDX particles are intentionally or unintentionally dispersed into the air, the resulting suspensions can be detonable. Understanding the detonation properties is very important in view of the destructive effects.
Here, we used numerical simulation to study the detonation processes of RDX particles suspended in the air. In order to capture the strong discontinuity in detonation waves, we applied the space-time conservation element and solution element (CESE) method to discretize the equations.
The CESE method originally proposed by Chang[1] provides a new way to solve the hyperbolic conservation equation. It has many features differing from other traditional numerical schemes, such as unified treatment of space and time, new shock-capturing strategy, and satisfaction of both local and global flux conservation in space and time by introducing conservation element (CE) and solution element (SE). Simplicity and accuracy are the distinguished advantages of the CESE method.
In this paper, we first simulated the detonation of RDX dust with the concentration of 750g/m^3 and the particle diameter of 40μm. By continually reducing the dust concentration in simulation, we obtained the lower limit of explosion. Finally we calculated the detonation process in a wavy channel.

2 Model

A two-phase mixture model was adopted. It assumes that each phase has independent hydrodynamic and thermodynamic properties. These two phases transfer their mass, momentum, and energy by the interphase terms. The governing equations can be written as:
Gaseous phase

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

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

Solid phase

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

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

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

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

Where the subscripts 1 and 2 denote the variables of the gas and particles. The ρ is the apparent density with $\rho_1=\rho_g\varphi_g$ and $\rho_2=\rho_s\varphi_s$ in which the φ is the volume fraction and yields $\varphi_g+\varphi_s=1$. The Y_j is the gaseous mass fraction of species j due to chemical reactions, and the ω_j is the relevant mass production rate. In our model j=1~5 corresponds with O_2, N_2, CO_2, H_2O, and CO, respectively. The other variables are as follows: u is the velocity, p the pressure, e the specific internal energy, N the particle number per unit volume, q_{chem} the heat of reaction, m the mass production rate, f the interphase drag force, and q the convective heat transfer from gas to particles.

When the temperature rises to melting point, the particle surface begins to melt. We suppose that the melting part is peeled off by the gas and decomposes immediately. The mass change rate is defined as

$$m = q / L$$

Where the L is the melting energy of RDX.

The interphase drag force is

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

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

$$q = N \cdot \pi d_p \cdot Nu \cdot \lambda_g (T_1 - T_2)$$

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.

A simplified combustion model of RDX was used. The RDX particles first decompose:

$$C_3H_6N_6O_6 \rightarrow 3H_2O + 3CO + 3N_2$$

The product CO then reacts with the oxygen

$$2CO + O_2 \leftrightarrow 2CO_2$$

The forward and backward reaction rates are

$$\omega_f = \min(1.0, 7.93e^{-2.48\Phi}) \times 1.5 \times 10^{13} [CO]^{1.0} [O_2]^{0.25} [H_2O]^{0.5} e^{-40/RT_1}$$

$$\omega_b = 4.16 \times 10^{16} [CO_2]^{1.0} [O_2]^{-0.25} [H_2O]^{0.5} e^{-106.95/RT_1} T_1^{-0.5}$$

In which the Φ is the equivalence ratio, the [X] denotes the concentration of the substance X.

The equation of state for the gas production is

$$p = \rho_g R T_1 \sum_{j=1}^{5} \frac{Y_j}{W_j}$$

In our simulation, we first use the CESE scheme to calculate the governing equations without the source terms, and then use the fourth-order Runge-Kutta method to calculate the source terms.

3 Results

We simulated the dust detonation of RDX particles with apparent density of 750g/m^3 and diameter of 40μm in a shock tube. A uniform mesh of Δx=2.5mm is used. The dust was ignited from the left wall with the condition of φ_g=1, u_l=1000m/s, and T_l=3600K. Fig. 1 shows the pressure profiles at different time with intervals of 150μs. It shows the transient process from initiation to steady detonation. The steady detonation forms after 0.6m with the velocity of 1910m/s and the Von Neumann peak pressure of 4.66MPa. The theoretical CJ detonation values are p_{cj}=3.28MPa, u_{cj}=848m/s, and T_{cj}=3200K, respectively. Fig. 2 shows the velocity and temperature profiles of the gas and particles near the detonation front. We can observe that the particles are always dragged and heated by the gas.

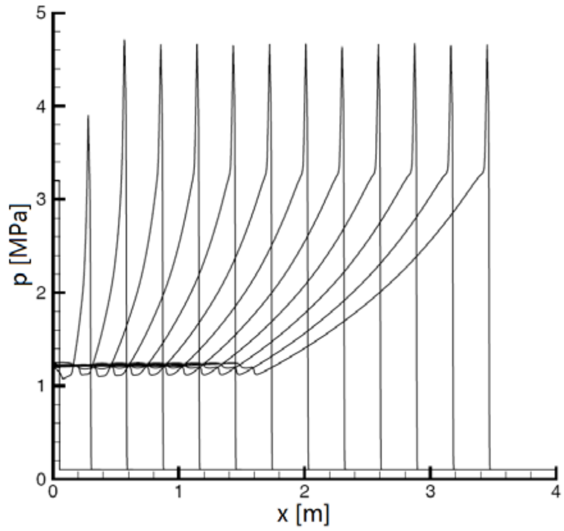

Figure 1. Gas pressure profiles at 0~1.8ms with intervals of 150μs.

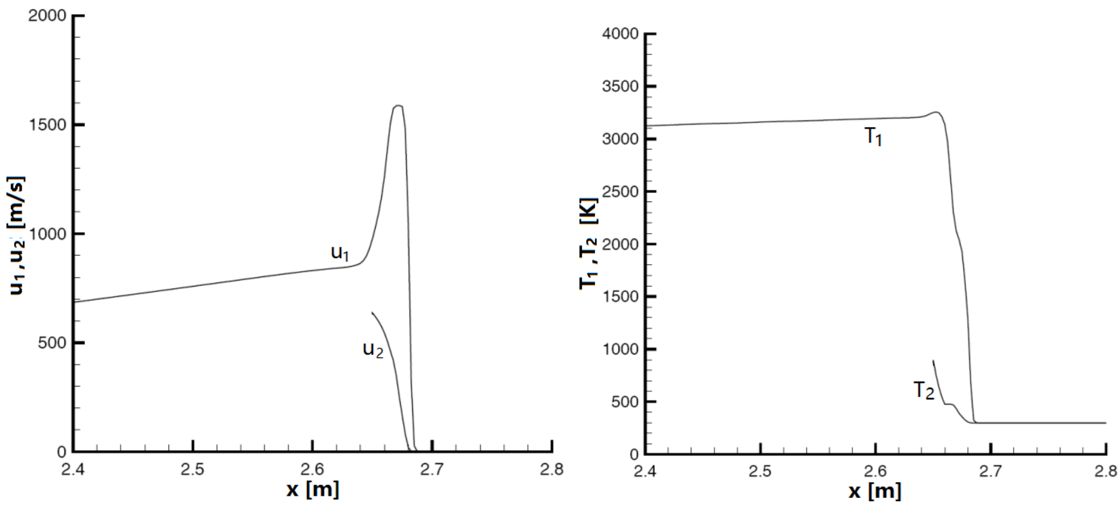

Figure 2. Velocity (Left) and temperature (Right) profiles of the gas and particles near the detonation front.

To explore properties of the detonation process, we simulated additional cases by changing the particle diameter and apparent density independently. Fig. 3a shows the histories of the peak pressure with the particle diameter increasing from 30μm to 60μm. The run distance to steady detonation increases from 0.5m to 1.7m. That is because the combustion slows as the specific surface area decreases with the rise of the diameter. However, the same steady detonations are reached at last due to the same apparent density. Fig. 3b shows the histories of the peak pressure with the particle apparent density decreasing from 750g/m^3 to 300g/m^3. The run distance to steady detonation increases from 0.6m to 2.0m, and the steady-state peak pressure decreases from 4.66MPa to 2.91MPa. We further reduced the apparent density to examine the lower limit of explosion. Fig. 4 shows the peak pressure with the densities of 80g/m^3 and 70g/m^3. The combustion can be maintained in the 80g/m^3-density RDX suspension, but will be extinct in the 70g/m^3-density suspension. This result agree well with the experiment [2].

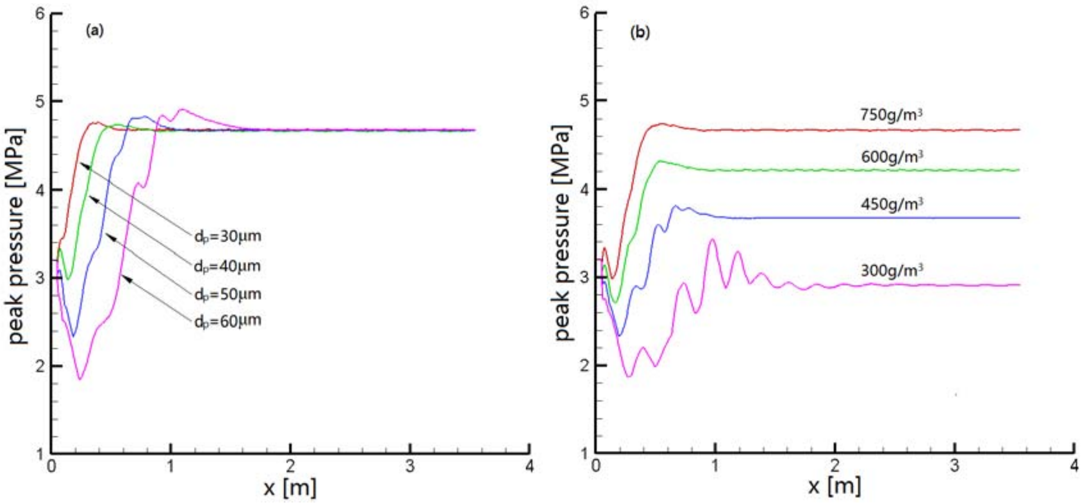

Figure 3. Peak pressure histories with different particle diameters and densities. (a): The particle diameter increases from 30μm to 60μm, the apparent density is 750g/m^3. (b): The apparent density decreases from 750g/m^3 to 300g/m^3, the particle diameter is 40μm.

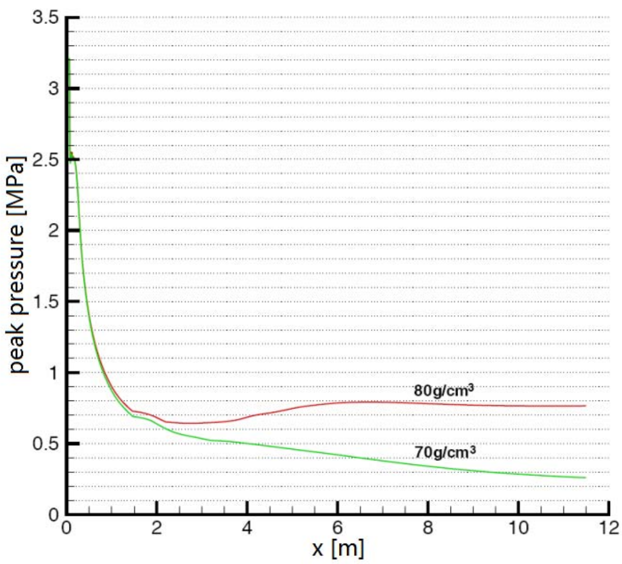

Figure 4. Peak pressure histories with apparent densities of 80g/m^3 and 70g/m^3.

We further simulated the first detonation case in a wavy channel. The length of the tube is 4m and the width is 0.8m. The length and width of the grooves are 0.3m and 0.1m. The right boundary is open outlet and others are solid walls. The 0.1m-long and 0.8m-wide area at left is ignited. The computational mesh is 2.5mm×2.5mm. Fig. 5 shows the pressure and temperature contours at different time. The flow pattern is very complex due to the dispersion and reflection. We can see the transverse waves moving along the detonation front in longitudinal direction. The results demonstrate that the CESE method is capable to catch the salient features of complex suspension detonations.

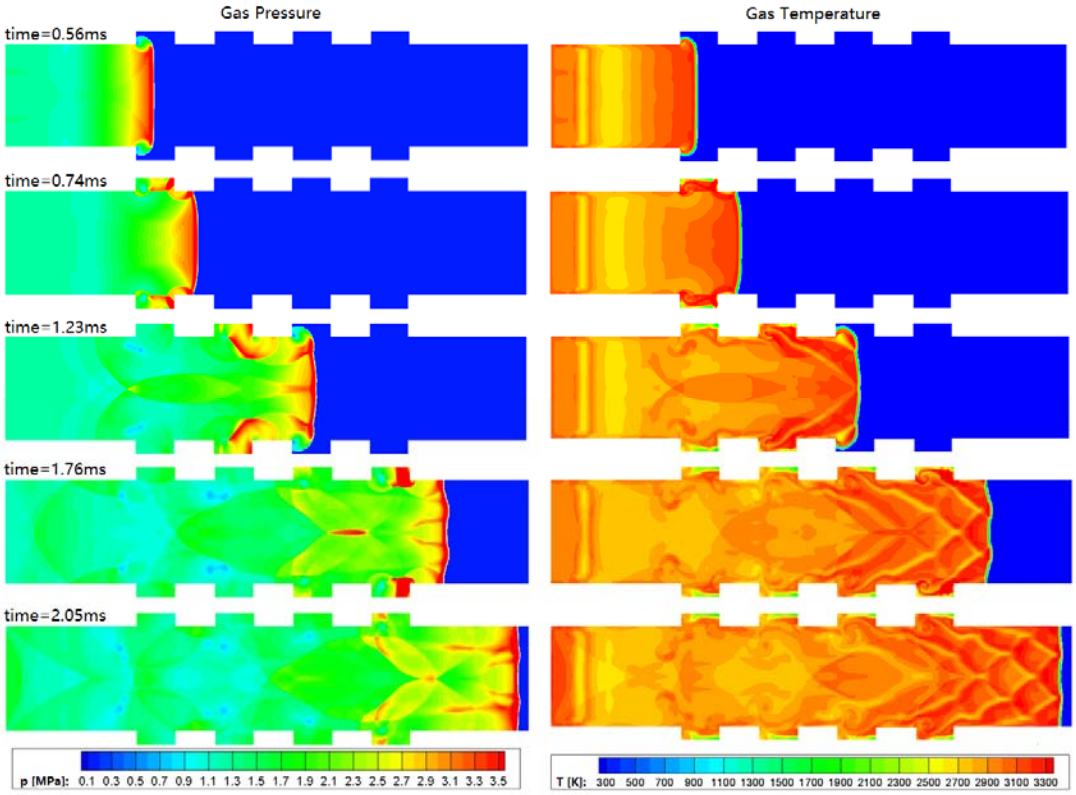

Figure 5. Contours of pressure (Left) and temperature (Right) at different time in the wavy tube. From top to bottom, the time is 0.56ms, 0.74ms, 1.23ms, 1.76ms, and 2.05ms.

4 Conclusions

Detonations of suspended RDX particles in air were simulated with two-phase flow model. Formation and propagation of detonations were examined. The parameters of detonations were obtained.

As the particle diameter increasing from 30μm to 60μm, the run distance to steady detonation increases from 0.5m to 1.7m.

As the particle apparent density decreasing from 750g/m^3 to 300g/m^3, the run distance to steady detonation increases from 0.6m to 2.0m, and the steady-state peak pressure decreases from 4.66MPa to 2.91MPa. When the density falls to 80g/m^3 the combustion still be maintained. However, the combustion will be extinct after the density falling to 70g/m^3.

The detonation process of the suspension in a wavy tube was simulated. The results demonstrate that the CESE method is capable to catch the salient features of complex suspension detonations.

Acknowledgement

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References

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[2] Fu w. (2008). Experimental study of the explosion characteristics of the RDX dust. Master's thesis in Nanjing University of science and technology, Nanjing, China. (*in Chinese*)