Numerical Simulation of Aluminum Dust Detonations with Different Product Phases

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1 Introduction

Detonation waves are waves of supersonic combustion induced by strong coupling shock and heat release. Detonation research has attracted much attention in recent years owing to its potential applications in hypersonic propulsion. Aluminum (Al) particle detonation is a type of dust detonation, and its research is important in the prevention of industrial explosions. Al dust detonations for flake and spherical particles have been studied , which is found to be very sensitive to the specific area[1]. Zhang et al.[2]investigated transverse waves in dusty detonations and calculated, using a detonation model, the minimum tube diameter for generating detonation. Fedorov et al.[3] applied a non-equilibrium model of steady Al-oxygen detonations to calculate parameters for one- and two-dimensional cellular detonations. One-dimensional and two-dimensional cellular structures of Al-oxygen detonation are also simulated and the influence of particle diameters are discussed[4].

In previous research, the combustion of Al dust ia assumed to be diffusion-controlled. However, Tanguay et al.[5] claimed that Al particle combustion is kinetics-controlled in the detonation products, even for a particle on the scale of $100\mu m$. This is due to the high speed of the detonation products, which has been neglected before. Then a hybrid combustion model that includes the kinetics-controlled combustion is proposed[6]. This model is used in cellular detonation simulations, and their results are compared with those obtained with the classic diffusion model[7] . The effect of realistic heat capacities used for the Al particle internal energy is studied to improve the accuracy[8]. However, the inclusion of both kinetic- and diffusion-controlled combustion introduces unresolved problems. Diffusion-controlled combustion produces solid alumina $Al_2O_3(s)$, while the diffusion-controlled combustion produces gaseous alumina $Al_2O_3(g)$. In the research field of dust detonation, we are not aware of published results considering

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both the solid and gaseous products, and the effects on the detonation parameters are thus still unclear. In this paper, both $Al_2O_3(s)$ and $Al_2O_3(g)$ are simulated to study how the product phase affects dust detonation, and a variable heat release model dependent on the product phase is proposed and discussed.

2   Mathematical Model and Numerical Method

Governing equations can be written as

$$\frac{\partial U_g}{\partial t} + \frac{\partial E_g}{\partial x} = S_g + H_g \tag{1}$$

$$\frac{\partial U_p}{\partial t} + \frac{\partial E_p}{\partial x} = S_p + H_p \tag{2}$$

where the subscript $(*)_g$ denotes the gas terms and $(*)_p$ denotes the particle terms. S is the source term induced by chemical reactions and H is the source term induced by gas-particle interactions. Detailed expressions for each term can be found in previous papers[6]. Above equations are solved separately, and the gases and particles are coupled through the source terms. The gas-particle force is

$$f_x = C_d \sum_{i=1}^{m} n_i \frac{\pi d_{pi}^2}{4} \rho (u - u_p) \sqrt{(u - u_p)^2}/2 \tag{3}$$

where n_i is the number density of each solid specie, d_{pi} is the particle diameter, ρ is gas density, u is velocity, and . C_d is drag coefficient.

The hybrid combustion model, proposed by [6], includes not only diffusion-controlled but also kinetics-controlled combustion. Al combustion rate k in this model is defined as

$$k = \frac{k_d k_s}{k_d + k_s} \tag{4}$$

where k_d and k_s are the reaction rates of diffusion- and kinetics-controlled combustion, respectively[6]. The shock-capturing method is the dispersion controlled dissipation scheme[9], which is one kind of the TVD schemes. In this simulation, both $Al_2O_3(s)$ and $Al_2O_3(g)$ are included. Generally three gas species $O_2(g)$, $N_2(g)$ and $Al_2O_3(g)$, and two solid species, $Al(s)$ and $Al_2O_3(s)$, are included in the simulation. In order to focus on the product phase effects, another type of gas species AlO is not considered in the current one-step heat release research.

3   Numerical Results and Discussion

3.1   Effects of Different Product Phases

To examine the effects of heat capacity, Al dust detonation is first simulated with solid alumina $Al_2O_3(s)$. Following previous experiment[10], initial pressure is
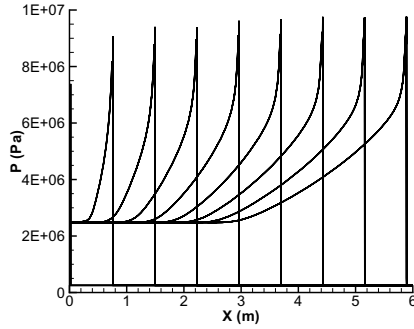
Fig. 1 Pressure profiles of Al dust detonation with solid product.

2.5*atm* and initial temperature is 300*K*. The average density of Al particles, with the diameter 2μm, are 1250g/m^3 and there is no $Al_2O_3(s)$ in the initial stage. Gaseous $O_2(g)$ and $N_2(g)$ have a ratio of mole concentrations of 1:4, initially. The pressure profiles are shown in Fig.1, with the grid scale being 0.5*mm* and the calculation domain being 6.0 m in length. The detonation is initiated by a small zone having a high temperature and pressure near the left side of the domain. Self-sustained detonation occurs and a constant speed of detonation of 1828m/s is gradually reached. This result has been shown in our previous research, including discussion on its physics, resolution test, and comparison with experimental results[8].
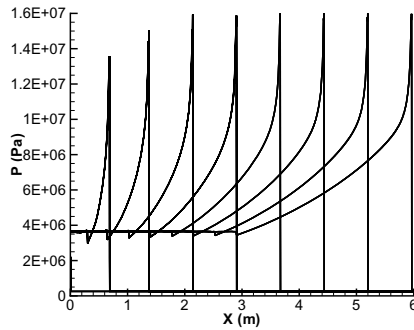

Fig. 2 Pressure profiles of Al dust detonation with solid product.

If the product is assumed to be gaseous rather than solid, the dust detonation is significantly different, as shown in Fig.2. The maximum pressure is about 16.0MPa, 64.0 times of pre-shock pressure, compared with 9.4MPa for the solid product. Additionally, the detonation velocity reaches approximately 2145m/s, which is much higher than the velocity of 1828 m/s for the solid product. To verify the numerical results, a resolution test is carried out using different grid scales by doubling the grids. The grid 0.5*mm* is found to be sufficient for both the gaseous and solid products, and is used in the paper.

Comparing results above, the effects of the product phase on the detonation parameters can be concluded. For given parameters, the gaseous product will induce higher pressure and velocity, meaning stronger dust detonation, while the solid product will induce weaker dust detonation. This is because the solid product, which does not contribute to the pressure, is driven by the gas-particle force. In general, there is strong detonation in the case of gaseous product, and weak detonation in the case of solid product.

3.2   Heat Release Model Dependent on the Product Phase

Although the effects of different product phases have been clarified, a new problem has emerged. When the gaseous product is introduced, the results deviate from, rather than approach to experimental results. However, gaseous products are used in almost all previous models, and most of our knowledge on Al dust detonation from the diffusion-controlled combustion model. Therefore, we must revisit previous models and examine how the close-to-experiment results were simulated.

Generally speaking, there are no widely accepted Al dust detonation models. Because Al multi-phase combustion is complicated, the combustion is usually simplified into one-step irreversible heat release, with several empirical parameters. This introduces the uncertainty to the simulation results, but ensures the detonation velocity or pressure is close to experimental results. The heat release is usually set to approximately 800KJ/mol, but in reality the heat release is not constant. The heat release from the solid alumina formation is not the same as the release from the gaseous alumina formation. Previous simulations with gaseous alumina usually used the heat release from the solid alumina formation, approximately 800KJ/mol. This induces the inconsistency, and the reaction rate thus needs to be adjusted to get close-to-experiment results. Furthermore, the constant heat release introduces problems as reported in our previous research[8]. To model the Al dust detonation accurately, the constant heat release must be abandoned.

Here, one model with two heat release values is proposed as the primary step. The first value Q_s is heat release from the solid alumina formation, and the second value Q_g is heat release from the gaseous alumina formation. Referring to the results before, Q_s is chosen to be 638KJ/mol without latent heat roughly. This value may produce results similar to those shown in Fig.1, and the latent heat release is not used to exclude unnecessary uncertainty. Q_g is the heat release of $Al_2O_3(g)$ formation and is set to be 273KJ/mol, the heat of formation for standard state. In this model, the fractions of the gaseous and solid product are prescribed, and the heat release is calculated according to the fractions, that is

$$Q = f_s Q_s + f_g Q_g, f_s + f_g = 1 \tag{5}$$

where f_s is the fraction of solid product and f_g is the fraction of gaseous product. We stress here that our intention is not to develop an accurate model to simulate Al particle detonation, but to ascertain key factors to develop advanced Al detonation models. Therefore, these heat release values Q_s and Q_g are not exact, but in a

reasonable range. There are too many uncertainties in the current models, and in this study we focus on the choice of heat release related with the product phase.

The detonation wave with $f_s = 0, f_g = 1$,which corresponds to purely gaseous product, is simulated first. The maximum pressure is 10.5MPa and the velocity is 1796m/s. These results are close to the results shown in Fig.1, for only solid product. Indeed, this is the extreme case because the solid product is absent, but the results are much better than the results shown in Fig.2. The underlying reason is that the heat release Q_g, which corresponds to the formation heat of gaseous alumina, is consistent with the product phase. In most previous models, the heat release is approximately 800KJ/mol, but the product is gaseous. We note that those models are inconsistent, although some close-to-experimental results can be produced.
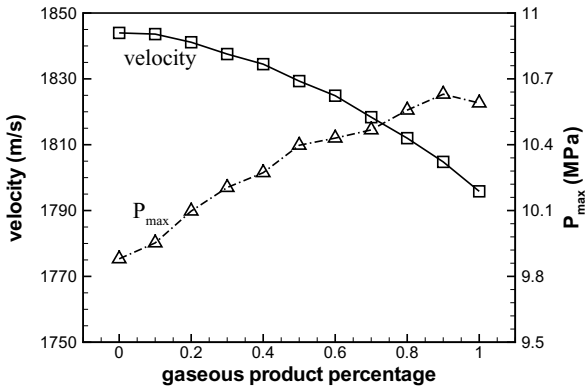

Fig. 3 Detonation velocity and maximum pressure of Al dust detonation as a function of the gaseous product percentage.

Al dust detonation waves with various fractions of gaseous alumina are simulated, as shown in Fig.3. When the gaseous product ratio increases, the velocity decreases and the maximum pressure increases. This demonstrates the effect of different product phases, because the velocity and pressure change in the same manner in the case of single product phase. However, the velocity variation is less than 3%, and the velocity variation is less than 8%. This variation is not of the same order as the difference in results shown in Fig.1 and Fig.2. It is thus concluded that the detonation parameters are insensitive to the product phases, if the values of heat release values are chosen properly.

4   Conclusion

Al dust detonations are simulated numerically to study the effects of product phases and the choice of heat release. Recent experimental results indicate that both gaseous and solid product may appear in the detonation, but effects of different product

phases on the detonation parameters have not yet been studied. Numerical results demonstrate that gaseous product will induce high velocity and pressure, while solid product will induce low velocity and pressure. When revisiting previous models, the inconsistency between the product phase and heat release is found, and a new model with variable heat release dependent on the product phase is proposed. Simulations with both solid and gaseous products are carried out, which reveals the necessity of establishing a relationship between the heat release and reaction products.

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