Effects of Particle Size Distribution on Cell Size Prediction in Al-Air Detonation

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1 Introduction

Aluminum (Al) powder, a high energetic metal material, is common in processing factories of various Al products and bears a great danger of explosion [1, 2]. Experimental investigations of Al-gas detonation are rather difficult due to the requirements of large tubes and strong initiation sources, and experimental conditions are hard to control and reproduce as well due to dispersion problems of solid particle suspensions, which makes numerical simulation an important aspect of studying Al-gas detonations [3,4].

It is found in literatures [5-7] that quantitative relationships of particle size, in the form of power laws, exist in many characteristic lengths of Al-gas detonation, including the induction length, two-phase relaxation lengths, detonation cell size, et al. Recently, the authors have developed a Eulerian-Lagrangian algorithm to take particle size distribution into account in gas-particle two-phase detonation simulations [8], and significant differences in detonation front structure and cell size between monodisperse and polydisperse Al-air detonations have been found [9]. As realistic reactive dust in industries and experiments is always polydisperse in size, it is of great importance to consider particle size distribution in realistic gas-particle detonation modelling and simulate this type of flow under a Eulerian-Lagrangian framework.

However, as two-dimensional or three-dimensional simulation is always needed in detonation cell size predictions, it is rather expensive when considering particle size distribution under a Eulerian-Lagrangian framework, especially for fine reactive particles. A simple idea is to introduce an effective particle size of the polydisperse suspension to take particle size distribution into account in detonation cell size predictions and conduct numerical simulations still through the classical Eulerian-Eulerian algorithm. To achieve this, following things must be confirmed first. Whether an effective particle size of a polydisperse suspension exists in two-phase detonation cell size predictions? How to obtain this effective particle size through the statistical characteristics of the polydisperse suspension? And what is the physical meaning of this effective

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particle size? The efforts made in this study are trying to address these questions by taking Al-air detonations as examples.

2 Computational Details

In this study, heterogeneous detonation propagating in an air suspension of small spherical Al particles is under consideration, and the suspension is assumed to be diluted enough to neglect the volume fraction of Al particles and particle-particle collisions. As it is a highly transient two-phase flow with strong shock waves, thermal and mechanical non-equilibrium between gas and solid particles is taken into account, which means that the momentum exchange and heat transfer between gas and particles are both modelled in simulations. Under the Eulerian-Lagrangian framework, the motion of every particle is tracked by Newton's laws of motion. The motion of gas is still described by the Euler equations, and gas-particle interactions, including mass, momentum and energy transfers, are presented as source terms. The detailed expressions of 2D governing equations can be found in our previous studies [8,9].

For the combustion of Al particles, the single-step global combustion model has been well developed, and is successful in predicting many key features of Al-gas detonation [5-10]. Therefore, it is employed to model the combustion of Al particles in this study, with the product Al_2O_3 presented as solid state,

$$2\mathrm{Al}(\mathrm{s})+3/2\,\mathrm{O}_2(\mathrm{g})\rightarrow \mathrm{Al}_2\mathrm{O}_3(\mathrm{s}). \tag{1}$$

Then, the reaction heat release is implicitly given by the formation enthalpies of Al, O_2 and Al_2O_3.

To model the combustion rate of the Al particles, the hybrid combustion model proposed by Zhang et al. [10] is employed in this study. The Lagrangian form of Al combustion rate can be easily derived from the original Eulerian form, as follow,

$$I_{pk}=\pi d_{pk}^2 C_{oxi}\frac{\nu_p W_p}{\nu_{oxi}W_{oxi}}\cdot\frac{k_{dk}k_{sk}}{k_{dk}+k_{sk}}. \tag{2}$$

The basic case simulated is the same as that experimentally investigated by Zhang et al. [11]. The tested material is a micrometric grade of atomized Al with a mean diameter of 2 μm suspended in air. The dust concentration is c_p = 1.25 kg/m^3, and the initial pressure and temperature of the suspension are respectively p_0 = 2.5 atm and T_0 = 300 K. The 2D computational domain is 1.6×0.1 m in length and width, and particles are set to be uniformly distributed in the computational domain. The mesh size is 0.05 mm, which has been well validated by convergence tests. Moreover, detonation is directly initiated by a small zone of high temperature and pressure at the left end of the computational domain. The 2D Al-air two-phase detonation problems are solved by our in-house space-time conservation element and solution element (CE/SE) code with Message Passing Interface (MPI) implementation [8,12].

3 Particle Size Distribution

Realistic Al-gas suspension involved in industries and experiments is always polydisperse in size, and it can be represented by a log-normal particle size distribution via the following number frequency distribution function $f_n(d_p)$,

$$f_n(d_p)=\frac{1}{\sqrt{2\pi}\sigma_0}\exp\left[-\frac{1}{2}\left(\frac{\ln d_p-\ln d_{nM}}{\sigma_0}\right)^2\right]\frac{1}{d_p}, \tag{3}$$

where d_{nM} and σ_0 are the number median diameter and standard deviation of the distribution, respectively. In numerical simulations, particle diameters of the polydisperse Al suspension can be set by a random number generator via Eq. (3).

The two mean diameters most often used to describe the statistics characteristics of the polydisperse suspension are the volume-average diameter, $\overline{d}$, and the mass-weighted-average particle diameter, $\overline{d}_m$,

$$\begin{cases} \overline{d} = \left[\int_0^\infty s^3 f_n(s) ds \right]^{1/3} = d_{nM} e^{\frac{3}{2}\sigma_0^2} \\ \overline{d}_m = \left[\int_0^\infty s^4 f_n(s) ds \right] / \left[\int_0^\infty s^3 f_n(s) ds \right] = d_{nM} e^{\frac{7}{2}\sigma_0^2} \end{cases}. \tag{4}$$

Then, the two parameters describing the log-normal distribution function, d_{nM} and σ_0, can be easily obtained through $\overline{d}$ and $\overline{d}_m$ via Eq. (4). In Zhang's experiment [11], $\overline{d}$ = 2 μm and $\overline{d}_m$ = 3.3 μm, which yields d_{nM} = 1.37 μm and σ_0 = 0.50.

Notably, $f_n(d_p)$ would reduce into a Dirac delta function $\delta(d_{nM})$ when $\sigma_0 \rightarrow 0$. Therefore, a suspension with σ_0 = 0 corresponds to a monodisperse suspension that consists of only one particle size, and $\overline{d} = \overline{d}_m = d_{nM}$ at that time.

4 Results and Discussions

To begin, cellular detonations of the monodisperse Al-air suspension with a uniform particle diameter of 2 μm and the polydisperse Al-air suspension with $\overline{d}$ = 2 μm and σ_0 = 0.5 that corresponds to Zhang's experiment [11] are respectively shown in Fig. 1 via peak pressure contours. It can be revealed that stable and regular cellular detonation structures have been obtained and the estimated cell sizes of them are $\lambda_{monodisperse}$ = 10.5 ± 0.5 mm and $\lambda_{0.5}$ = 13.3 ± 0.8 mm, respectively. $\lambda_{0.5}$ is 27% larger than $\lambda_{monodisperse}$. As realistic Al-gas suspension involved in industries and experiments is always polydisperse in size but monodisperse suspension is always used in Al-gas detonation modelling in previous studies [5-7,10], the difference in detonation front structures indicates the great importance of considering particle size distribution in heterogeneous detonation modelling and simulating this type of flow under a Eulerian-Lagrangian framework.

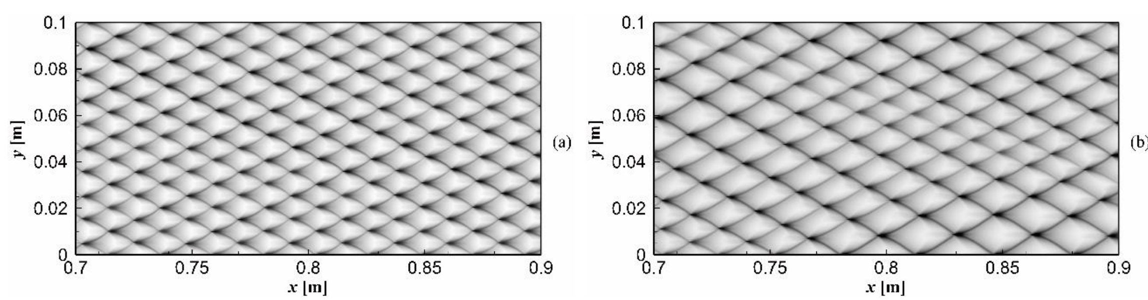

Figure 1. Peak pressure contours of Al-air detonations, (a) monodisperse with d_p = 2 μm and (b) polydisperse with $\overline{d}$ = 2 μm and σ_0 = 0.5.

However, it can be rather expensive when considering particle size distribution under a Eulerian-Lagrangian framework to simulate detonation cellular structures, especially for fine reactive particles. For example, there are 64 million Eulerian grids within the 2D computational domain with a grid size of 0.05 mm, while there are about 370 million Lagrangian particles in the Al suspension with a dust concentration of 1.25 kg/m^3 and a mean particle size of 2 μm in this 2D simulation, resulting in about 8500 CPU hours needed to complete the simulation. When nano-aluminum particles are under consideration, such as 100 nm in size, the number of Lagrangian particles can reach 150 billion, leading to impossible implementation of simulation with such large scale. This motivates us that if we can find an effective particle size of the polydisperse suspension, we may be able to conduct simulations of monodisperse detonation still through the classical Eulerian-Eulerian algorithm to predict detonation cell sizes of polydisperse suspension with high accuracy and save computational sources in the meanwhile.

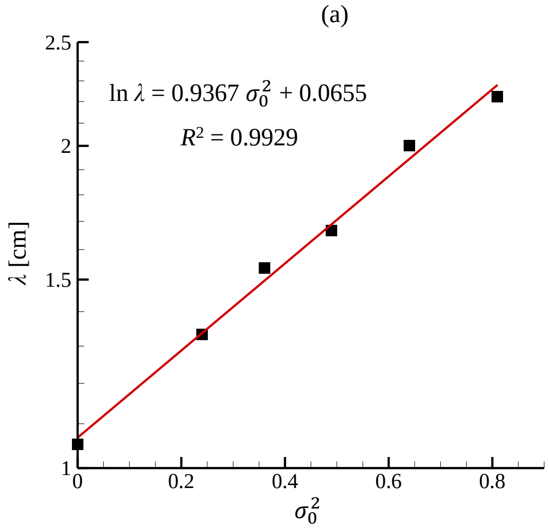

Figure 2. Detonation cell sizes of Al-air suspension as functions of (a) square of standard deviation σ_0^2 and (b) particle diameter d_p.

To do this, the quantitative relationship between detonation cell size and particle size distribution should be determined first. Figure 2a shows the cell sizes estimated by polydisperse detonation simulations with different σ_0 but fixed $\overline{d}$ = 2 μm, where R^2 is the square of correlation coefficient of fitting. It can be revealed that the relation between λ and σ_0 is

$$\lambda \sim e^{0.9367\sigma_0^2}. \tag{5}$$

Further, to determine the effective particle size, the quantitative relationship between detonation cell size and particle size of monodisperse suspension should be used as well. Indicated by Fig. 2b, the relation between λ and d_p in monodisperse suspensions is

$$\lambda \sim d_p^{1.1968}. \tag{6}$$

Combining Eq. (5) with Eq. (6), the effective particle diameter appears as

$$d_p \sim e^{0.7827\sigma_0^2}. \tag{7}$$

In Eq. (7), the relationship is obtained with a fixed value of $\overline{d}$, and $\tilde{d}_p$ can be reduced into the particle diameter of monodisperse suspension when $\sigma_0 = 0$. It is easy to reveal that the proportional constant must be $\overline{d}$, and the final expression of the effective particle diameter for polydisperse detonation cell size predictions is

$$d_p = \bar{d} \cdot e^{0.7827\sigma_0^2} = d_{nM} e^{1.5\sigma_0^2} \cdot e^{0.7827\sigma_0^2} = d_{nM} e^{2.2827\sigma_0^2}. \tag{8}$$

There is another way to find the effective particle diameter for detonation cell size predictions with particle size distributions. Assuming that the heterogeneous detonation cell size depends on the mean combustion rate of particles. As for the kinetic-controlled combustion model, the particle combustion rate is proportional to the square of particle diameter, while it is proportional to the particle diameter in the diffusion-controlled model. Therefore, the effective diameters of these two models can be determined through

$$\tilde{d}_p = \begin{cases} \left[\int_0^\infty s^3 f_n(s)\,ds\right] / \left[\int_0^\infty s^2 f_n(s)\,ds\right] = d_{nM} e^{2.5\sigma_0^2}, & \text{for kinetic-controlled} \\ \left\{\left[\int_0^\infty s^3 f_n(s)\,ds\right] / \left[\int_0^\infty s f_n(s)\,ds\right]\right\}^{1/2} = d_{nM} e^{2\sigma_0^2}, & \text{for diffusion-controlled} \end{cases}. \tag{9}$$

Comparing Eq. (9) with Eq. (8), difference only exists in the constant of exponent, and $2 < 2.2827 < 2.5$. As a hybrid combustion model is used in this study, the expression of Eq. (8) is thought to be reasonable.

To validate Eq. (8), an example is carried out with a polydisperse suspension with $\bar{d}$ = 4 μm and σ_0 = 0.8. From Eq. (4), d_{nM} = 1.53 μm is obtained, which yields an effective particle diameter of $\tilde{d}_p$ = 6.6 μm. Therefore, the detonation cellular structures of the polydisperse suspension and the monodisperse suspensions with d_p = 4 and 6.6 μm are shown in Fig. 3. The estimated detonation cell sizes are respectively $\lambda_{\text{polydisperse}}$ = 50.0 ± 10.0 mm, $\lambda_{4\mu\text{m}}$ = 28.6 ± 3.6 mm and $\lambda_{6.6\mu\text{m}}$ = 50.0 ± 10.0 mm. The result predicted by the effective particle diameter agree well with the result obtained by the polydisperse detonation simulation, whereas the monodisperse result of d_p = 4 mm is 43% under-predicted.

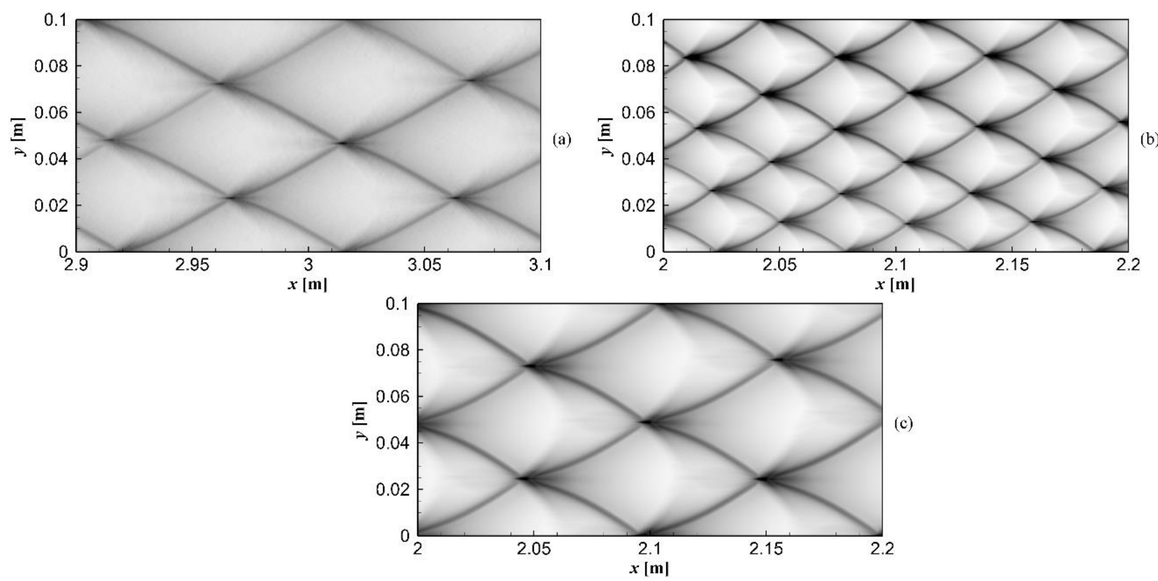

Figure 3. Al-air detonation cellular structures, (a) polydisperse with $\bar{d}$ = 4 μm and σ_0 = 0.8, (b) monodisperse with d_p = 4 μm and (c) monodisperse with d_p = 6.6 μm.

5 Conclusion

In this study, we construct an important quantitative relationship between the effective particle diameter for polydisperse detonation cell size predictions and the characteristic parameters in particle size distribution, i.e., $\tilde{d}_p = d_{nM} e^{2.2827\sigma_0^2}$. Using this effective particle diameter to take particle size distribution into account, predictions of detonation cell size in polydisperse suspensions can be easily implemented by monodisperse detonation simulations through the classical Eulerian-Eulerian algorithm with high accuracy and saving computational sources in the meanwhile.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Grant Nos. 11672312, 11772284 and 11532014), the Research Grants Council, Hong Kong (Grant No. 152151/16E), the Department of Mechanical Engineering, The Hong Kong Polytechnic University (Grant No. G-YBYJ) and the opening project of State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology (Grant No. KFJJ18-12M).

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