Research paper

Numerical analysis on combustion characteristics of nano aluiminum particle-oxygen two-phase detonation

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Abstract

Numerical simulation of nano size aluminum particle-oxygen two-phase detonation is performed using two-dimensional compressible Euler equations with a two-step combustion model. The present study is conducted to investigate numerically detonation characteristics of nano-size aluminum particles. The numerical results show that the detonation cell size becomes small when the aluminum particle size decreases, but this tendency becomes quite different from the micro-size particle case. Furthermore detonation in nano-size aluminum particle-oxygen mixture propagates at the near C-J value when its size becomes smaller.

Keywords : detonation, two-phase flow, aluminum dust, oxygen, nano-size particle

1. Introduction

Gas-solid two-phase detonation has been studied experimentally[1] and numerically[2)-4)] from the point of view of coal mine explosion to that of the recent new propulsion systems for detonation engine. Recently, nano-size particles become attractive as their material source, then their combustion characteristics study has been started by many scientists. Especially the combustion characteristics of nano-size particles are quite different from that of micro-size particles and have not been studied much yet. For example nano-size aluminum particle ignition delay time is shorter ; its ignition temperature is lower ; and its flame propagation speed is higher than that of micro-size aluminum particles. As for detonation, detonation velocity of nano-size aluminum particles is faster than that of micro-size aluminum particles and can be used for micro detonation engine fuel and other small propulsion systems efficiently. On the other hand we must also know the safety characteristics of nano-size particles such as detonability limit. The purpose of this study is to investigate numerically combustion characteristics of nano-size aluminum-oxygen two-phase detonation.

2. Numerical analysis

The present analysis of mathematical model system uses a continuous mixture approach ; non-compressible solid-phase and two-velocity and two-temperature model for solid and gas phases. But diffusion, heat conduction, and viscous terms are neglected. This system of equations is developed by Benkiewicz et al.[3]. Method of numerical analysis for this study is as follows : the governing equations are compressible two-dimensional two-phase Euler equations ; the source term is integrated using a second-order Strang-type fractional step method ; for the gas-phase convection term, Harten-Yee TVD scheme is applied ; and for the solid-phase convection term, the MUSCL Hancock TVD scheme is applied.

2.1 Aluminum combustion model

Aluminum particles are uniformly distributed in oxygen environment. The considered gas-phases of chemical reaction species include oxygen (O_2), aluminum (Al), aluminum monoxide (AlO), and aluminum oxide (Al_2O_3). The aluminum combustion model is applied using a two-step chemical reaction mechanism with an evaporation model, where solid aluminum particles and evaporated aluminum burn along with the reaction mechanism.

Although Al_2O_3 does not exist in gas-phase, it is assumed that it can be present in the form of very fine particles.

Solid particles are heated by surrounding gases, evaporate, and burns when the solid-phase becomes gas-phase. The inter-phase mass exchange factor Δc for an aluminum evaporation model has the following form :

$$\Delta c = \frac{3\rho_S \phi_S}{\tau}\left(1 + 0.276\sqrt{\mathrm{Re}}\right), \text{ for } T_S \geq T_{ign} \quad (1)$$

where combustion starts when the solid-phase temperature T_s exceeds its ignition temperature T_{ign} (1350 K). ρ_S is the solid density ; ϕ_S is the solid-phase volume fraction ; Re is the relative Reynolds number ; and τ is the characteristic combustion time described by a d^2-law :

$$\tau = K_r d_0^2 \quad (2)$$

K_r is the constant burning rate and d_0 is the initial diameter of aluminum particles. The d^2-law has a simple style, but the computations using this law provide a good agreement with the experimental one : for example, the computations conducted by Khasainov and Veyssiere[2] gave a successful result in two-phase aluminum-oxygen mixture. We have been using this characteristic combustion time model since our group started to use it[3]. This model does not consider for nano-size aluminum particles but does for micro-size aluminum particles so far. Hence we need to adopt a new characteristics combustion rate model for nano-size aluminum particles. Many research groups reported that the combustion characteristic time of this model for nano-size aluminum particles is different from the one we have been using for micro-size aluminum particles. In the present study, the Huang's model[5,6] was adapted because it can be applied to a wide range of nano-size aluminum particles and oxidizer mole fraction and it also shows a good agreement with the experimental results of combustion characteristic time. For micro-size aluminum particles the particle burning time τ_μ is

$$\tau_\mu = \frac{C_1 d_0^{1.8}}{T_0^{0.2} p^{0.1} X_{eff}} \quad (3)$$

and for nano-size aluminum particles the particle burning time τ_n is

$$\tau_n = \frac{d_0^{0.3}}{C_2 e^{\frac{E_b}{RT}} \cdot X_{eff}} \quad (4)$$

$$X_{eff} = C_{O_2} \quad (5)$$

where X_{eff} is the oxidizer mole fraction, C_1 and C_2 are constant, E_b is the constant energy, and R is the universal gas constant.

For the reactions of the product species, two mechanisms are used depending on gas-phase temperature. If the gas-phase temperature T_g is lower than the decomposition temperature T_{dec} (3500K) at the pressure between 0.1 – 10 MPa, then the combustion product is aluminum oxide due to an exothermic reaction

$$Al + \frac{3}{4}O_2 \Rightarrow \frac{1}{2}Al_2O_3 - 810.3 \times 10^3 [J\,mol^{-1}] \quad \text{for } T_g \leq T_{dec}, \quad (6)$$

but at the temperature higher than the decomposition temperature, aluminum is burned to aluminum monoxide due to an endothermic reaction.

$$Al + \frac{1}{2}O_2 \Rightarrow AlO + 66.9 \times 10^3 [J\,mol^{-1}] \quad \text{for } T_g > T_{dec} \quad (7)$$

The energetic effect by the reactions is related to the number of moles of aluminum (Al). However if this effect is related with the number of moles of aluminum oxide (Al_2O_3), then the aluminum oxide is decomposed to aluminum monoxide according to the following reaction :

$$Al_2O_3 \Rightarrow 2AlO + \frac{1}{2}O_2 + 1754.5 \times 10^3 [J\,mol^{-1}] \quad (8)$$

And these reactions are infinitely fast.

2.2 Numerical conditions

Numerical calculation using nano aluminum particles must not give an answer when a low grid resolution is used. But it is difficult to use a high grid resolution for a large tube due to numerical cost. Hence the numerical calculation is performed for two different numerical domain sizes : Case 1 is that the tube length is 3750 mm and its width is 250 mm and Case 2 is that the tube length is 1875 mm and its width is 125 mm. The present analysis applies for a block adaptive mesh refinement method and a moving grid method (Figure 1).The initial grid size is 2.6 mm for Case 1 and 1.3 mm for Case 2. The fine grid size is 650 μm in Case 1 and 325 μm in Case 2. The moving grid speed is 800 m s^{-1} since the detonation head can be kept in the grid system. As for the boundary conditions, the top, bottom, and left walls are adiabatic and the right boundaries are free flow condition as follows :

$$\begin{cases} f_{imax,j} = f_{mixture} & u < 0 \\ f_{imax,j} = f_{imax-1,j} & u \geq 0 \end{cases} \quad (9)$$

The initial pressure is 0.1 MPa ; initial temperature is 300 K ; and the initial particle diameter range is from 100 nm to 2.5 μm at the constant concentration of 0.25 kg m^{-3}.

3. Nano aluminum particle detonation calculation results

Detonation velocity is one of important physical values which are useful for safety and application such as detonation engine. The present study will focus on investigating the effect of particle size and particle concentration on detonation velocity as well as detonation cell size.

3.1 Effect of particle diameter on detonation velocity

Figure 2 shows the detonation velocities for the different particle diameters. In the figure detonation velocity increases when the particle diameter becomes smaller mainly due to particle drag coefficient explained

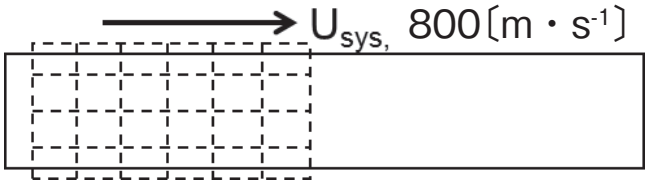

Figure 1 AMR and moving computational grid concept.

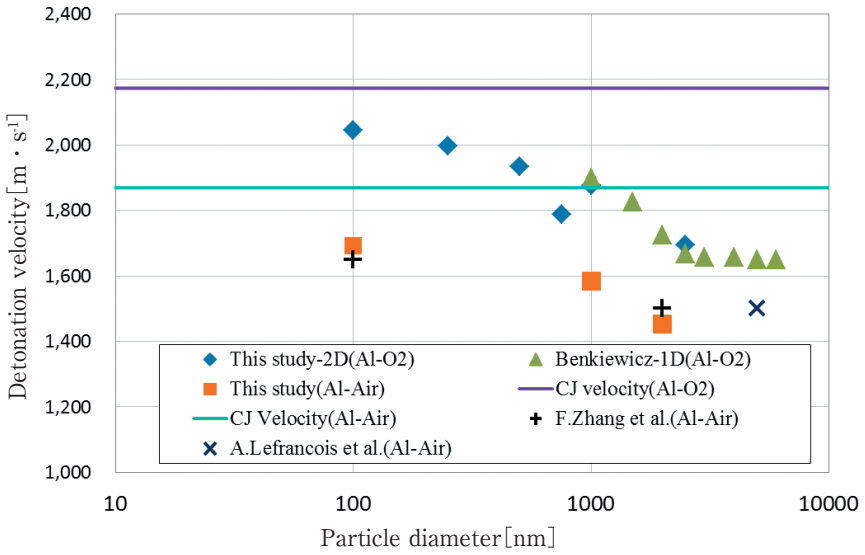

Figure 2 Detonation velocities for different particle diameter: Benkiewicz−1D[3], C−J velocity[7], F. Zhang et al.[8], A. Lefrancois et al.[9].

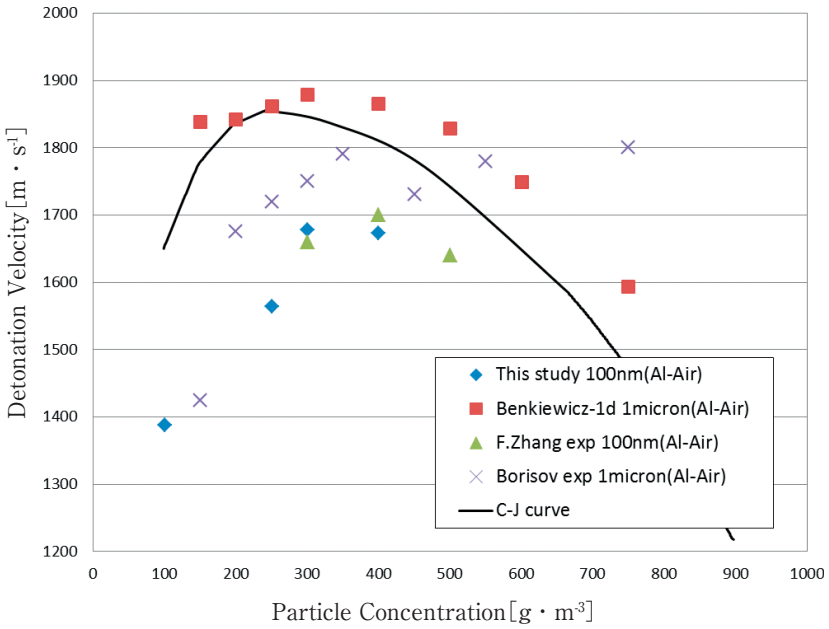

Figure 3 Detonation velocities for different particle concentration: Benkiewicz−1 d[3], F. Zhang[8], Borisov et al.[10].

below. The detonation in the nano-size aluminum particle-oxygen mixture propagates at the velocity closer to the C-J value[7], which is obtained using a gas-phase Al, when its size becomes smaller. One of the reasons is such that when the particle diameter becomes ten times smaller, the effect of the drag coefficient on particles is at least three times smaller and the efficiency of heat transfer on particles is at least ten times higher. Then the mixture becomes close to gaseous phase. Hence detonation velocity becomes faster.

One thing we have to check when the aluminum particle size becomes nano-size is the Knudsen effect due to using the continuous model for particles. Knudsen number, $Kn = \lambda/d$ where λ is mean free path and d is a representative length in flow such as particle diameter, explains the limit which can be treated as a continuous model or not. When the Knudsen number exceeds 0.01, the analysis cannot be treated as a continuous model. If the continuous condition is assumed in the present calculation, our numerical results show the values close to the ones Zhang[8] obtained experimentally within three percents of error (Figure 2). Hence in the aluminum particle size range of this study our two-phase model can be treated as a continuous model although the Knudsen number in our analysis, 0.74, is larger than 0.01.

3.2 Effect of particle concentration on detonation velocity

The influence of particle concentration on detonation velocity is presented in Figure 3. Our numerical results are close to Zhang's experimental ones[8] and become close to the C-J curve[7]. However, in this comparison, the particle concentrations at the peak detonation velocity for the data of Zhang[8] and Borisov et al.[10] are different from

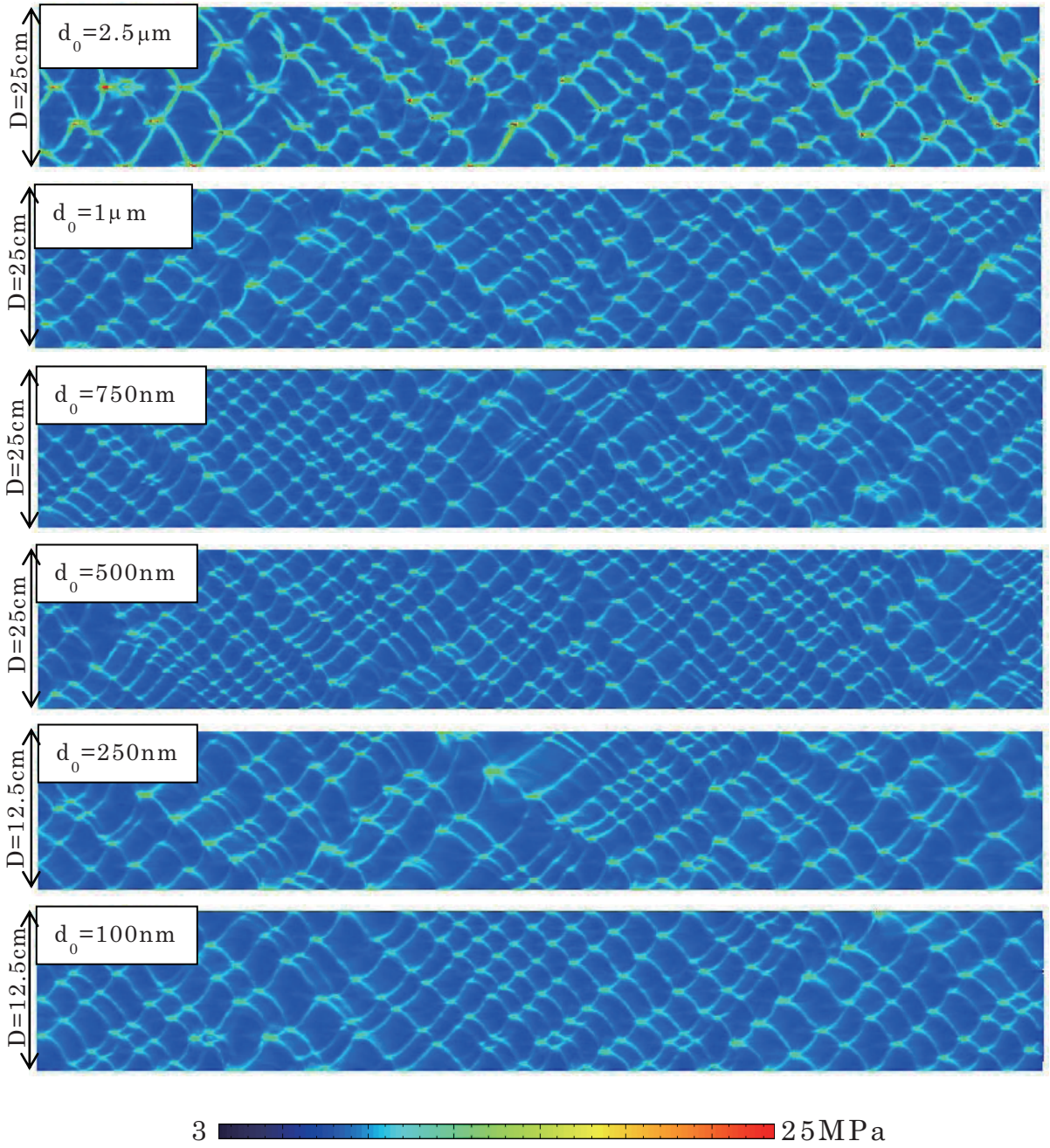

Figure 4 Maximum pressure history for different particle diameter.

the one we obtained from our calculation. This means that the initial particle concentration in their experiments might be different from the real particle concentration in the measurements due to sedimentation and adhesion of particles to the tube wall during dispersion. It is clear in our numerical results that when the particle size becomes smaller (from 1μm to 100 nm), the detonation velocity becomes close to the C-J value[7] because Al particle behaves like gas.

3.3 Detonation cell sizes

Detonation cell size is one of the important characteristics to see whether detonation is stable and within a detonability limit or not. Figure 4 shows the maximum pressure history which corresponds to the numerical cell structure for each particle diameter. Figure 5 shows the cell size vs. particle diameter. Detonation cell size which usually shows like a diamond structure is measured in the channel width direction.

But the present results show a different relationship between particle size and detonation cell size from the ones using the d^2-law model and the ones using the empirical equation computed from the cell size in micro-size particles obtained using d^2-law model by Fedrov and Khmel[6]. Huang's model provides a longer combustion characteristics time than that using the d^2-law, hence this causes a decrease of the mass change from solid-phase to gas-phase. As the result, it takes a longer time to terminate a reaction to make the detonation cell size larger. So the cell size might be correlated with the characteristic combustion time. Moreover, the comparison of our aluminum-air detonation cell size with that of Zhang's experiments[8] does not agree with each other quantitatively, but it does qualitatively. Hence the Huang's

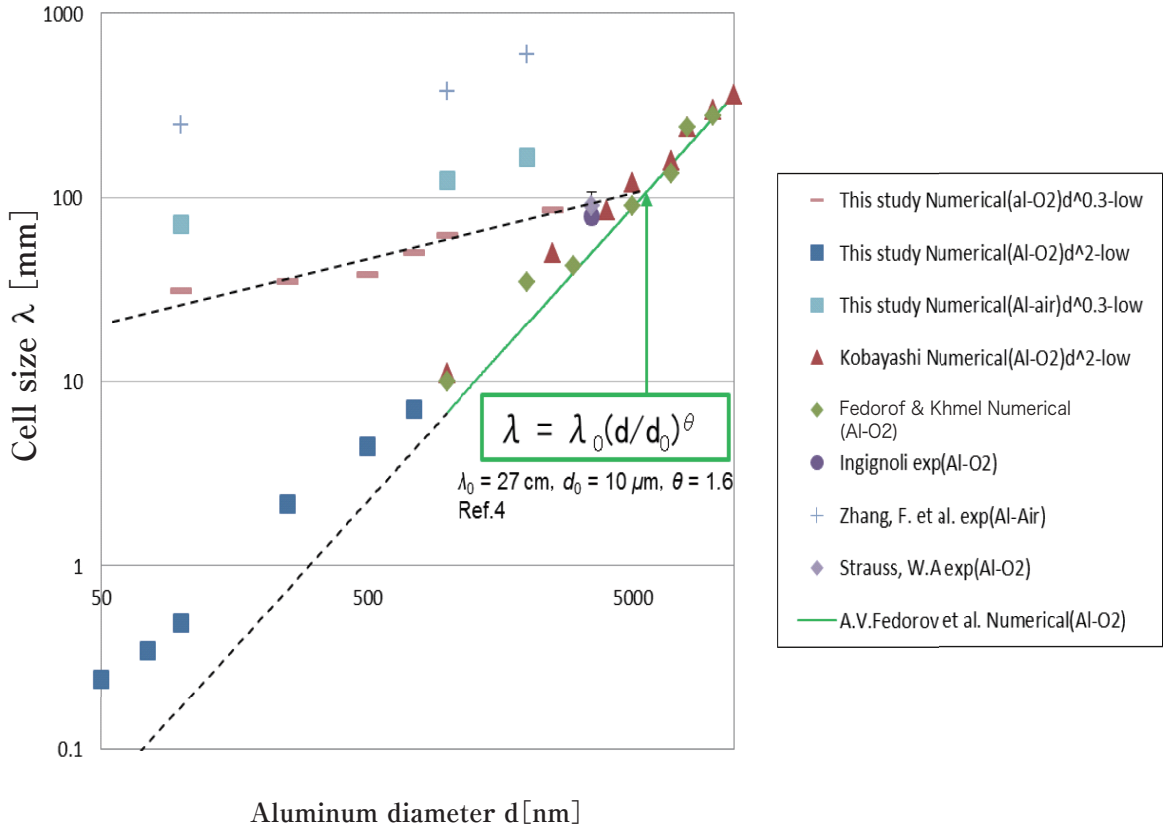

Figure 5 Cell size for different particle diameter : Kobayashi[11], Fedorov & Khmei[4], Ingignali[12], Zang, F. et al.[8], Strauss, W.A.[13], A. V. Feddorov et al.[4].

model shows a better tendency for the real case than that for the d^2-law model when the particles are smaller than micro size.

Figure 6 shows the several physical quantities of nano- and micro-size aluminum particles/oxygen detonation structure in the present study. In this case two-phase detonation propagates with a multi-headed structure with triple points similar to that using micro-size aluminum particles. However a difference between the case using micro-size particles and that using nano-size particles can also be seen from Figure 6. It can be proved from the solid temperature distribution that the distance of the solid particle evaporation for the case of 2.5 μm of aluminum particle size is shorter than that for cases of 500 nm of aluminum particle size. Moreover, it can be seen from the gas-phase temperature distribution that a mushroom type whirlpool, which is peculiar to the solid-gas two phase detonation, is smaller when the particle size is smaller. And in the case of particle size even smaller than micro-size, the temperature gradient and the slope of mass concentration are smaller than that of micro-sizes. Hence the nano-sige particle case of detonation apparently becomes similar to the gas-phase detonation.

4. Conclusions

We performed the numerical simulation of aluminum –oxygen two-phase detonation focused on the nano-scale particle sizes

- When particles become smaller, detonation velocity becomes close to the C-J value where the two-phase becomes a single-phase
- The numerical results show a value close to Zhang's experimental results and become close to the values of the CJ curve
- Detonation cell size becomes smaller when particle is smaller. The Huang's model provides a better result than that using the d^2-low model in the case of particles even smaller than micro-size

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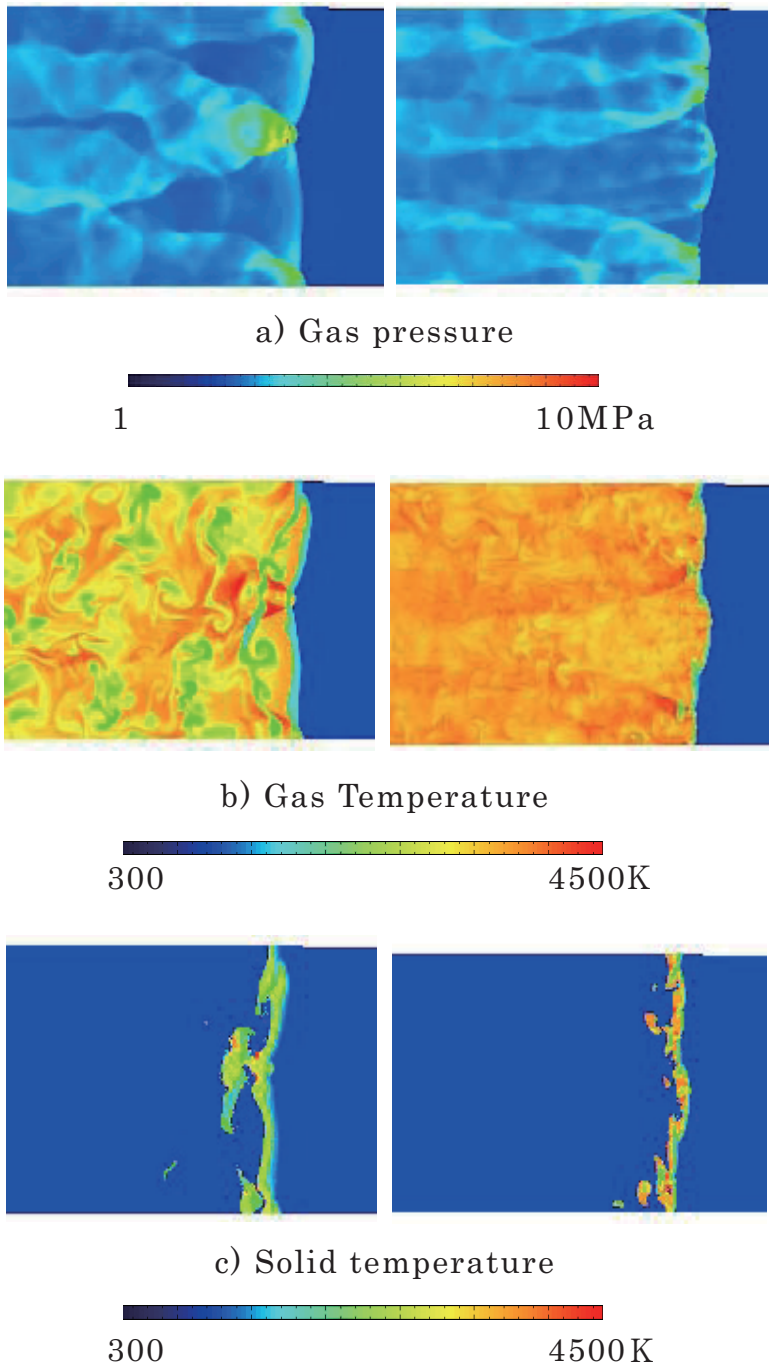

Figure 6 a) pressure, b) gas−phase temperature, c) solid−phase temperature distribution in the aluminum oxygen mixture at 2.5μ (lert) m and 500nm (right)

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ナノアルミニウム粒子―酸素二相デトネーションの燃焼特性に関する数値解析

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二次元圧縮性オイラー方程式と二段階総括化学反応モデルを用いて，ナノサイズ粒子と酸素の二相デトネーションの数値シミュレーションを行った。本研究の目的は，ナノサイズのアルミニウム粒子のデトネーションの燃焼特性を調べることにある。特に，アルミニウム粒子の径や濃度がデトネーション速度にどの様に影響を与えるのかとか，デトネーションのセルサイズがどのような値なのかを，以前行われたマイクロサイズのアルミニウム粒子の場合と比較しながら調べた。数値解析の結果として，アルミニウム粒子の径が小さくなればなるほど，その二相デトネーションの速度はC-J値（気相デトネーションの場合のデトネーションの速度）に近づくことが分かった。また，アルミニウム粒子と酸素の混合気中の濃度に対するデトネーション速度の関係では，今回の計算結果がZhangの実験結果に近い値となっていることが確認された。アルミニウム粒子―酸素の混合気中のデトネーションセルサイズについては，アルミニウム粒子径に対して，約５ミクロン以下になると，特性燃焼時間が粒子径の二乗則でなく三乗則に比例した式を使った計算によるセルサイズに合うことが確認された。

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