Modeling of Aluminum Combustion in Air-breathing Combustor

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Abstract
In order to increase specific impulse and thrust and suppress combustion instability, metal particle, such as aluminum can be used as energetic material. In this study, combustion mechanism of aluminum is modeled to investigate combustion characteristics of air-breathing combustor. Aluminum combustion is applied to numerical simulation and validated with experimental results of other researchers.

1. Introduction

Aluminum particle has been long used as additional energy source for hydrogen generation and thermite used for welding as well as additives of solid rocket propellant. Since after serious and comprehensive research on aluminum combustion was conceived by Glassman[1] in the late 1950s, numerous researchers have expended their efforts to this theme. A summary of the current understanding of aluminum particle combustion can be found in the review by Beckstead.[2]

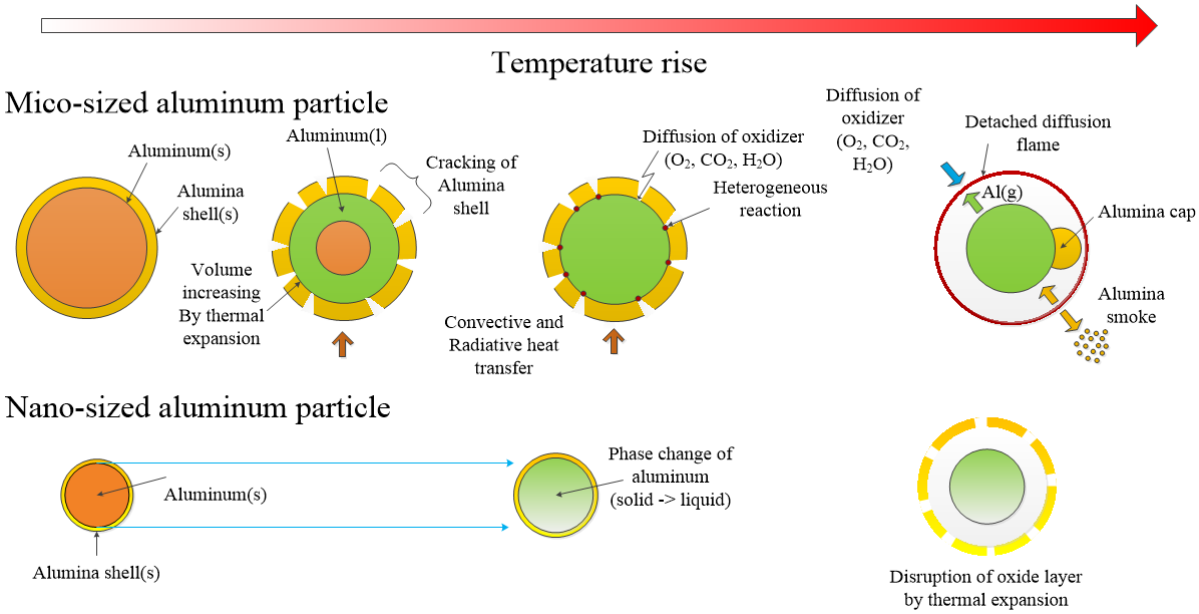


Figure 1. Combustion mechanism of micro and nano-sized aluminum particle

Combustion phenomena of aluminum particle differ markedly as its size. Research of aluminum combustion up to present is mainly focused on micro-sized particle. As a result, combustion phenomena of micro-sized particle is revealed in many specific parts. As seen in Fig.1, in the case of micro-sized particle, upon heating, pure aluminum contents is transformed to aluminum oxide by heterogeneous reaction, and this process thicken the oxide shell. When the particle temperature reach melting temperature of aluminum which has the value of 933 K, the volume of internal aluminum content is getting expanded by thermal expansion. Hence, aluminum oxide shell is cracked due to its internal shear stress, and ignition is started subsequently. After that particle is heated up to melting point of aluminum oxide, then molten oxide may form a cap. Above vaporization temperature of aluminum, finally, detached spherical flame which is controlled by diffusion is positioned off the particle surface.

Nano-sized particle, on the other hand, has lower melting point compared with micro-sized particle resulting from oxidation reaction of aluminum and polymorphic phase transformation of oxide shell, thus phase change is completed at relatively low temperature comparing with micro-sized particle. Furthermore, disruption of oxide shell is occurred at lower temperature on account of large curvature. Also many researchers reported that combustion of nano-sized particle is dominated by kinetically controlled reaction not diffusively controlled reaction. The evidence of this change in combustion mechanism has been observed experimentally in elsewhere.[3]
As can be seen above explanation, nature of combustion phenomena of aluminum particle is quite complex, and it has evident regimes distinguished by the size of particle. There are a few studies about combustion modeling of aluminum by several researchers.[4,5] However, methods which they applied are limited to the particle size of micron, so nano-sized particle is not concerned. Also, their methods have iterative routine calculating for mass fraction of aluminum vapor on the particle surface. Thus, these methods are expensive for massive numerical simulation containing thousands or millions of reacting discrete particles. Furthermore, formerly developed model is limited and insufficient to represent effect of other oxidizer, H_2O and CO_2.
This paper focused on development of the combustion modeling of aluminum, which has explicit calculation routine, covers wide particle diameter regimes, and simply but physically expresses intricate combustion mechanism of aluminum. In order to validate the model, experiment results of combusting and free falling single particle and air-breathing combustion suspended nano particles are compared to the simulation results. The aluminum combustion model has been imported to ANSYS FLUENT 12 using UDF(User Defined Function).

2. Model Formulation

2.1 Modeling of preheating stage

Aluminum particle is affected by convective heat transfer from the outside as well as heterogeneous reaction before being ignited. This heterogeneous reaction is considered because this effect conducts important role to the ignition delay.[5] Reaction rate of the heterogeneous reaction is proposed by Roberts et al.[6] as follow :

$$k_s = A \cdot \exp(-E_a / RT_p) \tag{1}$$

where the values represent that pre-exponent factor, A is 200 [kg/m^2], activation energy, E_a is 95,395 [J/mol], R is Gas constant, and T_p is particle temperature. Roberts et al. conducted experimental study for heterogeneous reaction rates of mechanical alloy consisted of aluminum and magnesium. Arrhenius parameters are experimentally obtained in the case of pure aluminum, atmospheric environment. In the air-breathing combustor, aluminum particles mostly reacts with oxygen, thus using these parameters to the simulation is acceptable convincingly.

2.2 Modeling of ignition onset

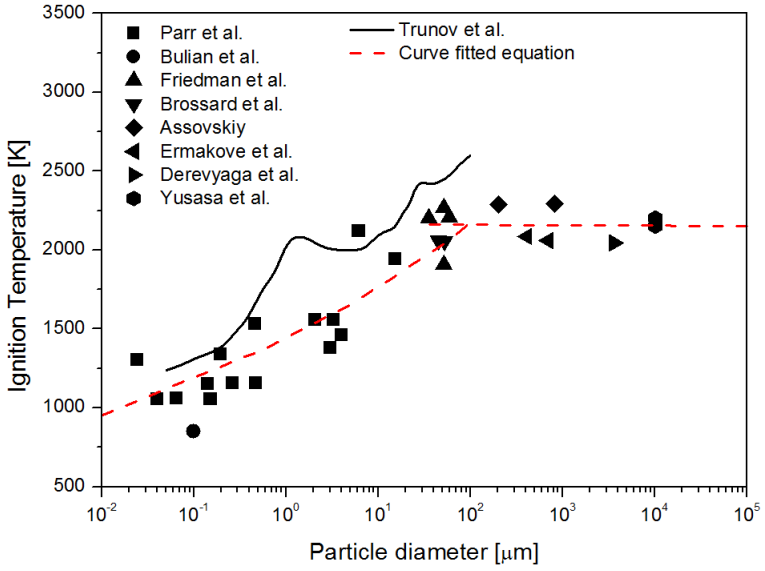


Figure 2. Ignition temperature of aluminum particle [10]

In order to simulate combustion behavior of aluminum particle, ignition temperature should be determined precisely. Studies on ignition temperature of aluminum particle in oxygen-containing environment have been conducted by many researchers. Sundaram et al. suggested ignition temperature as a function of particle diameter summarizing various experiment data.[7], and become as follow :

$$\begin{aligned} T_{ign} &= \exp(0.087 \times \log(d_p \times 10^6) + 7.28) \quad \left(d_p < 100\mu m\right) \\ &= 2350\,K \qquad\qquad\qquad\qquad\quad \left(d_p \geq 100\mu m\right) \end{aligned} \tag{2}$$

where d_p represents particle radius. As shown in Fig. 1, ignition occurs at about the melting point of aluminum oxide which has value of 2350 K for micro-sized particle (>100μm), and particle with diameter below 100 μm has wide range of ignition temperature. Bazyn et al. [3] and Trunov et al. [8] speculated that lowered ignition temperature of nano-sized particle is caused by polymorphic phase transformation and aluminum oxidation. Detailed and physical explanation can be found in elsewhere.[9]

2.3 Modeling of combustion process

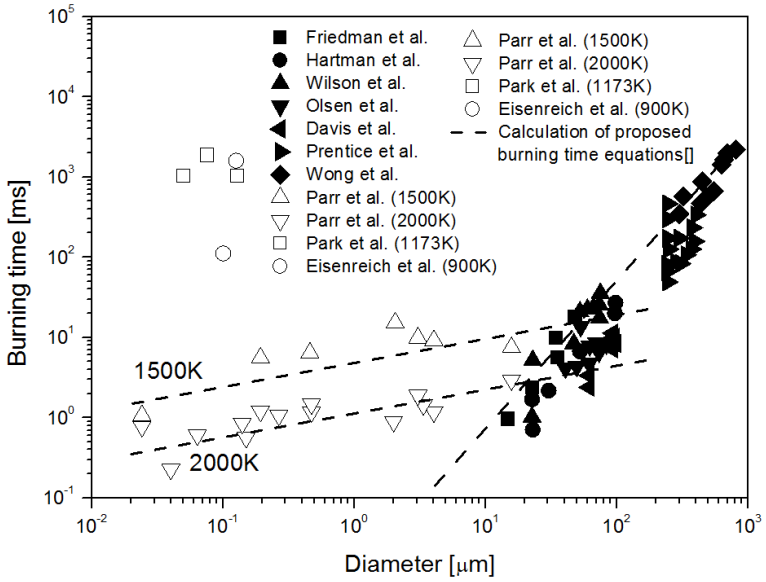


Figure 3. Burning time of aluminum particle as a function of particle diameter [12]

In order to model combustion of aluminum particle which can embrace various and complex processes as stated above, reaction rate based on correlation of particle combustion time is adopted for enhancing computational efficiency in larger scale numerical simulation. Beckstead et al. summarized experimental data of combustion time of aluminum particle, and proposed correlation which is available for particle size above 10 μm.[11] The correlated equation is given by :

$$\tau_b = \frac{0.00735 \cdot d_p^{\,1.5}}{X_{eff}\, p^{0.1} T_0^{\,0.2}} \quad \left(d_p \geq 10\mu m\right) \tag{3}$$

$$X_{eff} = X_{O_2} + 0.6\,X_{H_2O} + 0.22\,X_{CO_2} \tag{4}$$

where τ_b is combustion time, p is ambient pressure, T_0 is ambient temperature, and X_{eff} is effective oxidizer mole fraction defined in Eqn. 4. Effective oxidizers for aluminum combustion are O_2, H_2O and CO_2, and calculated by its mole fraction. As mentioned earlier, micro-sized particle is controlled by diffusion flame, thus combustion time could be modeled to d^n-law, which is generally used in droplet combustion. Unlike droplet combustion using n=2.0, in aluminum combustion, n is proposed 1.8 because of existence of aluminum oxide shell.
Recently, Huang et al. suggested combustion time for particle size below 10 μm based on experiment results for nano-sized particle performed by Parr et al.[12] Proposed equation become as follow:

$$\tau_b = \frac{d_p^{0.3}}{C \cdot \exp\left(-E_b / RT_0\right) \cdot X_{eff}} \quad \left(d_p < 10\mu m\right) \tag{5}$$

In Eqn. 5, activation energy, E_b is 73.6 [kJ/mol] and C is 5.5×10^4. As seen in Fig.3, reaction of nano-sized particle is kinetically controlled, thus environmental temperature has greater effect to combustion time compared with micro-sized particle. However, effect of particle size is found to be relatively small. Mass consumption rate of aluminum particle is applied as a function of burning time of aluminum particle, and given by :

$$\dot{m}_b = -\frac{m_p}{\tau_b} \tag{6}$$

where m_b is mass burning rate of aluminum particle, m_p is particle mass. Similar approach is utilized in [7,10,12], and they calculated burning speed of homogeneous mixture consisted of nano and micro-sized aluminum particle and oxidizer, such as air, steam, ice and CO_2. Their results were in good agreement comparing to experiment data.

3. Validation results

3.1 Free falling and combusting particle

Experimental studies on single falling particle for micro-sized aluminum were conducted by Williams et al.[13] and Dreizin[14]. Williams et al. measured particle diameter of a burning aluminum droplet by short photographic exposure with backlighting varying particle sizes of 20~90 μm and oxygen partial pressure, and particle was ignited by high power laser. In experiment of Dreizin, particle was produced and ignited using pulsed micro-arc discharge device, called GEMMED (GEnerator of Monodisperse MEtal Droplets), and quenched at a certain distance and then measured particle diameter.

In the focus of combustion modeling, Attili et al. conducted numerical simulation of aluminum combustion in solid rocket motor.[15] They used corrected Hermsen's model which is proposed by Widner[16], and become as followings :

$$\dot{m}_b = C \cdot \left(\rho_{Al}\right)\left(T_p^{1.57}\right)\left(p^{0.2}\right)\left(X_{eff}^{0.39}\right) \cdot D_{rel} \cdot \left(d_p^{1.1}\right) \cdot \psi_{Al} \tag{7}$$

$$D_{rel} = 1 + 2.7 X_{H_2} \tag{8}$$

$$\psi_{Al} = \frac{\phi_{Al}\rho_{Al_2O_3}}{\phi_{Al}\rho_{Al_2O_3} + (1-\phi_{Al})\rho_{Al}} \tag{9}$$

$$\phi_{Al} = \frac{m_{Al}}{\left(m_{Al} + m_{Al_2O_3}\right)} \tag{10}$$

where C has a value of 2.885×10^{-13} in SI units, ρ_{Al} and ρ_{Al2o3} are density of aluminum and alumina at each, Tp is particle temperature, X_{eff} is oxidizer mole fraction, X_{H2} is mole fraction of hydrogen. The term ψ_{Al} represents volume fraction of aluminum which is determined by mass fraction of aluminum, ϕ_{Al}. This parameter include particle distortion caused by aluminum oxide cap.

Figure 4 shows squared diameter history for initial diameter of 165 μm at ambient pressure of 1 atm, ambient temperature of 1500 K, and initial particle temperature is 300 K. Analytic result of Desjardin et al. [4] is in a quite good agreement with experiment of Dreizin [14], however the results by using the model of Attili et al. predicted relatively long combustion time. Current result shows nearly identical tendency to experiments result of Dreizin, and of course, located between slope range of William. Figure 5 represents calculated particle properties, temperature and mass. Particle mass is slightly increased just before ignition, because aluminum is oxidized transforming to alumina which has higher density by heterogeneous reaction. Particle temperature is sharply increased, and remains constant at around melting point of alumina. This result is also observed by experimental result of Butcher et al. [17] Figure 6 shows calculated mass fraction of aluminum and alumina. Aluminum content within the particle is decreased after being ignited, and mass fraction of alumina shows contrary trend.

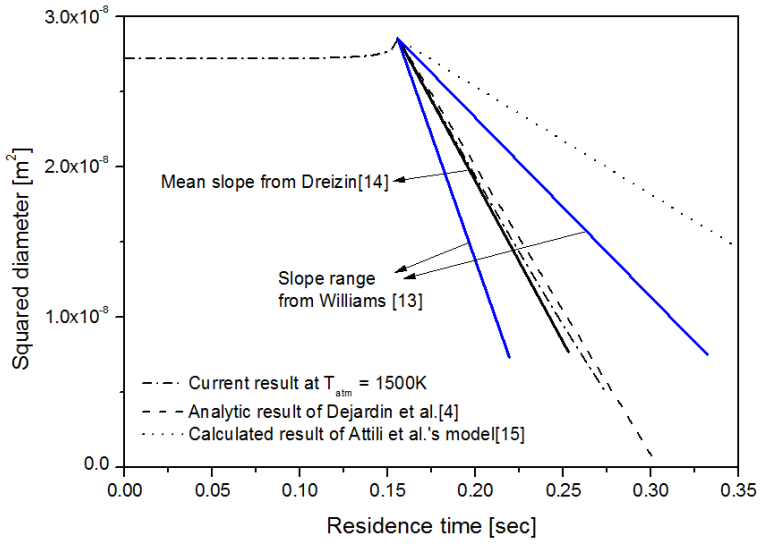


Figure 4. Comparison of squared diameter history for 165 μm free falling particle

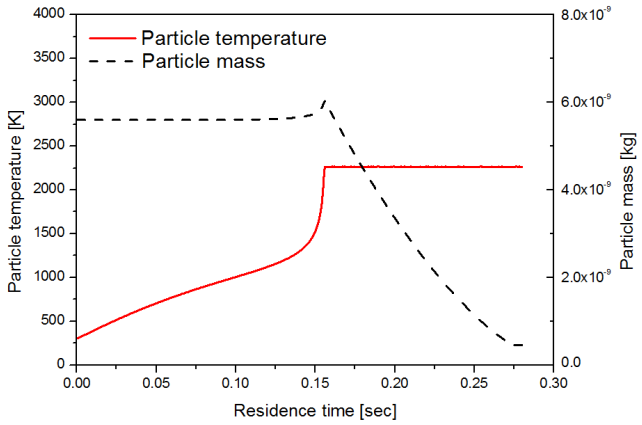


Figure 5.Calculated particle temperature and mass

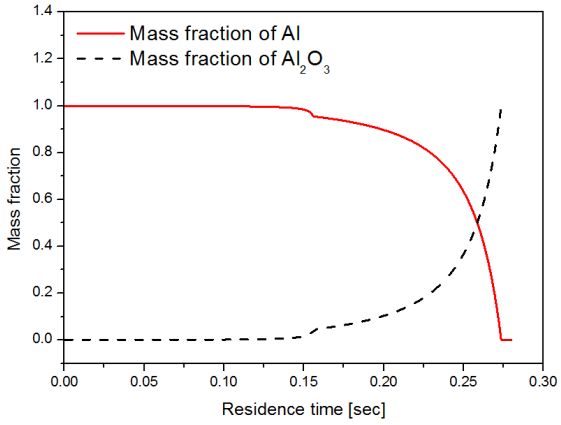


Figure 6. Calculated mass fraction of aluminum and alumina

3.2 Air-breathing combustion containing aluminum particles

Experimental studies on aluminum combustion in air-breathing combustor were conducted by Young et al.[18,19]. They used dumped combustor that the fuels are mainly ethylene and partially aluminum particle, and oxidizer is air. Aluminum particles of size of 50 nm and 2 μm are used to the experiment.

Figure 5 represents computational domain of validation case. The combustor has 38 mm height and 45 mm width, and backward step of 16 mm height. Premixed air and ethylene are entrained from ① in Fig. 5 , and pilot flame for igniting the main stream is injected at ②. Aluminum particles with carrying gas, ethylene, are injected at ③, and ④ is atmospheric outlet. Properties of pilot flame flow is calculated by CEA(Chemical Equilibrium Application), and calculated adiabatic temperature is 3271 K. Detailed boundary conditions are shown in Table 1. Ethylene combustion is modeled as one step reaction, and parameters for Arrhenius equation were referenced in [20].

A standard $k-\epsilon$ turbulence model, finite rate/eddy dissipation combustion model, and structured mesh of total of 8×10^5 cells are used for the simulation. Also particle behavior is calculated by using lagrangian approach, Discrete Phase Model (DPM).

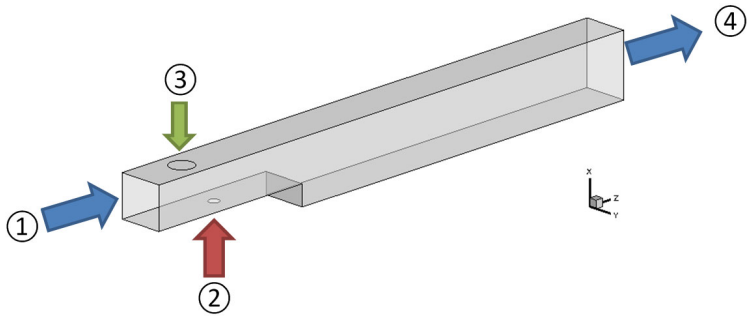
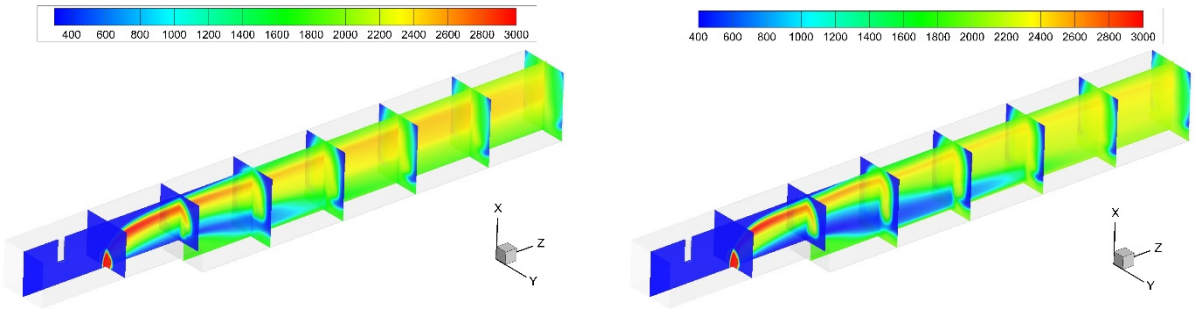


Figure 5. Computational domain of validation case

Table 1. Boundary conditions of validation case

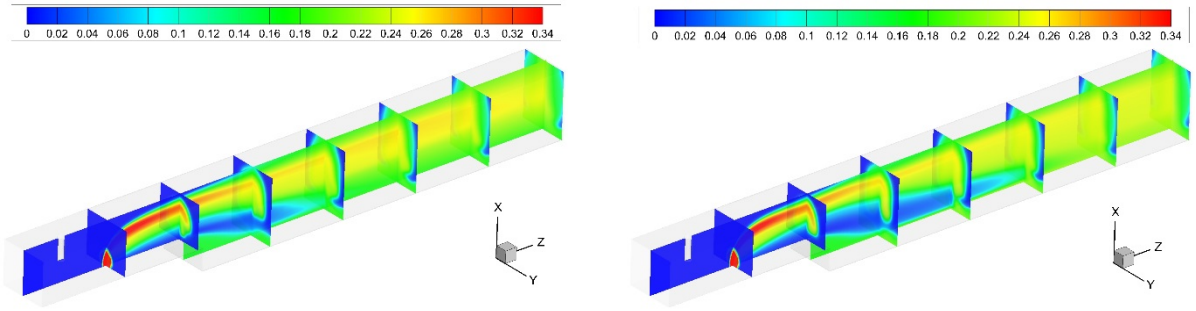
Location	Boundary type	Constituent	Temperature / Pressure
①	mass flow inlet	C_2H_4 (2.39 gm/sec) Air (83 gm/sec)	288 K 1 atm
②	mass flow inlet	Product gas of C_2H_4 (0.53 gm/sec) and O_2 (1.7 gm/sec) Product gas mole fraction (from CEA) Species: mole fraction CO_2: 0.15 CO: 0.28 H_2O: 0.27 OH: 0.12 O_2: 0.12 H_2: 0.06	3271 K (from CEA) 1.272 atm (4 psig)
③	mass flow inlet	C_2H_4 (1.27 gm/sec) Aluminum (0.39 gm/sec, 50 nm)	300 K 1 atm
④	pressure outlet	-	300 K 1 atm

Figure 6 represents temperature contours with only ethylene combustion and with suspension of 50 nm aluminum particles. There are two significant differences between two cases according to combustion of aluminum. The first is that, in the case with 50 nm aluminum particle, the area of temperature at around 3000 K is decreased. In other words, pilot flame thickness is thinner than other case, because in the earlier section in the combustor, entrained heat flux of pilot flame is used to heat up aluminum particle. At second, aluminum particle has relatively low reaction rate comparing with gas phase fuels, so effect of aluminum particle combustion is observed in the downstream of the flow direction. As can be seen in Fig. 8, at the outlet surface, upper section has slightly low temperature considering case with aluminum particles, and at the lower section in the combustor, tendency of temperature is reversed. Namely, temperature of lower section is increased by aluminum combustion. This observation is also represented in the experiment result. Figure 7 shows product mole fraction sliced contour which is sum of H_2O and CO_2. It also indicates similar trend of temperature.



(a) (b)

Figure 6. Temperature contours of cases of without (a) and with (b) 50nm aluminum particles



(a) (b)

Figure 7. Product mole fraction contours of cases of without (a) and with (b) 50nm aluminum particles

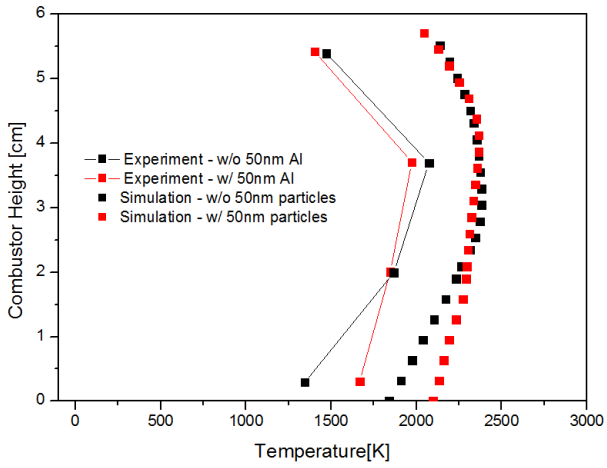


Figure 8. Comparison of combustor outlet temperature

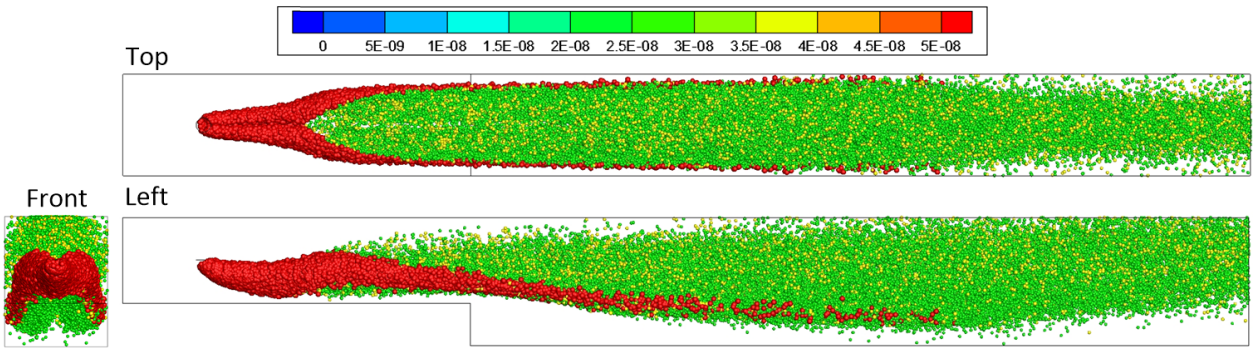


Figure 9. Particle diameter distributions with suspension of 50nm aluminum particles

Figure 9 indicates particle diameter distribution. Particle diameter is decreased from where impacted pilot flame, and unburned particles are separated to the side walls. Aluminum particles are shrunk up to the diameter of around 25 nm which of the half of initial diameter at the combustor outlet.

4. Conclusion

In this paper, a combustion modeling of aluminum particle are proposed and validated with experiment data of other researchers. This modeling is focused on usages for wide range of particle diameter, from nano to micro size, availability for multiple oxidizer, such as CO_2, H_2O, and it weightily aimed for developing simple and computationally efficient modeling for numerical simulation. In the validation case of free falling, combusting particle, history of squared diameter is almost identical to the experimentally obtained data of Dreizin, and located within slope range of William. In the case of air-breathing combustor, trend of the temperature at the outlet surface is in good agreement with experiment. However, the case with combusting aluminum particle differs from the magnitude of temperature. In further studies, multiple step ethylene reaction or Probability Density Function (PDF) using detailed reaction mechanism will be considered, and thermophysical particle behavior, such as melting process, will be included to the modeling.

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