Effects of ambient pressure, gas temperature and combustion reaction on droplet evaporation

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ABSTRACT

The effects of ambient pressure, initial gas temperature and combustion reaction on the evaporation of a single fuel droplet and multiple fuel droplets are investigated by means of three-dimensional numerical simulation. The ambient pressure, initial gas temperature and droplets' mass loading ratio, ML, are varied in the ranges of 0.1–2.0 MPa, 1000–2000 K and 0.027–0.36, respectively, under the condition with or without combustion reaction. The results show that both for the conditions with and without combustion reaction, droplet lifetime increases with increasing the ambient pressure at low initial gas temperature of 1000 K, but decreases at high initial gas temperatures of 1500 K and 2000 K, although the droplet lifetime becomes shorter due to combustion reaction. The increase of ML and the inhomogeneity of droplet distribution due to turbulence generally make the droplet lifetime longer, since the high droplets' mass loading ratio at local locations causes the decrease of gas temperature and the increase of the evaporated fuel mass fraction towards the vapor surface mass fraction.

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1. Introduction

Spray combustion is utilized in many industrial devises such as gas turbine engine and diesel engine. Recently, the spray combustion behavior has been studied by means of two- or three-dimensional direct numerical simulation (DNS) (e.g., [1–17]) or large-eddy simulation (LES) (e.g., [18–22]). However, the mechanism of spray combustion has not been fully understood yet. In particular, the effects of ambient pressure on the spray combustion behavior have not been well clarified yet mainly because the combustion conditions and the acquired properties are extremely limited due to the difficulty of the measurements (e.g., [23–25]).

Droplet evaporation is one of the most important factors which strongly depends on ambient pressure and therefore changes the spray combustion behavior in high ambient pressure conditions. Miller et al. [26] examined the validity of evaporation models by comparing them with experimental results in detail. Also, Miller and Bellan [27] performed a three-dimensional DNS and discussed the effects of the initial liquid mass loading ratio, initial Stokes number, and initial droplet temperature on the droplet evaporation in a turbulent mixing layer. In these studies, however the ambient pressure was fixed at the atmospheric pressure of 0.1 MPa and therefore the effects of the ambient pressure on the droplet evaporation were not studied.

The effects of the ambient pressure on the droplet evaporation have been investigated for a single droplet or an array of droplets. Nomura and Ujiie [28] experimentally studied the evaporation rate of a single droplet at various ambient pressures in the range of 0.1–5.0 MPa, and showed the pressure dependence of droplet lifetime. Yang and Wong [29] performed a numerical simulation of a flow around a single evaporating droplet under the same conditions as the Nomura and Ujiie's experiments. They suggested that the heat conduction from a fiber used in the experiment to suspend the droplet and the radiation from the furnace wall strongly affect the droplet evaporation rate. Similarly, Harstad and Bellan [30] numerically investigated the evaporation rate of a single droplet at various ambient pressures in the range of 0.1–10.0 MPa, and validated the evaporation models in sub- and supercritical conditions. They stated that precise estimation of Lewis number is essential in supercritical conditions. On the other hand, Mikami et al. [31] studied the burning lifetime of interacting two droplets at various ambient pressures in the range of 0.1–6.0 MPa by experiments, and showed that the pressure dependence of the burning lifetime for the interacting droplets is similar to that of a single droplet. That is, the total interaction coefficient, which is the ratio of the burning lifetime of the interacting droplets to that of a single droplet, slightly changes. In these studies, however, the evaporation characteristics of multiple droplets have not been discussed.

The purpose of this study is therefore to investigate the effects of ambient pressure, initial gas temperature and combustion reaction on the evaporation characteristics of both a single fuel droplet

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and multiple fuel droplets by means of three-dimensional numerical simulation. The ambient pressure, initial gas temperature and mass loading ratio are varied in the ranges of 0.1–2.0 MPa, 1000–2000 K and 0.027–0.36, respectively.

2. Numerical simulation

2.1. Governing equations

Present numerical simulation is performed based on the Euler–Lagrange framework. The governing equations for the gas phase are the conservation equations of mass, momentum, energy and mass of each species as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = S_\rho, \tag{1}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla P + \nabla \cdot \boldsymbol{\sigma} + S_{\rho u}, \tag{2}$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \boldsymbol{u}) = \frac{\partial P}{\partial t} + \boldsymbol{u} \cdot \nabla P + \nabla \cdot (\rho a \nabla h) + S_{\rho h}, \tag{3}$$

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \boldsymbol{u}) = \nabla \cdot (\rho D_k \nabla Y_k) + S_{comb,k} + S_{\rho Y_k}, \tag{4}$$

and the equation of state for ideal gas [2,5–7]. Here ρ is the density, $\boldsymbol{u}$ the gas phase velocity, P the pressure, $\boldsymbol{\sigma}$ the viscous stress tensor, h the specific enthalpy, and a the gaseous thermal diffusivity given by $\rho a = \lambda/c_p$, respectively. Here λ is the heat conductivity. Y_k and D_k are the mass fraction and the mass diffusion coefficient of the kth species which is given under the unity Lewis number assumption as $\rho D_k = \lambda/c_p$, respectively.

The phase coupling between the gas and dispersed-droplets phases is calculated by a Particle-Source-In-Cell (PSI-Cell) method [32], and the source terms, S_ρ, $S_{\rho u}$, $S_{\rho h}$, and $S_{\rho Y_k}$, are given as

$$S_\rho = -\frac{1}{\Delta V} \sum_N \frac{dm_d}{dt}, \tag{5}$$

$$S_{\rho u} = -\frac{1}{\Delta V} \sum_N \frac{dm_d \boldsymbol{u}_d}{dt}, \tag{6}$$

$$S_{\rho h} = -\frac{1}{\Delta V} \sum_N \frac{dm_d h_d}{dt}, \tag{7}$$

$$S_{\rho Y_k} = -\frac{1}{\Delta V} \sum_N \frac{dm_d}{dt} \quad \text{for } Y_k = Y_F, \tag{8}$$

where ΔV is the volume of the control volume for the gas phase calculation, m_d the droplets' mass, $\boldsymbol{u}_d$ the droplet velocity, h_d the specific enthalpy of a fuel droplet, and N the number of fuel droplets in the control volume. $S_{comb,k}$ is the source term due to the combustion reaction, as described later.

Concerning the evaporation of fuel droplets, a non-equilibrium Langmuir–Knudsen evaporation model [26,27,33] is employed. The governing equations for each droplet's position, $\boldsymbol{x}_d$, velocity, $\boldsymbol{u}_d$, temperature, T_d, and mass, m_d, are given by

$$\frac{d\boldsymbol{x}_d}{dt} = \boldsymbol{u}_d, \tag{9}$$

$$\frac{d\boldsymbol{u}_d}{dt} = \frac{f_1}{\tau_d}(\boldsymbol{u} - \boldsymbol{u}_d), \tag{10}$$

$$\frac{dT_d}{dt} = \frac{Nu}{3Pr}\left(\frac{c_p}{c_{p,d}}\right)\left(\frac{f_2}{\tau_d}\right)(T - T_d) + \frac{1}{m_d}\left(\frac{dm_d}{dt}\right)\frac{L_V}{c_{p,d}}, \tag{11}$$

$$\frac{dm_d}{dt} = \dot{m}_d. \tag{12}$$

Here T is the gas temperature, c_p the specific heat of mixture gas, $c_{p,d}$ the specific heat of the droplet, L_V the latent heat of evaporation at T_d, and τ_d the particle response time defined by

$$\tau_d = \frac{\rho_d d_d^2}{18\mu}, \tag{13}$$

where ρ_d is the droplet density, μ the viscosity and d_d the droplet diameter. The Prandtl and Nusselt numbers in the gas phase are given by

$$Pr = \frac{\mu}{\rho a}, \quad Nu = 2 + 0.552Re_{sl}^{1/2}Pr^{1/3}. \tag{14}$$

The droplet Reynolds number based on the slip velocity, $U_{sl} = |\boldsymbol{u} - \boldsymbol{u}_d|$, is defined as

$$Re_{sl} = \frac{\rho U_{sl} d_d}{\mu}. \tag{15}$$

The corrections of the Stokes drag and heat transfer for an evaporating fuel droplet, f_1 and f_2, are given as [2,26,34].

2.2. Evaporation model

Recently, various evaporation models have been proposed and validated [26,27,33,35–39]. In this study, a non-equilibrium Langmuir–Knudsen evaporation model is used [26,27,33]. The effect of the temperature gradient inside the droplet is neglected here due to its small effect [26]. As the liquid fuel, *n*-heptane and *n*-decane are used. Evaporation rate in Eq. (12) is given as

$$\dot{m}_d = -\frac{m_d}{\tau_d}\left(\frac{Sh}{3Sc}\right)\ln(1 + B_M), \tag{16}$$

[26,27,33], where Sc and Sh are the Schmidt and Sherwood numbers given as

$$Sc = \frac{\mu}{\rho D_k}, \quad Sh = 2 + 0.552Re_{sl}^{1/2}Sc^{1/3}, \tag{17}$$

and B_M is the mass transfer number given by

$$B_M = \frac{Y_{F,s} - Y_F}{1 - Y_{F,s}}. \tag{18}$$

Here Y_F is the mass fraction of fuel vapor in the far-field condition for a fuel droplet which is represented by the value in the cell where the fuel droplet is located (this condition is the same for $\boldsymbol{u}$ and T), and $Y_{F,s}$ is the vapor surface mass fraction (i.e., saturated vapor mass fraction) given as

$$Y_{F,s} = \frac{X_{F,s}}{X_{F,s} + (1 - X_{F,s})\overline{W}/W_F}, \tag{19}$$

$$X_{F,s} = \frac{P_{sat}}{P} - \left(\frac{2L_k}{d_d}\right)\beta, \tag{20}$$

where $X_{F,s}$ is the mole fraction of fuel vapor at the droplet surface, P_{sat} the saturated vapor pressure discussed later, P the pressure of the carrier gas, and $\overline{W}$ and W_F the averaged molecular weight of the carrier gas and the molecular weight of the fuel vapor, respectively. In Eq. (20), the non-equilibrium effect is considered using the Langmuir–Knudsen evaporation law, in which the non-dimensional evaporation parameter, β, is given by

$$\beta = -\left(\frac{\rho_d Pr}{8\mu}\right)\frac{dd_d^2}{dt}. \tag{21}$$

The value of the Knudsen layer thickness, L_k, is estimated by

$$L_k = \frac{\mu\{2\pi T_d(R/W_F)\}^{1/2}}{ScP}. \tag{22}$$

Here R is the universal gas constant.

2.3. Saturated vapor pressure

In many cases, the saturated vapor pressure, P_{sat}, in Eq. (20) is calculated by

$$P_{sat} = P\exp\left\{\frac{L_V W_F}{R}\left(\frac{1}{T_B} - \frac{1}{T_d}\right)\right\}. \tag{23}$$