



Evaporation and combustion of multicomponent fuel droplets



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HIGHLIGHTS

- We investigate effects of fuel components on droplet evaporation and combustion.
- Three kinds of surrogate fuels of Jet-A are considered.
- Differences are evident in the early period after ignition.

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ABSTRACT

The effects of difference in fuel components on the droplet evaporation and combustion are numerically investigated. Jet-A is used as liquid fuel, and one (*n*-decane)-, two (*n*-decane and 1,2,4-trimethylbenzene)- and three (*n*-dodecane, iso-octane and toluene)-component fuels are used as the surrogate fuels of Jet-A. The results show that the evaporation of the three-component surrogate fuel becomes faster and slower than those of the one- and two-component surrogate fuels in the initial and subsequent evaporating periods, respectively. The differences in the gas temperature evolution among these three different surrogate fuels are remarkable right after the ignition, but become small with time.

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1. Introduction

Spray combustion is utilized in many industrial devices such as gas turbine engines and diesel engines. Recently, the spray combustion behavior has been studied by means of two- or three-dimensional direct numerical simulations (DNSs) (e.g., [1–18]) or large-eddy simulations (LESs) (e.g., [19–23]). However, the mechanism of spray combustion has not been fully understood yet.

Evaporation of fuel droplets is one of the most important factors in the spray combustion and strongly depends on the fuel components. Therefore it is important to take the fuel components into account in order to precisely predict the combustion phenomena by numerical simulations. Daïf et al. [24] performed an experiment using a single and a few droplets of multicomponent fuel composed of *n*-decane and *n*-heptane, and compared the evaporation rate and droplet temperature with the results calculated by the evaporation model of Abramzon and Sirignano [25]. They showed that the evaporation model extended to multicomponent droplet evaporation in forced convection gave good results on the droplet

radius regression and the droplet surface temperature evolution. For multiple droplets, Le Clercq and Bellan [26] performed a direct numerical simulation of a mixing layer laden with evaporating droplets of multicomponent fuel (i.e., gasoline and diesel) and compared the results with those of the one-component fuel. They pointed out that the one-component fuel could be substituted for the multicomponent fuel, but it caused the increased evaporation time.

Very recently, Borghesi et al. [17] performed a direct numerical simulation of *n*-heptane spray autoignition in a turbulent flow. They found that higher turbulence intensity in the carrier gas enhanced the droplet evaporation and air/fuel mixing, and then ignition. In this study, however, only a one-component fuel was used and the effects of fuel component was not discussed.

The purpose of this study is to numerically investigate the effects of difference in fuel components on the droplet evaporation and combustion. Jet-A is used as liquid fuel, and a one-component fuel (*n*-decane), a two-component fuel (*n*-decane and 1,2,4-trimethylbenzene) and a three-component fuel (*n*-dodecane, iso-octane and toluene) are used as the surrogate fuels of Jet-A. For the calculation of the reaction, 113 species and 891 reactions for the one- and two-component fuels and 273 species and 2322

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Nomenclature

B_M	mass transfer number (-)	X	mole fraction (-)
c_p	heat capacity (J/(K kg))	Y	mass fraction (-)
D	diffusion coefficient (m ² /s)	ϵ	partial evaporation rate (-)
d	droplet diameter (m)	μ	viscosity (Pa s)
L	Knudsen layer thickness (m)	ρ	density (kg/m ³)
L_V	latent heat (J/kg)	τ	particle response time (s)
m	mass (kg)	0	initial value
P	pressure (Pa)	avg	averaged
Pr	Prandtl number (-)	c	at critical point
R	universal gas constant (J/(K mol))	d	droplet's
Re_{sl}	slip Reynolds number (-)	k	k th species
Sc	Schmit number (-)	nb	at normal boiling point
Sh	Sherwood number (-)	s	at droplet surface
T	temperature (K)	sat	saturated
W	mole weight (kg/mol)	V	vapor's

reactions for the three-component fuel are considered, respectively. The ambient pressure ranges from 0.1 MPa to 1.0 MPa, and the evaporation model for the multicomponent fuels in the high pressure conditions is extended based on our previous work [27].

2. Numerical simulation

2.1. Numerical method

The set of governing equations of the carrier gas and dispersed droplets phases and the numerical procedure are described in our previous paper [27]. To remove grid resolution dependency, source terms for gas phase are calculated for cells surrounding each droplet by using distance function from droplet position [17].

The evaporation model used in this study is mainly based on a non-equilibrium Langmuir–Knudsen evaporation model [28,29] and validated by comparing with the experiment by Nomura and Ujiie [30]. Multicomponent evaporation is taken into account using the discrete multicomponent method [31,32], in which each component individually evaporates according to its volatility. It is assumed that the temperature and composition are uniform inside the droplet. It is also assumed that the entire evaporation rate of multicomponent fuel is calculated in analogous way to that of a one-component fuel.

The entire evaporation rate of multicomponent fuel, \dot{m}_d , is expressed as

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

where

$$B_M = \frac{\sum_k Y_{V,s,k} - \sum_k Y_{V,k}}{1 - \sum_k Y_{V,s,k}}, \quad (2)$$

$$\tau_d = \frac{\rho_d d^2}{18\mu}, \quad (3)$$

$$Sc = \frac{\mu}{\rho \sum_k Y_{V,k} D_k}, \quad Sh = 2 + 0.552 Re_{sl}^{1/2} Sc^{1/3}. \quad (4)$$

Here Sc is the averaged Schmit number, Sh the averaged Sherwood number, B_M the mass transfer number, τ_d the particle response time, $Y_{V,k}$ the vapor mass fraction of k th species, ρ_d the density of liquid fuel, d the droplet diameter, μ the viscosity of gas and Re_{sl} the slip Reynolds number, respectively. $Y_{V,s,k}$ is the surface vapor mass fraction of k th species calculated as

$$Y_{V,s,k} = \frac{X_{V,s,k}}{X_{V,s,k} + (1 - X_{V,s,k}) \bar{W}/W_{V,k}}, \quad (5)$$

$$X_{V,s,k} = X_{k,d} \frac{P_{sat,k}}{P} - \left(\frac{2L_k}{d} \right) \beta. \quad (6)$$

Here $X_{V,s,k}$ is the surface vapor mole fraction of k th species, $X_{k,d}$ the mole fraction of fuel in the liquid phase, P the ambient pressure, \bar{W} the averaged mole weight and $W_{V,k}$ the mole weight of k th species, respectively. $P_{sat,k}$ is the saturated vapor pressure calculated by Sato's empirical equation [33] as

$$P_{sat,k}^{0.119} = 11.9T^{0.119} + C. \quad (7)$$

Here the unit of $P_{sat,k}$ is (mmHg) and C is the empirical constant calculated from values in a standard condition. L_k and β are the Knudsen layer thickness of k th species and the non-dimensional constant calculated as

$$L_k = \frac{\mu \{2\pi T_d (R/W_{V,k})\}^{1/2}}{ScP}, \quad (8)$$

$$\beta = -\left(\frac{\rho_d Pr}{8\mu} \right) \frac{d}{dt} d^2, \quad (9)$$

respectively. Here T_d is the droplet temperature, Pr the Prandtl number and R the universal gas constant, respectively.

The evaporation rate of k th species, $\dot{m}_{d,k}$, is calculated as

$$\dot{m}_{d,k} = \epsilon_k \dot{m}_d. \quad (10)$$

Here ϵ_k is the non-dimensional partial evaporation rate calculated as follows [31,32]. The conservation equation of each component around the droplet leads another form of \dot{m}_d which is expressed by using k -th species properties as

$$\dot{m}_d = -\frac{m_d}{\tau_d} \left(\frac{Sh_k}{3Sc_k} \right) \ln(1 + B_{M,k}), \quad (11)$$

where

$$B_{M,k} = \frac{Y_{V,s,k} - Y_{V,k}}{\epsilon_k - Y_{V,s,k}}, \quad (12)$$

$$Sc_k = \frac{\mu}{\rho D_k}, \quad Sh_k = 2 + 0.552 Re_{sl}^{1/2} Sc_k^{1/3}. \quad (13)$$

Here $B_{M,k}$ is the mass transfer number of k th species, Sh_k the Sherwood number of k th species and Sc_k the Schmit number of

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