



Title	Development and validation of evaporation model for a multi-component fuel considering volume-average internal mass and enthalpy
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9 **Highlights**

- 10 • A droplet evaporation model was developed for multi-component fuel.
- 11 • Internal distributions of the mass fraction and the enthalpy were developed.
- 12 • Internal distributions are satisfying the conservation of mass and enthalpy.
- 13 • The predicted results are in good agreement with the experimental results.
- 14 • Internal distributions have a major impact on the results at practical conditions.

Nomenclature

C_p	Heat capacity, J/mol/K
D	Diffusion coefficient, m ² /s
D_{eff}	Effective diffusion coefficient defined by Eq.(19), m ² /s
h	Sensible enthalpy for Eq.(22), J/kg
H_{latent}	Latent heat, J/kg
k	Thermal conductivity, W/(m K)
k_{eff}	Effective thermal conductivity defined by Eq.(20), W/(m K)
m	Mass of droplet, kg
MW	Molecular weight, g/mol
\dot{m}	Mass evaporation rate, kg/s
N	Number of chemical species in gas phase
N_l	Number of chemical species in liquid phase
P	Pressure, Pa
\dot{q}	Heat energy, W
R	Distance from the droplet center, m
R_d	Droplet diameter, m
Δt	Time step, s
T	Temperature, K
u	Velocity, m/s
u^c	The modified Stephan velocity, m/s
v	Diffusion velocity, m/s
x	Mole fraction
y	Mass fraction

Subscripts:

a	Average
amb	Ambient
c	Critical
g	Gas
i	i species
l	Liquid
m	Mixture system
ref	Reference value
s	Surface
v	Vapor

Greek symbols:

ε	Normalized mass fraction
η	Viscosity, kg/m/s
ρ	Density, kg/m ³
σ	Stefan-Boltzmann constant (5.67×10^{-9}), W/m ² /K ⁴
Ω	Dimensionless temperature

16 **Abstract**

17 We developed a droplet evaporation model for a multi-component fuel, considering the
18 nonuniform distributions of both mass fraction and temperature inside multi-component
19 fuel droplet. The distribution equations satisfy the conservation of droplet mass and
20 enthalpy. We proposed mass fraction and temperature distribution equations inside a
21 droplet to accurately determine variations between the numerical assumptions of a liquid
22 phase and a gas phase. We found that an obvious gradient appears in the mass fraction
23 and temperature distribution profiles at various ambient temperatures. To verify the
24 accuracy of the developed model, we further compared the predicted droplet lifetimes
25 with the experimental results at various ambient temperatures. The consideration of the
26 pre-evaporation process led to more accurate droplet lifetime prediction using the present
27 model. We also investigated the differences between the present model and the uniform
28 distribution model. The difference in the predicted droplet lifetime becomes more than
29 10% at practical spray combustion conditions. Thus, internal distribution of mass fraction
30 and temperature must be considered in practical spray combustion simulations.

31

32 **Keywords:** Droplet evaporation; Multi-component fuel; Internal distribution;
33 Numerical model; Spray combustion

34

35 **1. Introduction**

36 Computational fluid dynamics (CFD) provides remarkable advantages for the
37 prediction of combustion characteristics in a combustion chamber. Many researchers have
38 performed CFD studies to clarify the characteristics of complex spray flames encountered
39 in combustor design. Especially, the droplet evaporation process is an important

40 parameter in the design of spray combustors. Nomura *et al.* [1] investigated the droplet
41 evaporation characteristics in subcritical and supercritical environments. Moriai *et al.* [2]
42 revealed the differences between the predicted and the measured droplet diameters in a
43 subscale aircraft jet engine combustor. They found that the selection of the droplet
44 evaporation model affects the differences between the predicted and measured droplet
45 diameters. Furthermore, Noh *et al.* [3] compared the droplet evaporation models for a
46 turbulent non-swirling jet flame and found that different droplet evaporation models
47 predicted the different locations of lifted flame and droplet distributions. Thus, the
48 accuracy of the droplet evaporation model may affect the prediction of the spray flame
49 structure. A high-precision droplet evaporation model can help to optimize spray
50 combustor design.

51 For a precise simulation of the practical spray combustion field, droplet evaporation
52 models for multi-component fuel, such as practical fuel, have been developed. Some
53 researchers have suggested droplet evaporation models considering uniform internal
54 distributions [4-7]. However, the formation of gradient distributions for both
55 concentration and temperature inside a droplet is expected because of various fuel
56 volatility in multi-component droplet evaporation. Some droplet evaporation models
57 assuming unsteady diffusion inside the droplet have also been developed [8,9]. Torres *et*
58 *al.* [9] suggested the droplet evaporation model for multi-component fuels using interior
59 discretization, which is used in engine CFD codes. Although the one-dimensional model
60 can provide precise evaporation information, the discretization method for droplets
61 comprising large numbers of chemical species requires an unrealistic central processing
62 unit time. To decrease the calculation cost, a continuous thermodynamic model (CTM)
63 has been developed to analyze droplet evaporation for multi-component fuels by using a

64 continuous function of either the normal boiling temperature or molecular weight [10,11].
65 Despite the improved computational efficiency, however, CTMs cannot calculate the
66 evaporation rate of each fuel species.

67 The droplet evaporation model for multi-component fuels considering the internal
68 distributions for mass fraction and temperature has been developed without using
69 numerical grids. Yi *et al.* [12] have suggested the droplet evaporation model considering
70 the internal distributions of mass and temperature inside a droplet. Their model
71 approximated the mass and temperature distributions inside a droplet by a quadratic
72 polynomial function. As a theoretical model for multi-component droplet evaporation,
73 Sazhin *et al.* suggested various models on the basis of the discrete multi-component
74 (DMC) approach. Their droplet evaporation model introduces the mass fraction and
75 temperature distributions inside a droplet as a function of two variables which are the
76 length from droplet center and time. The equations are given by the analytical solutions
77 of a stationary spherically symmetric multi-component droplet. The model takes into
78 account droplet heating by convection from the ambient gas, the distribution of
79 temperature and diffusion of liquid species inside the droplet [13,14]. Furthermore, they
80 suggested a new multi-dimensional quasi-discrete model in terms of heating and
81 evaporation of Diesel fuel. This model takes into account the contribution of various
82 groups of hydrocarbons in Diesel fuels and quasi-components are formed within
83 individual groups [15]. The difference in the predicted evaporation times between the
84 multi-component and single component models has been also investigated for f biodiesel,
85 Diesel and gasoline droplet heating and evaporation [16]. Recently, a new model for
86 puffing and micro-explosions in water-fuel emulsion droplets is suggested [17]. However,
87 their droplet evaporation models have not satisfy the mass and enthalpy conservation

88 inside the droplet in overall droplet evaporation process even though the conservation of
89 mass and energy inside droplet have been satisfied in each time step. This is because
90 quasi-steady-state mass and enthalpy diffusions were assumed in the gas phase, whereas
91 the diffusions of mass and enthalpy in unsteady states were considered in the liquid phase.
92 In a quasi-steady state, the amount of diffused mass from the droplet is overestimated
93 compared with that in an unsteady state. Hence, the differences in the numerical
94 simulation assumption for the liquid and gas phase may result from the violation of
95 conservation. Furthermore, the effect of the droplet evaporation on the gas phase is
96 ignored in their model.

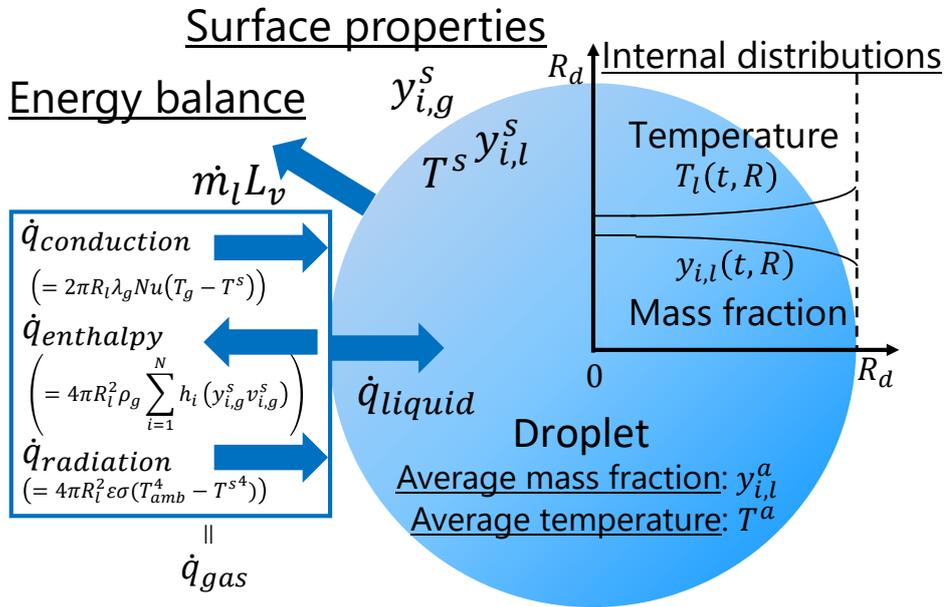
97 In this study, we developed a droplet evaporation model for multi-component fuels,
98 which can satisfy the conservation of mass and enthalpy inside the droplet and is intended
99 for spray combustion simulations. We derived the internal distributions of mass and
100 enthalpy which can simulate mass and enthalpy conservation during the droplet
101 evaporation process. To satisfy the conservation of mass and enthalpy, the volume-
102 average internal mass and enthalpy expressed by $y_{i,l}^a \int_0^{R_d} 4\pi R^2 dR =$
103 $\int_0^{R_d} y_{i,l}(t, R) 4\pi R^2 dR$ and $T^a \int_0^{R_d} 4\pi C_{p,l} R^2 dR = \int_0^{R_d} T(R, t) 4\pi C_{p,l} R^2 dR$ were applied
104 to the distribution equations. To consider the coexistence of the unsteady state along with
105 the quasi-steady state, mass fraction distribution, which has a boundary between the
106 gradient and uniform distribution, was introduced. Furthermore, the present model take
107 account for the effect of gases on droplet without considering the coupling and the concept
108 of region between the droplet and gas. Finally, the accuracy of the developed model was
109 verified at various ambient temperatures in comparison with experimental results. In [15],
110 the model was applied to bi-component fuel (ethanol and acetone) when ambient

111 temperature is room temperature. Even though the accuracy of the model is not verified
 112 at high ambient temperature in [15], the accuracy of the present model is verified at both
 113 low and high ambient temperature.

114

115 2. Numerical Model

116 2.1 General description of the numerical model



Mass vaporization rate (kg/s):

$$\dot{m}_l = \sum_{i=1}^{N_l} \dot{m}_{i,l} = \sum_{i=1}^{N_l} 4\pi R_l^2 \rho_g y_{i,l}^s (v_{i,g}^s + \sum_{i=1}^N y_{i,g}^s v_{i,g}^s)$$

Fig. 1. Schematic of the droplet evaporation model for multi-component fuel.

117

118 Figure 1 shows the schematic of our droplet evaporation model for multi-component fuels.

119 In the liquid phase, we consider the mass fraction distribution, $y_{i,l}(t, R)$, and the

120 temperature distribution, $T_l(R, t)$, inside a droplet, which are given by the analytical

121 solutions of a partial differential equation with spherical coordinates. The average mass

122 fraction of each species ($y_{i,l}^a$) is given by the mass balance of each species and updated

123 every timestep. The average temperature is also given by the energy conservation inside

124 the droplet. There is no need to consider the coupling of heat and mass transfer in the
125 present model. This is because the heat transfer and mass transfer are separately
126 considered in both liquid and gas phase. According to the mass transfer in the gas phase,
127 the present model applies the mass diffusion in multi-component system as the mass
128 evaporation rate of multi-component fuel of each species. The heat transfer is assumed as
129 the quasi-steady diffusion in the gas phase. In preset model, not only the effect of heat
130 transfer from the gas phase to the droplet but also the effect of heat transfer from the
131 droplet to the gas phase are considered. The enthalpy from the gas phase to the liquid
132 phase (\dot{q}_{gas}) comprises three terms, the heat conduction from the gas phase ($\dot{q}_{conduction}$),
133 the enthalpy diffusion from the liquid phase ($\dot{q}_{enthalpy}$), and the radiation from the gas
134 phase ($\dot{q}_{radiation}$). The mass evaporation rate of each species ($\dot{m}_{i,l}$) is given by the multi-
135 component system analysis of the equation of continuity. At the droplet interface, the
136 energy balance, $\dot{q}_{liquid} = \dot{q}_{gas} - \sum_{i=1}^{N_l} \dot{m}_{i,l} H_{i,latent}$, is considered. In the present model,
137 we assumed that (1) the fuel droplet is spherically symmetric, (2) Dufour and Soret effects
138 are neglected, (3) the droplet interface follows the thermodynamic equilibrium, and (4)
139 the gas-phase follow the quasi-steady-state assumption. Note that the dimensionless
140 number and thermodynamic properties used in the present model are described in
141 Appendix A-C.

142

143 *2.2 Liquid phase*

144

145 *2.2.1 Diffusion of species inside a droplet*

146 We assume that part of the droplet has a uniform species distribution to improve the

147 accuracy of modeling the mass diffusion. This is because there is a possibility that the
 148 mass does not diffuse completely from the droplet surface to the droplet center during a
 149 short time step, especially when the ambient temperature is high such as practical
 150 combustion field. Figure 2 shows the distribution of the mass concentration of each
 151 species in the uniform-gradient domain. The boundary x between the uniform distribution
 152 ($\varphi_{i,l}(t, R)$) and the gradient distribution ($\psi_{i,l}(t, R)$) is defined by the mass diffusion
 153 distance from the droplet surface. The mass diffusion distance is determined by the ratio
 154 of the effective mass diffusion coefficient $D_{eff,i}$ and the radius regression rate \dot{R}_d . Thus,
 155 the boundary is given by $x = R_d - \max\{D_{eff,i}|i \in N_l\}/\dot{R}_d$. The fuel species mass
 156 diffusion inside a spherically symmetric droplet can be expressed by the following
 157 equation:

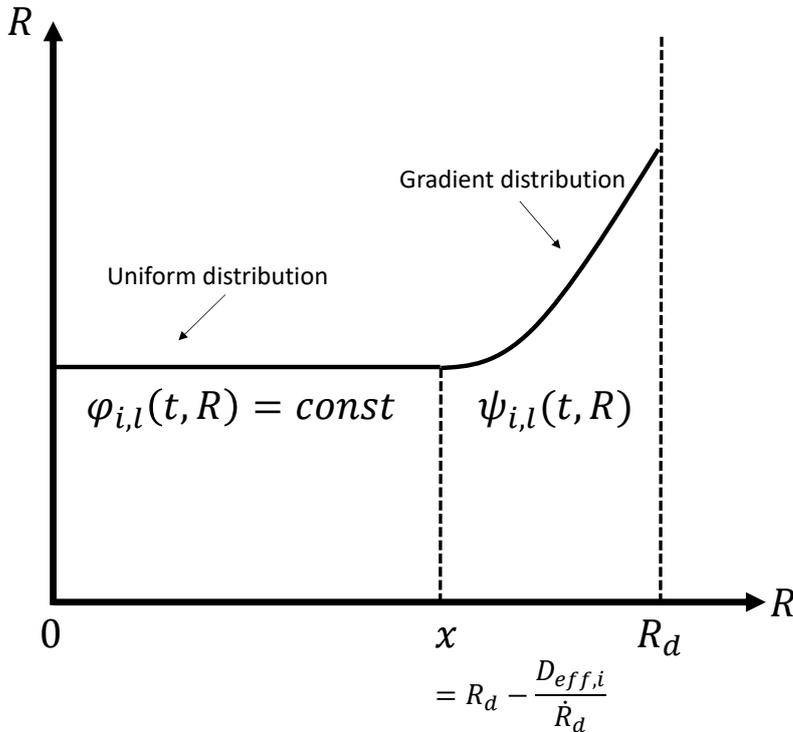


Fig. 2. Diagram showing the boundary x between the uniform distribution ($\varphi_{i,l}(t, R)$) and the gradient distribution ($\psi_{i,l}(t, R)$).

158

$$\frac{\partial y_{i,l}}{\partial t} = D_{eff,i} \left(\frac{\partial^2 y_{i,l}}{\partial R^2} + \frac{2}{R} \frac{\partial y_{i,l}}{\partial R} \right) \quad (1)$$

159

160 Sazhin *et al.* [14,16] previously suggested an analytical solution for Eq. (1) with the
 161 boundary conditions at the droplet center and surface. In our model, the boundary
 162 conditions based on the two-layer concepts shown in Fig.2 is described as

163

$$\begin{aligned} \frac{\dot{m}_l}{4\pi\rho_l R_d^2} (\varepsilon_i - y_{i,l}^s) &= -D_{eff,i} \frac{\partial y_{i,l}}{\partial R} & (R = R_d) \\ \frac{\partial y_{i,l}}{\partial R} &= 0 & (R = 0) \\ y_{i,l}(t, x^-) &= y_{i,l}(t, x^+), \frac{\partial y_{i,l}}{\partial R} \Big|_{R=x^+} = \frac{\partial y_{i,l}}{\partial R} \Big|_{R=x^-} = 0 \end{aligned} \quad (2)$$

164

165 where ε_i is the normalized fuel vapor fraction, defined as $\varepsilon_i = y_{i,g}^s / \sum_{i=1}^{N_l} y_{i,g}^s$. The
 166 analytical solution of Eq. (1) with the boundary conditions given by Eq. (2) can be
 167 described as

$$\begin{aligned} Y_{i,l}(t, R) &= \varepsilon_i(t) + \frac{1}{R} \left\{ \exp \left[D_{eff,i} \left(\frac{\lambda_0}{R_d} \right)^2 t \right] [q_{i,n} - \varepsilon_i(0) Q_0] \sinh \left(\lambda_0 \frac{R}{R_d} \right) \right. \\ &\quad \left. + \sum_{n=1}^{\infty} \exp \left[-D_{eff,i} \left(\frac{\lambda_n}{R_d} \right)^2 t \right] [q_{i,n} - \varepsilon_i(0) Q_n] \sin \left(\lambda_n \frac{R}{R_d} \right) \right\} \end{aligned} \quad (3)$$

168

169 where $h_0 = - \left(1 + \frac{\dot{m}_l R_d}{4\pi\rho_l R_d^2 D_{eff,i}} \right)$ and

170

$$Q_n = \begin{cases} \frac{1}{\|v_0(R)\|^2} \left(\frac{R_d}{\lambda_0} \right)^2 \{ \lambda_0 \cosh(\lambda_0) - \sinh(\lambda_0) \} & (\text{when } n = 0) \\ \frac{1}{\|v_n(R)\|^2} \left(\frac{R_d}{\lambda_n} \right)^2 \{ \sin(\lambda_n) - \lambda_n \cos(\lambda_n) \} & (\text{when } n \geq 1) \end{cases}$$

$$q_{i,n} = \begin{cases} \frac{1}{\|v_0(R)\|^2} \begin{cases} \int_0^x R\varphi v_0(R)dR & (\text{when } 0 < R < x) \\ \int_x^{R_d} R\psi_{i,l_0}(0,R)v_n(R)dR & (\text{when } x < R < R_d) \end{cases} & (n = 0) \\ \frac{1}{\|v_n(R)\|^2} \begin{cases} \int_0^x R\varphi v_n(R)dR & (\text{when } 0 < R < x) \\ \int_x^{R_d} R\psi_{i,l_0}(0,R)v_n(R)dR & (\text{when } x < R < R_d) \end{cases} & (n \geq 1) \end{cases}$$

171

172 Next, the derivation processes of the eigenvalues λ_0 and λ_n ($n \geq 1$) are described. The
 173 following boundary conditions are given in the present study, instead of Eq. (52) in Ref.
 174 [14]:

175

$$\begin{cases} v|_{R=0} = \left(\frac{\partial v}{\partial R} + \frac{h_0}{R_d} v \right)_{R=R_d} = 0 \\ v|_{R=x^-} = v|_{R=x^+} \\ D_{eff,i} \left[x \frac{\partial v}{\partial R} - v \right] \Big|_{R=x^+} = 0 \end{cases} \quad (4)$$

176

177 When $p < 0$ in the Eq.(51) in Ref. [14], we can write the general solution assuming that
 178 $p = -\lambda^2 < 0$ as

$$179 \quad v(R) = A \cosh\left(\lambda \frac{R}{R_d}\right) + B \sinh\left(\lambda \frac{R}{R_d}\right)$$

180 where A and B are arbitrary constants. The boundary conditions obtained using Eq. (4)
 181 lead to the following equations:

182

$$\begin{cases} v(0) = A \cosh\left(\lambda \frac{0}{R_d}\right) + B \sinh\left(\lambda \frac{0}{R_d}\right) = A = 0 \\ \left(\frac{\partial v}{\partial R} + \frac{h_0}{R_d} v \right)_{R=R_d} = \frac{B}{R_d} (\lambda \cosh(\lambda) + h_0 \sinh(\lambda)) = 0 \\ D_{eff,i} \left[x \frac{\partial v}{\partial R} - v \right] \Big|_{R=x^+} = B \left(\frac{\lambda}{R_d} x \cosh\left(\lambda \frac{x}{R_d}\right) - \sinh\left(\lambda \frac{x}{R_d}\right) \right) = 0 \end{cases} \quad (5)$$

183 B in this equation is not equal to 0 because the present study does not assume a trivial
 184 solution where $v = 0$. Thus, Eq. (5) can be rearranged as

185

$$\lambda \cosh(\lambda) + h_0 \sinh(\lambda) - \lambda x \cosh\left(\lambda \frac{x}{R_d}\right) + R_d \sinh\left(\lambda \frac{x}{R_d}\right) = 0 \quad (6)$$

186 Then, the solution of Eq. (6) gives only one eigenvalue $\lambda = \lambda_0 > 0$ and the corresponding
 187 eigenfunction.

$$188 \quad v_0(R) = \sinh\left(\lambda_0 \frac{R}{R_d}\right)$$

189 where the normalization leading to $B = 1$ is chosen. Furthermore, the direct calculation
 190 of the integrals leads to the following description for the norm of the eigenfunction v_0 .

$$191 \quad \|v_0\|^2 = \int_0^{R_d} v_0^2(R) dR = \frac{R_d}{4\lambda_0} (\sinh(2\lambda_0) - 2\lambda_0)$$

192 Furthermore, when $p > 0$ in Eq. (51) in Ref. [14], we can write the general solution
 193 assuming that $p = \lambda^2 > 0$ as

$$194 \quad v(R) = A \cos\left(\lambda \frac{R}{R_d}\right) + B \sin\left(\lambda \frac{R}{R_d}\right)$$

195 where A and B are arbitrary constants. The boundary conditions obtained using Eq. (4)
 196 lead to the following equations:

197

$$\begin{aligned} v(0) &= A \cos\left(\lambda \frac{0}{R_d}\right) + B \sin\left(\lambda \frac{0}{R_d}\right) = A = 0 \\ v(R_d) &= \frac{B}{R_d} (\lambda \cos(\lambda) + h_0 \sin(\lambda)) = 0 \end{aligned} \quad (7)$$

$$D_{eff,i} \left[x \frac{\partial v}{\partial R} - v \right] \Big|_{R=x^+} = B \left(\frac{\lambda}{R_d} x \cos\left(\lambda \frac{x}{R_d}\right) - \sin\left(\lambda \frac{x}{R_d}\right) \right) = 0$$

198 B in this equation is not equal to 0 because the present study does not consider the trivial
 199 solution $v = 0$. Therefore, Eq. (7) can be rearranged as

200

$$\lambda \cos(\lambda) + h_0 \sin(\lambda) - \lambda x \cos\left(\lambda \frac{x}{R_d}\right) + R_d \sin\left(\lambda \frac{x}{R_d}\right) = 0 \quad (8)$$

201 Then, the solution of Eq. (8) gives a countable set of positive solutions λ_n which are
 202 arranged in ascending order such as $0 < \lambda_1 < \lambda_2 < \lambda_3 < \dots$, and the corresponding
 203 eigenfunction can be described as

$$204 \quad v_n(R) = \sin\left(\lambda_n \frac{R}{R_d}\right)$$

205 where the normalization leading to $B = 1$ is chosen. Furthermore, the direct calculation
 206 of the integrals leads to the following description for the norm of the eigenfunction v_n .

207

$$208 \quad \|v_n\|^2 = \int_0^{R_d} v_n^2(R) dR = \frac{R_d}{\lambda_n} \left\{ \frac{\lambda_n}{2} - \frac{1}{4} \sin(2\lambda_n) \right\}$$

209

210 The analytical solution given by Eq. (3) is uniquely determined in mathematics.
 211 However, the disadvantage of using the analytical solution in numerical simulations is
 212 that it necessitates interactive calculation (e.g., Ref. [18]), which increase the calculation
 213 cost. Thus, the variables can be assumed constant during a short time step, which has been
 214 applied in numerical studies using the analytical solution [13].

215 In this study, we assumed that ε_i is constant during the short time step and used the
 216 distributions obtained at the previous time step, which are described as $\psi_i(t, R)$ and
 217 $\varphi_i(t, R)$. Assuming that ε_i , $\psi_i(t, R)$, and $\varphi_i(t, R)$ are constant during the short time step,
 218 the authors deform Eq. (3) to satisfy mass conservation inside the droplet as the follows:

219

$$y_{i,l}^a \int_0^{R_d} 4\pi R^2 dR = \int_0^{R_d} y_{i,l}(t, R) 4\pi R^2 dR \quad (9)$$

220

221 Note that the calculation for $y_{i,l}^a$ is introduced in Section 2.4. Eq. (9) has not been reported

222 in Sazhin's former studies (e.g. Ref. [16]). Substituting Eq. (3) into Eq. (9), we obtained
 223 the following identical equation:

224

$$\begin{aligned} \frac{1}{3}y_{i,l}^a R_d^3 = \frac{1}{3}\varepsilon_{i,l} R_d^3 + A_0 \left\{ \frac{R_d^2}{\lambda_0} \cosh(\lambda_0) - \left(\frac{R_d}{\lambda_0}\right)^2 \sinh(\lambda_0) \right\} \\ + \sum_{n=1}^{\infty} A_n \left\{ -\frac{R_d^2}{\lambda_n} \cos(\lambda_n) + \left(\frac{R_d}{\lambda_n}\right)^2 \sin(\lambda_n) \right\} \end{aligned} \quad (10)$$

225

226 where $A_0 = \exp\left[D_{i,l}\left(\frac{\lambda_0}{R_d}\right)^2 t\right][q_{i0} - \varepsilon_{i,l}(0)Q_0]$, and $A_n = \exp\left[-D_{i,l}\left(\frac{\lambda_n}{R_d}\right)^2 t\right][q_{in} -$
 227 $\varepsilon_{i,l}(0)Q_n]$. Eq. (10) can be rearranged as

228

$$\varepsilon_{i,l} = y_{i,l}^a - \frac{3A_0}{R_d \lambda_0^2} \{\lambda_0 \cosh(\lambda_0) - \sinh(\lambda_0)\} - \sum_{n=1}^{\infty} \frac{3A_n}{R_d \lambda_n^2} \{\sin(\lambda_n) - \lambda_n \cos(\lambda_n)\} \quad (11)$$

229

230 Equation (11) has no variable because ε_i is constant during the short time step. By
 231 substituting Eq. (11) into Eq. (9), the distribution equation of each fuel species can be
 232 given by

233

$$\begin{aligned} y_{i,l}(t, R) = y_{i,l}^a + \frac{1}{R} \left[\exp\left[D_{eff,i}\left(\frac{\lambda_0}{R_d}\right)^2 t\right] (q_{i0} - \varepsilon_i Q_0) \left\{ \sinh\left(\lambda_0 \frac{R}{R_d}\right) - \frac{3R}{R_d \lambda_0^2} (\lambda_0 \cosh(\lambda_0) - \sinh(\lambda_0)) \right\} \right. \\ \left. + \sum_{n=1}^{\infty} \exp\left[-D_{eff,i}\left(\frac{\lambda_n}{R_d}\right)^2 t\right] [q_{in} - \varepsilon_i Q_n] \left\{ \sin\left(\lambda_n \frac{R}{R_d}\right) - \frac{3R}{R_d \lambda_n^2} (\sin(\lambda_n) - \lambda_n \cos(\lambda_n)) \right\} \right] \end{aligned} \quad (12)$$

234

235 2.2.2 Droplet heating

236 According to former study [19], it has been pointed out that the thermal diffusivity is
 237 much larger than the mass diffusivity inside droplet in conventional hydrocarbon fuels.

238 This leads that the temperature is easier to form a distribution along the whole droplet

239 than the mass concentration inside droplet. This is why we focused on the precise theory
 240 of the mass diffusion inside droplet in the present model. The heat transfer inside a
 241 spherically symmetric droplet can be expressed by the following equation:

$$242 \quad c_{p,l}\rho_l \frac{\partial T}{\partial t} = k_{eff} \left(\frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right) \quad (13)$$

243

244 The boundary conditions at the center and surface of the droplet can be described as:

245

$$246 \quad \begin{aligned} 2\pi R_d k_g Nu (T_{amb} - T^s) - \dot{q}_{enthalpy} + \dot{q}_{radiation} - \dot{m}_l H_{latent} &= k_{eff} \frac{\partial T}{\partial R} \quad (R = R_d) \\ \frac{\partial T}{\partial R} &= 0 \quad (R = 0) \end{aligned} \quad (14)$$

246

247 Some conventional models (e.g. [16]) have not considered the enthalpy diffusion term.

248 However, the enthalpy diffusion flux in a multi-component energy balance is well-known,

249 yet it is a frequently neglected term [20]. Furthermore, our previous study [21] clarified

250 that the consideration of the enthalpy diffusion term results in a slower evaporation rate.

251 On the basis of Refs. [16] and [18], the solution of Eq. (13) with the boundary conditions

252 (Eq. (14)) can be given by

253

$$254 \quad T(t, R) = \frac{R_d}{R} \sum_{n=1}^{\infty} q_n \exp[-\kappa \lambda_n^2 t] \sin\left(\lambda_n \frac{R}{R_d}\right) + T_{eff} \quad (15)$$

254

255 where $\kappa = \frac{k_{eff}}{c_{p,l}\rho_l R_d^2}$, $\|v_n\|^2 = \frac{1}{2} \left[1 + \frac{H}{H^2 + \lambda_n^2} \right]$, $H = \frac{k_g Nu}{2k_l} - 1$, $T_{eff} = T_{amb} +$

256 $\frac{1}{2\pi R_d k_g Nu} (-\dot{q}_{enthalpy} + \dot{q}_{radiation} - \dot{m}_l H_{latent})$, and

257 $q_n = \frac{1}{R_d^2 \|v_n\|^2} \int_0^{R_d} R T_0(R) \sin\left(\lambda_n \frac{R}{R_d}\right) dR - \frac{(1+H)T_{eff}}{\lambda_n^2 \|v_n\|^2} \sin(\lambda_n)$. Note that T_{eff} is a
 258 function of time because \dot{m}_l and T_{amb} are time-dependent. The estimation of
 259 $C_{p,l}$ and ρ_l is described in Appendix A. The estimation of k_g and is described in
 260 Appendix B.

261 Assuming that T_{eff} and $T_0(R)$ are constant during a short time step, as in Ref. [18] , and
 262 $T_0(R)$ is obtained at the previous time step, the authors deform Eq. (15) to satisfy enthalpy
 263 conservation inside the droplet as the following:

264

$$T^a \int_0^{R_d} 4\pi C_{p,l} R^2 dR = \int_0^{R_d} T(R, t) 4\pi C_{p,l} R^2 dR \quad (16)$$

265

266 We assumed that the heat capacity inside the droplet ($C_{p,l}$) is constant, although heat
 267 capacity is a function of temperature. Substituting Eq. (15) into Eq. (16), we obtain the
 268 following identical equation:

269

$$\frac{4}{3} \pi T^a = 4\pi \left\{ - \sum_{n=1}^{\infty} \frac{q_n \exp[-\kappa \lambda_n^2 t]}{\lambda_n} \cos(\lambda_n) + \sum_{n=1}^{\infty} \frac{q_n \exp[-\kappa \lambda_n^2 t]}{\lambda_n^2} \sin(\lambda_n) \right\} + \frac{4}{3} \pi T_{eff} \quad (17)$$

270

271 Similar to the derivation process of the mass distribution equation, the temperature
 272 distribution equation can be given by

273

$$T(t, R) = T^a + \sum_{n=1}^{\infty} q_n \exp[-\kappa \lambda_n^2 t] \left\{ \frac{R_d}{R} \sin\left(\lambda_n \frac{R}{R_d}\right) - 3 \frac{(1+H) \sin(\lambda_n)}{\lambda_n^2} \right\} \quad (18)$$

274

275 To consider effect of internal circulation caused by the internal vortex on the droplet
 276 evaporation characteristics, the effective mass diffusivity (D_{eff}) [22] and the effective
 277 thermal diffusivity (k_{eff}) [23] were applied, instead of the normal mass diffusivity and
 278 the normal thermal diffusivity as

279

$$D_{eff,i} = \left\{ 1.86 + 0.86 \tanh \left[2.225 \log_{10} \left(\frac{Re_l Sc_l}{30} \right) \right] \right\} D_{l,i} \quad (19)$$

$$k_{eff} = \left\{ 1.86 + 0.86 \tanh \left[2.225 \log_{10} \left(\frac{Pe_l}{30} \right) \right] \right\} k_l \quad (20)$$

280

281 Note that the effective mass and thermal diffusivity have been applied to some droplet
 282 evaporation model for multi-component fuel (e.g. [13]) without using a detailed and
 283 analytical approach such as [24]. The estimation of $D_{l,i}$ and k_l is described in Appendix

284 A.

285

286 2.3 Gas-phase

287

288 2.3.1 Mass evaporation rate

289 In this study, the mass evaporation rate (\dot{m}_l) for each fuel species was expressed on the
 290 basis of the continuity equation for fuel vapor at the droplet surface in ambient gas.

291 According to Ref. [25], the total mass evaporation and the mass evaporation of species i
 292 in quiescent conditions were given by

293

$$\dot{m}_l = \sum_{i=1}^{N_l} \dot{m}_{i,l} = \sum_{i=1}^{N_l} 4\pi R_d^2 \rho_g^s y_{i,g}^s (v_{i,g}^s - \sum_{i=1}^N y_{i,g}^s v_{i,g}^s) \quad (21)$$

294

295 The estimation of ρ_g and is described in Appendix B.

296

297 2.3.2 Heat transfer

298 Three distinct terms were considered when analyzing the gas-phase heat flux: the heat
299 flux of conduction from the gas phase to the liquid phase ($\dot{q}_{conduction}$), that of enthalpy
300 diffusion from the liquid phase to the gas phase ($\dot{q}_{enthalpy}$), and that of heat radiation
301 from the phase to the liquid phase ($\dot{q}_{radiation}$). Although the enthalpy diffusion flux in a
302 multi-component energy balance is well-known, it is a frequently neglected [20].
303 However, our previous study using internal distribution formulas approximated by the
304 quadratic polynomial functions [21] elucidated that the consideration of the enthalpy
305 diffusion term reduces the evaporation rate. Moreover, the evaporation model calculation
306 results agreed better with the experimental results when the enthalpy diffusion term was
307 considered [21]. Thus, the total heat flux from the gas phase can be described as

308

$$\begin{aligned}\dot{q}_{gas} &= \dot{q}_{conduction} + \dot{q}_{enthalpy} + \dot{q}_{radiation} \\ &= 2\pi R_d k_g Nu (T_{amb} - T^s) - 4\pi R_d^2 \rho_g \sum_{i=1}^N h_{i,g} (y_{i,g}^s v_{i,g}^s) + 4\pi R_d^2 \varepsilon \sigma (T_{amb}^4 - T^{s4})\end{aligned}\quad (22)$$

309

310 Note that dimensionless numbers used in this work are summarized in Appendix C. The
311 estimation of ρ_g and $h_{i,g}$ is described in Appendix B.

312

313 2.4 Gas-liquid interface

314

315 2.4.1 Thermodynamic equilibrium

316 On the basis of Raoult's law, the vapor mole fraction at the droplet surface ($x_{i,g}^s$) was
 317 calculated as

318

$$x_{i,g}^s = \frac{P_{i,v}}{P_{amb}} x_{i,l}^s \quad (23)$$

319

320 where $x_{i,l}^s$ is the liquid mole fraction at the droplet surface, P_{amb} is the ambient pressure
 321 [Pa], and $P_{i,v}$ is the vapor pressure of species i [Pa] calculated using the Antoine equation
 322 as

323

$$\log_{10} P_{i,v} = A_{i,p} - \frac{B_{i,p}}{C_{i,p} + T^s} \quad (24)$$

324

325 where $A_{i,p}$, $B_{i,p}$, and $C_{i,p}$ are Antoine constants [26].

326

327 2.4.2 Energy equilibrium

328 The energy balance at the gas–liquid interface can be expressed as

329

$$\dot{q}_{gas} - \dot{q}_{liquid} = \sum_{i=1}^{N_l} \dot{m}_{i,l} H_{i,latent} \quad (25)$$

330

331 2.4.3 Energy and mass conservations within a droplet

332 The average temperature inside the droplet (T^a) at the n th time step can be calculated
 333 from the governing equation for energy in the liquid phase as

334

$$C_{p,l}m_l \frac{dT^a}{dt} = \dot{q}_{liquid} \Leftrightarrow T_{n+1}^a = T_n^a + \frac{\dot{q}_{liquid}}{C_{p,l}m_l} \Delta t \quad (26)$$

335

336 The droplet radius (R_d) [m] was calculated on the basis of the droplet mass at each time
337 step.

338

$$R_d = \left(\frac{m_l - \dot{m}_l \Delta t}{\frac{4}{3} \pi \rho_l} \right)^{\frac{1}{3}} \quad (27)$$

339

340 Moreover, the average mass fraction of species i inside the droplet ($y_{i,l}^a$) [-] was calculated
341 on the basis of the droplet mass and mass evaporation rate as

342

$$y_{i,l}^a = \frac{m_{i,l} - \dot{m}_{i,l} \Delta t}{m_l - \dot{m}_l \Delta t} \quad (28)$$

343

344 *2.6 Numerical algorithm*

345 The calculation code of the present model was developed using Fortran 90. Figure 3
346 shows the numerical algorithm of the present model. The calculation procedure can be
347 described as follows:

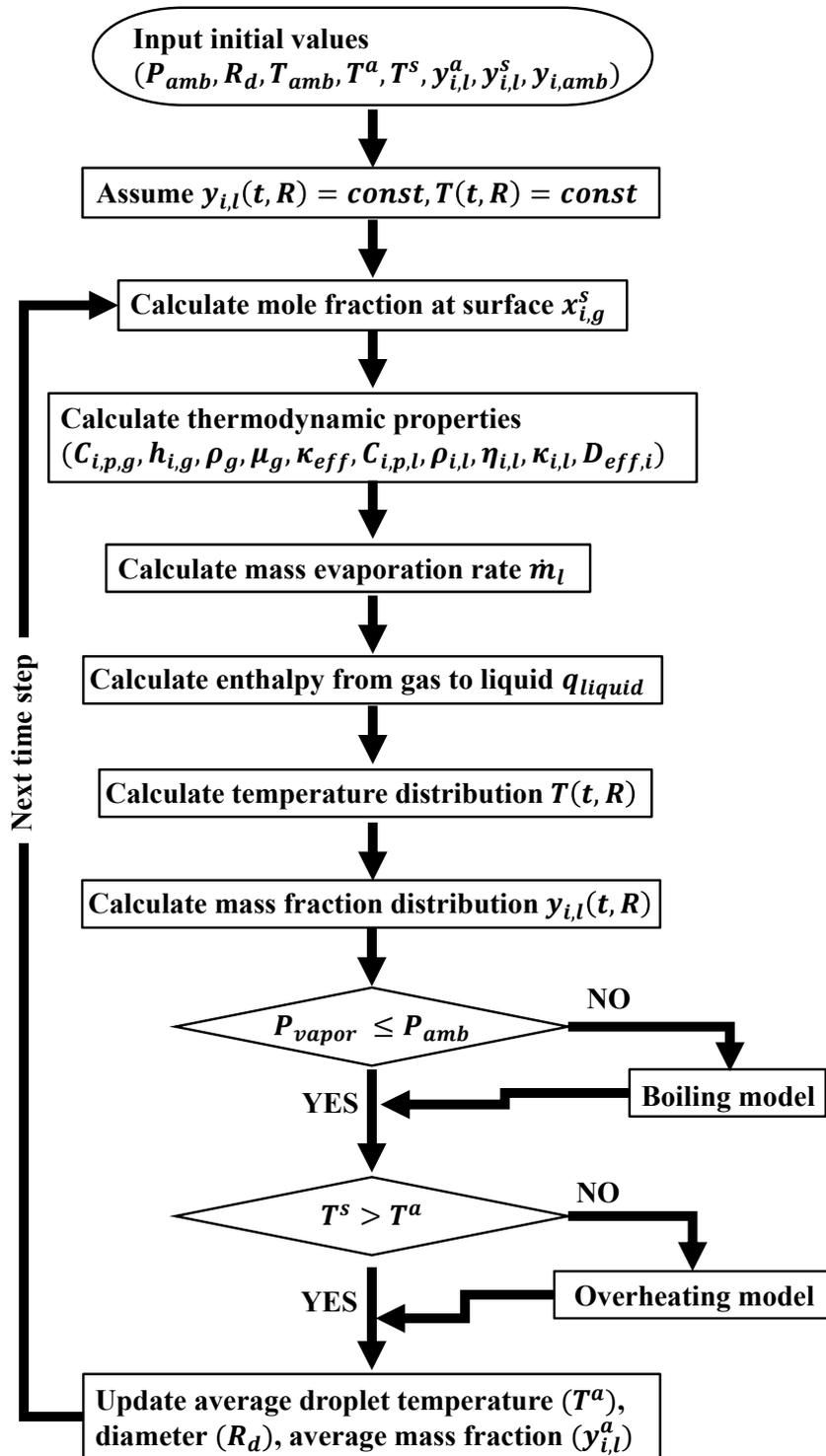


Fig.3 Numerical algorithm of present model

- 349 1. Input the initial values ($P_{amb}, T_{amb}, R_d, T^a, T^s$, and $y_{i,l}^a$).
- 350 2. Assume uniform temperature and mass fraction distributions inside the
- 351 droplet at the initial step, or use the distributions from the previous time
- 352 step.
- 353 3. Calculate thermodynamic equilibrium at the gas–liquid interface given
- 354 by Eq. (23).
- 355 4. Calculate thermodynamic properties in liquid and gas phases.
- 356 5. Calculate the mass evaporation rate given by Eq. (21).
- 357 6. Calculate the energy balance at the droplet interface given by Eq. (25).
- 358 7. Calculate the droplet temperature distribution given by Eq. (12).
- 359 8. Calculate mass fraction distributions inside the droplet given by Eq.
- 360 (18).
- 361 9. Update average droplet temperature (T^a) given by Eq. (26), the droplet
- 362 diameter (R_d) given by Eq. (27), and average mass fraction of species
- 363 i ($y_{i,l}^a$) given by Eq. (28). Repeat steps 2-9 until the droplet total mass
- 364 becomes 0.

365 Note that the explanations for the boiling model and the overheating model are described
366 in Appendix D and E, respectively. In the conditions shown in Section 3.2, the total vapor
367 pressure does not exceed the ambient pressure. In other word, the droplet temperature
368 does not exceed the temperature equivalent to boiling point. The droplet average
369 temperature given by Eq. (26) also does not exceed the surface temperature in the
370 conditions shown in Section 3.2. This is why the both the boiling model and the
371 overheating model were not activated. On the other hand, both the boiling model and the
372 overheating model were activated in the conditions shown in Section 3.3. However, the

373 boiling model and the overheating model had little effect on the prediction results because
374 the boiling model and the overheating model were used very infrequently in calculations.

375

376 *2.7 Surrogate fuel*

377 For the validation of the present model, a surrogate fuel for light cycle oil (LCO) [27]
378 was used as a multi-component fuel, which includes eicosane ($C_{20}H_{42}$), n-hexadecane
379 ($C_{16}H_{34}$), 1-methylnaphthalene ($C_{11}H_{10}$), and tert-butylbenzene ($C_{10}H_{14}$) with initial
380 mass fractions of 0.0729, 0.1753, 0.4402, and 0.3116, respectively. We found that the
381 evaporation characteristics of this surrogate fuel were in good agreement with those of
382 the actual LCO.

383

384 **3. Results and Discussion**

385

386 *3.1 Internal distributions*

387 We investigated the internal distribution behavior of the involved species as a function
388 of ambient temperature (T_{amb}) first. To reproduce the experimental conditions [27], the
389 initial droplet diameter (D_0) was selected as 500 μm , nitrogen was used as the ambient
390 gas, and the ambient pressure was 0.1 MPa. Fig. 4 shows the history of the internal mass
391 distribution of each fuel species as a function of the nondimensional length from droplet
392 center to the surface during evaporation at $T_{amb} = 473$ K. In this figure, the color shows
393 the mass fraction, and the horizontal distributions describe the mass fraction distribution
394 at each moment. According to Fig. 4, the gradients of the mass fraction distributions of
395 all fuel species were found in the early evaporation stage. Fig. 5 shows the internal
396 distributions as a function of normalized length from the droplet center to the surface at

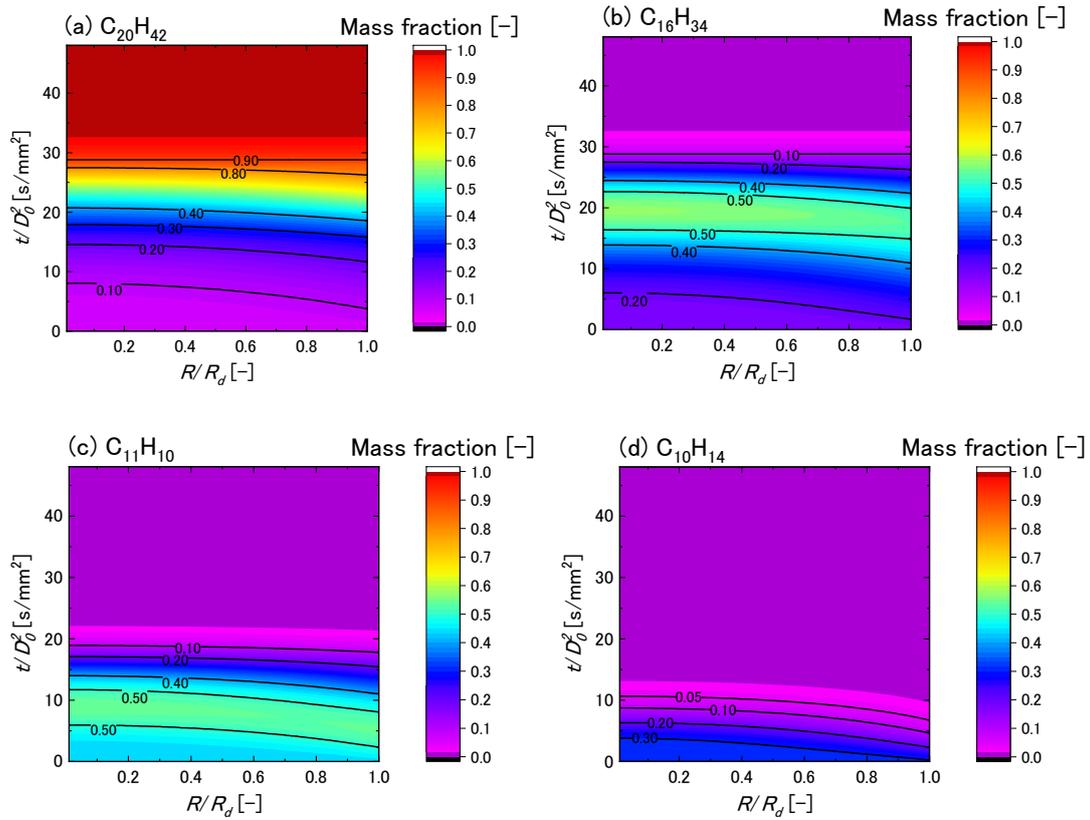


Fig. 4. History of internal mass distributions of each fuel species as a function of the nondimensional length from the droplet center to the surface during evaporation at $T_{amb} = 473$ K.

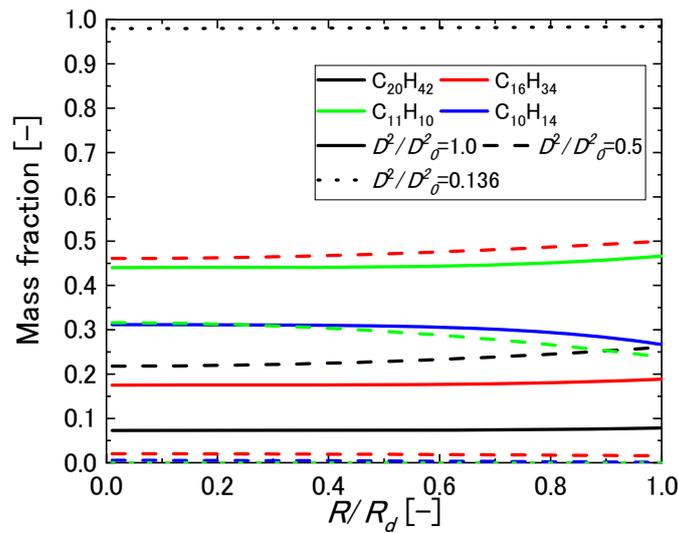


Fig. 5. Internal mass fraction distribution of each fuel species as a function of normalized length from the droplet center to the surface at early ($D^2/D_0^2 = 1.0$), middle ($D^2/D_0^2 = 0.5$), and late evaporation terms ($D^2/D_0^2 = 0.136$) at $T_{amb} = 473$ K

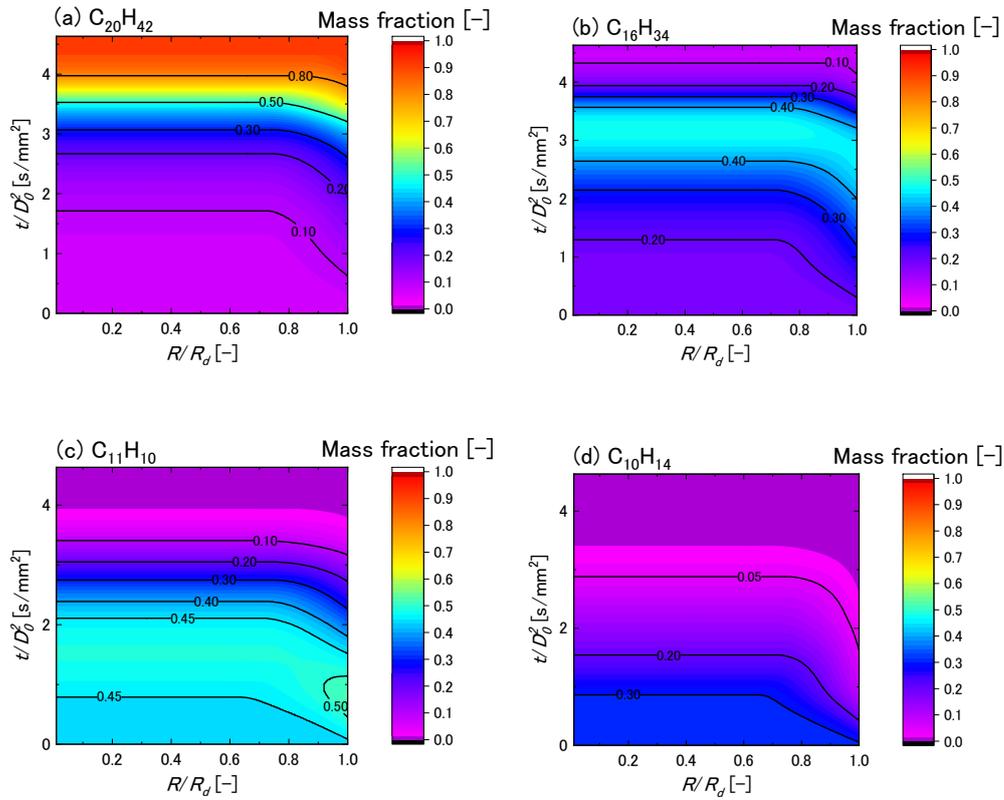


Fig. 6. History of internal mass distributions of each fuel species as a function of the nondimensional length from the droplet center to the surface during evaporation at $T_{amb} = 873$ K

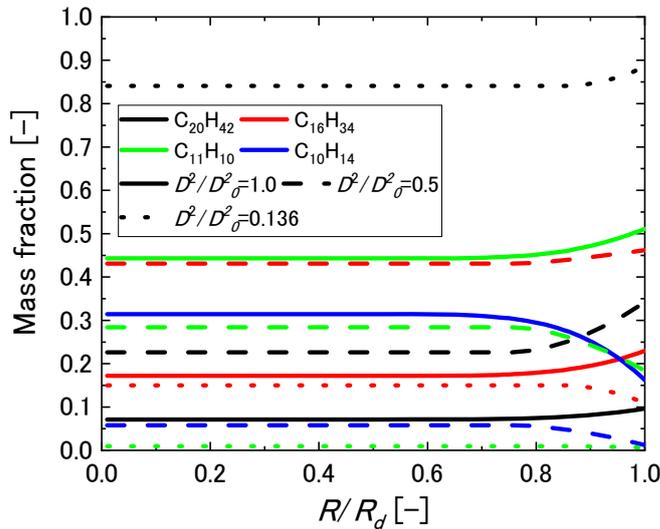


Fig. 7. Internal mass fraction distributions of each fuel species as a function of normalized length from the droplet center to the surface at early ($D^2/D_0^2 = 1.0$), middle ($D^2/D_0^2 = 0.5$), and late evaporation term ($D^2/D_0^2 = 0.136$) at $T_{amb} = 873$ K

399 early ($D^2/D_0^2 = 1.0$), middle ($D^2/D_0^2 = 0.5$), and late evaporation term ($D^2/D_0^2 = 0.136$)
400 at $T_{amb} = 473$ K. At the early evaporation term, the gradients of mass distribution for the
401 highly volatile species, $C_{11}H_{10}$ and $C_{10}H_{14}$, decrease, whereas those with low volatility,
402 $C_{16}H_{34}$ and $C_{20}H_{42}$, increase toward the droplet surface because the highly volatile
403 species evaporate more rapidly from the droplet surface than those with low volatility
404 species. However, the gradients of all fuel species become close to constant over time. At
405 the late evaporation term, the mass fraction distributions of $C_{16}H_{34}$ and $C_{20}H_{42}$ become
406 almost constant and $C_{20}H_{42}$ is dominant inside the droplet, including the effect of
407 considering internal mass fraction distributions is remarkable in the early evaporation
408 stage at a relatively low ambient temperature. A detailed discussion about the effects of
409 internal distributions on the evaporation behavior is provided in Section 3.3.

410 In the case of $T_{amb} = 873$ K, Fig. 6 shows more remarkable gradient distributions of all
411 fuel species during the whole evaporation term than Fig. 4 ($T_{amb} = 473$ K). As for the
412 case of $T_{amb} = 473$ K, Fig. 7 shows the internal distributions as a function of normalized
413 length from the droplet center to the surface at $T_{amb} = 873$ K. According to Fig. 7, the
414 gradients of mass distributions for all species around the droplet surface are steeper than
415 those in Fig.5. Then, the gradient becomes flat over time. Hence, the effect of considering
416 the gradient inside the droplet becomes larger as the ambient temperature increase.

417 Figure 8 shows the internal temperature distributions as a function of the
418 nondimensional length from the droplet center to the surface during evaporation at (a)
419 $T_{amb} = 473$ and (b) 873 K. According to Fig. 8-(a), the internal temperature distribution
420 becomes almost constant during the evaporation term. However, comparing Fig. 8-(b)
421 with Fig. 8-(a), we found that the internal temperature gradient becomes steeper in higher
422 ambient temperature as shown in Fig.8-(b). Thus, the consideration of temperature

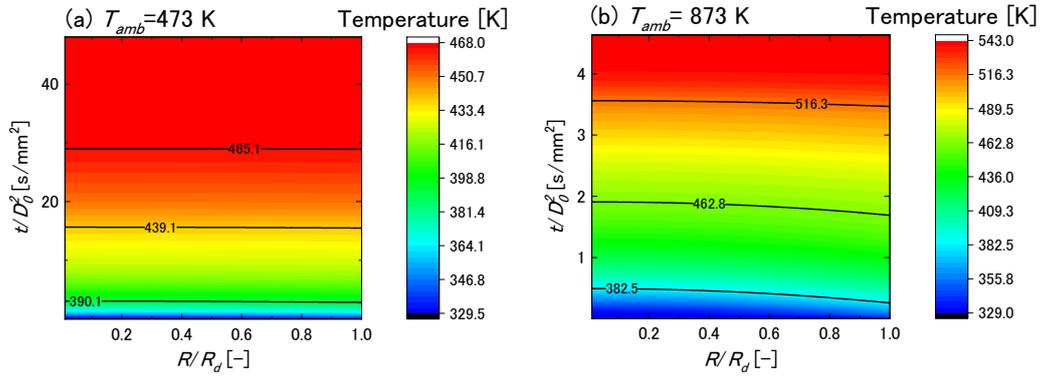


Fig. 8. Temperature distributions inside the droplet at (a) $T_{amb} = 473$ and (b) 873 K.

423

424 distribution inside a droplet plays an important role in the modeling of droplet evaporation

425 for a multi-component fuel at high ambient temperatures.

426

427 *3.2 Evaluation of model accuracy*

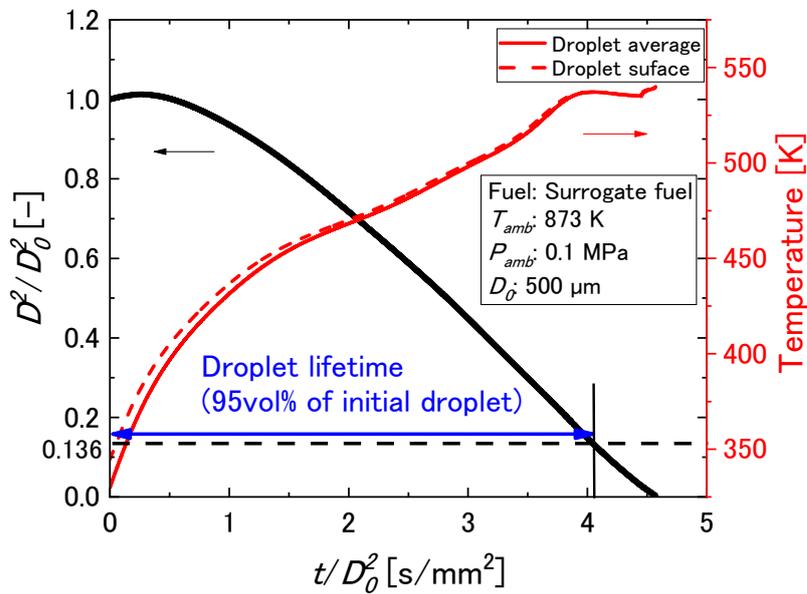


Fig. 9. Predicted droplet diameter and temperature.

428

429 Figure 9 depicts the history of the squared droplet diameter and the droplet average and

430 surface temperatures as functions of time, normalized by the squared initial droplet

431 diameter. The conditions used were $T_{amb} = 873$ K and $P_{amb} = 0.1$ MPa, with a 500 μm
 432 initial droplet diameter (D_0) to reproduce the experimental conditions [27]. As
 433 demonstrated in Fig. 9, the developed model reproduced the droplet diameter increase
 434 due to thermal expansion diameter in the early evaporation period, which was also found
 435 in the experimental results [28]. The droplet lifetime is the normalized time required for
 436 the evaporation of 95% of the initial droplet volume ($D^2/D_0^2 = 0.136$) [29]. Meanwhile,
 437 Fig. 9 demonstrates differences between the droplet surface temperature and average
 438 temperature. We present the detailed results obtained by the developed model and verify
 439 its accuracy in the following sections.

440 Figure 10 shows the predicted droplet lifetime for every 10 K from $T_{amb} = 473$ to 873
 441 K and the experimental results at various ambient temperature [28] to verify the accuracy
 442 of the present model. In Fig.10, the plots of experimental data indicate the average droplet
 443 lifetime of three or more experiments, and the maximum and minimum value of error bar
 444 are the maximum and minimum value of three or more experiments, respectively. Before

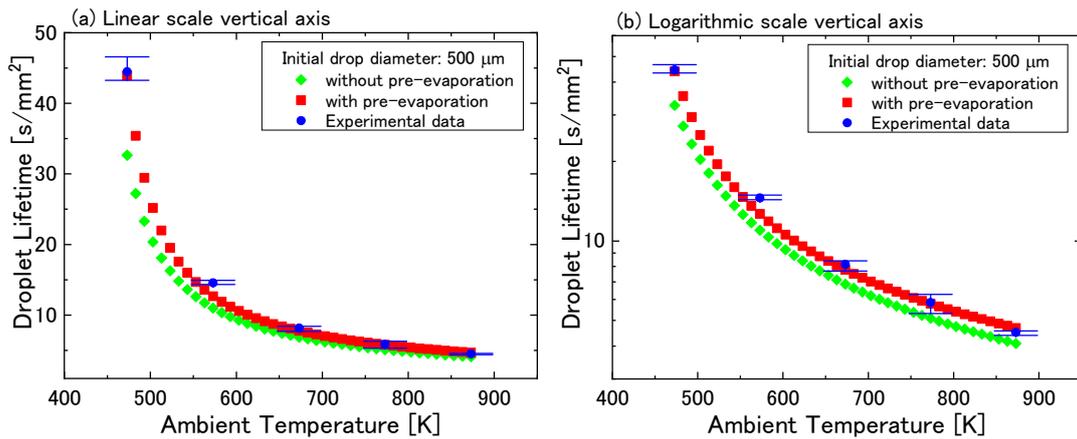


Fig. 10. Comparison between measured [28] and calculated droplet lifetimes at various ambient temperatures given by (a) linear scale in vertical axis and (b) logarithmic scale in vertical axis.

445

446 the detailed results are described, the meaning of pre-evaporation presented in Fig. 11 is
 447 explained as follows. Figure 11 depicts the experimental process of pre-evaporation. First,
 448 the fuel droplet was generated by a droplet generator on the tip of a droplet suspender
 449 (Fig. 11(a)). At that time, the surrounding gas temperature was 323 –353 K.
 450 Simultaneously, the fuel droplet, with a diameter in the range of $500 \mu\text{m} \pm 15\%$ was
 451 suspended at the intersection point of two fibers (Fig. 11(b)). Evaporation could begin
 452 soon after the droplet was suspended. The ambient gas was kept at 323 – 333 K (Fig.
 453 11(c)). The pre-evaporation occurred in the process shown in Fig. 11(c). Finally, the
 454 suspended droplet was inserted into the hot chamber, in which ambient temperatures were
 455 in the range of 473 –873 K, to record the droplet evaporation behavior using a high-speed
 456 camera (Fig. 11(d)). As Fig. 10 indicates, the calculated results without pre-evaporation
 457 differ from the experimental results at various ambient temperatures. Particularly, the

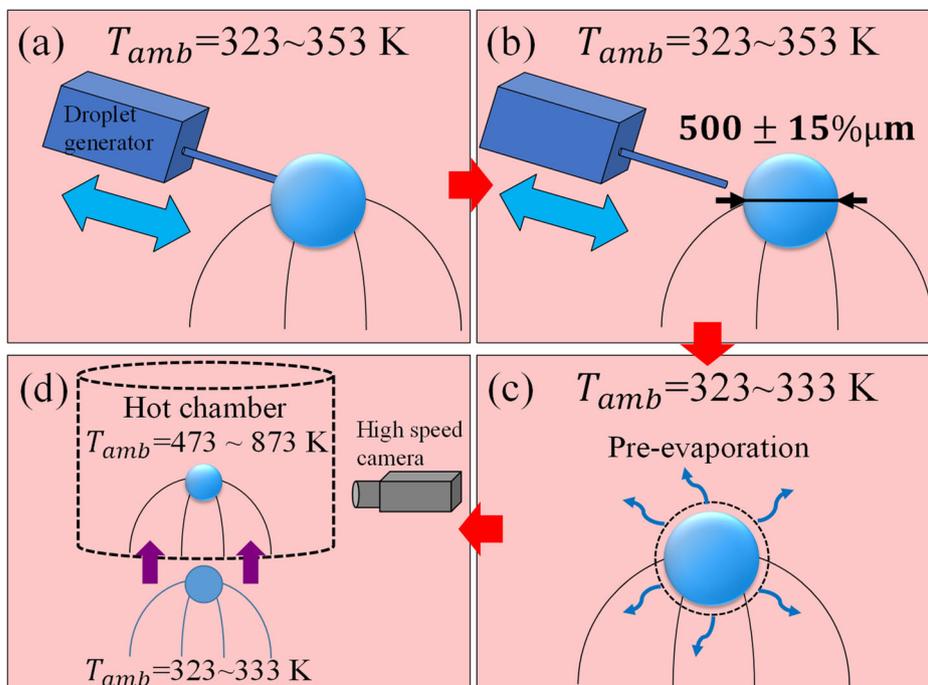


Fig. 11. Schematic of pre-evaporation process in experiments.

458

459 largest difference between the calculated and experimental results are found at $T_{amb} =$
 460 473 K. The differences between the calculated and experimental results may be caused
 461 by a change in the initial mass fractions of the surrogate fuel in the experiments due to
 462 the pre-evaporation. According to Fig.10(a), there are obvious differences
 463 between measured and predicted droplet lifetime without considering pre-
 464 evaporation term at $T_{amb} = 473$ K.

465 To increase the accuracy of the developed numerical model, this study also simulated
 466 pre-evaporation. The initial values for pre-evaporation term and main-evaporation term
 467 are shown in Table 1. In the calculation, the fuel droplet was assumed to remain at 330 K
 468 for 60 s before the droplet was inserted into a hotter chamber. Note that the initial droplet
 469 diameter in the calculation was set at 515 μm because the initial diameter before the pre-
 470 evaporation stage in the experiment was expected to be larger than the measured diameter
 471 in the hot chamber. Fig. 10 shows the comparison between measured and predicted
 472 droplet lifetime considering pre-evaporation term at various ambient temperature.
 473 According to Fig.10(a), the predicted droplet lifetime considering pre-evaporation term
 474 is in better agreement with the experimental results than the predicted droplet lifetime
 475 ignoring pre-evaporation term in low ambient temperature. Furthermore, it is found that
 476 the predicted droplet lifetime considering pre-evaporation term is in better agreement

Table 1 Initial values for pre-evaporation term and main-evaporation term

		Pre-evaporation term	Main-evaporation term
Ambient temperature	[K]	330	473 ~ 873
Ambient pressure	[MPa]	0.1	0.1
Droplet radius	[μm]	515	Value at end of pre-evaporation term
Droplet temperature	[K]	330	Value at end of pre-evaporation term
Ambient gas	[-]	N ₂	N ₂

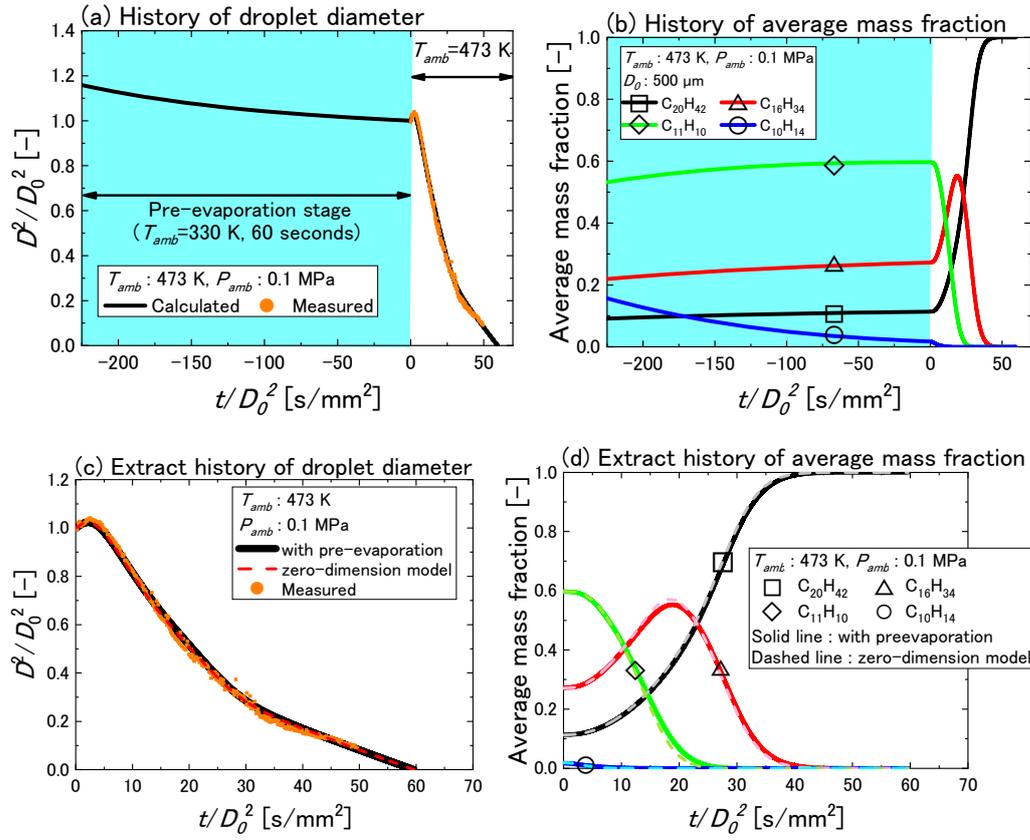


Fig. 12. Comparison between the experimental results and the simulated results considering the pre-evaporation process for (a) the history of the normalized squared droplet diameter, (b) the history of the average mass fraction of each species inside droplet, (c) extracted history of the normalized squared droplet diameter, and (d) extracted history of the average mass fraction of each species inside droplet at $T_{amb} = 473$ K.

477

478 with the experimental results than the predicted droplet lifetime ignoring pre-evaporation
 479 term in high ambient temperature as shown in Fig10(b). Figure-12(a) shows the history
 480 of the normalized square of the droplet diameter as a function of normalized time at
 481 $T_{amb} = 473$ K. During the pre-evaporation stage, the normalized square of the droplet
 482 diameter gently decreases. The predicted results of history of the normalized square of
 483 the droplet diameter are in good agreement with the experimental result. Figure 12(b)
 484 shows the average mass fraction values inside the droplet as a function of normalized

485 time. As seen in the pre-evaporation stage in Fig. 12(b), the species with the highest
486 volatility, $C_{10}H_{14}$, almost entirely evaporated before the droplet was inserted into the hot
487 chamber. To precisely compare the history of the normalized square of the droplet
488 diameter between the predicted results and measured results, the plots in Fig. 12(a) are
489 extracted as shown in Fig. 12(c). Furthermore, the history of the normalized square of the
490 droplet diameter predicted by the present model is compared with that predicted by the
491 zero-dimension model. Note that the zero-dimensional model is defined as the model that
492 has uniform temperature and mass fraction distribution in this paper. The plots in Fig.
493 12(b) are also extracted as shown in Fig. 12(d). In Fig. 12(d), the history of average mass
494 fraction predicted by the present model is compared with that predicted by the zero-
495 dimension model. According to both Fig. 12(c) and Fig. 12(d), there are few differences
496 in the history of predicted results between the present model and zero-dimension model.
497 However, it is found that there are clear differences between the present model and zero-
498 dimension model at practical spray combustion conditions. The detailed information will
499 be discussed in Section 3.3. Finally, the predicted droplet lifetimes considering pre-
500 evaporation are compared with the measured droplet lifetimes at various ambient
501 temperatures in Fig. 10. Table 2 shows the concrete value of both measured and predicted

Table 2 Differences in droplet lifetime between measurements and predictions at various ambient temperature

Ambient temperature [K]	Measurement [s/m ²]	Prediction ignoring pre-evaporation term [s/m ²]	Difference [%]	Prediction considering pre-evaporation term [s/m ²]	Difference [%]
473	44.480	32.652	36.225	43.977	1.145
573	14.561	10.992	32.472	12.661	15.010
673	8.151	6.860	18.816	7.768	4.929
773	5.843	5.092	14.745	5.783	1.043
873	4.503	4.088	10.156	4.681	-3.806

502 droplet lifetime and the differences in predicted droplet lifetime from measurements at
 503 various ambient temperatures. It is found that differences decreased when considering
 504 pre-evaporation term compared to when not considering pre-evaporation term in all
 505 ambient temperature.

506

507 *3.3 Effect of internal distributions at spray combustion conditions*

508 We investigated the effect of
 509 considering the internal temperature
 510 and mass concentration distributions
 511 inside the droplet. In previous
 512 section, we defined the zero-
 513 dimensional model. The zero-
 514 dimensional model has uniform
 515 temperature and mass fraction
 516 distribution. To elucidate the effect of
 517 considering the internal temperature

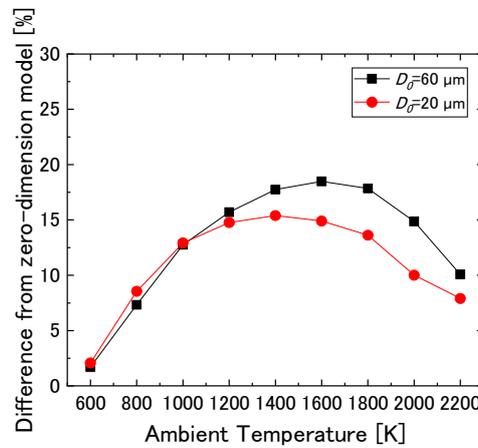
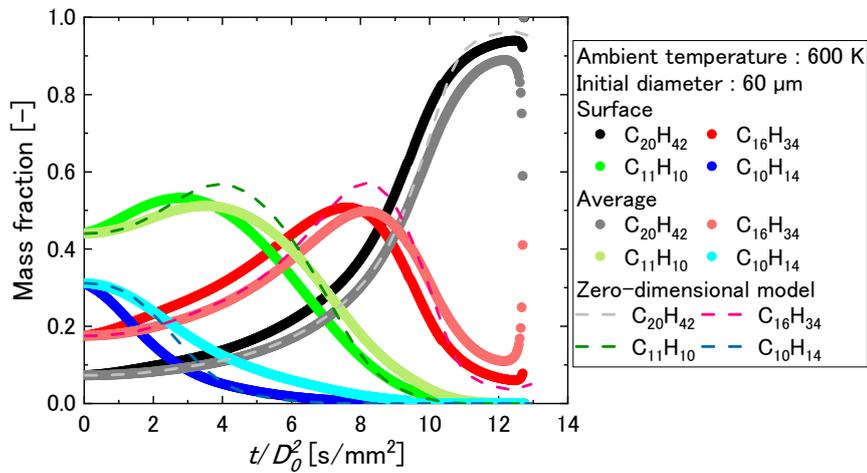
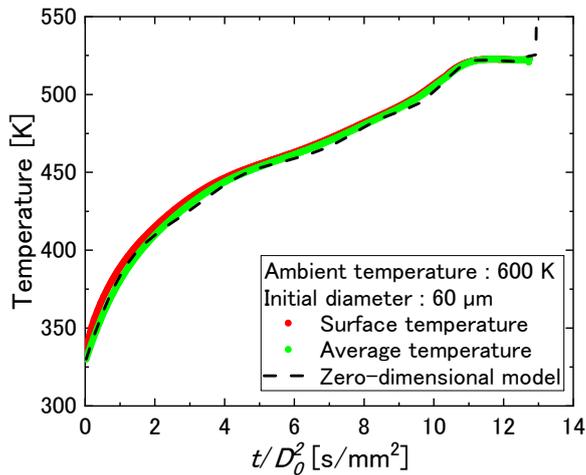


Fig. 13 Droplet lifetime differences between present model and zero-dimension model under various ambient temperature

518 and mass concentration distributions inside the droplet, the zero-dimensional model was
 519 compared with the present model. Furthermore, for the future use of the present model in
 520 practical spray combustion simulations, smaller initial droplet diameters were
 521 investigated. In this section, 60 and 20 μm were selected as initial droplet diameters on
 522 the basis of former experimental [30-32] and simulation studies [2]. To evaluate the effect
 523 of considering internal distributions quantitatively, the differences in predicted droplet
 524 diameter between the present model and the model assuming that internal distributions
 525 both temperature and mass concentrations are uniform. Figure 13 shows the



(a) History of liquid mass fraction

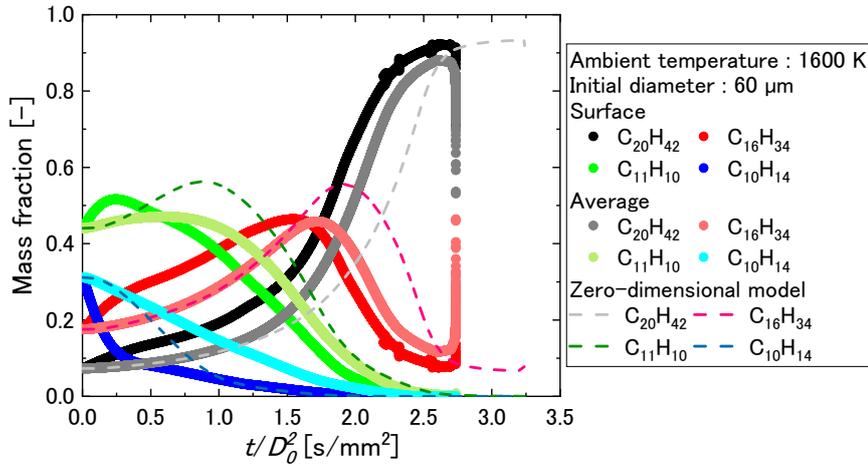


(b) History of droplet temperature

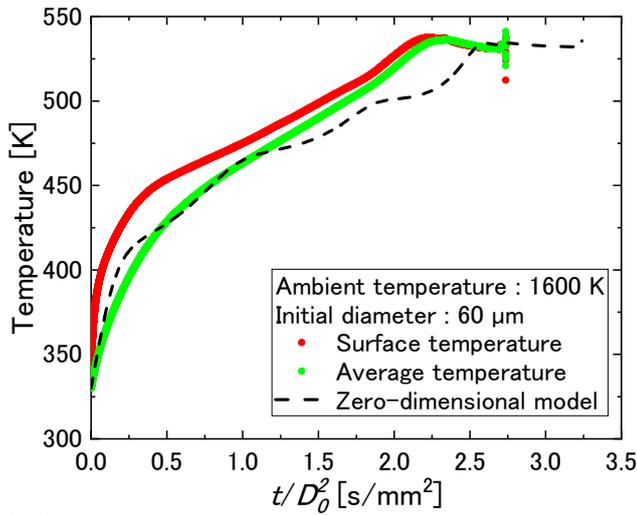
Fig.14 Comparison of the predicted results between the present model and the zero-dimensional model for (a) mass fraction and (b) temperature inside droplet at $T_{amb}=600$ K in $D_0=60$ μm .

526

527 comparison of the differences in droplet lifetimes formed by the present model and the
 528 zero-dimensional model at various ambient temperatures, which include both
 529 experimental and practical ambient temperatures. The divergence from the zero-
 530 dimensional model increases with the increased ambient temperature for both initial
 531 droplet diameters. Figure 14 shows the comparison of the predicted results between the



(a) History of liquid mass fraction



(b) History of droplet temperature

Fig.15 Comparison of the predicted results between the present model and the zero-dimensional model for (a) mass fraction and (b) temperature inside droplet at $T_{amb} = 1600$ K in $D_0 = 60$ μm .

532

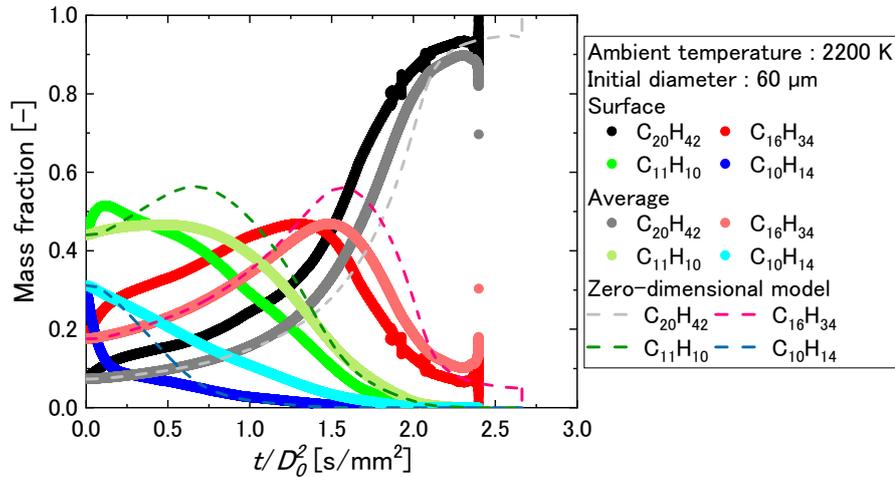
533 present model and the zero-dimensional model about the history of mass fraction (Fig.

534 14(a)) and temperature (Fig. 14(b)) inside the droplet at $T_{amb} = 600$ K in $D_0 = 60$ μm .

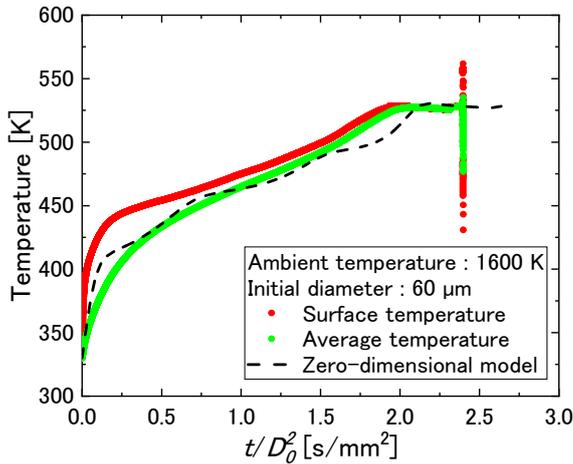
535 According to Fig. 14(a), little differences occur between the history of the mass fraction

536 at the droplet surface and the history of the average mass fraction in all fuel species.

537 Furthermore, minor differences can be seen for the time histories of mass fraction
538 obtained using the present model and the zero-dimensional model. Figure 14(b) shows
539 little difference between the surface temperature and the average temperature.
540 Additionally, the difference between the history of the droplet temperature between the
541 present model and the zero-dimensional model is insignificant, indicating that the effect
542 of considering internal distribution on the droplet lifetime diminishes at low ambient
543 temperature. On the other hand, Fig. 15 shows the comparison of the predicted results
544 between the present model and the zero-dimensional model regarding the history of mass
545 fraction (Fig. 15(a)) and temperature (Fig. 15(b)) inside the droplet at $T_{amb} = 1600$ K in
546 $D_0 = 60$ μm . Fig. 15(a) shows that the differences in the time history between the mass
547 fraction at the droplet surface and the average mass fraction at $T_{amb} = 1600$ K are larger
548 than those at $T_{amb} = 600$ K shown in Fig. 14-(a). Furthermore, the differences in the
549 history of mass fraction between the present model and the zero-dimensional model at
550 $T_{amb} = 1600$ K are also larger than those at $T_{amb}=600$ K. Fig. 15-(b) shows a large
551 difference between the surface temperature and the average temperature, especially from
552 the early evaporation stage to the middle evaporation stage. Furthermore, the difference
553 between the average droplet temperature given by the present model and the droplet
554 temperature given by the zero-dimensional model is large. This explains why the
555 differences in the droplet lifetime become larger as the ambient temperature increases.
556 Note that the average mass fraction of $\text{C}_{20}\text{H}_{42}$ suddenly decrease or that of $\text{C}_{16}\text{H}_{34}$
557 suddenly increase at the end of the evaporation process, as shown in Fig. 14(a) and Fig.
558 15(a). This is because the reduction in the effective mass diffusion coefficient ($D_{eff,i}$)
559 given by Eq. (19) due to the reduction in Re_l at the end of the evaporation process leads
560 to a steeper gradient inside the droplet. However, the effect of the increase or decrease in



(a) History of liquid mass fraction



(b) History of droplet temperature

Fig.16 Comparison of the predicted results between the present model and the zero-dimensional model regarding (a) mass fraction and (b) temperature inside droplet at $T_{amb} = 2200$ K in $D_0 = 60$ μm .

561

562 the average mass fractions at the end of the evaporation process is insignificant.

563 According to Fig. 13, the difference in the droplet lifetime between the present model

564 and the zero-dimensional model starts to decrease at higher ambient temperatures. In

565 $D_0 = 60$ μm , the difference in the droplet lifetime between the present model and the

566 zero-dimensional model decreases from $T_{amb} = 1600$ K to $T_{amb} = 2200$ K. Fig. 16 shows

567 the comparison of the predicted results between the present model and the zero-

568 dimensional model regarding mass fraction and temperature inside the droplet at $T_{amb} =$
 569 2200 K for $D_0 = 60 \mu\text{m}$. According to Fig. 16(a), the differences in the droplet surface
 570 mass fraction between the present model and the zero-dimensional model become small,
 571 especially for $\text{C}_{20}\text{H}_{42}$ and $\text{C}_{16}\text{H}_{34}$ at the late stage of the evaporation process. Figure
 572 16(b) also shows the small difference between the average droplet temperature given by
 573 the present model and the droplet temperature given by the zero-dimensional model.

574 To explain that the difference in the droplet lifetime between the present model and the
 575 zero-dimensional model decreases from $T_{amb} = 1600 \text{ K}$ to $T_{amb} = 2200 \text{ K}$ shown in Fig.
 576 13, Figure 17(a) shows the history of the difference in surface mass fraction for $\text{C}_{20}\text{H}_{42}$
 577 and $\text{C}_{16}\text{H}_{34}$ between the present model and the zero-dimensional model. Note that the
 578 vertical axis shows the absolute value of the differences between the surface mass fraction
 579 shown in Fig. 15(a) and that shown in Fig. 16(a). The horizontal axis shows the time
 580 normalized by the end time of droplet evaporation term given by the present study
 581 ($\tau_{end,present model}$). According to Fig. 17(a), the differences between the absolute values
 582 at $T_{amb} = 1600 \text{ K}$ and that at $T_{amb} = 2200 \text{ K}$ are small from $t/\tau_{end,present model} = 0-0.7$
 583 for both $\text{C}_{20}\text{H}_{42}$ and $\text{C}_{16}\text{H}_{34}$. However, the differences at $T_{amb} = 2200 \text{ K}$ become smaller

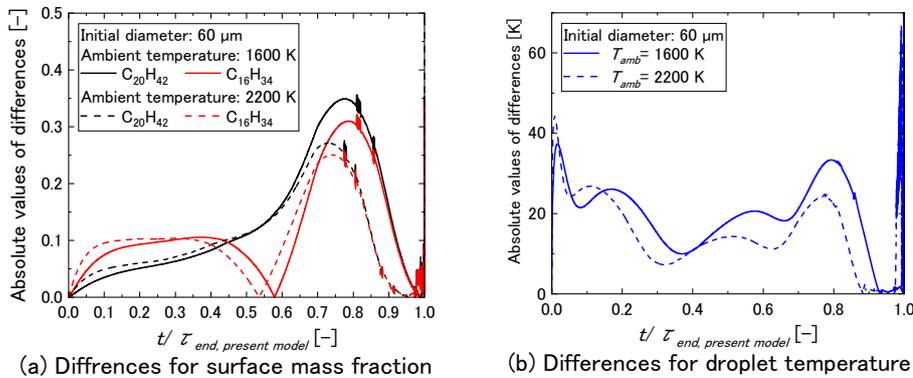


Fig. 17 Comparison of the predicted results between the present model and the zero-dimensional model regarding (a) mass fraction and (b) temperature at the droplet surface

584

585 than the differences at $T_{amb} = 1600$ K from $t/\tau_{end,present\ model} = 0.7-1.0$. Furthermore,
 586 the difference in the surface temperature between the present model and the zero-
 587 dimensional model at $T_{amb} = 1600$ K becomes larger than that at $T_{amb} = 2200$ K from
 588 $t/\tau_{end,present\ model} = 0.15-1.0$. Consequently, the differences in the droplet lifetime
 589 between the present model and the zero-dimensional model decrease from $T_{amb} = 1600$
 590 -2200 K as shown in Fig.13.

591 Figure 18 shows the history of the
 592 boundary x as a function of
 593 dimensionless time normalized by
 594 the end of the droplet evaporation
 595 term (τ_{end}). The boundary x
 596 between the uniform and gradient
 597 distributions is defined by the
 598 mass diffusion distance from the
 599 droplet surface. The mass

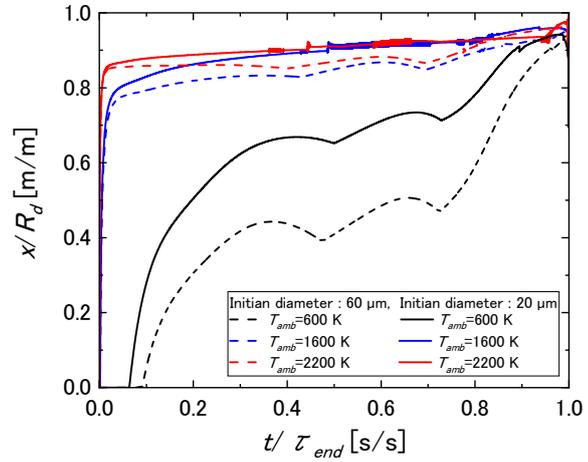


Fig.18 Behavior of the boundary between uniform and gradient distributions under various conditions

600 diffusion distance is determined by the ratio of the effective mass diffusion coefficient
 601 $D_{eff,i}$ and the radius regression rate \dot{R}_d . Therefore, the boundary is given by $x = R_d -$
 602 $max\{D_{eff,i}|i \in N_l\}/\dot{R}_d$. According to Fig. 18, the dimensionless boundary x/R_d
 603 approaches to unity over time in all ambient temperatures. This means that the boundary
 604 x moves to the droplet surface with time. Furthermore, the boundary x/R_d quickly rises
 605 to be close to unity as the ambient temperature increases. According discussed in the
 606 previous paragraph, it is expected that the behavior of the boundary x approaching to the
 607 droplet surface has two different effects on the evaporation characteristics. First, the

608 gradient distributions inside the droplet become steep because the area forming the
609 gradient distributions becomes narrow. This is why the difference in the droplet lifetime
610 between the present model and the zero-dimensional model increases from $T_{amb} = 600$
611 K to $T_{amb} = 1600$ K. Second, the overall distributions inside the droplet become closer
612 to being uniform because the area of forming the gradient distributions becomes narrow.
613 Thus, the difference in the droplet lifetime between the present model and the zero-
614 dimensional model decreases from $T_{amb} = 1600$ – 2200 K.

615 Additionally, Fig. 13 shows that the difference in the droplet lifetime between the present
616 model and the zero-dimensional model decreases for $D_0 = 20$ μm compared with that for
617 $D_0 = 60$ μm as the ambient temperature increases. According to Fig. 18, the history of
618 the boundary x/R_d for $D_0 = 20$ μm becomes close to the uniform distribution faster than
619 that for $D_0 = 60$ μm in all ambient temperatures. Hence, the differences in the droplet
620 lifetimes between the present model and the zero-dimensional model start to decrease
621 faster than those for $D_0 = 60$ μm . This is why the maximum difference in the droplet
622 lifetime between the present model and the zero-dimensional model for $D_0 = 20$ μm
623 appears at $T_{amb} = 1400$ K, which is smaller than that for $D_0 = 60$ μm , as shown in
624 Fig. 13.

625

626 4. Conclusions

627 In this study, a droplet evaporation model was developed for multicomponent fuels by
628 considering internal mass fraction and temperature distributions. Our model considers the
629 volume-average mass, $y_{i,l}^a \int_0^{R_d} 4\pi R^2 dR = \int_0^{R_d} y_{i,l}(t, R) 4\pi R^2 dR$, and enthalpy,
630 $T^a \int_0^{R_d} 4\pi C_{p,l} R^2 dR = \int_0^{R_d} T(R, t) 4\pi C_{p,l} R^2 dR$, to simulate the mass and enthalpy

631 conservation inside the droplet during droplet evaporation process. Additionally, the
632 simulated results were compared with the experimental results at various ambient
633 temperatures to verify the accuracy of the developed model. The main findings are
634 summarized as follows:

635 1. The internal gradients of both the mass concentration of fuel species and
636 temperature distributions become steeper at higher ambient temperatures. Mass
637 distributions inside the droplet play an important role in droplet evaporation
638 modeling for a multi-component fuel at high ambient temperatures.

639 2. The droplet lifetimes predicted by the developed model were compared with the
640 experimental results. The droplet lifetimes predicted by the model without the pre-
641 evaporation consideration differed from those measured by the experiment at
642 various ambient temperatures because of the influence of pre-evaporation in the
643 experiments. The droplet lifetimes predicted by the model with the pre-evaporation
644 consideration were in good agreement with the measured droplet lifetimes at
645 various ambient temperatures.

646 3. The difference in the droplet lifetime between the present model and the zero-
647 dimensional model, which assumes uniform temperature and mass fraction
648 distributions inside the droplet, is more than 10% at various practical spray
649 combustion conditions.

650

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 656 Center, faculty of Engineering, Hokkaido University.

657

658

659 **Appendix A. Physical properties of the liquid phase**

660 The liquid thermal conductivity of hydrocarbons is approximated as

$$661 \quad k_{i,l} = 10^{(A_i + B_i \left(1.0 - \frac{T^a}{T_{i,c}}\right)^{\frac{2}{7}})}$$

662 where, $\begin{cases} A_i = 0.002911 \times n_i^2 - 0.07139 \times n_i - 1.319595 \\ B_i = -0.002498 \times n_i^2 + 0.05872 \times n_i + 0.710698 \end{cases}$, and $T_{i,c}$ and n_i are the

663 critical temperature [K] and the carbon number of species i , respectively. This

664 approximation is reasonable for the hydrocarbons with $5 \leq n_i \leq 25$. The mixed liquid

665 thermal conductivity k_l is given by Pauer Law method [26]:

$$666 \quad k_l = \left(\sum_{i=1}^{N_l} \frac{y_{i,l}^a}{k_{i,l}^2} \right)^{-0.5}$$

667 The diffusion coefficient $D_{i,l}(= D_{i,m})$ [m²/s] can be given by the expansion of the

668 binary diffusion coefficient to the multi-component system by using the methods

669 developed by Perkins and Geankoplis *et.al.* [26]:

$$670 \quad D_{i,m} \eta_m^{0.8} = \sum_{\substack{j=1 \\ j \neq i}}^{N_l} x_{j,l}^a D_{i,j} \eta_j^{0.8}$$

671 where the binary diffusion coefficient $D_{i,j}$ [m²/s] is given by Hanyduk and Minhas *et.al.*

672 [26]:

673
$$D_{ij,b} = 8.93 \times 10^{-8} \frac{V_j^{0.267}}{V_i^{0.435}} \left(\frac{T^a}{\eta_{j,l}} \right)$$

674 The viscosity of the liquid mixture η_m [kg/m/s] can be given by the expansion of the
 675 viscosity of species i $\eta_{i,l}$ [kg/m/s] to the multi-component system using the Grunberg and
 676 Nissan method.

677
$$\eta_m = \sum x_{i,l}^a \ln(\eta_{i,l})$$

678 where the viscosity of species i $\eta_{i,l}$ [kg/m/s] can be estimated by the method developed
 679 by Orrick and Erbar *et.al.* [26] method as

680
$$\ln \left(\frac{\eta_{i,l}}{\rho_{i,l} MW_i} \right) = A_i + \frac{B_i}{T^a}$$

681 where A_i and B_i are the molecular structure-dependent coefficient, $\rho_{i,l}$ is the liquid
 682 density of species i [kg/m³], MW_i is the molecular weight [g/mol], T^a is the average
 683 temperature inside the droplet [K].

684 The liquid density of species i can be given by

685
$$\rho_{i,l} = a_i b_i \left(-\left(1 - \frac{T^a}{T_{i,c}}\right) \right)^{n_i}$$

686 The liquid heat capacity of species i $C_{i,pl}$ [J/kg/K] can be given using the Ruzika and
 687 Domalski method [26].

688
$$C_{i,pl} = R \left[\sum_{i=1}^k n_i a_i + \sum_{i=1}^k n_i b_i \frac{T^a}{100} + \sum_{i=1}^k n_i d_i \left(\frac{T^a}{100} \right)^2 \right]$$

689 where $n_i a_i$, $n_i b_i$, and $n_i d_i$ are the coefficients calculated from molecular structures. The
 690 average heat capacity of droplet $C_{p,l}$ can be calculated by $C_{p,l} = \sum y_{i,l}^a C_{i,pl}$. The values

691 used in this study are shown in Table A.1.

692

693 **Table A.1 List of coefficients for physical property estimation in the liquid phase**

Component		n- eicosane	n- hexadecane	1- methylnaphthalene	tert- butylbenzene
thermal conductivity	n_i	20.000	16.000	11.000	10.000
liquid viscosity	A_i	-11.150	-10.310	-7.1600	-8.7800
	B_i	2255.0	1859.0	414.00	992.00
liquid density	a_i	0.23759	0.24348	0.27189	0.27832
	b_i	0.24934	0.25442	0.22408	0.26103
	n_i	0.30880	0.32380	0.25709	0.28570
liquid heat capacity	$n_i a_i$	58.040	46.851	14.064	21.412
	$n_i b_i$	-1.6693	-1.4495	3.4380	-0.9781
	$n_i d_i$	2.3120	1.8848	0.3056	1.1408

694

695 **Appendix B. Thermodynamic properties of the gas phase**

696 The thermal conductivity for nitrogen gas k_g [W/m/K] can be estimated by

697
$$k_g = \frac{252 \times 10^{-5} \times T_{ref}^{1.5}}{T_{ref} + 200}$$

698 where T_{ref} is the reference temperature [K].

699 The diffusion coefficient of the gas phase $D_{i,g}$ [m²/s] can be given by the expansion of

700 the binary diffusion coefficient to the multi-component system using Blanc's law .[26].

701
$$D_{i,g} = \left(\sum_{\substack{j=1 \\ j \neq i}}^N \frac{x_{j,g}^s}{D_{ij,g}} \right)^{-1}$$

702 The binary diffusion coefficient of the gas phase $D_{ij,g}$ [m²/s] is given by the method

703 reported by Reid *et.al.* [26]:

$$704 \quad D_{ij,g} = \frac{0.0266T_{ref}^{1.5}}{P_{amb}MW_{ij}\sigma_{ij}^2\Omega_D}$$

$$705 \quad \text{where, } MW_{i,j} = 2 \left[\left(\frac{1}{MW_i} \right) + \left(\frac{1}{MW_j} \right) \right]^{-1}, \quad \sigma_{i,j} = \frac{\sigma_i + \sigma_j}{2}$$

$$706 \quad \Omega_D = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}$$

$$707 \quad \left(\begin{array}{l} T^* = \frac{k_B T_{ref}}{\sqrt{\varepsilon_A \varepsilon_B}} \\ A = 1.06036, \quad B = 0.15610 \\ C = 0.19300, \quad D = 0.48635 \\ E = 1.03587, \quad F = 1.52996 \\ G = 1.76474, \quad H = 3.89411 \end{array} \right)$$

708 The viscosity of the nitrogen gas mixture μ_g [kg/m/s] can be estimated by

$$709 \quad \mu_g = \frac{1457 \times 10^{-9} \times T_{ref}^{1.5}}{T_{ref} + 110}$$

710 where T_{ref} is the reference temperature [K].

711 The density of the gas mixture of the ambient gas (N_2) and fuel vapor ρ_g [kg/m³] can be

712 calculated using the equation of state for an ideal gas as

$$713 \quad \rho_g = \frac{\sum_{i=1}^N x_{i,ref} MW_i}{\sum_{i=1}^N x_{i,ref}} \left(\frac{P_{amb}}{RT_{ref}} \right)$$

714 The heat capacity for the nitrogen gas mixture $C_{ip,g}$ [J/mol/K] can be calculated as a

715 function of T_{ref}

$$716 \quad C_{ip,g}(T_{ref}) = R(a_{i,1} + a_{i,2}T_{ref} + a_{i,3}T_{ref}^2 + a_{i,4}T_{ref}^3 + a_{i,5}T_{ref}^4)$$

717 where R is the universal gas constant and $a_{i,1}, a_{i,2}, a_{i,3}, a_{i,4},$ and $a_{i,5}$ are the coefficients

718 of the fitting function.

719 The sensible enthalpy of the ambient gas and fuel vapor $h_{i,g}$ [J/mol] can be calculated

720 by.

$$\begin{aligned}
 721 \quad h_{i,g}(T_{ref}) &= \int_0^{T_{ref}} C_{ip,g}(T) dT \\
 722 \quad &= R(a_{i,1}T_{ref} + \frac{a_{i,2}T_{ref}^2}{2} + \frac{a_{i,3}T_{ref}^3}{3} + \frac{a_{i,4}T_{ref}^4}{4} + \frac{a_{i,5}T_{ref}^5}{5} + a_{i,6})
 \end{aligned}$$

723 The thermodynamic properties of the mixture of the ambient gas and fuel vapor around
 724 the droplet surface are a function of temperature. However, it is difficult to estimate not
 725 only the temperature but also the mass fraction of the gas mixture. For the droplet
 726 evaporation model, reference values are used on the basis of one-third law as the follows.

727

$$728 \quad \begin{cases} T_{ref} = T^s + \frac{1}{3}(T_{amb} - T^s) \\ y_{i,ref} = y_{i,g}^s + \frac{1}{3}(y_{i,g}^{amb} - y_{i,g}^s) \end{cases}$$

729 The values used in this study are shown in Table B.1.

730 **Table B.1 List of coefficients for physical property estimation in gas phase**

	n-eicosane	n-hexadecane	1-methylnaphthalene	tert-butylbenzene	nitrogen
$a_{i,1}$	-1.8392E+00	-1.4019E+00	-6.9950E+00	-7.7671E+00	3.2987E+00
$a_{i,2}$	2.2898E-01	1.8328E-01	1.0905E-01	1.2036E-01	1.4082E-03
$a_{i,3}$	-1.2799E-04	-1.0182E-04	-8.1241E-05	-8.6981E-05	-3.9632E-06
$a_{i,4}$	2.7278E-08	2.1553E-08	2.4223E-08	2.4680E-08	5.6415E-09
$a_{i,5}$	5.6826E-24	1.2795E-24	1.0332E-24	1.7691E-24	-2.4449E-12
$a_{i,6}$	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-1.0209E+03

731

732 **Appendix C. Nondimension number**

733 Liquid phase:

$$\text{Reynold's number: } Re_{i,l} = \frac{\rho_l^a u_r d_r}{\eta_{i,l}}$$

$$\text{Peclet number: } Pe_{i,l} = \frac{\rho_l^a u_r d_r C_{i,p,l}}{\lambda_{i,l}}$$

734 Gas phase:

$$\text{Reynold's number: } Re_g = \frac{\rho_g |u_r - u_d| d_r}{\mu_g}$$

$$\text{Grashof number: } Gr_g = \frac{8g_0 R_l^3 (T_{amb} - T^a)}{\left(\frac{\mu_g}{\rho_g}\right)^2 T_{amb}}$$

$$\text{Schmidt number: } Sc_{i,g} = \frac{\mu_g}{\rho_g D_{i,g}}$$

$$\text{Prandtl number: } Pr_{i,g} = \frac{\mu_g C_{i,p,g}}{\kappa_g}$$

Sherwood number [33]:

$$Sh_{i,g} = 2.0009 + 0.514 \left(\max \left(Re_g, \max(Gr_g, 0)^{\frac{1}{2}} \right) \right)^{\frac{1}{2}} Sc_{i,g}^{\frac{1}{2}}$$

Nusselt number [33]:

$$Nu_{i,g} = 2.0009 + 0.514 \left(\max \left(Re_g, \max(Gr_g, 0)^{\frac{1}{2}} \right) \right)^{\frac{1}{2}} Pr_{i,g}^{\frac{1}{2}}$$

735

736 The estimation of $\eta_{i,l}$ is described in Appendix A. The estimation of $C_{i,p,g}$, $D_{i,g}$ and μ_g is
737 described in Appendix B.

738

739 **Appendix D. Boiling model**

740 This section discusses fuel droplet evaporation model with boiling. In this model, the
741 boiling model will be applied when vapour pressure at droplet surface becomes larger
742 than ambient pressure.

743 It is very difficult to get the boiling point of multi-component fuel qualitatively. Hence,
744 the boiling model will get an approximate solution as the boiling point of multi-
745 component fuel by using Newton's method. First, when fuel droplet become boiling, the
746 vapor pressure at droplet surface become same with ambient pressure. The following
747 relationship can be given.

748

$$\sum_{i=1}^{N_l} p_{i,v} x_{i,l}^s = P_{amb} \quad (D.1)$$

749

750 Substituting Eq.(24) into Eq.(D.1), the vapour pressure can be calculated as a function of
751 boiling point.

752

$$\sum_{i=1}^{N_l} x_{i,l}^s 10^{\left(A_{i,p} - \frac{B_{i,p}}{C_{i,p} + T_b - 273.15}\right)} = P_{amb} \quad (D.2)$$

753

754 For Newton's method, the following function is defined.

755

$$g(T_b) = \sum_{i=1}^{N_l} x_{i,l}^s 10^{\left(A_{i,p} - \frac{B_{i,p}}{C_{i,p} + T_b - 273.15}\right)} - P_{amb} \quad (D.3)$$

756

757 Hence, convergence calculation for the boiling point of multi-component fuel can be
758 given by the following equation.

759

$$T_b^{n+1} = T_b^n - \frac{g(T_b)}{g'(T_b)} \quad (D.4)$$

$$\text{Convergence judgement: } \left| \frac{g(T_b)}{g'(T_b)} \right| < 10^{-3}$$

760

761 When fuel droplet become boiling, it is assumed that the droplet surface temperature (T^s)
762 is replaced as the boiling point (T_b) given by the above calculations, and droplet surface
763 is occupied by fuel vapour ($\sum_{i=1}^{N_l} y_{i,g}^s = 1$). According to algorithm of the boiling model,

764 the procedure 4. ~ 8. described in Section 2.6 will be conducted after the droplet surface
 765 temperature is replaced as the boiling point.

766

767 **Appendix E. Overheating model**

768 When the droplet average temperature becomes larger than the droplet surface
 769 temperature (overheating), the present model consider the heat up from inside droplet by
 770 using correction factor suggested by Adachi *et.al.* [34]. The following is the calculation
 771 procedure.

772 1. Calculate the difference between the droplet surface temperature and average
 773 temperature ($\Delta T = T^a - T^s$).

774 2. If overheat ($\Delta T \geq 0$) occurs, the enthalpy (\dot{q}_{liquid}) heat the droplet from inside
 775 droplet as the following.

$$776 \quad \dot{q}_{liquid} = 4\pi R_l^2 (h_{liquid} + \alpha_{sh}) \Delta T = 4\pi R_d^2 \left(-\frac{k_{eff} \frac{\partial T_l(r)}{R_l \partial r} \Big|_{r=1}}{T^s - T_{amb}} + \alpha_{sh} \right) \Delta T$$

777 Where the correction factor α_{sh} suggested by Adachi *et.al.* can be given by the
 778 followings.

$$779 \quad \alpha_{sh} = 0.76 \Delta T^{0.26} \quad (0 \leq \Delta T < 5)$$

$$780 \quad = 0.027 \Delta T^{2.33} \quad (5 \leq \Delta T < 25)$$

$$781 \quad = 13.8 \Delta T^{0.39} \quad (25 < \Delta T)$$

782 3. The mass evaporation rate of species i is decided by proportional distribution in
 783 response to a mass fraction.

$$784 \quad \dot{m}_l = \frac{\dot{q}_{gas} - \dot{q}_{liquid}}{H_{latent}}$$

785 $\dot{m}_{i,l} = y_{i,g}^s \dot{m}_l$

786

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