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雰囲気温度と初期液滴直径が正デカン単一液滴の冷炎直径及び中間生成物の濃度境界層に与える影響

Influence of Ambient Temperature and Initial Droplet Diameter on Cool Flame Diameter and Concentration Boundary Layer of Intermediate Species for Isolated *n*-Decane Droplet

鈴木太成 [1]，菅沼祐介 [2]，野村浩司 [2]，田辺光昭 [3]，齊藤允教 [3]

Taisei SUZUKI[1], Yusuke SUGANUMA[2], Hiroshi NOMURA[2], Mitsuaki TANABE[3], Masanori SAITO[3]

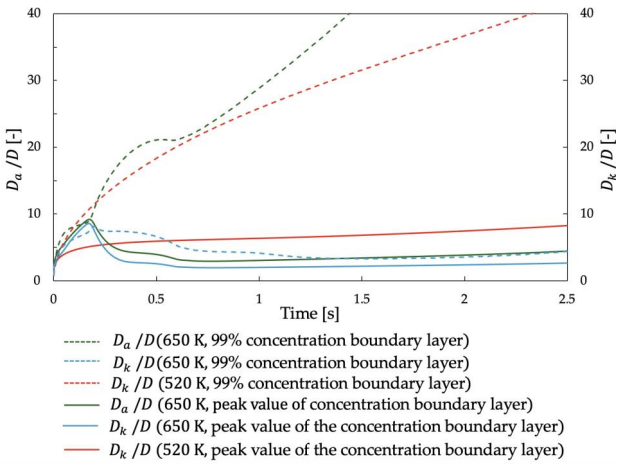
1 日本大学大学院理工学研究科航空宇宙工学専攻，Graduate School of Science and Technology, Nihon University

2 日本大学生産工学部，College of Industrial Technology, Nihon University

3 日本大学理工学部，College of Science and Technology, Nihon University

* Correspondence: csti25018@g.nihon-u.ac.jp

Abstract: The relationship between the concentration boundary layer of intermediate species and the cool flame diameter were investigated by numerical simulations for single *n*-decane droplet. This study's conditions, it was shown that the concentration boundary layer of intermediate speciesbecomes relatively larger with respect to the droplet diameter as the initial droplet size decreases. Therefore, the cool flame diameter is also considered to become relatively larger with respect to the droplet diameter. These results suggest that ambient temperature and initial droplet size may affect the extent and relative positioning of the cool flame diameter and the concentration boundary layer of intermediate species, with smaller droplets potentially increasing their relative spread.



Keywords: Cool flame, Droplet combustion, Spontaneous ignition

1. Introduction

Spray combustion is a combustion method that is widely adopted in internal combustion engines such as diesel engines and jet engines. In this method, the fuel is injected in a fine droplet, which subsequently atomises into a finer droplet. Which then go through evaporation, spontaneous ignition, and flame spread through various physical and chemical processes. Particularly in the case of higher hydrocarbon fuels, where low-temperature oxidation reactions generate excited formaldehyde (CH_2O) prior to the occurrence of high-heat release hot flame. This result in a relatively low-heat-release cool flame accompanied by weak chemiluminescence. Tanabe et al., experimentally demonstrated that cool flames occur during the spontaneous ignition process of a single droplet under high-temperature and high-

pressure conditions and reported that the timing of spontaneous ignition is governed by the cool flame[12]. Umemura et al., theoretically predicted hot flame spread modes and clarified through numerical simulations and experiments that multiple flame spread modes exist[3-5]. Mikami et al., using microgravity experiments, investigated the flame spread modes of *n*-decane droplet arrays under high-temperature conditions for various droplet spacings and initial ambient temperatures, and revealed that the flame spread mode of fuel droplet arrays changes depending on the nondimensional droplet spacing and ambient temperature[6]. Ikezawa et al., reported based on numerical simulations, that variations in ambient temperature and droplet spacing in *n*-decane droplet arrays affect the transition of cool flame spread modes[7]. Fujieda et al., using a forced ignition device, observed cool flame spread in *n*-decane droplet arrays under microgravity, reporting that the cool flame spread speed increases as droplet spacing increases[8]. Mikami et al., demonstrated that cool flame propagation can occur in multi-droplet systems, even when the droplet spacing is greater than the hot flame spread limit[9]. Saito et al., a microgravity experiment to elucidate the cool flame dynamics in a multi-droplet system was conducted using the TEXUS-60 sounding rocket. The cool flame position was successfully observed through formaldehyde chemiluminescence. Based on the experimental results, the cool flame propagation speed along *n*-decane droplet arrays was measured[10]. Dietrich et al., conducted microgravity experiments on the International Space Station and numerical simulations and measured the cool flame diameter after extinction based on CH_2O luminescence[11]. Takahata et al. clarified, using numerical simulations, the influence of ambient temperature and fuel droplet diameter on the cool flame diameter[12]. To classify the flame spread modes in cool flames, it is necessary to clarify the relationship between the intermediate species concentration boundary layer and the cool flame diameter in fuel droplets. In this study, the relationship between the concentration boundary layer of intermediate species and the cool flame diameter is evaluated using numerical simulations.

2. Calculation Conditions

Table 1 lists the calculation conditions. Numerical analysis was conducted using the software ANSYS Fluent 2023 R2. **Fig. 1** shows a schematic of the simulation domain and the boundary conditions for each boundary in the case of a single droplet. The calculation was performed in two-dimensional axisymmetric coordinates under steady-state conditions.

Table 1 Simulation conditions.

Fuel	*n*-decane
Initial droplet diameter [mm]	0.5, 1.0
Ambient pressure P_0 [MPa]	0.1
Initial droplet temperature [K]	300
Ambient temperature T_0 [K]	520, 650
Chemical reaction model[13]	77 species, 287 reactions
Ambient gas composition [mol%]	O_2:21, N_2:79

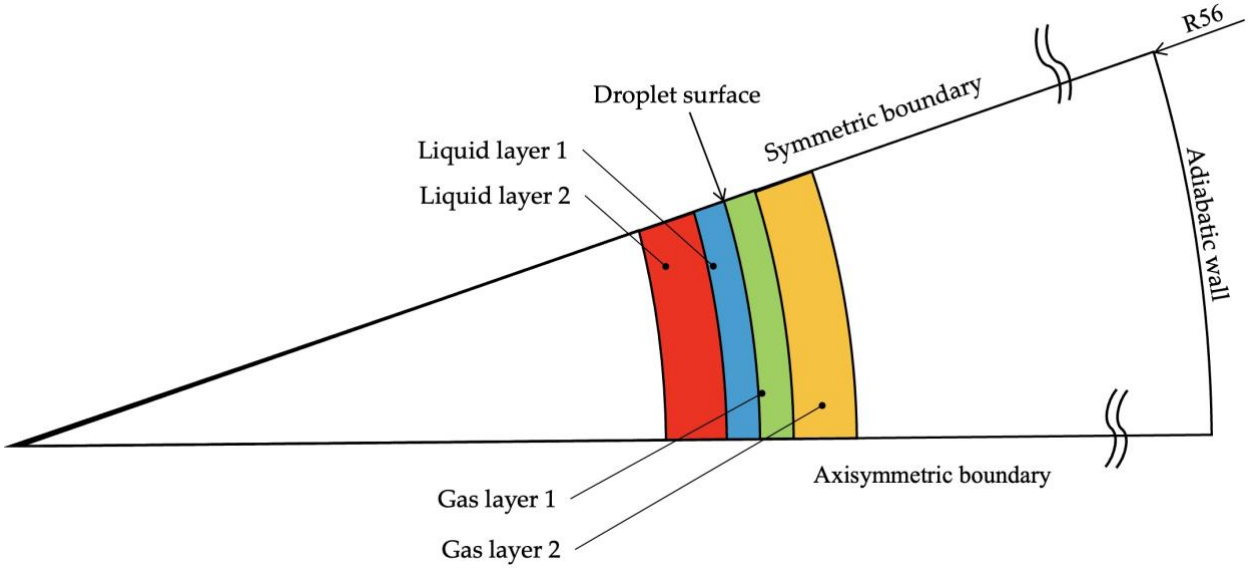


Figure 1. Numerical simulation domain for an isolated droplet.

3. Evaluation Method

Fig. 2 shows a schematic diagram of cool flame propagation. Droplets formed by spray combustion evaporate and spontaneously ignite, but they pre-vaporize depending on the ambient temperature. At this time, some of the fuel droplets exposed to high-temperature air vaporize, and a layer of fuel vapor surrounds the fuel droplets. When considering actual spray combustion, it is necessary to consider the effect of the fuel vapor layer formed by pre-vaporization on flame propagation between droplets. In the case of cold flames, it is expected that a layer of intermediate species will form around the droplets due to pre-vaporization in the temperature range where intermediate species are activated in low-temperature oxidation reactions, and that cool flames will propagate. Therefore, the relationship between cool flame diameter and concentration boundary layer of intermediate species is evaluated for isolated droplet.

Fig. 3 shows a schematic diagram of the chemical boundary layer. In regions where the cool flame reaction is active, the concentrations of the intermediate species C_{10}ket and the final product CH_2O are expected to be high. Dietrich et al., measured the distance between the maxima of CH_2O luminescence to determine the cool flame diameter[11]. Similarly, Takahata et al., assumed the distance between the maxima of CH_2O concentration after cool flame spontaneous ignition to be the cool flame diameter and calculated it[12]. In this study, the distance from the droplet center to the position of maximum CH_2O concentration is defined as $\boldsymbol{R_c}$, and twice this distance is defined as the cool flame diameter $\boldsymbol{D_a}$. Likewise, the distance from the droplet center to the position of maximum C_{10}ket concentration is defined as $\boldsymbol{R_k}$, and twice this distance is defined as the concentration boundary layer diameter $\boldsymbol{D_k}$. In addition, considering the possibility of cold flames propagating even in areas with low fuel concentrations. The cool flame diameter and the concentration boundary layer of intermediate species diameter based on the 99% concentration boundary layer are also calculated.

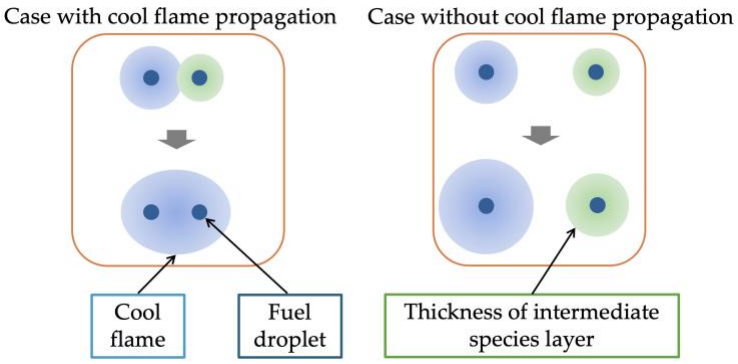


Figure. 2 Schematic diagram of cool flame propagation

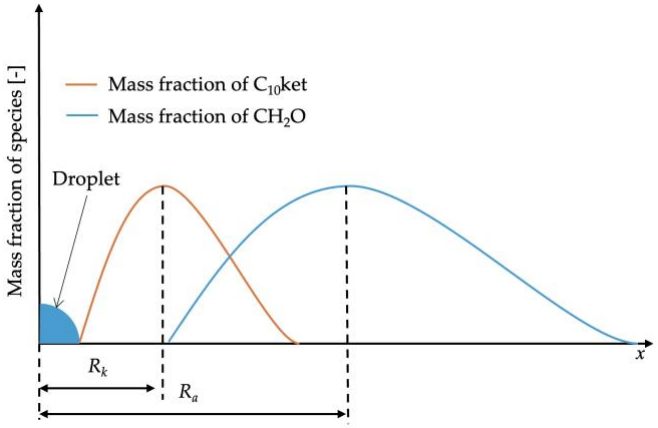


Figure 3. Schematic diagram of chemical boundary layer.

4. Results and Discussion

4.1 Influence of Ambient Temperature on Cool Flame Diameter and Intermediate Species Concentration. Boundary Layer.

Fig. 4 shows the time histories of the ratios $\boldsymbol{D_a/D}$ and $\boldsymbol{D_k/D}$ for different ambient temperatures and concentration boundary layer definitions. First, the peak values of the concentration boundary layer of intermediate species are compared. As a result, it was confirmed that the intermediate species layer expands more rapidly and over a wider region under higher ambient temperature conditions. In addition, the cool flame diameter under the condition with spontaneous ignition (650 K) is found to be larger than the intermediate species layer under the condition without spontaneous ignition (520 K). Next, when comparing based on the 99% concentration boundary layer, it is shown that the intermediate species layer becomes larger at lower ambient temperatures. This can be attributed to the fact that, under higher temperature conditions, early spontaneous ignition suppresses the formation of intermediate species. Regarding the cool flame diameter, it is found to be larger than the intermediate species layer at 520 K, except in the time of 0.1~0.2 s. From these results, it is suggested that, in considering flame propagation in droplet arrays, cool flame propagation speed may increase toward the rear part of the array, since the intermediate species layer is more widely formed around downstream droplets due to pre-vaporization. Furthermore, when discussing the flame spread limit, it is also suggested that the cool flame may propagate even in lower concentration regions outside the point where the CH_2O concentration peak reaches the intermediate species layer.

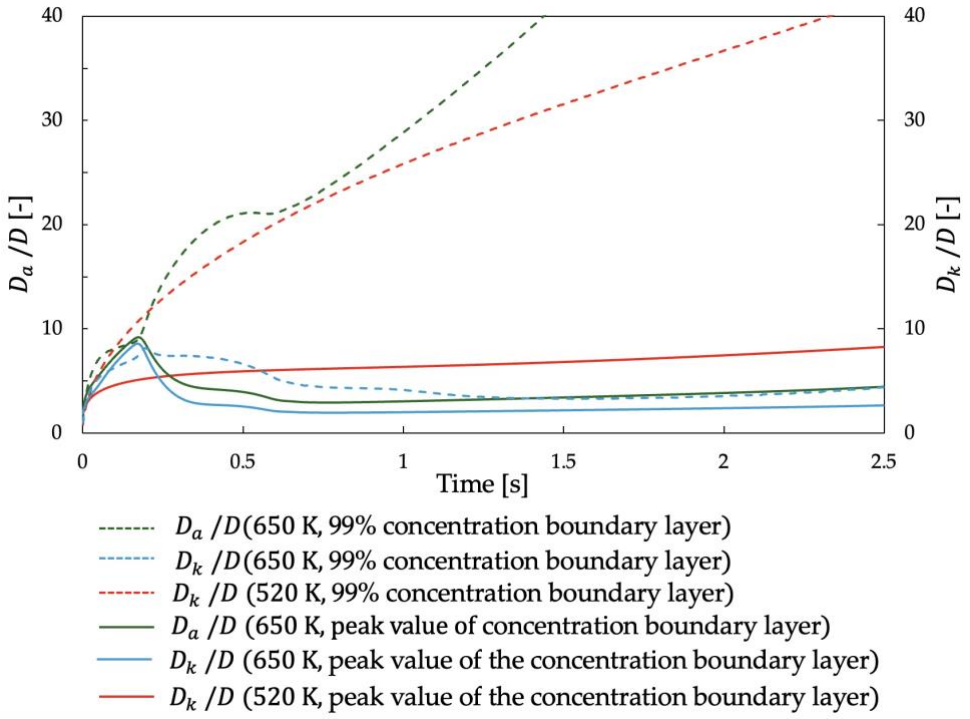


Figure 4. Time histories of the ratios $\boldsymbol{D_a/D}$ and $\boldsymbol{D_k/D}$ for different ambient temperatures and concentration boundary layer definitions（Initial droplet diameter = 1.0 mm）.

4.2 Influence of Initial Droplet Diameter on concentration boundary layer of intermediate species.

Fig. 5 shows the time history of the ratios $\boldsymbol{D_k/D}$ for two different initial droplet diameters at an initial ambient temperature of 520 K. $\boldsymbol{D_k/D}$ is larger for the initial droplet diameter of 0.5 mm compared to 1.0 mm. Indicating that a smaller initial droplet diameter results in a larger ratio of the C_{10}ket concentration boundary layer diameter to the droplet diameter.

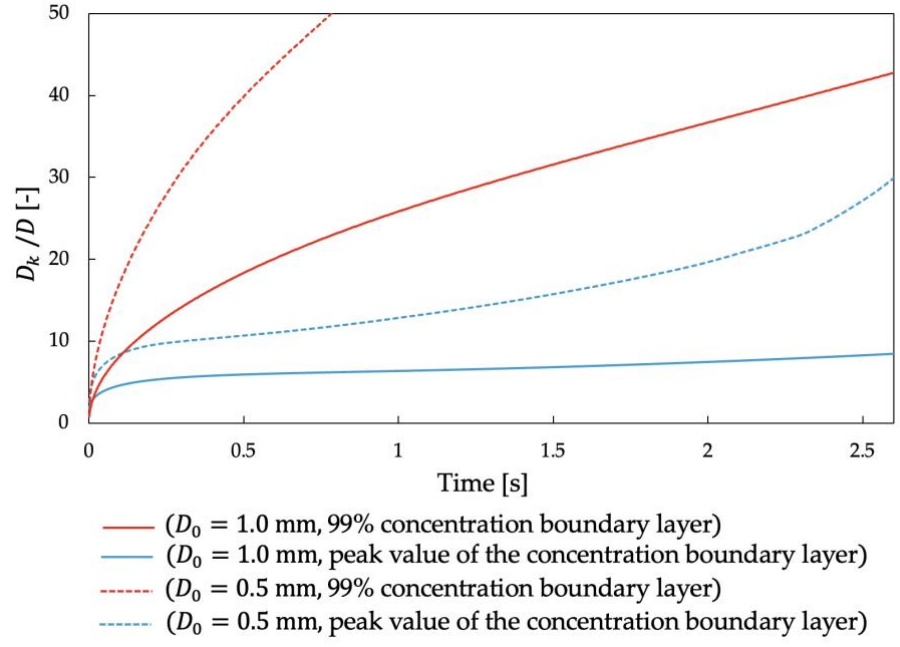


Figure 5. Time histories of the ratios $\boldsymbol{D_k/D}$ for different initial droplet diameters (T_0 = 520 K).

5. Conclusions

The relationship between the concentration boundary layer of intermediate species and the cool flame diameter was evaluated using numerical simulations by varying the ambient temperature and the initial droplet diameter, and the following findings were obtained.

1. The concentration boundary layer of intermediate species was observed to expand more rapidly and over a wider region at higher ambient temperatures.

2. It was confirmed that a smaller initial droplet diameter results in a larger ratio of the concentration boundary layer of intermediate species diameter to the droplet diameter.

Acknowledgements

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