## JASMAC



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燃料二液滴で生じる冷炎振動に関する 位相空間を用いた研究

# Study on cool flame oscillation occurred around a fuel droplet pair using phase space

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#### 1. Introduction

Spray combustion is used as one of the combustion methods in practical engines. The combustion involves the complex phenomena of droplet vaporization, spontaneous ignition, and flame spread. Tanabe et al. <sup>1),2)</sup> discovered the existence of cool flame in the spontaneous ignition of a single droplet. Cool flame is known to have oscillatory behavior. <sup>3),4)</sup> Cuoci et al.<sup>5)</sup> conducted a detailed simulation of a single fuel droplet of *n*-decane and reported cool flame oscillation of the droplet. Actual spray combustion involves interaction among droplets. Ohno et al.<sup>6)</sup> simulated a fuel droplet pair of *n*-decane and reported cool flame oscillation. Moriue et al.<sup>7)</sup> conducted an experiment of droplet interaction effects using the fuel droplet pair. They reported that the mutual cooling effect was affected to cool flame ignition delay increase, while the effect of duplicated fuel sources was affected to cool flame temperature increase. In this study, we used a Variational Auto-Encoder (VAE) to simultaneously train the physical quantities of a single fuel droplet and fuel droplet pair output from the numerical simulation that takes the spatial distribution into account. We will discuss the cool flame oscillation of single droplet and that of droplet pair, respectively, using a phase space output from the VAE.

#### 2. Method

#### 2.1. Numerical simulation model and data sampling area

The simulation was carried out by using Ansys Fluent 19.1 with a two-dimensional (2D) axisymmetric numerical domain. In this study, the single fuel droplet and the fuel droplet pair were simulated. **Figure 1** shows the schematic of the simulation domain. **Figure 1** also shows the zone (in red and blue dotted lines) at

which physical quantities (i.e., temperature and species fractions) are sampled to train the VAE. Considering the fields of temperature and species, we decided the zone. In the droplet pair case, the droplet was divided into the right and left sides at x = 4 mm. Please note that x > = 4 mm is defined as the right side of the droplet pair and that x < = 4 mm is defined as the left side of the droplet pair. These definitions enable simultaneously training by the VAE to distinguish between inter-droplet and non-inter-droplet. **Table 1** shows the model parameters. For the details of the model, refer to the previous study.<sup>8</sup>)



**Figure 1**. Simulation zone in black (The right figure is the single droplet and the left figure is the droplet pair) and VAE analysis domain (in red and blue dotted lines).

Chemical reaction model <sup>99</sup>	77 species
	287 reactions
Fuel	<i>n</i> -Decane
Time step size (s)	10-4
Inter droplet distance (mm)	∞(single), 8
Initial droplet diameter (mm)	1.0
Initial gas phase temperature (K)	600
Initial droplet temperature (K)	300
Initial gas phase pressure (MPa)	0.1
Initial gas composition (mol%)	O2 : 21
	N2:79

#### 2.2. Variational Auto-Encoder (VAE) design

The VAE is used as an analytical method. **Figure 2** shows the data flow through the VAE. The input data consists of three-time series data of physical phenomena (the single droplet, the right side of the droplet pair, and the left side of the droplet pair) combined into one data set. This data enables physical phenomena on the single droplet, on the right side of the droplet pair, and on the left side of the droplet pair to be trained simultaneously in the VAE. In the encoder part of the VAE, the dimension of the vectorized physical quantities is reduced to the lower order vector of latent variables. Layer 4 of the encoder is three dimensions for us to obtain a phase space. The layer enables mapping the trajectories of the single droplet, the right side of the droplet pair on the same space by condensing each physical phenomenon. An area around a point on the space output from Layer 4, the final layer, of the VAE has a similar distribution.

The decoder part of the VAE reconstructs physical phenomena reduced to three dimensions. For the details of the VAE, refer to the previous study.<sup>10</sup>



Figure 2. Data flow through the VAE.

#### 3. Making up input data to VAE

The input data used for training the VAE are a time series of the spatial distribution of physical quantities. **Figure 3** shows the time history of the maximum temperature in **Figure 1**. A VAE analysis intervals were from 1.172 s to 1.379 s (single droplet) and from 1.211 s to 1.418 s (droplet pair). During the VAE analysis interval, the cool flame is considered to be oscillatory, for the maximum temperature is oscillatory. The physical quantities that make up the data were selected from a large number of physical quantities: temperature and the mass fraction of the species, H, OH, HO<sub>2</sub>, HCHO, R, RO<sub>2</sub>, QOOH, O<sub>2</sub>QOOH, and OQ'OOH.



Figure 3. The time history of maximum temperature. (a) Single droplet, (b) Droplet pair

#### 4. Result

**Figure 4(a)** shows the trajectories on the phase space of the single droplet, the right side of the droplet pair, and the left side of the droplet pair, respectively. **Figure 4(b)** shows the phase plane spanned by the two latent variables  $\mu_0$  and  $\mu_1$ . **Figure 4(a)** shows that each trajectory does not intersect with their own trajectory. At the point that they intersect on their own trajectory, the state is not identified because of the multiple directions.<sup>10</sup>

Hence, Figure 4(a) suggests that each state is distinguished from each other. Figure 4(b) shows that the endpoints of the single droplet and of the right side of the droplet pair are almost at the same position. According to the characteristics of the VAE, the state at the endpoint of the single droplet and that of the right side of the droplet pair are considered to be similar. On the other hand, the state of the endpoint of the left side of the droplet pair is considered to be different from that of the single droplet and the right side of the droplet pair. Figure 5(a) shows the output points of the temperature and species distribution maps at each point on the space. Please note that each of the distribution planes was designed to be parallel to each other. Figure 5(b) shows the distribution maps of temperature and species at each output point. On the one hand, the figure shows that there is a difference in distribution between the upper left and lower right of the figure. The temperature and mass fraction are lower in the upper left than in the lower right. On the other hand, the temperature and mass fraction are higher on the lower right than on the upper left. The same thing can be said for the upper right and lower left. According to each distribution map, the temperature and mass fraction of HCHO are higher at the similar point, but OQ'OOH and OH show higher temperature and mass fractions at different points. Therefore, it is considered that the phase of each physical quantity is obtained by using a distribution map. Figure 4(a) shows that the trajectories on the space are from bottom to top, the left side of the droplet pair (in the blue), the single droplet (in the red), and the right side of the droplet pair (in the green). Here, considering that each distribution plane is parallel to each other, the vertical axis to that plane is defined as  $\mu_2$ '. Figure 5(b) shows that the temperature and mass fraction were lower as the order of the distribution progressed (from the left side to the right side in **Figure 5(b)**). It can be said that a positive direction of the  $\mu_2$ ' axis represents lower temperatures and mass fractions.



**Figure 4**. (a) Phase space and (b) Phase plane (The red indicates the single droplet, the green indicates the right side of the droplet pair and the blue indicates the left side of the droplet pair).

#### 5. Summary

①The physical quantities considering the spatial distribution of the single fuel droplet and the fuel droplet pair were simultaneously trained by the VAE. Each physical phenomenon could be mapped with its own trajectory on the same phase space. Each trajectory did not intersect with its own trajectory, and the states could be distinguished.

②Each distribution plane was designed to be parallel to each other. The axis vertical to the distribution plane is defined as  $\mu_2$ '. The positive direction of the  $\mu_2$ ' axis indicates the lower temperature and mass fraction.



(a) The output points of distribution maps on the phase space. The blue indicates the left side of droplet pair, the red indicates the single droplet and the green indicates the right side of droplet pair.



(b) The distribution maps of temperature and species at each output point on the phase space.

**Figure 5**. (a) The output points of the distribution map on the phase space. (b) The distribution maps of temperature and species at each output point on the phase space.

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