Three-dimensional Numerical Simulation of Spray Flame in Laminar Counterflow

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1 Introduction

The improvement of combustion efficiency and exhaust emission is the most important issue in the combustion engineering field in the last decade. Spray combustion is utilized in a number of combustion systems, such as gas turbine, diesel engine, and other energy converting machines. It is unfortunate that the developing of the commercial combustor is conducted on the basis of empirical knowledge of spray combustion, since spray combustion has a complex phenomenon in which dispersion of liquid fuel droplets, evaporation, and chemical reaction of fuel vapor with oxidizer take place simultaneously and interactively. Therefore, elucidation and modeling of spray combustion phenomena based on theoretical knowledge are needed to develop innovative combustors.

In order to reduce the computational load, some simplification models (e.g. the parcel model) are utilized into the computational analysis of spray combustor. The parcel model, which is a typical example of the simplification, can decrease computational load by replacing a number of droplets by one hypothetical droplet. However, the parcel model can not take the droplet group combustion into account because of loss of the spacial distribution of droplets in droplet cluster. As a result, computational result of spray combustion using parcel model shows different combustion phenomena from the actual spray combustion, especially on the droplet group combustion phenomenon [1], [2]. The droplet group combustion is an important characteristic in spray combustion phenomenon.

To verify the presence of the droplet group combustion in the actual flames, some numerical and experimental study has been conducted [3], [4], [5]. Nakamura et al. [5] conducted two-dimensional direct numerical simulation (DNS) about spray combustion in counterflow. They showed that premixed-like and diffusion-like combustion regions appear in spray combustion field and that the droplet group combustion tends to reduce the gaseous temperature. However, two-dimensional analyses can not deal with droplet clusters that have three-dimensional structure. Aims of this study are to reveal combustion phenomena of droplet cluster and to develop highly accurate physical model of droplet cluster combustion. Effects of equivalence ratio of fuel spray, droplets diameter distribution, and gravity on spray flame structure were investigated using a three-dimensional DNS in the first stage of these aims.

2 Theoretical Formulation and Numerical Method

A time-dependant three-dimensional simulation of spray flames formed between two opposed circular ducts of finite dimensions is developed. In this study, external forces, Soret effect, Dufour effect, pressure gradient diffusion, bulk viscosity, and radiative heat transfer are ignored. Governing equations for gas

phase and dispersed phase are solved in Eulerian coordinate and Lagrangian one. Governing equations for gas phase were mass, momentum, energy, and mass fraction of chemical species conservation equations. The heat source terms due to chemical reaction and diffusion of chemical species in energy conservation equation of temperature form are considered [6].

Governing equations for dispersed phase are position, velocity, temperature, mass of droplet [5]. The droplets collision, rotation, and breakup are neglected in this study. Droplet temperature and mass were calculated by Langumuir-Knudsen evaporation model [7]. The interaction between gas phase and dispersed phase are concerned by using Eulerian-Lagrangian method. Coupling terms in gas phase equations were treated by PSI-CELL model [8].

The convective terms in gas phase equations are discretized and solved by CIP method [9]. Finite difference method and second-order central difference schemes are used to discrete the diffusion terms in governing equations for gas phase. For time integration of all equations, Euler explicit scheme is used. Thermodynamic and transport properties are calculated with CHEMKIN-II [10] and TRANFIT [11]; the original programs are modified to be vectorized. A one-step global reaction model of n-Decane with 5 reactive species $(C_{10}H_{22}, O_2, H_2, N_2, H_2O)$ is adopted [5].

The computational domain and inlet duct geometry are shown in Fig. 1. The cylindrical computational domain of 60 mm in diameter and 30 mm in height was used. The equivalence ratio of n-Decane vapor and air premixed gas which is set to $\phi_q = 0.6$ and the air that is composed of 21% oxygen and 79 % nitrogen issued from lower and upper inner ducts to the computational domain, respectively. From upper and lower outer ducts, pure nitrogen flowed in. Initial velocity of each gas is 0.8 m/s. For the computation, a $100 \times 72 \times 100$ grid system was used in the radial and circumferential and axial directions. A uniform grid spacing of 0.3 mm was used in the radial and axial directions, respectively. All inlet gases flowed from each ducts with a uniform axial velocity of 0.8 m/s and a temperature of 298 K. Outflow boundary conditions were applied for all quantities on the exit boundary. The time was set to t = 0, when fuel droplets are injected in computational domain from upper inner duct after premixed gas flame is stabilized near the stagnation plane. The computations are performed for three different Sauter mean diameter (SMD) conditions of $66.2\mu m$, $82.0\mu m$, and $104\mu m$. Those SMD and its dropletsize distributions are measured experimentally at the same configuration by using phase Doppler anemometry (PDA) [12].

3 **Results and Discussion**

3.1Validation of the computational result

The computed spray flame position was compared to experimental measurement to validate the computational model. The instantaneous result of spray flame computation and the direct image of spray flame in experiment are shown in Fig. 2, respectively. The luminous flame represents diffusion flame region and the flame surface could be consider to be near the isosurface of $\phi_g = 1.0$. The computed spray flame location agrees with that of the experimental one shown in the Fig. 2. Accordingly, the quantitative validity of the developed model was demonstrated.







(a)Simulation (b)Experiment Figure 2: (a)Isosurface of equivalence ratio of $\phi_g = 1.0$, (b)Direct

Figure 1: Schematic drawing of computational domain.

photograph of spray flame at $\phi_l = 0.106$, SMD=104 μ m.

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3.2 Effects of droplet size distribution on flame structure

Fig. 3 shows the time-averaged mass fractions of n-Decane and oxygen and the time-averaged gas temperature on the center axis of counterflow for each condition of droplet size distribution at $\phi_l = 1.06$. The mass fraction and the gas temperature are averaged during from 250 ms to 500 ms. The height on the center axis of counterflow is nondimensionalized by dividing the distance between upper duct and lower duct. Fuel spray is supplied from outlet of the inner upper port at non-dimensional height Z = 0.

It is obvious that the time-averaged mass fractions of n-Decane for each droplet size distribution have peak value in high temperature region. It can be considered that these peaks in Fig. 3 are related to the behavior of group combustion phenomenon. The decrease of gas temperature in group combustion region is shown at SMD=104 μ m (see Fig. 3(c)). A heat transfer between gaseous phase and dispersed phase that cause temperature rising and evaporation of droplets is thought to be the reason for this phenomenon (evaporative cooling effect). At SMD=66.2 μ m, the small peak of mass fraction of n-Decane is seen near the value of Z = 0.37. This small peak is attributed to pre-vaporization of fuel droplets as a result of heat supply from downstream diffusion-like flame. The upstream fuel droplet evaporation leads to formation of premixed-like combustion region.



Figure 3: Time-averaged gas temperature and time-averaged mass fraction of fuel and oxygen on the center axis of counterflow at $\phi_l = 1.06$.

3.3 Effects of gravity on flame structure

The difference of flame structures between non-gravity field (0-g) and gravity field (1-g) are investigated. The time-averaged mass fraction of n-Decane and oxygen and time-averaged gas temperature at $\phi_l = 1.06$, SMD=104 μ m are shown in Fig. 4. In the 0-g condition, due to increased evaporation of fuel droplets at upstream of counterflow, the time-averaged mass fraction of n-Decane in the group combustion region is decreased by comparison with the 1-g condition. The enhanced evaporation is result of decrease in droplets velocity at upstream of counterflow due to reduction of gravity acceleration. The reason of shift to upstream of flame position is same to that as discussed above. The increase of peak value of time-averaged gas temperature in the 0-g condition is as a result of combustion of fuel generated by enhanced evaporation of droplets at upstream of counterflow.



Figure 4: Flame structures on the center axis of counterflow in zero gravity and normal gravity.

4 Conclusion

The three-dimensional DNS was applied to spray flames formed in the counterflow, and detail structure of spray flames was investigated. The Langmuir-Knudsen evaporation model and a global 1-step reaction model are used to simulate droplets evaporation and a chemical reaction for n-Decane, respectively. A computation result of the 1-g spray flame location showed good agreement with the experimental observation of flame location.

The 1-g spray flame was classified in two regimes; the diffusion-like flame and the premixed-like flame. In the diffusion-like combustion region, a group combustion phenomenon was observed. A heat transfer between gaseous phase and dispersed phase that cause temperature rising and evaporation of droplets leads to decrease of gas temperature (evaporative cooling effect). The premixed-like combustion region was generated by pre-vaporization of fuel droplets as a result of heat supply from downstream diffusion-like flame.

In the 0-g condition, the decrease of fuel mass fraction in group combustion region, the shift of flame position to upstream of counterflow, and the increase of peak value of gas temperature were observed by comparison with the 1-g condition. These phenomena can be explained through consideration of decrease in droplets velocity at upstream of counterflow due to reduction of gravity acceleration.

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