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Characteristics of flamelets in spray flames formed in a laminar counterflow

Hiroaki Watanabe [a,b], Ryoichi Kurose [b,*], Seung-Min Hwang [a], Fumiteru Akamatsu [c]

[a] *Energy Engineering Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), 2-6-1 Nagasaka, Yokosuka, Kanagawa 240-0196, Japan*
[b] *Department of Mechanical Engineering and Science, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto 606-8501, Japan*
[c] *Department of Mechanical Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan*

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Abstract

A two-dimensional numerical simulation of a spray flame formed in a laminar counterflow is presented, and the flamelet characteristics are studied in detail. The effects of strain rate, equivalence ratio, and droplet size are examined in terms of mixture fraction and scalar dissipation rate. *n*-Decane ($C_{10}H_{22}$) is used as a liquid spray fuel, and the droplet motion is calculated by the Lagrangian method without the parcel model. A one-step global reaction is employed for the combustion reaction model. The results show that there appear large differences in the trends of gaseous temperature and mass fractions of chemical species in the mixture fraction space between the spray flame and the gaseous diffusion flame. The gas temperature in the spray flame is much higher than that in the gaseous diffusion flame. This is due to the much lower scalar dissipation rate and the coexistence of premixed and diffusion-limited combustion in the spray flame. For the spray flames, gas temperature and mass fractions of chemical species are not unique functions of the mixture fraction scalar dissipation rate. This is because the production rate of the mixture fraction, namely evaporation rate of the droplets, in the upstream region is not in proportion to its transport-diffusion rate in the downstream region. The behavior shows marked differences as the strain rate decreases, the equivalence ratio increases, or the droplet size decreases.

Keywords: Numerical simulation; Spray flame; Counterflow; Flamelet; Laminar flow

1. Introduction

Spray combustion is utilized in a number of engineering applications such as energy conversion and propulsion devices. It is, therefore, necessary to precisely predict the spray combustion behavior in designing and operating the equipment. However, since spray combustion is a complex phenomenon in which dispersion of the liquid fuel droplets, their evaporation, and chemical reaction take place interactively at the same time, the underlying physics governing these processes has not been well understood.

Akamatsu and co-workers [1–6] have conducted several kinds of measurements using optical techniques and obtained instantaneous and statistical

* Corresponding author. Fax: +81 75 753 9218.
E-mail address: kurose@mech.kyoto-u.ac.jp (R. Kurose).

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data describing spray combustion properties. They showed that spray flames do not consist only of single droplet combustion but contain group combustion; the spray flame structure differs depending on the boundary conditions and the spray characteristics.

Large-eddy simulation (LES) is becoming a standard tool to study and predict single-phase gaseous combustion fields in recent years [7–9], and may be valid for simulating spray combustion. In LES modeling of gaseous fuel combustion, the flamelet model [10–13] is widely used. In the flamelet model, mass, momentum, and mixture fraction (Z) conservation equations are solved in physical space. Enthalpy and concentrations at each position are identified by a lookup table that is called a chemtable. The chemtable is obtained by solving a one-dimensional flamelet equation in Z space, and Z and scalar dissipation rate (χ) are used as parameters to determine the values of the variables in physical space [12,14]. It is therefore essential to understand the detailed behavior of the variables such as enthalpy and concentrations as functions of Z and χ.

On the other hand, the number of LES studies of two-phase combustion is limited. Recently, Kurose and Makino [15] applied LES to a turbulent jet flame of solid fuel and investigated the interactions among the dispersion, evaporation, and combustion of the solid-fuel particles. Ham et al. [16] also performed LES of a spray combustion field in a realistic gas turbine combustor. The small number of LES studies is attributed not only to the high computational cost, but also to the lack of experimental data for the validation. In two-phase combustion, Z, which characterizes the mixing of vaporized fuel and oxygen, is no longer a conserved scalar because of the interphase mass transfer (evaporation) from the dispersed phase to the gaseous phase. Consequently, the dependence of enthalpy and concentrations on Z and χ becomes complicated.

A numerical simulation, which directly solves conservation equations for carrier gaseous phase and Lagrangian equations for dispersed droplet dynamics, is attractive not only for discussing the detailed spray combustion mechanism but also for validating models for LES [18,19]. The computational cost is, however, larger than for LES. Domingo et al. [20] compared two-dimensional simulations. Reveillon and Vervisch [21] described a two-dimensional numerical simulation of spray flames and proposed a classification of the spray flame structures. Our group [22] investigated aspects of spray combustion including the details of droplet group combustion using a two-dimensional simulation. However, the behavior of the flamelet has not been fully investigated in previous spray combustion studies.

The purpose of this study is to clarify the characteristics of flamelets within two-phase combustion. In this paper, spray combustion behavior is studied by performing a two-dimensional numerical simulation of spray flames in a laminar counterflow. The characteristics of the flamelet are discussed in detail. A one-step global reaction is employed to model the combustion of a liquid fuel (n-decane, $C_{10}H_{22}$). Effects of strain rate, equivalence ratio, and droplet size on the behavior of Z, χ, and the other variables are investigated.

2. Numerical simulation

2.1. Governing equations

The governing equations considered for the gaseous phase are mass, momentum, energy, species mass fraction, and mixture fraction conservation,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = S_m, \tag{1}$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j + P\delta_{ij} - \sigma_{ij}) - \rho g_i = S_{ui}, \tag{2a}$$

$$\sigma_{ij} = 2\mu\left[\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{1}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right], \tag{2b}$$

$$\frac{\partial (\rho h)}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j h - \rho\lambda\frac{\partial h}{\partial x_j} + \sum_{k=1}^{n} h_k(\rho\lambda - \rho D_k)\frac{\partial Y_k}{\partial x_j}\right] = S_h, \tag{3}$$

$$\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j Y_k - \rho D_k\frac{\partial Y_k}{\partial x_j}\right) = S_{\mathrm{combu},k} + S_{Y_k}, \tag{4}$$

$$\frac{\partial (\rho Z)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j Z - \rho D_Z\frac{\partial Z}{\partial x_j}\right) = S_Z, \tag{5}$$

where u_i is the gaseous phase velocity, ρ is the density, μ is the viscosity, P is the static pressure, g_i is the gravitational force, h is the specific total enthalpy, λ is the gaseous thermal diffusivity, and h_k, Y_k, and D_k are the specific enthalpy, the mass fraction, and the mass diffusion coefficient of the kth species, respectively. δ_{ij} is the Kronecker delta function. S_i represents interactions between the gaseous and the disperse phases and $S_{\mathrm{combu},k}$ is the source term due to combustion, described later. Z is the mixture fraction. The diffusion coefficient of Z, D_Z, is given by diffusion coefficient of mixture gas. The gaseous phase density, ρ, is calculated from the equation of a state for an ideal gas.