Fuel 104 (2013) 515–525

Contents lists available at SciVerse ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Two-dimensional direct numerical simulation of spray flames - Part 1: Effects of equivalence ratio, fuel droplet size and radiation, and validity of flamelet model

Akitoshi Fujita [a], Hiroaki Watanabe [b], Ryoichi Kurose [a,*], Satoru Komori [a]

[a] Department of Mechanical Engineering and Science, and Advanced Research Institute of Fluid Science and Engineering, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto 606-8501, Japan

[b] Energy Engineering Research Laboratory, Central Research, Institute of Electric Power Industry (CRIEPI), 2-6-1 Nagasaka, Yokosuka, Kanagawa 240-0196, Japan

HIGHLIGHTS

- ▶ We investigate effects of equivalence ratio, fuel droplet size, and radiation.
- ▶ Contribution of premixed flame increases as fuel droplet size decreases.
- ▶ Heat transfer between droplets and ambient fluid is captured by flamelet model.

ARTICLE INFO

Article history:
Received 16 December 2011
Received in revised form 26 April 2012
Accepted 27 August 2012
Available online 18 September 2012

Keywords:
Numerical simulation
Spray combustion
Jet flame
Radiation
Flamelet model

ABSTRACT

The effects of equivalence ratio, fuel droplet size, and radiation on jet spray flame are investigated by means of two-dimensional direct numerical simulation (DNS). In addition, the validity of an extended flamelet/progress-variable approach (EFPV), in which heat transfer between droplets and ambient fluid including radiation is exactly taken into account, is examined. *n*-decane ($C_{10}H_{22}$) is used as liquid spray fuel, and the evaporating droplets' motions are tracked by the Lagrangian method. The radiative heat transfer is calculated using the discrete ordinate method with S_8 quadrature approximation. The results show that the behavior of jet spray flame is strongly affected by equivalence ratio and fuel droplet size. The general behavior of the jet spray flames including the heat transfer between droplets and ambient fluid with radiation effect can be captured by EFPV.

1. Introduction

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

Recently, the spray combustion behavior has been studied by direct numerical simulations (DNSs) [e.g., 1–8] or large-eddy simulations (LESs) [e.g., 9–12]. However, since these computations are still so expensive that the effects of the changes in combustion conditions such as equivalence ratio, fuel droplet size and ambient pressure on the spray combustion behavior have not been sufficiently discussed yet. Moreover, in most of these studies, radiative heat transfer was neglected or significantly simplified, because the computation of radiation further increases the computational cost. Watanabe et al. [5] studied the effects of radiation on the spray flame characteristics and soot formation by performing a two-dimensional DNS of spray flames formed in a laminar counterflow, in which the radiative interaction between the gas and dispersed droplets is taken into account, and found that the radiative heat transfer strongly affects the spray flame and soot formation behaviors. However, since the radiation effect is discussed only on the spray flames formed in a laminar counter flow, there remains uncertainty as to how the radiative heat transfer affects the characteristics of jet spray flames.

In LES and RANS (Reynolds-Averaged Navier–Stokes) simulations of gaseous combustions, flamelet models [e.g., 13,14] have been widely used as the turbulent combustion model. However, in the original flamelet model in which the energy equation is not solved in the physical space, not only the radiative heat transfer but also convective heat transfer between the gas and droplets for the spray combustion cannot be taken into account.

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

0016-2361/$ - see front matter
http://dx.doi.org/10.1016/j.fuel.2012.08.044

Nomenclature

C	progress variable, –	Z	mixture fraction, –
c_L	specific heat of liquid fuel, J kg^{-1} K^{-1}	α	Plank mean gas absorption coefficient, m^{-1}
c_p	specific heat of mixture gas, J kg^{-1} K^{-1}	ϕ	equivalence ratio, –
D	non-dimensional initial droplet diameter, –	ρ	density, kg m^{-3}
FI	flame index, –	BL	boiling point
h	total enthalpy of mixture gas, J kg^{-1}	F	fuel gas
L	length, m	lib	flamelet library
L_V	latent heat of droplet evaporation, J kg^{-1}	max	maximum value
P_k	partial pressure of kth species, Pa	min	minimum value
P_p	contribution of premixed flame, –	O	oxidizer
T	gaseous temperature, K	0	reference value
U	velocity, m s^{-1}		
Y_k	mass fraction of kth species, –		

Recently, Ihme and Pitsch [12] extended the flamelet/progress-variable approach [15] (referred to as FPV, in this paper) to account for the radiative heat transfer, and investigated the effects of radiation on the gas temperature and NO formation on LES of Sandia flame D and a realistic aircraft engine. However, they considered the radiation only in the gas phase using the optically thin approximation [16] and still neglected the heat transfer between droplets and ambient fluid including radiation.

The purpose of this study is therefore to investigate the effects of equivalence ratio, fuel droplet size, ambient pressure and radiation on the spray combustion behavior by means of two-dimensional DNS of spray jet flames. In addition, FPV coupled with the radiation model, which can account for the heat transfer between droplets and ambient fluid including radiation, (referred to as EFPV, in this paper) is proposed and validated by comparing with the results using the direct combustion model based on the Arrhenius formation (referred to as ARF, in this paper). n-decane ($C_{10}H_{22}$) is used as liquid spray fuel, and the evaporating droplets' motions are tracked by the Lagrangian method. The radiative heat transfer is calculated using the discrete ordinate method [17] with S_8 quadrature approximation. The present paper provides the first part of two investigations. In this part 1, the effects of equivalence ratio, fuel droplet size and radiation on the spray combustion behavior are investigated. In addition, the validity of EFPV in various equivalence-ratio and fuel-droplet-size conditions and in the presence of the radiation are examined. In part 2 [18], the effect of ambient pressure on the spray combustion behavior and the validity of EFPV in high-pressure condition will be discussed. Originally, combustion models such as FPV are intended for use in connection with SGS models for LES or RANS of the carrier gaseous phase. However, in order to avoid discussion of the effect of the SGS contributions on numerical accuracy, a numerical method using fine resolution without the SGS models is chosen here. In these papers, we simply call this method DNS, regardless of the combustion model.

2. Numerical simulation

2.1. Numerical methods for ARF and EFPV

In ARF, the Arrhenius formation is directly solved in the physical space as well as the flow field. In EFPV, on the other hand, the Arrhenius formation is solved in generating a lookup table called flamelet library. Therefore, the detailed spray combustion behavior is investigated based on ARF, and the validity of EFPV is discussed by comparing with the results obtained by ARF.

The set of governing equations of the carrier gaseous phase and dispersed droplets phase for ARF and EFPV are described in our previous papers [3–7]. n-decane ($C_{10}H_{22}$) is used as liquid fuel, and the combustion reaction of the evaporated n-decane with oxygen is described by a one-step global reaction model [19] as

$$C_{10}H_{22} + \frac{31}{2}O_2 \rightarrow 11H_2O + 10CO_2. \tag{1}$$

In this study, the treatment of the radiative heat transfer for ARF is modified from Watanabe et al. [5]. Computation of radiative heat transfer tends to be much expensive due to procedure of estimating non-gray gas absorption coefficient and solving the radiation intensity balance equation. A common and straightforward way to account for radiation in gaseous flames is to ignore the radiation effect or to employ the optically thin approximation [16] which can effectively reduce the computational cost of solving the radiation intensity transport equation. Moreover, even in the optically thin approximation [16], most researchers use gray gas approximation because it is still very expensive to estimate non-gray gas absorption coefficient. In this study, in order to take into account the non-gray gas absorption coefficient, a tabulated library which is pre-computed and parameterized as a four-dimensional function by partial pressures of fuel, CO_2 and H_2O gases, P_F, P_{CO_2} and P_{H_2O}, and gas temperature, T, is employed. Namely, the local value of the Plank mean gas absorption coefficient of the medium, α, is determined by the interpolation among these four variables as

$$\alpha = \alpha(P_F, P_{CO_2}, P_{H_2O}, T). \tag{2}$$

More than 80 % of the computational cost for the total computation can be effectively reduced by the presented method. The value of α is calculated using a detailed narrow-band model RADCAL [20]. The radiative heat transfer is computed based on the discrete ordinate method [17]. For the standard FPV, the heat transfer between droplets and ambient fluid including radiation cannot be taken into account, as described earlier. Therefore, in the present EFPV, the total enthalpy is solved in the physical space in order to account for the heat transfer between droplets and ambient fluid including radiation similarly to ARF and the gas temperature obtained from the flamelet library is corrected by

$$\Delta T = \frac{h - h_{lib}}{c_p}, \tag{3}$$