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Large-eddy simulation of ethanol spray combustion using a SOM combustion model and its experimental validation

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ABSTRACT

In this paper, large-eddy simulation of ethanol spray-air combustion was made by using an Eulerian–Lagrangian approach, a sub-grid-scale kinetic energy stress model, and a filtered finite-rate combustion model with a sub-grid scale reaction rate, called second-order moment (SOM) combustion model, proposed by our research group. The simulation accounts for the sub-grid turbulence–spray–combustion interactions and the coupling between the temperature fluctuations and species concentrations fluctuations. The simulation results are validated in detail by experiments. It is found that the LES-SOM statistical results are in better agreement with the experimental results than those obtained by LES accounting for only the filtered finite-reaction rate (LES-FA) neglecting the SGS reaction rate, and are in much better agreement than those obtained by RANS modeling using the most complex PDF equation combustion model with detailed chemistry. The instantaneous LES results show the earlier production of the coherent structures in the two-phase jet combustion than that in the single-phase jet combustion. The instantaneous temperature map indicates the existence of small flame islands, expressing the droplet-group combustion, which is not observed in single-phase jet combustion.

1. Introduction

Large-eddy simulation (LES) of liquid spray combustion, which is becoming a more advanced Computational Dynamic Fluid (CFD) tool and is extensively studied in recent years, can give the detailed instantaneous flow and flame structures and more exact statistical results than those given by the Reynolds averaged Navier Stokes (RANS) modeling. Recent advances in LES of turbulent spray combustion were reviewed by the present author [1]. For engineering application the LES is mainly applied to rocket-engine combustors, ram-jet engine combustors, gas turbine combustors and internal combustion engines. However, it is still a challenging task to understand the complex physical phenomena involved the interactions of combusting droplets, the turbulence and chemical reaction. One of the key problems is to develop sub-grid scale (SGS) models, including SGS stress models and combustion models.

Kong et al. did LES of spray combustion in diesel engines [2]. An Eulerian–Lagrangian simulation with a sub-grid-scale (SGS) kinetic energy equation stress model and a combustion model based on a detailed chemistry mechanism of *n*-heptane–air reaction with 30 species and 65 elementary reactions was used, and the SGS reaction rate was omitted. The

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Nomenclature

a, c, C_v, C_ε	empirical model constants
B	pre-exponential factor
D	dissipation term
E	activation energy
g	sub-grid scale mass flux
k	turbulent kinetic energy
h	enthalpy
K	reaction rate constant
M	molecular weight
p	pressure
P	production term
Pr	Prandtl number
q	sub-grid scale heat flux
r	radius
R	universal gas constant
S	source term
u	velocity component
T	temperature
w	reaction rate
x, y, z	space coordinate
Y	mass fraction

Greek alphabets

ε	dissipation rate
κ	Von Kármán constant
β	stoichiometric ratio
μ	dynamic viscosity
ν	kinematic viscosity
ρ	density

Subscripts

i, j, k	components; coordinates
ox	oxygen
fu	fuel
sgs	subgrid scale value
t	turbulent

Superscripts

-	filtered value
′	subgrid scale value

instantaneous temperature, CO concentration, NO concentration and soot formation were obtained, the predicted statistical results are compared with the change of pressure and heat release in the cylinder with the crank angle. No experimental validation was made for the flow field, temperature and species concentration inside the combustion chamber. The grid size is in the same order as that for RANS modeling. It is actually near to unsteady RANS modeling. Similarly, LES of spray combustion in a diesel engine was made by Banerjee et al. [3], using a dynamic SGS energy equation stress model and a detailed chemistry model and the CHEMKIN code without accounting for the effect of sub-grid-scale reaction rate. Also, no detailed experimental validations of the LES statistical results are given. Chrigui et al. [4] investigated the predictive capability of combustion large eddy simulation approach coupled to Lagrangian droplet dynamic model for an ethanol spray flame using the Eulerian–Lagrangian approach with dynamic sub-grid scale Germano models and a detailed reaction mechanism consisting of 56 species and 351 reversible reactions. Droplets are injected in polydisperse manner and the chemistry is described by a tabulated detailed chemistry based on the flamelet generated manifold approach. Overall the simulation results including gas temperature, droplet velocities and corresponding fluctuations, droplet mean diameters and spray volume flux at different distances from the exit plane show good agreement with experimental data. Moin et al. [5] reported the LES of spray combustion in a gas-turbine combustor using a dynamic eddy-viscosity SGS stress model and a laminar-flamelet combustion model with presumed PDF. The statistical results for isothermal gas-particle flows are validated by experiments. The LES statistical results for combustion case were validated for the temperature distribution at a cross section. No other experimental