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Proceedings of the Combustion Institute xxx (2014) xxx–xxx

Proceedings of the Combustion Institute

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LES of a methanol spray flame with a stochastic sub-grid model

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Abstract

This paper describes the Large Eddy Simulation (LES) of a methanol/air turbulent nonpremixed spray flame. An Eulerian stochastic field method is employed for the turbulence-chemistry interaction of the gas phase while a Lagrangian formulation is used for the liquid phase. A reduced reaction mechanism (18 species and 14 reactions) is adopted and stochastic models are used to account for the influence of sub-grid scale (*sgs*) motions on droplet dispersion and evaporation. Comparisons of the predicted gas phase and droplet statistics with measurements show a good agreement confirming that the droplet dispersion and evaporation models used in this work are adequate. The general features of the spray flame such as the occurrence of external group combustion and its development into separate combusting islands are well captured.

Keywords: Large Eddy Simulation; Turbulent spray combustion; Stochastic field method; PDF method

1. Introduction

Combustion systems with liquid fuel sprays have been extensively used in various engineering applications such as industrial furnaces, internal combustion engines, rocket propulsion and gas turbines. The modelling of such systems requires a good understanding of both physical and chemical processes taking place in these two phase flows. However, the numerical simulation of liquid spray flames is challenging because it is difficult to simulate their multi-scale nature. The ability to model and simulate particle-laden flows could result in significant advances in the design of various spray combustion systems in terms of their efficiency and reduction in pollutant emissions.

LES is an effective tool for predicting the properties of turbulent reactive flows. In LES, the equations of motion are solved directly for the large-scale energetic turbulent motions while the influence of the sub-grid scale (*sgs*) motions on the resolved flow field are modelled. In the present work, the liquid phase is described using a Lagrangian formulation whilst an Eulerian approach is employed for the gas phase. In the context of LES, the size of droplets is assumed to be sufficiently small so that they can be treated as point sources of mass, momentum and energy. Stochastic models are used to account for the influence of *sgs* motions on particle dispersion, i.e. acceleration, and particle vaporisation. Previous studies

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http://dx.doi.org/10.1016/j.proci.2014.06.086
1540-7489/

have investigated different experimental configurations, e.g. a swirl stabilised burner with liquid kerosene [1], an aeronautical type combustor, which is the DLR Generic Single Sector Combustor, [2] and a methanol fuelled spray burner in a hot coflow experiencing turbulent auto-ignition [3].

The overall aim of the present research is to conduct LES simulations of a turbulent spray flame possessing multiple length and time scales involving chemical reactions and interactions between gas phase turbulence and particle motions. The predictive capabilities of LES with major improvements regarding liquid phase modelling are validated by reproducing the turbulent flame structures of an experimental burner [4]. The spray flame configuration studied in the present paper has also been the subject of a previous numerical study [5]. A Reynolds averaged approach was adopted with a Reynolds stress transport equation model being used in conjunction with a probability density function (*pdf*) equation method. Account was taken of droplet evaporation and two-way coupling of mass and momentum exchange. It appears, however, that the present work represents a first attempt at applying LES to the configuration under consideration.

The structure of this paper is as follows. First, the experimental apparatus investigated in the current work is described. The mathematical formulation of the LES filtered equations for physical variables of the continuous phase flow and the methods used to predict the particle dispersion and evaporation in a stochastic manner are presented. The numerical set-up and initial/boundary conditions are then explained. The numerical results are compared with experimental measurements and discussed in detail. The conclusions of the current investigation are made in the last section.

2. Experimental configuration

The experimental burner is a canonical turbulent methanol/air spray flame designed by Karpetis and Gomez [4]. The liquid fuel, methanol, is fed into the burner housing using a commercial ultrasonic atomizer (Sono-Tek) which produces particles at minimal velocity. The drops are carried upwards by air through a number of primary holes. Furthermore, around 4% of the total air flow rate is diverted around the atomizer in order to carry the drops past its tip and create a small region of recirculation where the flame is attached.

In the experiments, two methanol spray flames with Reynolds numbers based on cold conditions between 21,000 and 28,000 are examined and referred to as flame I and II respectively; in the present work, only flame I is examined. The total mass flow rates of air and methanol are 1.6×10^{-3} kg/s and 8.5×10^{-5} kg/s respectively. The measurements are performed at 0.1D, 0.5D and at every half burner exit diameter (D = 12.7 mm) thereafter up to 6.5D in the axial direction. Phase Doppler Anemometry (PDA) is used to measure spray properties, i.e. droplet number density and size and velocity statistics. Chemiluminescence imaging and Raman spectroscopy are adopted to obtain the spray flame images and the gas phase temperature respectively.

3. Numerical modelling

3.1. Filtered gas phase equations

The density-weighted filtered governing equations of low-Mach number, variable density flows with point sources of mass, momentum, species or energy contributions from the dispersed phase are:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = \bar{\dot{S}}_{mass} \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} + \frac{\partial \tilde{\tau}_{ij}^{sgs}}{\partial x_j} + \bar{\dot{S}}_{mom,i} \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{\phi}_\alpha}{\partial t} + \frac{\partial \bar{\rho}\tilde{\phi}_\alpha\tilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu}{\sigma}\frac{\partial \tilde{\phi}_\alpha}{\partial x_j}\right) - \frac{\partial \tilde{J}_j^{sgs}}{\partial x_j} + \overline{\rho\dot{\omega}_\alpha(\underline{\phi}, T)} + \bar{\dot{S}}_\alpha \tag{3}$$

where ρ, u_i, p and ϕ_α represent the fluid density, velocity vector, pressure and scalar quantities, i.e. species mass fraction and enthalpy. Equal diffusivities are assumed for the species and enthalpy equations so that σ is the Schmidt and Prandtl number as appropriate.

A dynamic version of Smagorinsky model [6] is adopted to close the unresolved residual stresses $\tilde{\tau}_{ij}^{sgs}$. Equation (3) involves the sub-grid scalar flux $\tilde{J}_j^{sgs}$ and the filtered chemical source term $\overline{\rho\dot{\omega}_\alpha(\underline{\phi}, T)}$ which represents the net formation rate of species α due to chemical reactions or heat sources and sinks. Since the chemical source term $\dot{\omega}_\alpha$ is highly non-linear, it is accounted for through a joint sub-grid *sgs* in conjunction with the Eulerian stochastic field method [7]. The source terms of mass, momentum and relevant scalar, i.e. $\bar{\dot{S}}_{mass}, \bar{\dot{S}}_{mom,i}$ and $\bar{\dot{S}}_\alpha$, are obtained from the volume-averaged contribution of every particle within a specific control volume (see e.g. [8] for more detail).

3.2. Modelling of liquid sprays

Following the work of Bini [9,10], a stochastic Markov model is used to account for the effect of the *sgs* velocity fluctuations on the *p*th particle over a time *dt*. The evolution of the particle velocity $\boldsymbol{u}_p$ is determined by:

Please cite this article in press as: W.P. Jones et al., *Proc. Combust. Inst.* (2014), http://dx.doi.org/10.1016/j.proci.2014.06.086