Available online at www.sciencedirect.com

ScienceDirect

Proceedings of the Combustion Institute 36 (2017) 1705–1712

Proceedings of the Combustion Institute

www.elsevier.com/locate/proci

Large-eddy simulation of piloted diffusion flames using multi-environment probability density function models

Wei Zhao

Combustion Engineering, GE Power, GTTL 1256, 300 Garlington Rd, Greenville, SC 29615, USA

Received 4 December 2015; accepted 15 July 2016
Available online 26 July 2016

Abstract

Two piloted partially premixed jet flames (Sandia Flames D and F) are calculated using large-eddy simulation. A multi-environment turbulent combustion model, which depicts the sub-grid probability density function (pdf) as a weighted summation of a small number of Dirac delta functions in composition space, is used for modeling of turbulence chemistry interaction. It was coupled with a 19-species reduced mechanism and an *In Situ* adaptive tabulation algorithm for chemical source term integration. The impact of number of environments is investigated in this study. While predictions of Flame D by both two- and three-environment models are in good agreement with experimental data, only the three-environment model correctly captures the strong extinction and re-ignition in Flame F. The current study highlights the capability of the multi-environment pdf model for modeling of turbulent flames that feature strong local extinction and re-ignition.

Keywords: Multi-environment model; Pdf; Piloted diffusion flames; Sandia flame

1. Introduction

Large-eddy simulation (LES) has become a powerful method to describe the turbulent flow and turbulence chemistry interaction. In LES, the energy-containing large turbulent structures are directly resolved and only the scales smaller than the filter width are modeled. The small scales tend to be more uniform and isotropic than the large ones and can be modeled with models that are more universal and simpler than their counterparts for Reynolds averaged fluxes. However, since chemical reactions occur only on the smallest scales of all sub-grid scales, the combustion process has to be modeled entirely. An overview of the combustion models that have been proposed in the past can be found in Pitsch [1] and Pope [2].

The one-point joint probability density function (pdf) for all of the reactive scalars provides a means to close the filtered chemical reaction source terms in LES. Derivation of the transport equation of the pdf was given by Pope in [6]. One of the advantages of the pdf approach is that the chemical source terms appear exactly in the equation and require no further modeling. The most commonly used approach to solve the pdf equation in turbulent reacting flows is the Lagrangian stochastic particle method, where an ensemble of particles is used to represent the joint pdf. While early works [16,17] on

E-mail address: wei4.zhao@ge.com

http://dx.doi.org/10.1016/j.proci.2016.07.064
1540-7489

these methods often included the velocity vector as a stochastic variable in order to minimize errors associated with spatial discretization, the recent trend has been to use a Lagrangian solver for the composition joint pdf coupled with a standard Eulerian method for momentum equations [3,7,11], especially in the context of LES. More recently, methods aimed at solving the pdf transport equation in a fully Eulerian manner have been proposed. Among them are the stochastic field method [8–10] and multi-environment model [3,21]. The former is based on stochastic Eulerian fields, which evolve according to stochastic partial differential equations equivalent to the joint pdf transport equation. The multi-environment pdf (MEPDF) model, on the other hand, employs a presumed form for the joint composition pdf, which is represented by a small number of Dirac delta functions in composition space. The direct quadrature method of moments (DQMOM) is then used to find the transport equations for the weights and nodes of the environments, which depict the presumed pdf. Like the stochastic field method, the MEPDF model can be incorporated into existing CFD codes without undue difficulty. Notice that the MEPDF model is deterministic, so it does not have the stochastic errors that come with the Lagrangian particle and stochastic field pdf methods. Examples of recent application of the MEPDF model to LES of turbulent reacting flows can be found in [13,15,27].

In this study, the same LES-MEPDF approach described in Zhao et al. [27] is applied to simulate the Sandia Flames D and F [18,19]. The Sandia flame series have been numerically studied by many researchers using a variety of combustion models, such as flamelet models [4,5,24], pdf methods [10,16,20,25,31], conditional momentum closure [23], and others [12,22,26], to name a few. Noticeably for Flame F, Xu and Pope [16] used a joint velocity-composition pdf model in the context of Reynolds averaging and successfully predicted the strong extinction and re-ignition that agree very well with experimental data. Jones and Prasad [10] used LES and a stochastic field model approach that showed a reasonable local extinction level. However, the predicted mean temperature profiles at the extinction zone were significantly higher than the experiment. The objective of the current study is to examine the capability of the MEPDF model to predict the local extinction and re-ignition in turbulent flames and the impact of number of environments on the accuracy and computational cost of the model.

2. Multi-environment pdf model

The development of the MEPDF model was detailed in Fox [3], and is only briefly repeated here. It begins with a transport equation for a one-point one-time joint composition PDF, f_ϕ:

$$\frac{\partial f_\phi}{\partial t} + \nabla\cdot\left(\langle\mathbf{u}\rangle f_\phi\right) - \nabla\cdot\left(\Gamma_e\nabla f_\phi\right) = -\frac{\partial}{\partial\psi_i}\left[\left(\Omega_m(\langle\phi_i\rangle - \psi_i) + S_i(\psi)\right)f_\phi\right]$$

where $\langle\mathbf{u}\rangle$ is the filtered velocity vector, $\Gamma_e = \frac{\mu_l}{s_c} + \frac{\mu_t}{s_{c_t}}$ is the effective diffusion coefficient, S_i is the reaction source term, and $\Omega_m = c_\phi(\mu_t + \mu_l)/(\rho\Delta^2)$ is the SGS mixing frequency, where Δ is the filter width and c_ϕ is the micro-mixing model constant. Notice that the interaction-by-exchange-with-the-mean (IEM) mixing model is used to close the equation. In the MEPDF model, the joint pdf for N_s scalars is assumed to be of the form:

$$f_\phi(\psi;\mathbf{x},t) = \sum_{n=1}^{N_e} p_n(\mathbf{x},\ t)\prod_{\alpha=1}^{N_s}\delta[\psi_\alpha - \langle\phi_\alpha\rangle_n(\mathbf{x},\ t)]$$

where N_e is the number of environments, $p_n(\mathbf{x},t)$ is the mass weight of environment n, and $\langle\phi_\alpha\rangle_n(\mathbf{x},t)$ is a component of the composition vector (of length N_s) of environment n.

The transport equations for mass weight, p_n, and mass weighted species mass fraction, $p_n\langle\phi_\alpha\rangle_n$, of environment n can be defined as

$$\frac{\partial p_n}{\partial t} + \nabla\cdot(\langle\mathbf{u}\rangle p_n) - \nabla\cdot(\Gamma_e\nabla p_n) = a_n$$

and

$$\frac{\partial(p_n\langle\phi_\alpha\rangle_n)}{\partial t} + \nabla\cdot(\langle\mathbf{u}\rangle p_n\langle\phi_\alpha\rangle_n) - \nabla\cdot[\Gamma_e(\nabla p_n\langle\phi_\alpha\rangle_n)] = b_{\alpha n}$$

The source terms, a_n and $b_{\alpha n}$ are determined using DQMOM to match the desired moments of the scalars. In this study, two- and three-environment models are considered. The source terms a_n and $b_{\alpha n}$ for the two-environment model that matches the first and the second moments (mean and variance) of each scalar is given in Tang et al. [14]. For a three-environment model, the first three moments of each scalar are matched. The source terms a_n and $b_{\alpha n}$ are given by:

$$a_1 = a_2 = a_3 = 0$$

$$b_{\alpha1} = \frac{D_\alpha - C_\alpha(\phi_{\alpha2}+\phi_{\alpha3})}{(\langle\phi_\alpha\rangle_1 - \langle\phi_\alpha\rangle_2)(\langle\phi_\alpha\rangle_1 - \langle\phi_\alpha\rangle_3)} - \Omega_m p_1(\langle\phi_\alpha\rangle_1 - \psi_\alpha) + p_1 S_\alpha(\langle\phi\rangle_1)$$

$$b_{\alpha2} = \frac{D_\alpha - C_\alpha(\phi_{\alpha1}+\phi_{\alpha3})}{(\langle\phi_\alpha\rangle_2 - \langle\phi_\alpha\rangle_1)(\langle\phi_\alpha\rangle_2 - \langle\phi_\alpha\rangle_3)} - \Omega_m p_2(\langle\phi_\alpha\rangle_2 - \psi_\alpha) + p_2 S_\alpha(\langle\phi\rangle_2)$$

$$b_{\alpha3} = \frac{D_\alpha - C_\alpha(\phi_{\alpha1}+\phi_{\alpha2})}{(\langle\phi_\alpha\rangle_3 - \langle\phi_\alpha\rangle_1)(\langle\phi_\alpha\rangle_3 - \langle\phi_\alpha\rangle_2)} - \Omega_m p_3(\langle\phi_\alpha\rangle_3 - \psi_\alpha) + p_3 S_\alpha(\langle\phi\rangle_3)$$

where $C_\alpha \equiv \sum_{n=1}^{3}\Gamma_e p_n(\nabla\langle\phi_\alpha\rangle_n)^2$ and $D_\alpha \equiv \sum_{n=1}^{3}\Gamma_e p_n\langle\phi_\alpha\rangle_n(\nabla\langle\phi_\alpha\rangle_n)^2$.