Combustion and Flame 162 (2015) 1464–1476

Contents lists available at ScienceDirect

Combustion and Flame

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

Multi-environment probability density function approach for turbulent CH_4/H_2 flames under the MILD combustion condition

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ARTICLE INFO

Article history:
Received 28 March 2014
Received in revised form 6 November 2014
Accepted 12 November 2014
Available online 8 December 2014

Keywords:
Multi-environment PDF
Auto-ignition
Flame liftoff
CH_4/H_2 flame
NOx formation
MILD combustion

ABSTRACT

The multi-environment probability density function approach has been applied to simulate turbulent CH_4/H_2 flames under moderate or intense low-oxygen dilution (MILD) conditions. In order to circumvent excessive computational burden, the direct quadrature method of moments (DQMOM) has been adopted as an alternative approach to solve the transported probability density function (PDF) equation. The multi-environment PDF approach has the form of a conventional Eulerian scheme and retains the desirable property of a particle-based method. In this study, the joint-composition PDF is approximated using the two-environment PDF, expressed via the combination of weights and abscissas on the composition and physical space. Micromixing is represented by the IEM model, and the chemical mechanism is based on detailed chemistry. In terms of the unconditional means and conditional statistics for temperature and mass fractions of species and pollutants, the predicted profiles are in reasonable agreement with experimental data. Numerical results clearly indicate that the two-environment PDF transport model has the capability to realistically predict the effects of oxygen mass fraction on the flame lift-off, auto-ignition, flame structure, and NOx formation characteristics in turbulent CH_4/H_2 jet flames issuing from a jet in hot coflow (JHC). It was also found that the two-environment PDF approach reproduces the sensitivity of the CO and CO_2 peak levels versus the O_2 concentration variation, as well as the peak levels of NO conditional fluctuations under the MILD combustion condition. Even if considerable discrepancies in the unconditional means exist mainly due to inconsistent treatment of weight combination and shortcomings of singularity treatment procedure, the present three-environment PDF model well captures the measured high-level conditional temperature and CO fluctuations on the fuel-lean side where the local extinction occurs via mixing of the shrouded cold air and the vitiated flame field.

1. Introduction

Increasingly strict requirements for the environmental regulation of combustion-generated pollutants coupled with stronger demands for energy economy have led to increased interest in new combustion technology that ensures high combustion efficiency and low pollutant emission. MILD (Moderate and Intense Low oxygen Dilution) combustion is the one of new combustion technologies that can offer a feasible solution to these problems. MILD combustion occurs when reactants are preheated above their auto-ignition temperature and enough inert combustion products are entrained to dilute the flame zone. As a result, a flame front is no longer identifiable, so that MILD combustion is often denoted as flameless combustion or flameless oxidation (FLOX) [1,2]. This technology is also known as high temperature air combustion (HiTAC) due to the common practice of preheating the oxidizer [3]. Unlike conventional diffusion or premixed combustion, MILD combustion regimes have unique features such as volumetric enlargement of the reaction zone and a more uniform temperature distribution [3,4]. Compared to conventional combustion technology, the use of this technology can provide an energy savings of approximately 30%, and hence CO_2 reduction, a 30% reduction in furnace size, and a 25% reduction in pollutant emission [5]. According to Arghode et al. [6], high temperature air combustion technology (HiTAC) [3], with significantly higher combustion intensity and shorter residence times, is classified as a colorless distributed combustion (CDC). Colorless distributed combustion has found the useful application to achieve ultra-low levels of NOx and CO in gas turbine combustors. Recently, Cho et al. [7,8] experimentally studied the behavior of heat transfer and emissions in a practical natural-gas-fired furnace with regenerative flameless oxidation. Based on experimental results, they identified the optimum MILD combustion

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http://dx.doi.org/10.1016/j.combustflame.2014.11.014
0010-2180/

condition in terms of combustion efficiency, flame stabilization, pollutant emissions (NO, CO) and temperature uniformity.

Although the concept of MILD combustion has been extensively investigated, mathematical modeling of the flameless combustion regime has received less attention [9]. In fact, MILD combustion does not feature the high-density gradients and complex turbulence–chemistry interaction processes that are prominent in conventional turbulent jet flames. However, the conditions of uniform temperature distribution and low oxygen concentration lead to slower reaction rates and enhance the influence of molecular diffusion on flame characteristics, particularly when hydrogen is contained in the fuel. In terms of these aspects, it is quite desirable to systematically assess the capability of state-of-the-art turbulent combustion models to predict the flame field under the MILD combustion process [9].

There have been several research efforts [10–16] for modeling turbulence–chemistry interaction in MILD combustion conditions. Christo and Dally [10,11] numerically investigated the turbulent flame field of the JHC burner using the steady flamelet, eddy dissipation concept (EDC) and transported PDF models. These validation studies [10,11] considered three levels of oxygen concentration in the vitiated coflow and concluded that the EDC model produced better results than the flamelet model. The transported PDF approach had a prediction capability comparable to that of the EDC model [11], but it was sensitive to the level of velocity fluctuations. Christo and Dally [11] also reported that differential diffusion played an important role in these JHC flames due to the composition of the fuel (CH_4/H_2 in a ratio of 50/50 by volume).

Several other simulation studies on benchmark flames [12] in the MILD combustion environment were previously performed. Kim et al. [13] simulated the same JHC flames using the conditional moment closure (CMC) model. Their results well reproduced the effects of oxygen concentration on flame structure and NO formation however, their approach is based on the single mixture formulation, which has limitations when analyzing non-premixed flames with three-feeding inlets encountered in the MILD combustion. Frassoldati et al. [14] numerically investigated the same burner to study the effect of inlet turbulence, and applied a detailed NOx post-processor. Mardani et al. [15] studied the sensitivity of predictions for different models for differential diffusion in context with the EDC model. Ihme and See [16] applied a large eddy simulation using the flamelet/progress variable model to benchmark cases [12], and the three-stream JHC flame field was described via two mixture fractions. The first mixture fraction is associated with the mixing of fuel and coflow, while the second mixture fraction describes both the entrainment of surrounding air and non-homogeneity of the radial oxygen profile in the coflow region. This procedure properly handles the complexity of three-stream flamelet modeling for JHC burners emulating MILD combustion behavior.

MILD combustion was also studied in laboratory-scale furnaces [17–27] and semi-industrial scale furnaces for the purpose of practical application. Orsino and Weber [24] investigated a semi-industrial-scale burner using three turbulent combustion models: the eddy break-up model (EBU), the EDC model and the presumed PDF model with equilibrium chemistry. They reported that all three of these models are capable of properly predicting the overall flame characteristics such as temperature fields and low pollutant emission. Mancini et al. [25] found that the realistic prediction of entrainment via jets is a crucial element for successful modeling of MILD combustion burners. Kim et al. [26] investigated the effects of various global reaction mechanisms for modeling MILD combustion of natural gas. More recently, the experimental and numerical investigation by Danon et al. [27] reported an industrial-scale FLOX burner which fired the low calorific gases. Parente et al. [28] adopt the EDC model together with the KEE-58 kinetic scheme to numerically simulate the flameless processes encountered in a micro-cogeneration system of heat and power. Their analysis showed that a combination of an EDC combustion model and a skeletal chemistry mechanism predicted the axial profiles of mean temperature and species concentration in the flue gas with reasonable accuracy when compared to experimental values. However, the EDC model is unable to predict the extinction and re-ignition processes often encountered in MILD combustion conditions. Moreover, the EDC approach is not able to realistically describe the jet flame stabilization [29,30].

Among the state-of-art turbulent combustion models, the transported PDF model could be the most reliable approach for modeling the complex turbulent reacting flows that accompany auto-ignition, local extinction, re-ignition and pollutant formation [31,32] in MILD combustion conditions. The transported PDF model has the inherent capability to directly treat non-linear chemical source terms without any assumptions. However, the stochastic Lagrangian PDF (SLPDF) model [33] based on the Monte Carlo method is computationally excessive when used to simulate the turbulent flame encountered particularly in large-scale practical combustors. Recently, Haworth [34] extensively reviewed the progresses in the transported PDF approaches for turbulent flames. Based on the Eulerian frame, two alternative approaches are proposed to solve the transported PDF equation: the multi-environment probability density function (MEPDF) approach [35], and the stochastic Eulerian PDF (SEPDF) method [36,37].

In the SEPDF method [36,37], the joint composition PDF transport equation is solved using a set of Eulerian stochastic fields defined over the entire spatial domain. The SEPDF method specifies equi-weighted fields, which evolve according to a stochastic partial differential equation by remaining statistically equivalent to a one-point joint composition PDF. In the multi-environment PDF (MEPDF) approach [35], the joint composition PDF transport equation is approximated using a weighted discretization in composition space and the IEM micromixing model [38] and the evolution of PDFs is expressed as the set of simultaneous equations of weights and weighted abscissas. The MEPDF method has the form of a conventional Eulerian scheme and retains the desirable properties of a particle-based method.

Wang et al. [39] applied the MEPDF method to numerically investigate the reactive precipitation process in non-ideal plug-flow reactors. The direct quadrature method of moments (DQMOM) was applied to calculate the turbulent spurious dissipation rate for multi-environmental micromixing models, and the solution sensitivity for the environment number was consistently monitored. Comparisons between the MEPDF and SLPDF methods were also reported for simulations of reactive precipitation in a plug-flow reactor [39]. In context with the DQMOM-IEM approach, Gavi et al. [40] numerically studied the interaction between mixing and reaction in a confined impinging turbulent jet reactor. Akroyd et al. [41] systematically addressed essential issues of the MEPDF model to treat the diffusion term. In order to eliminate singularity and enforce boundedness, they suggested a filter function for general cases, and an analytical solution for special cases. For turbulent scalar mixing and reacting flows [42], Akroyd et al. [43] systematically compared the MEPDF and SEPDF methods in terms of formulations and computational performance. Their numerical results indicate that the MEPDF method yields better agreement with experimental data than the SLPDF approach, while the SEPDF model retains minor grid-dependence. On the other hand, for three non-premixed, piloted, methane–air turbulent jet flames [44] with the distinctly different levels of local extinction and turbulence–chemistry interactions, Jaishree and Haworth [45] made an extensive comparison of three composition PDF transport models, SLPDF, SEPDF and MEPDF, in terms of numerical accuracy and computational efficiency. According to Jaishree and Haworth [45], the numerical results of two stochastic methods (SLPDF and SEPDF)