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The influence of chemical mechanisms on PDF calculations of nonpremixed piloted jet flames ☆

Renfeng Richard Cao *, Stephen B. Pope

Mechanical and Aerospace Engineering, Cornell University, 245 Upson Hall, Ithaca, NY 14853, USA

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Abstract

Seven different chemical mechanisms for methane are used in PDF model calculations of the Barlow and Frank flames D, E, and F in order to investigate the ability of these mechanisms to represent the local extinction, reignition, and other chemical phenomena observed in these nonpremixed piloted jet flames. The mechanisms studied range from a 5-step reduced mechanism to the GRI3.0 mechanism which involves 53 species. As in several other recent studies, we use the PDF method based on the joint probability density function of velocity, turbulence frequency, and composition. Extensive tests are performed to ensure the numerical accuracy of the calculations, to relate them to previous calculations based on the same model, and to reexamine the sensitivity of the calculations (especially of flame F) to uncertainties in the pilot temperature and the treatment of radiation. As has been observed in other studies of laminar and turbulent nonpremixed flames, we find that the GRI3.0 mechanism overpredicts the levels of NO, typically by a factor of 2. Apart from this, the GRI3.0 and GRI2.11 mechanisms yield comparably good agreement with the experimental data for all three flames, including the level of local extinction and the conditional means of major and other minor species. Two augmented reduce mechanism (ARM1 and ARM2) based on GRI2.11 and containing 16 and 19 species are slightly less accurate; while the 5-step reduced mechanism and two C_1 skeletal mechanisms containing 16 species display significant inaccuracies. An examination of the autoignition and laminar-flame behavior of the different mechanisms confirms (with some exceptions) expected trends: there is an association between long ignition delay times, small extinction strain rates, and high levels of local extinction. This study again demonstrates the ability of the joint PDF method to represent accurately the strong turbulence–chemistry interactions in these flames, and it clarifies the necessary level of description of the chemical kinetics.

Keywords: PDF methods; Turbulent flames; Detailed chemistry; Mixing models

1. Introduction

In this work we use PDF methods to study the performance of seven different chemical mechanisms in the calculation of turbulence–chemistry interactions in nonpremixed turbulent flames. The calculations are compared to the experimental data of Barlow

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* Corresponding author. Fax: +1 (607) 255 1222.
E-mail address: rc239@cornell.edu (R.R. Cao).

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and Frank [1] which were obtained using the Sydney burner. This burner consists of a central fuel jet and a substantial annular pilot, and it is surrounded by a coflowing air stream. It is most fitting to describe these results in this special issue of Combustion and Flame honoring Bob Bilger. The Sydney burner was developed 20 years ago by Stärner and Bilger [2], with the aim of creating strong turbulence–chemistry interactions in a stable flame with relatively simple fluid mechanics and turbulence structure [3]. The demonstration of local extinction and reignition in these flames earned Masri and Bilger [4] the silver medal of the Combustion Institute in 1988. Single-point laser diagnostics were then applied to these flames (as reviewed by Masri et al. [5]), culminating in the experiments of Barlow and Frank [1] which are the focus of the current work. The subsequent line-imaging measurements of Karpetis and Barlow [6] yielded, in 2004, a second silver medal for work based on the Sydney burner.

The flow parameters and the pilot temperature for the nonpremixed piloted jet methane–air flames D, E, and F are listed in Table 1. The fuel, consisting of 25% methane and 75% air, with a temperature of 294 K, forms the inner fuel jet with a diameter of $D = 7.2$ mm. The flame is stabilized using a pilot with a diameter of $D_\mathrm{p} = 18.2$ mm. The pilot is a burnt lean mixture of C_2H_2, H_2, air, CO_2, and N_2, chosen to have the same elemental composition as methane/air at 0.77 equivalence ratio. The coflowing air stream has a temperature of 291 K. Flame D has a small degree of local extinction, while flames E and F have significant and increasing amount of local extinction, with flame F being quite close to global extinction. (The jet velocity in flame F is over 90% of the estimated blowoff velocity [7].)

In 2000, fifteen years after the development of the Sydney burner, the first modeling studies appeared [8–10] which convincingly and quantitatively described local extinction and reignition in these nonpremixed piloted jet methane flames. These two sets of calculations from Imperial College [10] and from Cornell [8,9] also raised questions about the two modeling ingredients at the core of turbulence–chemistry interactions, namely, the chemical mechanisms and the turbulent mixing model. The two sets of calculations use different mechanisms and different mixing models. The EMST mixing model [11] with model constant $C_\phi = 1.5$ is used in [8,9], whereas the modified Curl model [12,13] with $C_\phi = 2.3$ is used in [10].

Some recent investigations [14–16] have shed light on the relative performance of different mixing models, although our understanding remains incomplete. In general, the calculated amount of local extinction decreases with increasing C_ϕ, and EMST yields less local extinction than modified Curl (for the same value of C_ϕ). The present study aims at advancing our understanding of the issues related to chemical mechanisms.

There are some recent studies of the Barlow and Frank flame D using PDF methods with detailed chemistry [17,18]. Raman et al. [17] calculated the mean profiles and conditional means in flame D using the joint velocity–composition PDF method with the detailed GRI mechanisms (GRI3.0 and GRI2.11) and a 16-species reduced mechanism. In this work, we present PDF calculations of flames D, E, and F using seven different mechanisms. These range from a 5-step reduced mechanism [19,20], to the GRI3.0 detailed mechanism [21] which involves 53 species and 325 reactions. The principal results considered (which are compared to the experimental data [22,23]) are the burning index [8] and means of temperature and species mass fractions conditional on mixture fraction.

In previous work [8,10], it has been found that the calculated level of local extinction (particularly in flame F) is sensitive to the value of the mixing model constant C_ϕ. The base case considered here uses $C_\phi = 1.5$, the value used in conjunction with the EMST [11] model in the previous studies of these flames [8,9]. The present calculations, using the most comprehensive detailed methane mechanisms (i.e., GRI2.11 and GRI3.0), verify that this value of C_ϕ is appropriate. We also investigate the sensitivity of PDF calculations using different chemical mechanisms to the mixing model constant C_ϕ.

Previous calculations [9] have revealed that some flames exhibit a strong sensitivity to the temperature

Table 1
Flow parameters of flames D, E, and F

Flame	Re_jet	$U_\mathrm{j,b}$ (m/s)	$U_\mathrm{p,b}$ (m/s)	U_c (m/s)	T_p (K)	Local extinction
D	∼22,400	49.6	11.4	0.9	1880	Little
E	∼33,600	74.4	17.1	0.9	1880	Moderate
F	∼44,800	99.2	22.8	0.9	1860	Severe

$U_\mathrm{j,b}$ is the bulk velocity for the fuel jet; $U_\mathrm{p,b}$ is the bulk velocity for the pilot; U_c is the coflow velocity; T_p is the pilot temperature.