Combustion and Flame 166 (2016) 113–124

Contents lists available at ScienceDirect

Combustion and Flame

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

Two-dimensional flow effects on soot formation in laminar premixed flames

Y. Xuan[a,*], G. Blanquart[b]

[a] Department of Mechanical and Nuclear Engineering, Pennsylvania State University, University Park, PA 16802, USA
[b] Department of Mechanical Engineering, California Institute of Technology, Pasadena, CA 91125, USA

ARTICLE INFO

Article history:
Received 22 July 2015
Revised 28 December 2015
Accepted 11 January 2016
Available online 18 February 2016

Keywords:
Soot
Laminar premixed flames
Two-dimensional flow effects

ABSTRACT

Experimental measurements on axisymmetric laminar premixed flames have been used extensively for chemical and soot model validation. Numerical simulations of these flames always rely on the assumption of one-dimensionality. However, the presumed one-dimensionality has not been justified in general, and may not be valid under all circumstances. In the current work, two-dimensional flow effects are investigated in four representative ethylene/air laminar premixed flames, which have been selected as validation targets for the International Sooting Flame workshop. These flames cover all typical experimental arrangements, namely stabilizing plate, steel plate with centered hole, and enclosed chamber. To assess the assumption of one-dimensionality, detailed numerical simulations with finite-rate chemistry are performed with the exact experimental set-ups. It is shown that flow entrainment and acceleration are significant for all four flames. Further, it is found that the flame centerlines cannot be approximated as one-dimensional, since the mass flow rates vary substantially along the centerlines. As a consequence, non-negligible differences are found between the soot profiles predicted in two-dimensional simulations and in simulations where one-dimensionality is assumed. Using data extracted from the two-dimensional simulations, a modified one-dimensional model is derived on the flame centerline to include two-dimensional effects. Results from the modified one-dimensional model are compared against detailed, two-dimensional simulation results and experimental measurements.

1. Introduction

The combustion of fossil fuels in practical devices is responsible for the generation of a wide range of pollutants including soot particles. Due to the strong adverse effects of soot on human health and the environment, stricter legislation governing soot emission in engineering applications has been adopted since the past decade. This makes the development of low emission combustion systems a necessity. The design of such devices relies on the accurate prediction of soot yield in combustion environments, which requires a more fundamental understanding of the various soot formation mechanisms.

Our current understanding of the chemical kinetics, structure, and transport of soot has been achieved through comparisons between predictions of different models against experimental data in a variety of flame configurations, including both laminar flames [1–26] and turbulent flames [27–34], as well as both premixed flames [1–19,27–29] and non-premixed flames [20–26,30–34]. However, the lack of coordination among the experimental flame configurations makes it difficult to assess the predictive capability of the various soot models. It is only until recently that a structured database of well-characterized target sooting flames has been established, within the framework of the International Sooting Flame (ISF) workshop [35]. In this workshop, series of burner-stabilized laminar premixed flames, laminar co-flow non-premixed flames, turbulent sooting flames, and pressurized flames were selected as validation targets for numerical models. The major advantage of burner-stabilized laminar premixed flames over other flame types is that the fluid flows are relatively simple. Therefore, the effects of soot transport become secondary, and the soot yield is primarily governed by the soot formation chemistry. Another advantage of this flame configuration is that these "flat" flames are typically assumed to be one-dimensional, which makes the numerical prediction of soot formation computationally efficient, even when relatively large chemical kinetic mechanisms are employed [4,6,7].

The experimental arrangements of these laminar premixed flames generally involve porous plate burners to produce a flat flame, and some flame stabilization mechanisms. For instance, it

* Corresponding author.
E-mail address: yux19@psu.edu, yxuan.caltech@gmail.com (Y. Xuan).

http://dx.doi.org/10.1016/j.combustflame.2016.01.007
0010-2180/

Table 1
Physical parameters and experimental details on the four representative premixed flames.

	Flame 1 (ISF Flame 1a)	Flame 2 (ISF Flame 2a)	Flame 3 (ISF Flame 3a)	Flame 4 (ISF Flame 4b)
Fuel/oxidizer	C_2H_4/air	C_2H_4/air	C_2H_4/air	C_2H_4/air
Equivalence ratio	2.07	2.34	2.1	2.5
C/O ratio	0.69	0.78	0.7	0.834
Pressure	1 atm	1 atm	1 atm	1 atm
Unburnt injection velocity	5.88 cm/s	6.73 cm/s	6.44 cm/s	7.84 cm/s
Burner diameter	56 mm	60 mm	60 mm	41.3 mm
Burner temperature	320 K	320 K	320 K	320 K
Stabilization mechanism	Wire grid	Holed aluminum plate	Steel plate	Pilot flame
Co-flow stream	C_2H_4/air flame	Nitrogen flow	Nitrogen flow	CH_4/air flame and air flow
Co-flow diameter	75 mm	70 mm	70 mm	61.3 mm and 150 mm
Enclosed chamber	Yes	No	No	No
References	[1–4]	[5–7]	[8–13]	[17]

is quite standard to introduce a steel plate downstream above the burner to stabilize the flame [8–14]. Such plate perturbs significantly the flame, introduces a stagnation point on the flame centerline, and may have non-negligible effects on soot formation at upstream locations. Other flame stabilization set-ups include the implementation of holed steel plates [5–7] and wire grids [1–4] above the flame. All these flame stabilization apparatus make the experimentally measured flames inherently multi-dimensional. Further, buoyancy effects in these flames may be important, especially as the injection velocity for the fuel/air mixtures is generally small. The hot plume downstream of the flame front, where soot dynamics is still active, is essentially buoyancy-driven and could cause substantial flow entrainment which would further enhance the multi-dimensional nature of these flames. Finally, shielding co-flow air streams or leaner premixed flames are frequently employed in these flames [1–13,17] to prevent perturbations from the environment. The presence of these co-flow streams may substantiate heat transfer in the radial direction, especially when shielding flames are used [17]. Since these laminar premixed flames are all axisymmetric, the multi-dimensional effects stated above will be referred to as two-dimensional in the rest of the paper.

These burner designs have been used for many years for laminar premixed flame studies without any major issue related to two-dimensional flow effects, since the major flame characteristics and the oxidation chemistry of hydrocarbon fuels are resilient to such effects. However, due to the high sensitivity of soot formation to residence time and local temperature, the two-dimensional flow effects in these burner-stabilized flames, as discussed above, are expected to be more important for soot research. Despite these potentially strong two-dimensional effects, the comparison between experimental data and numerical predictions, where one-dimensionality is assumed, is still a common practice for chemical kinetic and soot model validation. The one-dimensionality assumption has not been validated previously and the two-dimensional flow effects on soot yield have not been quantified in these flames.

The objective of this work is two-fold. The first objective is to assess the importance of two-dimensional effects on soot formation in a few selected representative burner-stabilized flames. The second objective is to derive a simplified numerical framework for these flames, including the two-dimensional effects, based on a budget analysis using detailed, two-dimensional flame simulation results. The intent of this paper is *not* to achieve accurate soot predictions in these flames or to develop new physical models, but to establish an appropriate and efficient numerical framework that allows for fair comparisons between experimental data and simulation results, which can be used for chemical and soot model validation.

The paper is organized as follows. The experimental configurations of the selected representative flames are presented and discussed in Section 2. The numerical methods and models employed are described in Section 3. Predictions of soot formation from both two-dimensional and one-dimensional simulations are compared to experimental measurements in Section 4. In Section 5, a budget analysis is carried out on species and temperature equations, from which a simplified one-dimensional numerical framework accounting for two-dimensional flow effects is derived and validated.

2. Representative laminar premixed flames

Four representative laminar premixed flames are selected in this work, covering all experimental arrangements typically employed for flame stabilization. All four flames are target flames selected by the ISF workshop. More specific details about these flames and the experimental set-ups are included in Table 1 and summarized below. Sketches depicting all four flame configurations are included in Fig. 1.

The first flame selected in this work is Flame 1a in the laminar premixed flame series from the ISF workshop. A 56 mm diameter, water-jacketed tubular steel capillary burner is used. The central flat flame burner is surrounded by a flat shielding burner. This two-burner-setup is protected against convection of the surrounding air by a glass tube with two wire grids placed 80 mm and 100 mm above the burner, respectively.

The second flame selected in this work is Flame 2a in the laminar premixed flame series from the ISF workshop. This flame is produced by a 60 mm diameter porous-plate laminar premixed flat-flame burner at atmospheric pressure (McKenna model). The reactant mixture at the burner exit is surrounded by an annular nitrogen flow to eliminate peripheral diffusion. The burner is cooled using water at room temperature with a flow rate sufficiently high. The flame is stabilized using a 125 mm diameter circular aluminum plate with a 30 mm hole in the center that is mounted 32 mm above the burner surface.

The third flame selected in this work is Flame 3a in the laminar premixed flame series from the ISF workshop. This flame burns on a water-cooled, McKenna burner, which has a sintered bronze plug with a diameter of 60 mm. An outer co-flow of nitrogen shields the flame from room air entrainment. The flame is stabilized with a stainless steel plate (same diameter as the burner) located 21 mm above the burner. This burner, together with the stabilization mechanism, has also been proposed as a standard test case for the International Workshop and Meeting on Laser-Induced Incandescence [36].

The last flame selected is Flame 4b in the laminar premixed flame series from the ISF workshop. The central, sooting flame (ethylene/air) is stabilized above a water-cooled sintered bronze matrix. This flame is surrounded by a non-sooting shielding flame of methane/air with an equivalence ratio ϕ=1.68. This shielding