Available online at www.sciencedirect.com

ScienceDirect

Proceedings of the Combustion Institute 35 (2015) 821–829

Proceedings of the Combustion Institute

www.elsevier.com/locate/proci

Direct numerical simulations of probe effects in low-pressure flame sampling ☆

Vyaas Gururajan [a,*], Fokion N. Egolfopoulos [a], Katharina Kohse-Höinghaus [b]

[a] Department of Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, CA 90089-1453, USA

[b] Department of Chemistry, Bielefeld University, Universitätstrasse 25, D-33615 Bielefeld, Germany

Available online 9 July 2014

Abstract

Speciation studies of low-pressure flames using intrusive sampling and molecular beam mass spectrometry analysis are essential towards developing and validating combustion models. In order to assess potential probe-induced effects, direct numerical simulations of a realistic experimental configuration were carried out using a finite-volume fully compressible code as well as detailed descriptions of chemical kinetics and molecular transport. A 50 mbar rich propene/oxygen/argon flame was modeled for which experimental data are available. The effects of the probe and supporting flange, non-adiabaticity, sampling location, and compressibility when there is suction through the sampling orifice were assessed. Results showed that even under adiabatic conditions, the presence of the probe-flange assembly affects the flow field two-dimensionally. Furthermore, the effects of heat loss and compressibility were found to be significant at the sampling location. Important radicals for fuel oxidation such as OH and HCO, and for soot formation such as C_3H_3 are affected by the sampling procedure and their concentrations at the sampling location can differ notably compared to unperturbed one-dimensional flames.

Keywords: Low-pressure flames; Flame sampling; Flame structure; Flame chemistry; Premixed flames

1. Introduction

Data obtained in laminar flames are key towards the development and validation of kinetic models. Although experimental methods have advanced over the past few decades (e.g., [1]), there are still uncertainties associated with standard experiments (e.g., [2]) that could have a major effect on kinetics given the relatively low sensitivity of flame properties to rate constants [3]. Minimizing experimental uncertainties requires the in-depth understanding of the controlling physics of the experimental approach as well as rigorous assessment of the assumptions of the hydrodynamic model that is used in the numerical simulations.

☆ Accepted for presentation at the 35th International Symposium on Combustion, San Francisco, California, USA, August 3–8, 2014.

* Corresponding author. Fax: +1 213 740 8071.
E-mail address: gururaja@usc.edu (V. Gururajan).

http://dx.doi.org/10.1016/j.proci.2014.06.046
1540-7489/

Molecular beam mass spectrometry (MBMS) [4] is among the leading techniques in measuring species concentrations in chemically reacting flows. The method mainly comprises probing a low-pressure (40–100 mbar) burner-stabilized premixed laminar flame with a conical quartz nozzle at various depths in order to characterize the chemical structure. Having been a staple in combustion chemistry studies for more than fifty years and serving as an invaluable tool in kinetics studies [5], the method nonetheless suffers from an inescapable drawback, namely the potential distortion by the probe of the flame from its one-dimensional adiabatic structure that is assumed in numerical simulations. This issue of probe-induced effects on flames is not limited to the MBMS technique. For instance, gas chromatography measurements are just as prone to these distortions [6]. Efforts in the past [7–9] have focused on quantifying these systematic errors to be able to "subtract" them out. Recently, Struckmeier et al. [10] published the results of a comprehensive experimental investigation on the effects of probe angle, orifice diameter, and other experimental parameters of the flame structure. Skovorodko et al. [11] developed a code to model the entire experimental domain including the expansion section in the nozzle. However, this was done using single-step chemistry and by spatially fixing the source terms in the energy and species conservation equations.

A systematic and rigorous computational study of probe effects in low-pressure flame sampling that delineates the effects of all the relevant boundary conditions while incorporating detailed chemistry has yet to appear. One possible reason for this is the lack of freely available, open-source numerical codes that could be modified to describe the exact laboratory conditions and used by experimentalists. Recently, Cuoci et al. [12] have advanced the laminarSMOKE finite-volume based code built using the OpenFOAM [13] suite of CFD tools and the OpenSMOKE [14] library of functions that handles detailed chemistry and transport while offering an interface to various ODE solvers. The code also incorporates a robust algorithm for time stepping, making it amenable to the stiff chemistry normally encountered in combustion applications.

The goal of this investigation was to perform for the first time direct numerical simulations of the probe effects on the structure of a low-pressure laminar flame and to assess the deviations from results obtained in unperturbed flames; it should be noted that in direct numerical simulations all pertinent spatial and temporal scales are resolved without any simplifying assumption in any type of flow laminar or turbulent alike. Towards that goal, the laminarSMOKE [13] code was adopted to conditions that are close to the experimental ones. The simulations are considered as direct given that the fluid mechanics, chemical kinetics, and heat and mass transport processes were modeled based on the current state-of-the-art knowledge and without invoking any simplifying assumptions. This approach will lay the fundament for further study with the aim to provide correction rules for existing data and result eventually in an optimized probe design that would cause a minimum disturbance to the flame.

2. Modeling approach

Numerical simulations of the three-dimensional problem coupling fluid dynamics and full chemistry in this study are based on the laminarSMOKE code which addresses the stiff chemistry [15] component of reacting flows by employing the Strang splitting [16], a procedure founded on the premise that for suitably small time steps the processes of molecular transport and reaction can be separated into a sequence of time integrations wherein the final solution of the transport step is the initial condition for the reaction step. The reaction step is thus reduced to a spatial array of homogeneous reactors with appropriate initial conditions whose time integration is handled by standard ODE solvers such as DVODE [17] that was used in the present study. The Strang splitting layer is superimposed on the well-established PISO algorithm (Pressure Implicit with Splitting of Operators) [18] for the pressure-velocity coupling, to complete the algorithm for solving the discretized conservation equations [19].

The study was performed for a 50 mbar propene/oxygen/argon mixture at an equivalence ratio $\phi = 2.3$ with mole fractions 0.255/0.495/0.25, respectively, a C/O ratio of 0.773, and a velocity of 48 cm/s at the burner exit that is the inlet of the solution domain; matching the experiments in [9]. The USC Mech-II kinetic model [20] was reduced from 117 species to 34 species using the directed relation graph (DRG) method [21] to save computational cost while preserving the essential aspects of the flame structure; the reduced model can be found in Table S1 of Supplementary material along with comparisons of temperature and key species profiles with the detailed model. Thermal radiation and Soret diffusion were not included, and the thermodynamic, transport, and kinetic properties were evaluated using the OpenSMOKE library [14]. The Soret diffusion formulation is not available in the current version of laminarSMOKE. The code will be modified to account for it in subsequent studies in which the aim will be to perform quantitative comparisons against available experimental results.

The axisymmetric geometry of the solution domain as seen in Fig. 1 was enclosed by the surfaces whose boundary conditions are defined in Table 1 for all cases considered. These cases were