



ELSEVIER

Available online at www.sciencedirect.com

SCIENCE @ DIRECT®

Proceedings of the Combustion Institute 30 (2005) 383–390

Proceedings
of the
Combustion
Institute

www.elsevier.com/locate/proci

Further studies of the reaction kernel structure and stabilization of jet diffusion flames

Fumiaki Takahashi^{a,*}, Viswanath R. Katta^b

^a National Center for Microgravity Research on Fluids and Combustion, NASA Glenn Research Center, Cleveland, OH 44135, USA

^b Innovative Scientific Solutions, Inc., Dayton, OH 45440, USA

Abstract

The structure of axisymmetric laminar jet diffusion flames of ethane, ethylene, acetylene, and propane in quasi-quiet air has been studied numerically in normal earth gravity (1g) and zero gravity (0g). The time-dependent full Navier–Stokes equations with buoyancy were solved using an implicit, third-order accurate numerical scheme, including a C₃-chemistry model and an optically thin-media radiation model for heat losses. Observations of the flames were also made at the NASA Glenn 2.2-Second Drop Tower. For all cases of the fuels and gravity levels investigated, a peak reactivity spot, i.e., *reaction kernel*, was formed in the flame base, thereby holding a trailing diffusion flame. The location of the reaction kernel with respect to the burner rim depended inversely on the reaction-kernel reactivity or velocity. In the C₂ and C₃ hydrocarbon flames, the H₂–O₂ chain reactions were important at the reaction kernel, yet the CH₃ + O → CH₂O + H reaction, a dominant contributor to the heat-release rate in methane flames studied previously, did not outweigh other exothermic reactions. Instead of the C₁-route oxidation pathway in methane flames, the C₂ and C₃ hydrocarbon fuels dehydrogenated on the fuel side and acetylene was a major hydrocarbon fragment burning at the reaction kernel. The reaction-kernel correlations between the reactivity (the heat-release or oxygen-consumption rate) and the velocity, obtained previously for methane, were developed further for various fuels in more universal forms using variables related to local Damköhler numbers and Peclet numbers.

© 2004 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

Keywords: Diffusion flame; Flame stability; Flame structure; Reaction kernel; Microgravity combustion

1. Introduction

Diffusion flame holding and lift-off phenomena are of essential importance in relation to both earth-bound combustion systems and spacecraft fire safety. To elucidate flame stability mecha-

nisms, the structure of the flame-stabilizing region must be known. Numerous studies of the structure and stability of laminar diffusion flames have been conducted in both normal earth gravity (1g) and microgravity (μg) [1–12]. Although several attempts [1–3] were made to reveal the internal structure of the flame-stabilizing region experimentally, most previous works were limited to overall flame characteristics. Qin et al. [13] examined the local conditions of the lifted triple flame structure in a partially premixed methane jet.

* Corresponding author. Fax: +1 216 977 7065.

E-mail address: Fumiaki.Takahashi@grc.nasa.gov (F. Takahashi).

In previous papers [14–17], by using a comprehensive computational fluid dynamics code [18] with a detailed chemistry model for methane combustion, the authors have revealed the complex chemical kinetic structure of the stabilizing region of both jet and flat-plate diffusion flames, predicted the flame lifting limit, and proposed diffusion flame stability mechanisms. Because of the unique geometry of the flame-stabilizing region, forming an edge of a diffusion flame, back-diffusion of radical species in every downward direction into a surrounding oxygen-rich environment dramatically enhances chain-branching and exothermic reactions. As a result, a peak reactivity spot, i.e., *reaction kernel*, which is responsible for holding a trailing diffusion flame, is formed. In methane flames, the chain-branching reaction, $H + O_2 \rightarrow OH + O$ (R1), and the dominant exothermic reaction, $CH_3 + O \rightarrow CH_2O + H$ (R46), are particularly important in the fuel-lean reaction kernel. To obtain more universal results, we must address the following questions. How does the chemical kinetic structure of the reaction kernel vary for higher hydrocarbon fuels? How does it affect flame stabilization? What parameters determine the location of the reaction kernel? This paper reports the new results for various C_2 and C_3 hydrocarbons. It is of particular interest to investigate the fate of a distinct role of the methyl radical in methane flames.

2. Numerical methods

The numerical code (UNICORN) used in this study, developed by Katta et al. [18], is described in more detail elsewhere [14]. Time-dependent axisymmetric governing equations consist of continuity, axial and radial full Navier–Stokes momentum, energy, and species conservation equations with the ideal-gas equation of state. The momentum equations are integrated using an implicit QUICKST numerical scheme [18] for the convection terms, which is third-order accurate in both space and time and has a very low numerical-diffusion error. The finite-difference form of the species and enthalpy is obtained using the hybrid scheme with upwind and central differences. Viscosity, conductivity, and diffusivity are estimated using molecular dynamics and mixture rules. The enthalpy of each species is calculated from polynomial curve fits. A C_3 -chemistry model [19,20] used for all fuels consists of 33 species and 112 elementary steps, which include C_1 - and C_2 -chemistry used for methane previously [14–17]. A simple radiation model [21] based on an optically thin-media assumption was incorporated into the energy equation for radiative heat losses from CO_2 , H_2O , CH_4 , and CO .

The computational domain of 60×50 mm in the axial (z) \times radial (r) directions is represented

by a mesh of up to 601×201 with clustered grid lines near the axisymmetric jet exit and a minimum spacing of 0.05 mm. The inner diameter and lip thickness of the fuel tube are $d = 3$ and 0.5 mm, respectively. The fuel tube exit plane is placed 10 mm downstream from the inflow boundary in the open computational domain. Flat velocity profiles in the fuel tube and boundary layer velocity profiles outside the burner tube are prescribed. The initial and boundary conditions for the axial (U) and radial (V) velocities and species and energy at different flow boundaries are the same as in previous works [14–17].

The mass flow rate of each fuel is adjusted such that the total oxygen requirement based on the stoichiometric expression is equal to that of methane studied previously. The fuel type, the mean fuel jet velocity (U_j), the mean air velocity (U_a), and gravity level, in addition to the methane flames studied previously [17], are as follows:

Case 1: ethane, $U_j = 0.06857$ m/s; (a) $U_a = 0.001$ m/s, 1g, (b) 0g, (c) $U_a = 0.12$ m/s, 0g.

Case 2: ethylene, $U_j = 0.08$ m/s; (a) $U_a = 0.001$ m/s, 1g, (b) 0g, (c) $U_a = 0.12$ m/s, 0g.

Case 3: acetylene, $U_j = 0.096$ m/s; (a) $U_a = 0.001$ m/s, 1g, (b) 0g.

Case 4: propane, $U_j = 0.048$ m/s; (a) $U_a = 0.001$ m/s, 1g, (b) 0g.

3. Results and discussion

Observations of the flames in μg were made in the NASA Glenn 2.2-Second Drop Tower. Figure 1 shows video images of axisymmetric ethane jet diffusion flames (2.87 mm i.d.) in still air at the elapse time after ignition of $t = 3$ s in 1g (Fig. 1A) and $t = 2.2$ s in μg (Fig. 1B). The burner image is superimposed. The fuel mass flow rate (0.61 mg/s, $U_j = 0.077$ m/s at 294 K and 0.98 atm) was close to that for the computation. Blue flame emission in both 1g and μg was brighter than those in methane flames [17], and an orange flame tip due to soot formation in 1g was also brighter and expanded [this trend was more evident in propane flames (not shown)]. In 1g, the flame quickly reached a steady state. The visible (blue) flame width was 5.5 mm, and the height was ambiguous due to soot. The flame base location was 0.2 mm lower than the jet exit and 0.6 mm away from the burner wall. In μg , the flame expanded for the entire drop period. At $t = 1$ s (not shown), the visible flame width was 14.6 mm. At $t = 2.2$ s, soot formed initially at ignition almost disappeared. The flame width and height (from the jet exit) were 16.9 and 12.7 mm, respectively, and the flame base location was 4.1 mm lower than the exit and 3 mm away from the burner.

Download English Version:

<https://daneshyari.com/en/article/9637357>

Download Persian Version:

<https://daneshyari.com/article/9637357>

[Daneshyari.com](https://daneshyari.com)