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Structure of incipiently sooting partially premixed ethylene counterflow flames

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ABSTRACT

We perturbed an atmospheric-pressure ethylene diffusion flame by progressively adding oxygen in the fuel stream, while holding constant peak temperature and stoichiometric mixture fraction. The resulting partially premixed flames presented a well-defined double-flame structure, with a (lightly) sooting region sandwiched between a premixed flame component and a diffusion flame one. Temperature measurements were performed using fine thermocouples and thin filament pyrometry, whereas species concentrations profiles of CO₂, CO, N₂, O₂, H₂ and C1–C12 species, including aromatics, were determined by gas sampling through a quartz microprobe followed by GC–MS analysis. In addition to the diffusion flame, two of the flames, at equivalence ratio, $\Phi = 6.5$ and $\Phi = 5.0$, were probed in detail with these diagnostic techniques. A fourth flame at $\Phi = 3.0$ was examined only qualitatively because of excessive soot presence. The premixed flame component of the dual flame structure and the diffusion flame one are coupled both thermally and chemically. Soot formation increases with lowering equivalence ratio and increasing temperature, a trend that is consistent with that of purely premixed strained flames stabilized against a hot nitrogen counterflow, as confirmed computationally by comparing profiles of a critical soot precursor such as benzene. However, partially premixed flames, probably as a result of the back diffusion of key radicals such as H and OH from the diffusion flame component, have a lower tendency to soot as compared to purely premixed ones. Comparison of measurements with computational results using two detailed chemical kinetic mechanisms show good agreement for major species once the velocity boundary conditions are properly determined via 2-D modeling of the flow within the burner. In one case, the agreement is also good for some soot precursors such as benzene, despite mismatches in some critical intermediates. Reaction path analysis suggests an increasingly larger contribution of the C3 path to benzene formation with the lowering of the equivalence ratio. The database with the measurements of primary reactants, products and intermediates, including critical soot precursors up to 3-ring aromatics is available to developers of chemical reaction mechanisms.

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1. Introduction

Partially premixed flames (PPFs) are rich flames in which the fuel feed stream is premixed with some amount of oxidizer. If the equivalence ratio is above the rich flammability limit, the flame does not propagate; if it is below such a limit, it still retains its propagating capabilities. In either case the unburned fuel products can be further oxidized in a nonpremixed or diffusion-controlled regime yielding a dual flame structure. These flames are of relevance to turbulent combustion in which, even if the fuel and oxidizer are originally separated at their injection in the combustion chamber, turbulence may engender some level of premixing with combustion taking place in a stratified medium [1, 2], with a broad range of equivalence ratios from very rich to lean. This situation is relevant to gas turbine combustion and

internal combustion engines, especially in the near-injector region. Even in nonpremixed turbulent combustion one can envision conditions of local extinction with a break in the flame surface, which will cause mixing of fuel and oxidizer, with ensuing partial premixing. Lastly, PPFs intervene in the stabilization of lifted turbulent flames via edge flames and, in some cases, triple flames consisting of a rich branch, a lean one, with a trailing diffusion flame fed by unburned CO and H₂ from the premixed side [3].

In this study we examine PPFs in the soot context in the light of some work on compression ignition (CI) engines. Although such engines have been traditionally presented as a prototypical example of diffusion (nonpremixed) flames, the application of advanced laser diagnostic techniques challenged this concept [4]. The prevailing view is now that vaporization and mixing occur reasonably fast for the initial soot loading in the vicinity of the injector to be generated under rich *premixed* combustion [5]. Subsequently, soot grows and is oxidized across an envelope nonpremixed flame further downstream that is formed between the products of the rich

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premixed flame and the oxidizer. This scenario is very different from that typical of diffusion flames where soot is nucleated on the fuel side, under conditions of virtually infinitely large equivalence ratio. The simultaneous presence of oxidizing species with soot particulate affects the sooting process qualitatively and quantitatively by providing an opportunity for oxidation to act in parallel with soot formation [6]. As a result, a detailed understanding of soot formation in partially premixed flames is in order, especially under the high-pressure conditions that are typical of these engines.

The critical missing step in our understanding of soot formation is the inception (or nucleation) stage [7–12], where the transition from parent fuel gas molecules to soot nanoparticle occurs. To shed light on this step, a detailed chemical characterization of the flame is indispensable, which inevitably requires sampling followed by the application of analytical chemistry techniques. Engines are poorly suited to detailed probing. We chose instead well-controlled *laminar* flames in which the soot challenges can be decoupled from complications associated with turbulence and the presence of the droplet phase, without sacrificing the coupling of chemistry and transport.

With this in mind, we established a well controlled testbed consisting of a laminar counterflow with a rich mixture fed from one side, the oxidizer from the other and a mixed scenario of premixed-flame/diffusion flame in between, in what has been defined as two-stage combustion in one of the first studies of this type in counterflow [13]. This configuration is ideal to put in evidence the dual flame structure that had been observed in CI engines. It lends itself also to simple, mostly one-dimensional, computational modeling with well-specified boundary conditions, using detailed chemical kinetics, including soot precursors.

As a first step towards the characterization of these flames under high-pressure conditions of relevance to engines, we focus here on atmospheric pressure $C_2H_4/O_2/N_2$ premixed streams counterflow to a N_2/O_2 stream, with equivalence ratios ranging from infinite (diffusion flame) to $\Phi = 3$, under conditions of incipient or moderate sooting that are compatible with gas sampling by quartz microprobe. Sampling is followed by analysis with standard analytical chemistry techniques to quantify chemical growth to soot precursors such as polyaromatics, as in our previous work [14–17].

There have been several studies on soot formation in PPFs. The most relevant ones in the present context are those with two ingredients: (a) a two-stage combustion, with a premixed flame and a diffusion flame sandwiching a lightly sooting region, in an “interdependent regime” [18] and (b) chemical speciation including aromatics and other soot precursors. A broad study on this type of flames using heptane as a diesel fuel surrogate was conducted in [19,20], but these authors’ experimental emphasis was not on soot formation, even though they did consider numerically the effect of strain rate and equivalence ratio on critical soot precursors. A computational follow-up study from the same lab, partially validated with the experimental data in [19,20] on purely diffusive flames, focused on the effect of the parent fuel molecular structure on soot formation [21].

2. Experimental methods

Burner geometry and experimental techniques are extensively discussed in previous articles [16,17] and only a brief description will be provided here. Combustion is established in a counter flow burner, including a nitrogen shroud that shields the flame from room drafts and ensures burning in the controlled atmosphere that is determined by the composition of the feed streams. The combustor consists of two identical opposed converging nozzles with an area ratio of 9, and an internal diameter of 6.35 mm at the outlet. The premixture is issuing from the bottom nozzle, the oxidizer from the top one and each convergent section is preceded by a short straight section containing glass beads and meshes to uniformize the flow coming from the feed lines. Sampling starts by drawing gas through a small silica capillary

tube (OD/ID = 0.14 mm/0.10 mm), connected to the GC–MS system by a heated metal tube. The probe tip is positioned near the flame axis and a motorized vertical stage displaces the combustor allowing for the scan of the entire flame structure. To collect a sample, a valve separating the GC–MS from the line is opened and the sample is drawn into the sample storage volume that had been initially kept under vacuum (< 1 mbar). The line and the valve are kept at 423 K to prevent condensation of heavy species. Once the sample is retrieved from the flame, it is split into three columns whose outlets are connected to different sensors: a thermal conductivity detector (TCD) for H_2 , O_2 and N_2 , a flame ionization detector (FID) for CO, CO_2 , and hydrocarbons up to C_2 , with a methanizer converting CO and CO_2 to CH_4 , and a mass spectrometer (MS) for larger hydrocarbons and aromatics up to acenaphthylene. Gaseous calibration is performed with calibrated bottles (Scotty®) for CO, CO_2 , C_2H_2 , C_2H_6 , while calibrated flows are obtained with flow controllers for CH_4 , C_2H_4 , H_2 , O_2 and N_2 . The MS is calibrated both with reference gas mixtures (Scotty®) and with liquid mixtures of the compound of interest, atomized with an electrospray in a stream of hot nitrogen that allows vaporization and perfect mixing. Knowledge of the mass flow rate of the mixture (through a syringe pump) and of the nitrogen stream leads to the production of a calibrated flow of heavy hydrocarbons. The analysis is run on-the-fly while the probe is kept in idle state until the subsequent sample is drawn. The cumulative error in measured concentrations is estimated at $\pm 7.5\%$ for light species (up to 32 AMU) and $\pm 15\%$ for the heavier ones by considering the uncertainties associated with calibration, sampling and analysis procedures. Temperature measurements are performed with a 50 μm Pt/Pt-13% Rh cylindrical bead thermocouple and by thin filament pyrometry using a 13 μm SiC wire. Standard corrections for radiative losses are applied to the thermocouple measurements.

The relative position between the probe measuring point and the blue chemiluminescent layer of the diffusion flame is recorded with a digital camera. This distance is measured with an accuracy of $\pm 50 \mu m$ by image processing and is used to reconstruct the spatial profiles and correct for the probe intrusiveness, in case it did affect the actual position of the flame with respect to the boundaries. As reported in [17], this approach yields spatially resolved measurements even in thin flames under high-pressure conditions.

2.1. Computational modeling

The experimental study is supplemented with one dimensional computational modeling of the flames using the OPPDIFF code [22] integrated with the CHEMKIN [23] and the transport [24] subroutine libraries. The detailed chemistry is modeled with two chemical mechanisms: USC-MechII [25] that is optimized for the prediction of laminar flame speed of flames fueled by C1–C4 hydrocarbons, and the mechanism in [26], heretofore referred to, in brief, as Pitsch mechanism, tracking the aromatic growth up to relatively large species. Multicomponent diffusion coefficients and thermal diffusion are accounted for in the transport model provided with the mechanisms. In registering the experimental profiles with the computational ones the blue chemiluminescence of the diffusion flame is overlapped with the position of the computed peak concentration of CH_2^* on the oxidizer side of the gas stagnation plane (GSP).

To account for possible departures in the boundary conditions from the ideal plug flow ones, we model the baseline diffusion flame with a two-dimensional axisymmetric model including the flow in the burner nozzles and shroud housing, using COMSOL Multiphysics (Comsol Inc.). A simplified chemical reaction mechanisms using 10 species and 5 reactions [27] is used for these simulations. The model yields modified boundary conditions in terms of both value and axial gradient of the axial velocity component along the centerline. Once these modified boundary conditions are used in the one-dimensional Chemkin calculations, the temperature profile along the centerline is

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