THE EFFECT OF OXYGENATED FUELS ON ETHYLENE LAMINAR PREMIXED FLAME: AN EXPERIMENTAL AND NUMERICAL STUDY

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Abstract

This study explores the impact of doping ethylene/air premixed flames with ethanol (EtOH) or OME_3, each contributing 20% of the total carbon, across equivalence ratios $\Phi = 2.01–2.46$. Through combined experimental and numerical analysis, the work offers a detailed understanding of how these oxygenated additives influence soot formation and flame chemistry in rich combustion conditions.

Introduction

In the context of the global shift from fossil fuels to sustainable energy sources, this study explores the impact of oxygenated fuels—specifically ethanol (EtOH) and oxymethylene ether (OME_3)—on gas-phase chemistry and particle formation in ethylene/air laminar premixed flames. EtOH, the most common biofuel, and OME_3, a promising e-fuel with high oxygen content and no C–C bonds, are both known to influence combustion processes and emissions. The presence of oxygen in these fuels modifies oxidation and growth pathways, potentially reducing soot precursor formation and overall particulate emissions. However, the generation of oxygen-rich nanoparticles remains a concern due to their distinct reactivity and possible toxicity. This work analyzes flames with equivalence ratios ranging from $\Phi = 2.01$ to 2.46, covering a transition from near- to heavily-sooting regimes. A combined experimental and numerical approach is adopted to characterize the combustion behavior and elucidate the mechanisms driving soot and nanoparticle formation under these conditions.

Experimental setup

Premixed ethylene flames were stabilized at atmospheric pressure on a water-cooled McKenna burner, with a cold gas velocity of 10 cm/s and a preheat temperature of 200 °C. A stainless steel plate positioned above the burner aided flame stabilization. Ethanol (EtOH) and OME_3 were added via syringe pump to constitute 20% of the total carbon input, while nitrogen dilution was adjusted to maintain constant total carbon flow, equivalence ratio, and velocity. The burner was cooled to 80 °C to ensure full evaporation of the oxygenated fuels. The ethylene/OME3 blend at equivalence ratios of $\Phi = 2.16$ and 2.31 has been only numerically investigated so

far. An experimental investigation of these flames will be carried out in the future.
A water-cooled, stainless steel isokinetic probe with a conical tip was used to sample gas-phase and condensed-phase species from premixed ethylene flames. Vertical movement of the burner allowed for the acquisition of species concentration profiles. C_1–C_6 hydrocarbons were analyzed via GC-FID, while N_2, O_2, CO, and CO_2 were quantified using GC-TCD. Polycyclic aromatic hydrocarbons (PAHs) and particulates were collected at various heights above the burner using an ice-cooled trap and Teflon filter system, allowing simultaneous sampling of gas-phase and condensed species. Samples were extracted with dichloromethane to separate PAHs from soot and analyzed by GC–MS. Eighteen PAHs, including naphthalene, fluoranthene, pyrene, and coronene, were identified and quantified using a GC–MS system equipped with an HP-5MS column and electron impact ionization. Even though all the condensed-phase species and PAHs were analyzed, only Acenaphthylene, Anthracene, Pyrene, and Naphthalene are included as sum in the modeling and the experimental results for a consistent comparison.

Numerical modeling

Numerical simulations were carried out to assess the capability of the models in predicting the key flame characteristics and their sooting behavior. The numerical simulations were performed using the Cantera software, specifically employing the code for a burner-stabilized flame with an imposed temperature profile. The flame is solved using a mixture-averaged transport model for ideal gases, as described in Kee et al. [1]. For the ethylene and ethylene/EtOH mixtures, the mechanism (280 species, 17170 reactions) is the one developed by D'Anna and coworkers [2], where the kinetics for EtOH taken from the CRECK Modeling group are added. For ethylene/OME3 flames, we employed the OME1-3 mechanism (338 species, 17493 reactions) of Sun et al. [3]. For both mechanisms, heavy polycyclic aromatic hydrocarbons (PAHs) and soot particles are reported into 25 lumped pseudo-species, ranging from 24 to over $4x10^8$ carbon atoms, using a detailed sectional method. Five sections are used for H/C variation, namely 0, 0.25, 0.50, 0.75, 1; in this way, 92 lumped species (Ait1) for the stable form and 92 (Ajt1) for radicals are modeled. Species A1t1–A12t1 were treated as spheres, whereas larger lumped species were modeled as fractal aggregates (fractal dimension = 1.8 [4]); A12t1 represents the typical primary particle size considered as soot 'building block.'

Results

Figure 1 summarises the peak concentrations of the key species at each equivalence ratio. The reported trends indicate that the influence of ethanol and OME3 becomes more pronounced as the equivalence ratio increases. Specifically, as expected, CH_4 concentrations increase with rising equivalence ratio, reflecting the higher carbon content present under fuel-rich conditions and a more effective decomposition of the oxygenated additive. At the same time, OME3 doping inhibits the formation of C_2H_2 and C_6H_6 (relevant for particle formation and growth).

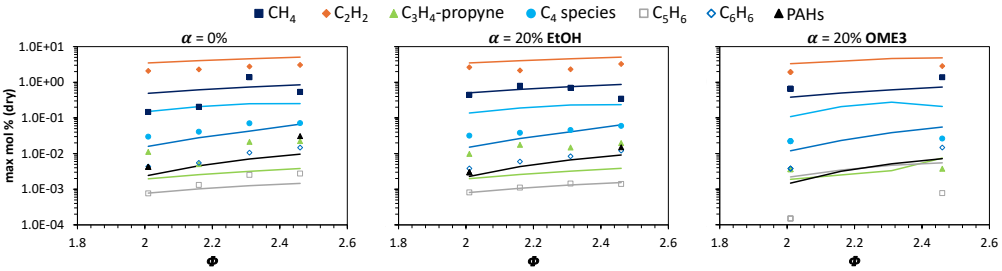

Figure 1. Maximum of the axial concentration profiles of CH_4, C_2H_2, C_3H_4-propyne, C4 hydrocarbons, C_6H_6, and GC-PAHs in ethylene, ethylene/EtOH, and ethylene/OME3 premixed flame at different equivalence ratios.

In particular, C_2H_2 concentration is higher in the pure ethylene flames across all the equivalence ratios because it mostly derived from ethylene dehydrogenation pathways [18].

Both models demonstrate good agreement with the experimental results for all species, except for CO_2, which exhibits the lowest predicted concentration among the species considered.

Conclusions

This work examines the impact of replacing 20% of ethylene carbon with ethanol or OME_3 in rich premixed flames ($\Phi = 2.01–2.46$) through experimental measurements and numerical modeling. Both additives reduce soot precursor concentrations, delay particle formation, and decrease nucleation-mode particle density, particularly under less sooting conditions. At higher equivalence ratios, the soot reduction effect weakens due to acetylene-driven surface growth. Simulations using D'Anna's sectional model and Sun OMEs mechanism confirm these trends, showing that oxygenates promote cleaner combustion by rerouting carbon from PAH pathways. The study underscores the soot-mitigation potential of oxygen-rich fuels and recommends further research under practical engine-relevant conditions.

References

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