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Kellie Ann Beall, Editor

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PARTICLE MEASUREMENTS IN $Fe(CO)_5$-INHIBITED FLAMES

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Introduction

Since iron pentacarbonyl ($Fe(CO)_5$) is among the most efficient flame inhibitors ever identified [1-4], research on flame inhibition by $Fe(CO)_5$ was recently started at NIST with the goal of understanding its mechanism [5]. Obtaining a detailed understanding of this super-effective chemical inhibitor will provide insights and approaches useful for development of the next generation of fire suppressants to replace the ozone-depleting suppressant CF_3Br. Our approach has been to use simple laboratory burners (premixed Bunsen-type flames and counterflow diffusion flames) to obtain global, yet fundamental, information on the action of $Fe(CO)_5$. The burning velocity and extinction strain rate, which provide a measure of the overall reaction rate, are determined with addition of $Fe(CO)_5$, while varying the stoichiometry, oxygen mole fraction, flame temperature, and flame location. Together with numerical modeling and kinetic model development, these data allow interpretation of the detailed chemical mechanism [6].

In previous research, we have shown that in premixed $CH_4/O_2/N_2$ flames, behavior at low and high $Fe(CO)_5$ mole fractions is distinctly different: at low $Fe(CO)_5$ mole fraction the burning velocity is strongly dependent on inhibitor mole fraction, whereas at high $Fe(CO)_5$ mole fraction, the burning velocity is nearly independent of inhibitor mole fraction. The behavior in counterflow diffusion flames is similar in that the inhibition effect becomes weaker as the mole fraction of agent increases (although it does not go to zero as in the premixed flames). A critical part of the research on $Fe(CO)_5$ is to understand iron pentacarbonyl's diminishing effectiveness at high mole fraction in order to avoid similar behavior in future fire suppressants. In recent work [5,6], it has been postulated that the diminished effectiveness of $Fe(CO)_5$ is due to loss of the active gas-phase iron species to the much less active condensed-phase compounds. The present work presents preliminary data on the light scattered by particles in premixed methane-air flames inhibited by iron pentacarbonyl.

Experiment

The premixed burner used for the data presented here has been described previously [7]. The laser scattering and extinction system consists of a laser; three detectors for the reference, extinction, and scattering signals; associated optics and a chopper; and lock-in amplifiers. A 3 W argon-ion laser provides a polarized beam at 488 nm, which is mechanically chopped at 1000 Hz. The burner is located in a chemical fume hood, and a polarization-preserving single-mode optical fiber brings the beam into the hood. After exiting the fiber, the beam is re-collimated to a diameter of approximately 2 mm, and passes through a polarizer to ensure near-complete vertical polarization, and a lens focuses the beam to a waist of approximately 0.1 mm. The transmitted power of the beam traversing the flame is measured using a silicon photodiode with neutral density, opal glass, and laser-line filters placed in front of the detector. The detection system for light scattered normal to the laser beam consists of a circular aperture, collection lens, pinhole aperture, laser-line filter, and 1P28 photomultiplier tube (PMT); the imaged control volume is about 1 mm in length. The reference signal also uses a 1P28 PMT, with a neutral density filter, a laser line filter, and opal glass. The signal from each photomultiplier tube is pre-amplified before entering a lock-in amplifier, which is controlled by a PC. A data acquisition card in the PC records the output from the lock-ins during the experiments. Typically, 500 readings are recorded over a time of about 1 s.

Results

The extinction and scattering signals have been obtained as a function of position above the conical Bunsen-type flame with varying amounts of $Fe(CO)_5$ added to the reactants of a stoichiometric methane-air flame. The attenuation of the laser passing through the flame is small, less than 2% for all beam positions above the flame and inhibitor mole fractions up to 500 ppm. The scattering signal appears to increases rapidly for $Fe(CO)_5$ mole fractions above 100 ppm, indicating that the scattering cross section for 488 nm light increases rapidly under these conditions. This may correspond to the presence of particles, or of new species or clusters with large scattering cross sections, or it may correspond to the growth of existing particles. In future work, we will refine the extinction system to allow measurement of the small attenuation in the flames, so that equivalent spherical diameters and number densities can be obtained, and thermophoretic samples will be obtained.

Acknowledgments

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