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Effects of m-xylene on aromatics and soot in laminar, N_2-diluted ethylene co-flow diffusion flames from 1 to 5 atm

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ABSTRACT

Experimental data and model results are presented for the effects of m-xylene on aromatic species and soot in a nitrogen-diluted ethylene flame over a range of pressures from 1 to 5 atm. The experimental approach was designed to investigate the effects of m-xylene as a perturbation to a base flame by keeping the amount of carbon added as m-xylene to 5% or less. The experimental results indicate that the maximum soot levels and those of small (1 or 2 rings) and large (3 or more ring) aromatic species are roughly first order with respect to the amount of m-xylene added. A chemical kinetic model was formulated, integrated into a 2-D modeling code, and used to simulate the effects of m-xylene addition and pressure on aromatic species and soot. The modeling results capture the general trends in concentration of soot and small aromatics as m-xylene concentration and pressure are varied. However, the model under-predicts the effect of m-xylene concentration and pressure on soot compared to the experimental results.

1. Introduction

The research summarized in this paper investigates the effect of the addition of m-xylene to a laminar N_2-diluted ethylene co-flow diffusion flame to determine the effects on aromatic hydrocarbons and soot. The work is part of a collaborative effort by a University, DoD, and Industry team to establish a validation database for soot formation and to test current soot models against that database[1]. The work of the team is focused on gas turbine engines with JP-8 as the practical fuel of interest.

The research team selected a two-component surrogate for JP-8 to match the Threshold Soot Index [2] of a typical JP-8. The surrogate consists of 77% dodecane and 23% m-xylene by volume. The use of m-xylene in the fuel was not optimal in terms of the boiling range of JP-8; however, it was chosen because of the need to have species for which chemical kinetic models were available. m-Xylene was chosen because a chemical mechanism was available in the literature at the time the study was conducted. Equally well developed kinetic models were not available for aromatic species typically found JP-8 such as diethylbenzene and tri-methylbenzene.

One of the goals of the collaborative research program was generating data relevant to gas turbine combustors, which can operate at pressures of 30 atm or more. Therefore, pressure was a key experimental parameter. Studying the soot production in flames of pure m-xylene at pressures of 1 atm or higher was not practical because of the large amount of soot that would form. Consequently, a test procedure was developed in which the m-xylene was added to a N_2-diluted, laminar, co-flow ethylene diffusion flame. The nitrogen flow rate was established such that the ethylene flame was nearly soot free at atmospheric pressure. The key parameters that were investigated in the study were the amount of m-xylene added to the flame and the pressure.

In these experiments, the N_2-ethylene co-flow flame establishes the base environment that is perturbed by the exchange of a small amount of the ethylene carbon, up to 5%, with carbon from the m-xylene. Therefore, the overall reaction conditions in terms of species and temperature as well as residence time will be nearly constant for all of the flames.

2. Previous research

2.1. m-Xylene combustion and kinetics

No experiments with m-xylene directly comparable to those conducted in the present study were found in the literature. The closest work was the determination of the sooting tendency of m-xylene in a N_2-diluted methane flame [3]. Other studies of m-xylene include experiments in shock tubes [4–6], a flow reactor

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[7], a jet-stirred reactor [8], a rapid compression machine [9], and premixed flames [10]. The flow reactor, jet-stirred reactor and the shock tube data of Battin-LeClerc et al. [4] were used to develop the kinetic model for the present study.

Four detailed m-xylene kinetic models appear in the literature. Battin-LeClerc et al. [4] published a model based on shock tube studies and flow reactor data of [7] in 2006. It was followed by a model created by Gail and Dagaut [8] based on their work in a jet-stirred reactor. Recently, two additional models have appeared. Narayanaswamy et al. have published an oxidation model that encompasses a number of monocyclic aromatic species including m-xylene [11]. The work of Brezinsky and Gudiyella [6] included formulation of a detailed kinetic model for m-xylene oxidation at high pressure. At the time that the work summarized in this paper was conducted, the available models were those of Battin-LeClerc et al. [4], Gail and Dugaut [8] and an earlier, unpublished mechanism of Gudiyella et al. [6b].

2.2. Effect of pressure on soot

The effect of pressure on soot volume fraction in laminar co-flow diffusion flames has been studied by a number of investigators. Unlike the present study, most of the work in the literature is performed without dilution by an inert gas. Work with neat fuels includes several studies of laminar co-flow flames of ethylene at pressures as high as 25 atm [12–14].

Charest et al. conducted an experimental and modeling study of soot formation in laminar ethylene co-flow diffusion flames at pressures from 10 to 35 atm [15]. They used nitrogen-dilution to reduce soot volume fractions and suppress smoke formation. The maximum soot volume fraction varied from 8 ppm at 10 atm to 62 ppm at 35 atm. They report a pressure exponent of 1.36 for the variation of carbon converted to soot. Their study also included modeling of the flames. They report generally good agreement between the simulations and experiments, although soot volume fractions were over-predicted.

3. Experimental approach

3.1. Experimental facility

The co-flow burner used in this study is based on the design of Santoro et al. [16], which has a central fuel jet (I.D. = 11.1 mm) surrounded by a co-flowing air stream (I.D. = 101.6 mm). The annular region for the co-flow air contains screens, glass beads, and a honeycomb to produce a uniform exit velocity profile. The fuel tube is partially filled with glass beads to condition the flow. This configuration proved to be unstable over much of the desired pressure range, so the fuel tube internal diameter was decreased to 6 mm, which resolved the stability problem. The fuel tube extends 5 mm above the top surface of the annulus for air flow. During the experiments, the fuel temperature was measured 2.5 cm below the tip of the fuel tube using a K-type sheathed thermocouple. The air temperature was monitored with a similar thermocouple located at the base of the honeycomb, which was position at the top of the co-flow air annulus.

This burner was housed inside a 20 cm I.D. pressure vessel constructed of Schedule 40 carbon steel. The burner had 2° of freedom, one along the vertical direction and the other in the horizontal direction, perpendicular to the laser beam path. Vertical motion was achieved by using a stepper motor (Velmex PK266) coupled to a lead screw (0.065 in/turn pitch), which was in turn attached to a linear bearing. The vertical translation system had an effective step resolution of 6.35 μm. Horizontal translation was achieved by coupling a weight-actuated linear bearing to a commercially available translation stage (Velmex BiSlide) that had a step resolution of 5 μm.

Optical access to the flame was facilitated by way of four ports, 6.25 mm in diameter, located at 90° intervals. For the laser extinction and laser-induced incandescence measurements, the ports were fitted with half-inch thick S1-UV fused silica windows, coated with a broadband anti-reflective (AR) material optimized for the visible spectrum. For the absorption measurements, an AR coating was necessary to eliminate interference fringes that can form as a result of the laser beam undergoing multiple reflections between diametrically opposite windows. For the laser-induced fluorescence measurements, the AR coated windows were replaced with uncoated S1-UV fused silica windows, since the AR material absorbs UV radiation.

The C_2H_4 and N_2 flows were delivered using calibrated mass flow controllers (Brooks Instruments 5850 series) that are rated for operation at pressures of up to 100 atm with an accuracy of ±1% of the set point. The ethylene gas used in these experiments was chemical purity grade (99.9%); the nitrogen was industrial grade with a purity of 99.98%. The two streams were mixed downstream of the mass flow controllers, the two lines were isolated with check valves.

During the course of the study, two different approaches were used to create the m-xylene vapor, a bubbler and a vaporizer, both of which worked well. The bubbler was used in the early phases of the work because it was a relatively simple approach. In the bubbler approach, the nitrogen was preheated to carefully controlled temperatures to match the vapor pressure to the m-xylene to the desired partial pressure in the system. The bubbler was eventually replaced by a vaporizer as the project transitioned to the study of higher boiling point compounds. A comparison of the two systems showed that the soot fields in flames with m-xylene added were identical within experimental uncertainty.

Energy for vaporization was delivered by an electrically heated, fluidized bed (Techne SBS-4). The liquid flow rate was controlled by a syringe pump (Chemyx Inc. Fusion 100 fitted with a gas-tight #1001 syringe from Hamilton). The N_2/C_2H_4 flowed into a stainless steel coil immersed in the fluidized bed. The liquid fuel was added to the stream in a T-fitting just before the fluidized bed. Heating tapes and a heated flexible line were used to maintain the temperature of the mixture above the dew point of m-xylene. A heated flexible line (Atmoseal with temperature controller and maximum temperature of 250 °C) was used to connect the outlet of the vaporizer to the entrance of the high pressure chamber. Heating tapes were also wrapped around the fuel lines inside the high pressure chamber. Thermocouples were placed between the fuel lines and the heating tapes to monitor the heating tape temperatures. The temperatures on the heated lines were set at 200 °C to avoid fuel decomposition.

3.2. Diagnostics methods

Three different laser-based diagnostic methods were applied to the flame – laser-induced incandescence (LII), laser-induced fluorescence (LIF) and light extinction.

The LII measurements were performed using a frequency-doubled Nd:YAG laser (Continuum Surelite III fitted with second harmonic generator). The laser provided a 9 mm diameter beam, with a pulse width of 7 ns at a flash lamp repetition rate of 10 Hz. The 532 nm beam was expanded into a vertical sheet using a fused silica cylindrical lens and focused at the center of the burner using a 500 mm focal length convex lens.

The LII signal was collected by an intensified CCD (Princeton Instruments ICCD) camera fitted with a 576 × 384 EEV chip. The LII radiation was focused on the CCD using an f2.8 105 mm UV lens (Nikon UV-Nikkor), fitted with a narrow band interference filter