Experiments and Model Development for the Investigation of Sooting and Radiation Effects in Microgravity Droplet Combustion

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INTRODUCTION

The spherically-symmetric burning of an isolated droplet is a dynamic problem that involves the coupling of chemical reactions, multi-phase flow (liquid, gas, particulate) with phase change. To this end, microgravity droplet combustion serves as an ideal platform for advancing the understanding the diffusion flame physics of liquid hydrocarbon fuels and additives that are typically used in internal combustion engines and gas turbines. Due to the complex and incomplete understanding of soot processes in the combustion of large molecular weight hydrocarbon droplets, theoretical/computational formulations have historically neglected sooting behavior. Testbed experiments in microgravity using droplet flames, used a mildly sooting fuel, n-heptane, and employed parameter adjustment techniques to minimize sooting for comparisons with and validations of numerical models. None of the experimental techniques, however, were entirely successful and sooting remains a critical component in the analysis of droplet combustion, commensurate with its importance in the burning of conventional fuels. *A thorough interpretation of droplet burning behavior cannot be accomplished without examining and incorporating the influences of sooting and radiation.* Concurrently, isolated droplet combustion studies offer an opportunity to investigate sooting phenomena on the dynamics of diffusion flames, and over parameter ranges not available in quasi-steady experiments such as annular jet diffusion flames. The current state of numerical modeling approaches for droplet combustion and diagnostics permits consideration of the transient nature of the sooting and radiation at a level of detail that is computationally prohibitive and experimental intractable for multi-dimensional configurations. Experimental measurements and numerical model development can provide a comprehensive test of their influence on the burning rate, flame structure, flame extinction, and soot aerosol properties. Thus, this problem is a logical extension of non-sooting droplet combustion experiments and numerical modeling efforts that have been previously conducted.

This study involves flight experiments (for droplets between 1.5 to 5 mm) and supportive ground-based experiments, with concurrent numerical model development and validation. The experiments involve two fuels: n-heptane, and ethanol. The diagnostic measurements include

light extinction for soot volume fraction, two-wavelength pyrometry and thin-filament pyrometry for temperature, spectral detection for OH chemiluminescence, broadband radiometry for flame emission, and thermophoretic sampling with subsequent transmission electron microscopy for soot aerosol property calculations.

ETHANOL EXPERIMENTS

Ethanol droplet combustion has been extensively studied by researchers using reduced-buoyancy techniques. In a classical investigation, Godsave [1953] analyzed the burning behavior of suspended ethanol droplet combustion. Kumagai and coworkers [Okajima and Kumagai, 1975; Hara and Kumagai, 1991] studied ethanol combustion using droptower facilities to measure burning rates and flame diameters of ethanol for various initial droplet diameters and investigate the importance of relative velocity of moving droplets. Lee and Law [1992] studied combustion of small, freely-falling methanol and ethanol droplets in which they reported droplet burning histories and time resolved bulk liquid-phase water mass fractions. Ethanol was also one of the primary fuels studied aboard the STS-94/MSL-1 Shuttle mission in the Fiber-Supported Droplet Combustion-2 (FSDC-2) program [Colantonio et al., 1998]. In those studies, the burning rate, flame diameter measurements, and extinction behavior for droplets ranging from 2.5 to 6 mm were measured and analyzed. In all of the studies mentioned above, experiments were performed for ethanol droplets burning in atmospheric pressure. Consequently, there were no observations of sooting in those experiments.

Soot formation in ethanol droplet combustion was first observed by Yap [1984] in his experiments using freely-falling droplets in a high-pressure drop-tube. In 2001, Urban et al. [2001] observed the formation of a sootshell for ethanol droplets burning in pressures of 2 atm in the NASA 2.2 sec. droptower. However, soot concentrations were not measured in these experiments due to a lack of appropriate diagnostic equipment.

In this work, we describe new experiments on the burning characteristics of isolated ethanol droplets and the environmental conditions leading to soot formation and luminous radiation. Experiments were performed by varying the pressure from 1 to 2.2 atm, the oxygen concentrations from 21% to 50%, and the initial diameters from 1mm to 2.5 mm. Experiments were performed at both the NASA Glenn 2.2 sec. drop tower and the JAMIC 10 sec. dropshaft.

Figure 1 displays the backlit images of ethanol droplets of 1.7 mm diameter burning in air at pressures ranging from 1.0 to 2.2 atm. The lack of the presence of a sootshell is clearly observed in the 1.0 and 1.5 atm experiments with slight attenuation caused by small concentrations of soot in the 2.2 atm experiment. In an effort to increase the likelihood of forming soot in ethanol experiments, ambient pressure and the oxygen concentration were varied in conjunction. Figure 2 displays the laser-backlit images of ethanol droplets burning in various oxygen concentrations in nitrogen at 2.2 atm. At 21% and 25% O_2 in N_2, there is no luminosity exhibited in the flame view and the attenuation of the laser beam in the backlit view was lacking. As the oxygen concentration is increased to 30% O_2 in N_2, the formation of a distinct sootshell and a luminous flame are observed. Another interesting behavior was noted in which the sooting propensity appears to decrease at 40 % O_2 in N_2 case compared to the 30% O_2 in N_2 case. Additional experiments and analysis are required to investigate this interesting behavior. From the experiments shown in figure 2, the maximum soot volume fraction, $f_{v,max}$, was measured the using tomographic inversion technique. These measurements clearly bear out the interpretation

from the visual observation – at 21% O_2 in N_2, there is no measurable soot concentration, while at 30% O_2 in N_2, the maximum soot volume fraction is approximately 13 ppm. These experiments clearly demonstrate the strong dependence of sooting behavior of ethanol droplets on ambient pressure and oxygen concentration.

DROPLET COMBUSTION COMPUTATIONAL MODEL DEVELOPMENT

In this project, the numerical computation of droplet combustion is performed using a moving finite-element chemically reacting flow model. The model simulates the transient, spherically symmetric combustion of a liquid droplet in an infinite oxidizing medium by solving the conservation equations of mass, species, and energy in both liquid and gas phases. The model includes detailed description of gas-phase chemical kinetics and transport. Radiative heat transfer is described using a Planck-mean absorption formulation for both the gas phase (non-luminous) and soot.

Recently, many improvements to the model have been made that include:

a. The code structure was entirely rewritten to improve speed, stability, expandability, and to simplify its future maintenance.

b. Numerical improvements include the use of hardware-optimized linear algebra subroutines, modern iterative solvers (GMRES-based), dynamic memory management.

c. Liquid phase thermal contraction/expansion is implemented (via supplied liquid-phase equation of state).

d. The transport sub-models were custom-coded for efficiency; calculation of transport coefficients is now (optionally) based on multicomponent formulation (as opposed to prior mixture-averaged formulae) with inclusion of thermal diffusion terms for light species (previously not available). The latter was shown to have a significant effect on soot predictions in counterflow diffusion flames.

e. Chemical reaction terms are computed with the fast custom package that can be produced from any CHEMKIN-formatted reaction mechanism; this approach offers drastic speed improvements over the use of standard CHEMKIN libraries.

f. The basic framework for *generic* soot model was implemented and coupled with the main components (the source terms for nucleation, coagulation, and surface growth/oxidation, and the transport terms for molecular and thermal diffusion) via third-order method of moments.

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ACKNOWLEDGMENTS

FIGURES
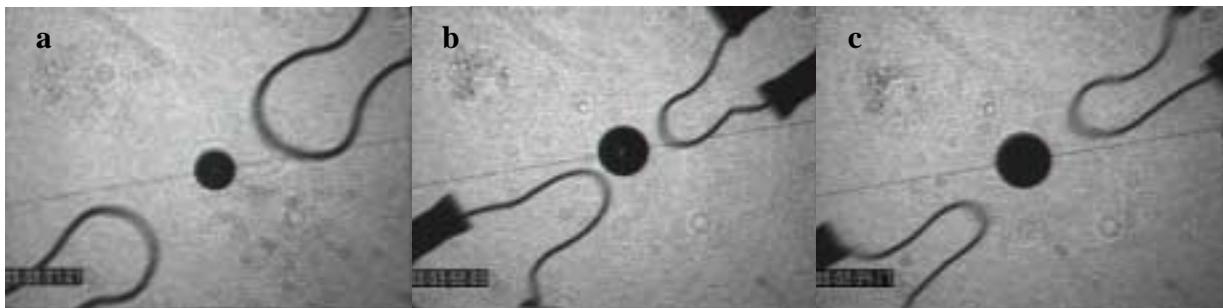
Fig. 1 Ethanol droplets burning at 21 % oxygen in nitrogen and elevated pressure a) 1 atm; b) 1.5 atm; c) 2.2 atm
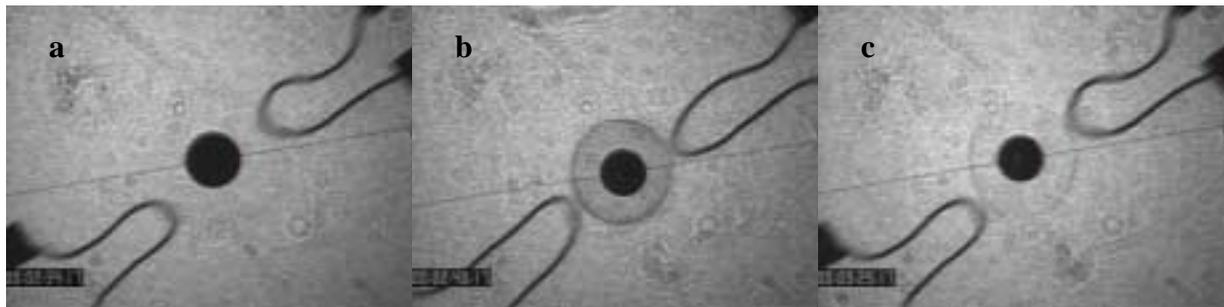
Fig 2 Ethanol droplets burning at elevated pressure and enhanced oxygen concentration a) 2.2 atm 21% O_2; b) 2.2 atm 30% O_2; c) 2.2 atm 40% O_2