

BI-COMPONENT DROPLET COMBUSTION IN REDUCED GRAVITY

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INTRODUCTION

This research deals with reduced-gravity combustion of bi-component droplets initially in the mm size range or larger. The primary objectives of the research are to study the effects of droplet internal flows, thermal and solutal Marangoni stresses, and species volatility differences on liquid species transport and overall combustion phenomena (e.g., gas-phase unsteadiness, burning rates, sooting, radiation, and extinction). The research program utilizes a reduced-gravity environment so that buoyancy effects are rendered negligible. Use of large droplets also facilitates visualization of droplet internal flows, which is important for this research.

In the experiments, droplets composed of low- and high-volatility species are burned. The low-volatility components are initially present in small amounts. As combustion of a droplet proceeds, the liquid surface mass fraction of the low-volatility component will increase with time, resulting in a sudden and temporary decrease in droplet burning rates as the droplet rapidly heats to temperatures close to the boiling point of the low-volatility component. This decrease in burning rates causes a sudden and temporary contraction of the flame. The decrease in burning rates and the flame contraction can be observed experimentally. Measurements of burning rates as well as the onset time for flame contraction allow effective liquid-phase species diffusivities to be calculated, e.g., using asymptotic theory [1]. It is planned that droplet internal flows will be visualized in flight and ground-based experiments. In this way, effective liquid species diffusivities can be related to droplet internal flow characteristics.

This program is a continuation of extensive ground based experimental and theoretical research on bi-component droplet combustion that has been ongoing for several years. The focal point of this program is a flight experiment (Bi-Component Droplet Combustion Experiment, BCDCE). This flight experiment is under development. However, supporting ground-based studies have been performed. This ground-based research is summarized below.

REDUCED GRAVITY EXPERIMENTS

Data have been obtained on droplet combustion behaviors in environments with various diluents. The diluents were selected to have significant variations in molecular weight, allowing investigation of variations in properties such as binary species diffusion coefficients on combustion behaviors such as transient flame diameters. The droplets were composed of either decane or decane-hexadecane mixtures. Experiments were performed at 0.1 MPa with ambient oxygen mole fractions, X_{O_2} , of 0.21 and 0.5.

Data for normalized droplet diameters and flame standoff ratios are shown in Fig. 1 for $X_{O_2} = 0.21$. Here, Y is the initial hexadecane mass fraction, d_0 is the initial droplet diameter, d is the instantaneous droplet diameter, d_f is the instantaneous flame diameter, and K_{ave} is an average burning rate constant (i.e., the negative of the slope on a plot of d^2/d_0^2 vs. t/d_0^2). Figure 1(a) shows that changing the inert species in the environment has a significant effect on K_{ave} . Helium produces the largest burning rate while burning rates for Xe and N_2 are about the same.

Flame unsteadiness is also influenced by the inert species. From Fig. 1(b), it is evident that using Xe as an inert species promotes quasisteady flame standoff ratios, while N_2 and He promote flame unsteadiness with He producing the least steady flames. To interpret this behavior, we will consider an effective O_2 diffusivity, D_{O_2} , between the environment and the

flame zone. Since droplets exist for only a finite time, quasisteady flame behaviors will be promoted when D_{O_2} values are increased. If it is assumed that $D_{O_2} = D_{I_{O_2}}$, where $D_{I_{O_2}}$ is the binary species diffusion coefficient for the inert species and O_2 , it is found that D_{O_2} increases as the inert molecular weight decreases, which should promote stronger flame unsteadiness for Xe relative to He (and N_2). However, this trend does not agree with the experimental results and it is likely that other phenomena influence flame unsteadiness

Other factors that can influence flame unsteadiness are Soret transport and differences between binary species diffusion coefficients [2,3]. Aharon and Shaw [2] provided theory to estimate these effects on transport of O_2 to droplet flames. When this theory is applied to environments containing O_2 with He, N_2 or Xe, it is found that D_{O_2} values are largest for Xe and smallest for He, with Soret effects being as important as differences in binary diffusion coefficients. Thus, stronger flame unsteadiness is predicted for He, with Xe predicted to exhibit the most quasisteady flames (N_2 is in between). These predictions agree with the present experimental results, suggesting that Soret transport and differences between binary species diffusion coefficients were important in the present experiments.

NUMERICAL MODELING OF PROPANOL-GLYCEROL DROPLET COMBUSTION

A one-dimensional computational model was developed to simulate reduced-gravity combustion of propanol-glycerol droplets. This model provides an intermediate step between asymptotic models and a 3-d code that is being developed as part of this research. The new code employs an implicit finite difference formulation with variable gridding. It allows for variable liquid properties, nonideal liquid effects, absorption of water, liquid radial velocity fields (from liquid density changes) and droplet swelling. The code has been used to model previous experimental results on combustion of propanol-glycerol droplets [4].

The code solves the liquid-phase conservation equations for temperature and mass fraction profiles within a droplet. The continuity equation is integrated to determine liquid radial velocities. Properties vary spatially and temporally and boundary conditions are evaluated using second order difference equations. Liquid properties and activity coefficients are evaluated using correlations and the UNIFAC method [5-7]. The gas phase is treated as quasisteady, allowing analytical results to be used for gas-phase profiles and droplet-flame standoff ratios [2,8]. The assumption of a quasisteady gas phase is consistent with experimental results that show quasisteady flame standoff ratios for these droplets [4].

Figure 2(a) shows experimental results for droplet size variations, with numerical results superimposed as solid lines. The calculations sought to provide a good match between experimental and theoretical results on burning rates so that the onset of flame contraction predicted by the model could be compared with experimental results. This was accomplished by adjusting the gas-phase thermal conductivity by relatively small amounts. Initial droplet swelling from droplet density changes is evident in the computational and experimental results. The swelling in the experiments was slightly larger than predicted by the computations, though the predicted swelling is essentially within the uncertainty of the measurements. In Fig. 2, E is an enhancement factor by which liquid thermal conductivity and species diffusivity were increased during a particular calculation. This factor was introduced to allow effects of internal circulation to be modeled. The value $E = 1$ predicted flame contraction much earlier than the experiments, while $E = 10$ provided a much closer prediction (Fig. 2(a)).

Figure 2(b) shows experimental flame size data as well as computational predictions of flame sizes. Agreement between calculations and experiment is reasonable, both qualitatively as well as quantitatively, when the value $E = 10$ is used. The E values required to match theory and

experiment typically ranged from 8 to 10, which are larger than what would be expected to apply to droplets with Hills-type vortex flows [9]. As a result, the droplets may have contained more than one vortex or perhaps chaotic flows may have been present, which can cause larger increases in effective diffusivities [10].

NUMERICAL MODELING OF FIBER-SUPPORTED DROPLETS

A computer code is being developed to simulate 3-d vaporization of droplets that are attached to thin fibers. This code, which is being developed in collaboration with Prof. H. A. Dwyer of UC Davis, includes multi-component liquids as well as Marangoni flows from temperature gradients and liquid concentration gradients. The present status of the code is as follows. Fully validated: gas and liquid fluid mechanics and heat transfer; mesh generation and interaction between the fiber, gas and liquid phases; gas phase chemical reactions; variable properties; interface forces. Partially validated: mass transfer between gas and liquid phases; multi-component liquid properties; thermal surface tension forces. Continuing development: concentration driven surface tension forces; adaptive mesh generation for resolution of flame structure; resolution of ignition processes. The code has been run for various validation cases.

Figure 3 shows representative results for a nonreacting fiber-supported droplet in a hot environment. In this case, the fiber diameter is 1/20 of the droplet diameter. Flows were observed to form within the droplet as a result of thermal Marangoni effects (see the dark streamlines in the droplet). The fiber and the droplet are cooler than the environment, and the location of the fiber on either side of the droplet can be seen by the thermal boundary layer over the fiber length (green coloring in Fig. 3(a)). For validation, this case was run with a cross flow, yielding temperature variations in Fig. 3(b).

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REFERENCES

1. I. Aharon and B. D. Shaw, *Combust. Flame* 113, 507 (1998).
2. I. Aharon and B. D. Shaw, *Micrograv. Sci. Tech.* X/2, 75 (1997).
3. D. E. Rosner, R. S. Israel and B. La Mantia, *Combust. Flame* 123, 547 (2000).
4. V. Dee and B. D. Shaw, AIAA paper 2001-0468 (2001).
5. S. I. Sandler, *Chemical and Engineering Thermodynamics* (2nd ed), John Wiley & Sons, New York (1989).
6. R. H. Perry, *Perry's Chemical Engineers' Handbook* (7th ed.), McGraw-Hill, New York (1997).
7. R. C. Reid, J. M. Prausnitz and B. E. Poling, *The Properties of Gases and Liquids* (4th ed), McGraw-Hill, New York, (1987).
8. B. D. Shaw, *Combust. Flame* 81, 277 (1990).
9. J.-P. Delplanque, R. H. Rangel and W. A. Sirignano, *Progress in Astronautics and Aeronautics* 132, 164 (1991).
10. M. D. Dryden and H. Brenner, *J. Fluid Mech.* 379, 319 (1999).

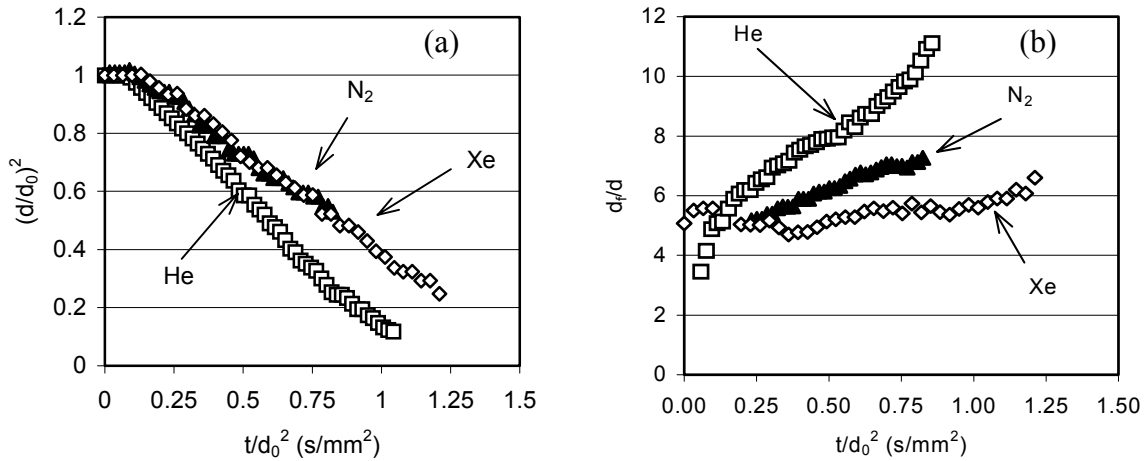


Figure 1. Data for a decane-hexadecane droplet ($Y = 0.2$): (a) normalized droplet diameters; and (b) flame standoff ratios. Ambient inert species are noted on the figures.

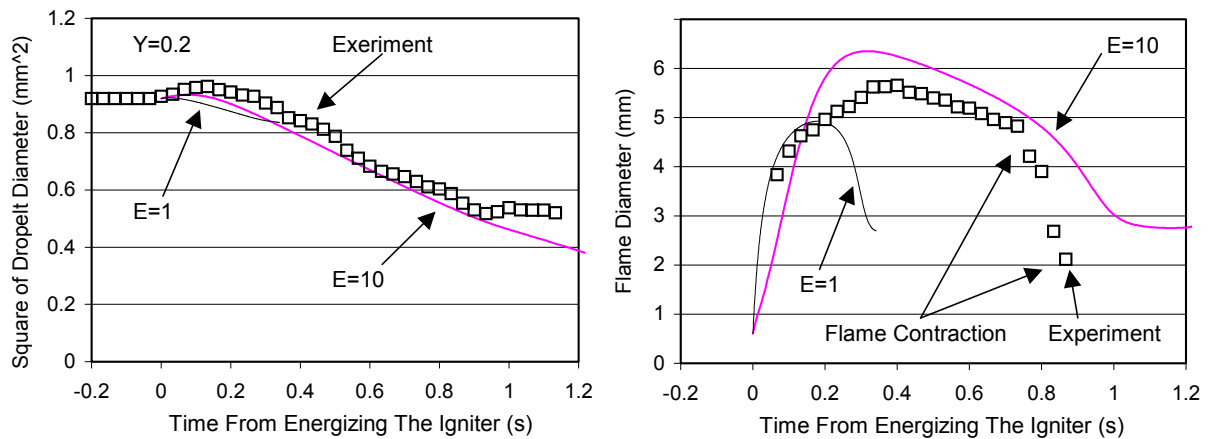


Figure 2 Histories for (a) droplet and (b) flame sizes ($Y = 0.2$). The symbols are from the experiments and the lines are from the computational model.

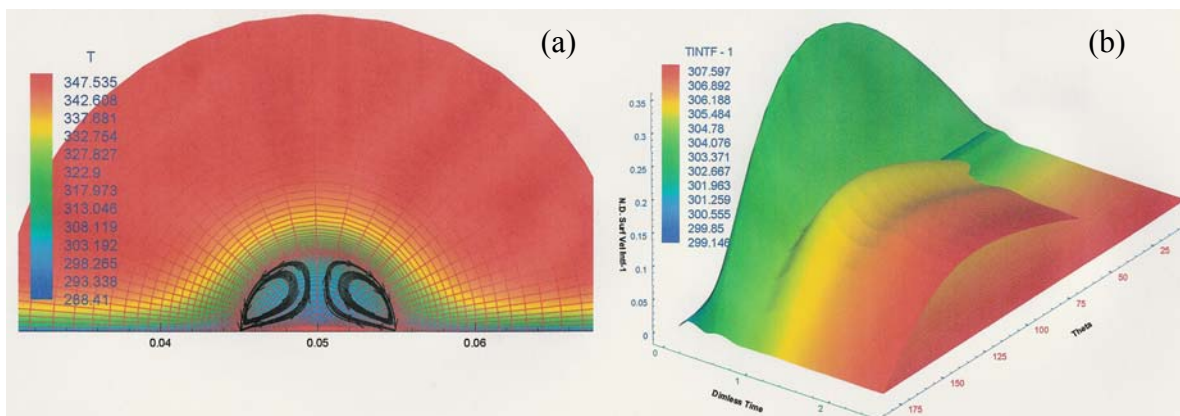


Figure 3 Numerical simulation of a droplet on a fiber: (a) grid, streamlines and temperature profiles; and (b) transient surface temperature development on a symmetry line.