BI-COMPONENT DROPLET COMBUSTION IN REDUCED GRAVITY

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ABSTRACT

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. Some of the most recent ground-based research is summarized below.

Reduced Gravity Experiments

Experiments on combustion of fiber-supported propanol droplets with initial droplet diameters of about 1 mm were conducted in air at standard temperature and with pressures ranging from 0.1 to 1.0 MPa [2]. The experiments were conducted using the 2.2 Second Drop Tower at the NASA John H. Glenn Research Center at Lewis Field in Cleveland, OH. The results indicate significant differences in combustion of propanol droplets at 0.1 MPa relative to higher pressures. The flame at 0.1 MPa is non-sooting with blue coloring during most of the combustion process. For higher pressures, flames exhibited somewhat non-spherical shapes as well as significant amounts of sooting during most of the combustion history. The non-spherical flame shapes were likely a

result of the increased importance of buoyant convection at elevated pressure as inferred from Grashof numbers that were calculated based on flame dimensions. Droplet burning rates were also observed to increase with increasing pressure. Theory indicates that these increases resulted mainly from decreases in liquid densities and enthalpies of vaporization, where these decreases are caused by increases in liquid saturation temperatures.

Analytical Modeling

Simplified analyses of spherically symmetrical combustion of an isolated fuel droplet were developed to account for fuel pyrolysis [3]. Fuel pyrolysis is modeled as a high activation-energy process that occurs within a thin zone between the droplet and the flame. Accounting for fuel pyrolysis changes classical expressions for the transfer number because the flame must supply energy for fuel pyrolysis, which requires the flame to be located closer to the droplet. Sample calculations for combustion of heptane droplets in air at one atm indicate that transfer numbers, burning rates and quasisteady flame standoff ratios can be appreciably reduced when fuel pyrolysis effects are included in the analyses.

Soot shell standoff ratios in reduced-gravity droplet combustion were also investigated analytically [4]. Analysis of energy conservation between the droplet and the flame shows that temperature gradients between the droplet and a flame are influenced by variations in specific heats as well as fuel pyrolysis, which influences thermophoretic soot transport. Analyses show that if endothermic fuel pyrolysis is neglected, soot shells are predicted to be close to the fuel oxidation zone where fuel mass fractions are small. Analyses that account for endothermic fuel pyrolysis indicate that the onset of fuel pyrolysis can be abrupt, leading to local increases in temperature gradients. These temperature gradient changes can be large enough to influence soot transport, causing soot-shell standoff ratios to be smaller than if fuel pyrolysis is neglected. Theoretical predictions of pyrolysis-controlled soot-shell standoff ratios compare favorably with experimental data on reduced-gravity combustion of n-heptane droplets in air at 1 atm

References

- 1. I. Aharon and B. D. Shaw, Estimates of Liquid Species Diffusivities from Experiments on Reduced-Gravity Combustion of Heptane-Hexadecane Droplets, <u>Combustion and Flame</u> 113, 507 (1998).
- 2. S. M. Dakka and B. D. Shaw, Combustion of Propanol Droplets in Reduced Gravity, paper 04S-46 presented at the 2004 Spring Meeting of the Western States Section of the Combustion Institute, University of California, Davis, March 29-30.
- 3. B. D. Shaw, Theory of Spherically Symmetrical Droplet Combustion with Gas-Phase Fuel Pyrolysis, <u>Combustion Science and Technology</u> (submitted).
- 4. Theory of Influence of Fuel Pyrolysis on Soot-Shell Standoff Ratios in Reduced-Gravity Droplet Combustion, paper 04S-50 presented at the 2004 Spring Meeting of the Western States Section of the Combustion Institute, University of California, Davis, March 29-30.

BI-COMPONENT DROPLET COMBUSTION IN REDUCED GRAVITY

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BI-COMPONENT FUEL DROPLETS

- Multicomponent liquid fuels are commonly used in practical applications
- Need to understand gasification behaviors of multicomponent droplets
 - Predict rates that particular species gasify from droplets
 - Gas behaviors
 - Determined by species that have gasified
 - Liquid behaviors
 - Determined by species that remain inside droplets

THIS RESEARCH IS COMPRISED OF

- Space-based experiments (future)
 - Up to 4 mm initial diameter
- Ground-based studies (current)
 - Drop tower experiments
 - Up to 1 mm initial diameter
 - Ground experiments at UC Davis
 - Analytical/numerical studies

SOME RECENT EFFORTS FROM THIS RESEARCH PROGRAM

- Numerical Modeling of Droplet Combustion
 - 1-Dimensional
 - 3-Dimensional
- Drop Tower Experiments
 - Propanol droplet combustion
 - Single-component droplets provide baseline data for comparison with bi-component droplets
 - Up to 10 atm in air
- Analytical Modeling
 - Effects of gas-phase fuel pyrolysis
 - Flame standoff ratios
 - Burning rates
 - Soot shell behaviors



0.6

Time From Energizing The Igniter/s

0.8

1

1.2

0.4

Histories for flame and droplet sizes (initial glycerol mass fraction, Y, of 0.2). The symbols are from experiments and the lines are from the computational model. The variable E is a liquid-phase transport enhancement factor, to account for liquid convection effects. Comparison of the computational and experimental results indicates that significant convective mixing was present in the experiments.

One-Dimensional Numerical Model

1. Variable properties with nonideal liquids

-0.2

0

0.2

0.4

0.6

Time From Energizing The Igniter/s

0.8

1.2

1

- 2. Spherical symmetry
- 3. Transient liquid phase
- 4. Quasisteady gas phase (in agreement with experimental data)
- 5. Implicit finite-difference formulation with variable gridding

-0.2

0

0.2

THREE-DIMENSIONAL DROPLET COMBUSTION MODELING (with H. A. Dwyer)

Marangoni flows; gas-phase chemistry; radiation; fiber effects; 3-dim flows; liquid-phase transport; moving gas phase (possible convective effects)

Method of Approach

- 1. Overset Grid (Chimera) Approach
- 2. Low-Mach-number reacting Navier-Stokes equations with variable liquid and gas properties
- 3. Projection solver with ADI preconditioned GMRES
- 4. Variable surface tension with temperature and concentration dependence
- 5. Multi-component and non-ideal liquid phase
- 6. Specified droplet shapes (can be relaxed with effort)
- 7. 3-Dimensional model

Finite-volume formulation Global or detailed chemistry





Mesh Schematic

Re=0.1, CH₃OH/Air

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REDUCED-GRAVITY COMBUSTION OF PROPANOL DROPLETS



Pressure Effects on Flames

Increasing the pressure increases soot formation and flame distortion

Pressure Effects on Burning Rates

1.6 1.4 1.2 $K_0(P)/K_0(P_{ref})$ 1 Experiment 0.8 - Theory 0.6 0.4 0.2 0 0.5 1 1.5 0 P (MPa)

Normalized Burning Rates

Burning rates increased as the ambient pressure increased

Increases in burning rates can be accounted for by considering influences of pressure on enthalpy of vaporization and liquid density

ANALYTICAL MODELING OF INFLUENCES OF FUEL PYROLYSIS

- Fuel pyrolysis reactions
 - Can be highly temperature sensitive
 - Significantly endothermic
 - Reaction sheet model employed here
- Gas-phase temperature profiles are influenced by fuel pyrolysis
 - Energy required for pyrolysis alters temperature profiles
- Burning rates decrease as a result of fuel pyrolysis
- Flame standoff ratios decrease as a result of fuel pyrolysis
- Soot shell standoff ratios are influenced by fuel pyrolysis



ANALYTICAL MODELING OF INFLUENCES OF FUEL PYROLYSIS



Predicted variations for the normalized burning-rate ratio K/K_0 , the normalized flame standoff ratio $(r_f/r_d)/(r_f/r_d)_0$ and the normalized effective transfer number ratio B_{eff}/B_0 as a function of the ratio H/L, where H is the enthalpy change associated with fuel pyrolysis and L is the droplet enthalpy of vporization. The solid line is for a pyrolysis temperature of 900 K ands the dashed line is for a pyrolysis temperature of 1000K. The calculations are for combustion of n-heptane droplets in air at one atm.

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