Soret transport, which is mass transport driven by thermal gradients, can be important in practical flames as well as laboratory flames by influencing transport of low molecular weight species (e.g., monatomic and diatomic hydrogen). In addition, gas-phase Soret transport of high molecular weight fuel species that are present in practical liquid fuels (e.g., octane or methanol) can be significant in practical flames (Rosner et al., 2000; Dakhlia et al., 2002) and in high-pressure droplet evaporation (Curtis and Farrell, 1992), and it has also been shown that Soret transport effects can be important in determining oxygen diffusion rates in certain classes of microgravity droplet combustion experiments (Aharon and Shaw, 1998). It is thus useful to obtain information on flames under conditions where Soret effects can be clearly observed.

This research is concerned with investigating effects of Soret transport on combustion of liquid fuels, in particular liquid fuel droplets. Reduced-gravity is employed to provide an ideal (spherically-symmetrical) experimental model with which to investigate effects of Soret transport on combustion. The research will involve performing reduced-gravity experiments on combustion of liquid fuel droplets in environments where Soret effects significantly influence transport of fuel and oxygen to flame zones. Experiments will also be performed where Soret effects are not expected to be important. Droplets initially in the 0.5 to 1 mm size range will be burned. Data will be obtained on influences of Soret transport on combustion characteristics (e.g., droplet burning rates, droplet lifetimes, gas-phase extinction, and transient flame behaviors) under simplified geometrical conditions that are most amenable to theoretical modeling (i.e., spherical symmetry). The experiments will be compared with existing theoretical models as well as new models that will be developed. Normal gravity experiments will also be performed.

Experimental research will involve performing reduced-gravity droplet combustion experiments in a NASA Glenn drop tower (the 2.2 s tower). Use will be made of an existing droplet combustion rig. Digital images of the drop rig are shown in Fig. 1. This rig will be used to provide results on Soret effects for droplets initially from about 0.5 mm to 1 mm in diameter. The pressure will range from subatmospheric to as high as about 1.2 MPa (and possibly higher).

The drop rig has a pressure vessel mounted on a NASA-supplied drop frame with associated control electronics and gas and liquid handling systems. Orthogonal views are used with the drop rig; one view is used to image droplets and the other view is used to image flames. The flame view is not backlit, and a Xybion intensified-array CCD camera can be used to image OH emissions in this view (CH emissions can also be imaged).
Theoretical modeling will employ further development of analytical models beyond that described by Aharon and Shaw (1998). Further development of analytical theory will involve accounting for transient effects as well as developing models of Soret effects and multicomponent diffusion effects between droplet and flames. A goal of this modeling will be to develop simplified analytical models that retain the essential physics of Soret transport. In this way, Soret effects can be illustrated in a transparent manner.

Use will also be made of a computer code being developed as part of a NASA-sponsored program to study combustion of bi-component droplets. The numerical modeling involves development of a three-dimensional model for combustion of a droplet on a fiber (as well as a free droplet). The code includes important effects such as gas-phase radiant losses, detailed chemical kinetics, and realistic fiber effects (e.g., a nonslip condition, and fiber radiation in the vicinity of the flame). Soret transport can be turned on or off in the model.

References


Figure 1. Digital images of the drop rig: (a) overall rig; and (b) closeup of the pressure chamber interior. The endcaps for the pressure chamber are not shown.
REDUCED GRAVITY STUDIES OF SORET TRANSPORT EFFECTS IN LIQUID FUEL COMBUSTION

B. D. Shaw
University of California, Davis
RESEARCH GOALS

Investigate effects of multicomponent diffusion and thermal (Soret) diffusion

These phenomena can be important when large differences exist between molecular weights of gas species

H or H₂ with other species

Liquid hydrocarbon fuel (e.g., C₈H₁₈) with air
(can be important with diffusion flames)

This research utilizes droplet combustion to gain information on how Soret transport and multicomponent diffusion influence liquid fuel combustion in general

The following topics will be investigated

Transport of O₂ to the flame zone around a droplet
Transport of fuel to the flame zone
Sooting behaviors
Flame unsteadiness
Burning rates
THEORY FOR TRANSPORT OF OXYGEN TO THE FLAME ZONE
(Aharon and Shaw, 1998)

\[ \frac{d_f}{d_d} = \frac{r_f}{r_d} \approx \frac{\rho_d K V_O}{8 W_F n D_0 x_{O,\infty}} \]

Standoff Ratio

\[ D_O = \beta \phi D_{IO} \]

Effective O_2 Diffusivity

\[ \beta = 1 - x_{I,\infty} \alpha_{T,O} \ln \left( \frac{T_f}{T_\infty} \right) \]

Soret Transport

\[ \phi = \left[ x_{I,\infty} - x_{O,\infty} \sum_{j \neq O} \Gamma_{Oj} \frac{\varepsilon_j}{\varepsilon_O} \right]^{-1} \]

Multicomponent Diffusion
FLAME UNSTEADINESS

$$\tau_d = \frac{4r_d^2}{K}$$  Characteristic Droplet Lifetime

$$\tau_g = \frac{(2r_f0)^2}{D_g}$$  Characteristic Gas-Phase Diffusion Time

$D_g = \text{Effective gas-phase species diffusivity.}$

Quasisteady Flame Behavior is Promoted if $\tau_g / \tau_d$ Decreases

$$\frac{\tau_g}{\tau_d} = \left( \frac{r_f0}{r_0} \right)^2 \frac{K}{D_g} \approx \left( \frac{\rho_d \nu_o}{8W_F nX} \right)^2 \left( \frac{K}{D_g} \right)^3$$

Reducing $D_g$ should increase flame unsteadiness.

$D_g$ is influenced by inert species in the gas phase by changes in Soret transport and multicomponent diffusion effects.
PREVIOUS EXPERIMENTS (Shaw and Dee, 2003)

Drop-tower experiments
   NASA Glenn 2.2 s Drop Tower
   NASA Glenn drop dig

Test conditions
   Fiber-supported droplets
   Ambients at 1 atm

   \( \text{O}_2/\text{He} \)
   \( \text{O}_2/\text{N}_2 \)
   \( \text{O}_2/\text{Xe} \)

   \( \text{O}_2 \) Mole Fraction
   \( X = 0.21, 0.5 \)

Heptane-hexadecane droplets
   Initial hexadecane mass fractions
   \( Y = 0, 0.05, 0.2 \)

Considered flame unsteadiness, burning rates and sooting
Increasing the inert molecular weight promoted flame unsteadiness
MLAME UNSTEADINESS INTERPRETATION

<table>
<thead>
<tr>
<th>Inert</th>
<th>$D_{IO}$ (cm$^2$/s)</th>
<th>$\phi$</th>
<th>$\beta$</th>
<th>$\tau_g/\tau_d$ ($D_g = D_{IO}$)</th>
<th>$\tau_g/\tau_d$ ($D_g = \beta \phi D_{IO}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>10.3</td>
<td>0.65</td>
<td>0.43</td>
<td>0.024</td>
<td>1.2</td>
</tr>
<tr>
<td>N$_2$</td>
<td>3.3</td>
<td>0.94</td>
<td>0.97</td>
<td>0.24</td>
<td>0.37</td>
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<tr>
<td>Xe</td>
<td>2.4</td>
<td>1.03</td>
<td>1.34</td>
<td>0.8</td>
<td>0.32</td>
</tr>
</tbody>
</table>

Multicomponent and Soret transport effects can reverse gas-phase unsteadiness trends with respect to inert species molecular weight.

SOOT FORMATION

<table>
<thead>
<tr>
<th>Inert</th>
<th>$Le$ ($D_g = D_{IO}$)</th>
<th>$Le$ ($D_g = \beta \phi D_{IO}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>1.4</td>
<td>5.0</td>
</tr>
<tr>
<td>N$_2$</td>
<td>1.05</td>
<td>1.15</td>
</tr>
<tr>
<td>Xe</td>
<td>0.64</td>
<td>0.46</td>
</tr>
</tbody>
</table>

Decreasing the effective O$_2$ Lewis number promoted sooting in the experiments.

Multicomponent and Soret transport effects can change effective Lewis numbers, which influence flame temperatures and sooting.
SUMMARY

Soret transport and multicomponent diffusion can influence combustion behaviors

- Oxygen transport to flames
- Flame unsteadiness
- Sooting
- Burning rates
- Fuel transport to flames

Previous experiments have provided a preliminary indication that Soret transport and multicomponent diffusion can significantly influence combustion of liquid fuel droplets

Further research is presently being pursued to provide more information about these effects.

This research will investigate Soret transport and multicomponent diffusion effects in significantly greater detail

- Future reduced-gravity experiments with different fuels and gas-phase compositions will be performed
- Analytical and numerical modeling will also be performed
ACKNOWLEDGEMENT

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