Experimental and Modeling Study of the Burning of an Ethanol Droplet in Microgravity

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Motivation

droplet studies in microgravity:

- simple geometric configuration - opportunity for testing/validating theory
- facile method to study the diffusive combustion of fuel molecular species similar to those in transportation fuels
- link to multi-droplet (spray) applications
- fire safety criteria in space

ethanol:

- relatively simple and established chemistry
- azeotropic behavior of mixtures with water
- change in sooting tendency with pressure
- important gasoline fuel additive
Earlier Studies - Small Droplets

Hara and Kumagai (1991)

- free (unsupported) ethanol droplets
- 1 atm, in air
- \( d_0 \sim 0.7-1.3 \) mm
- 1.5 s droptower
- reported burning history, flame position

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Extinction
• drops tethered on silicon-carbide fibers (80, 150 microns), 2 to 5 mm initial diameter
• fuels: Methanol, Methanol-Water, Ethanol, Ethanol-Water, n-Heptane, n-Decane, n-Heptane-Hexadecane
• burned in cabin air (1 atm, 22-25 C, 39-46% RH)
• quiescent (all), convective (n-Heptane, n-Decane), & multiple drop (n-Heptane, n-Decane) experiments
• backlighted drop, direct flame video, & dual radiometer measurements
Droplet burning history (FSDC-2)

pure ethanol, $d_0 = 3.41$ mm
Time-Dependent, Spherically Symmetric, Bi-component Model for Droplet Combustion
(Based on FEM approach of Cho, et al., 1992)

Gas Phase:
- Multicomponent molecular diffusion
- Detailed chemical kinetics
- Spectral (non-luminous) thermal radiation
- UV flame emission

Species Equations:
\[
\frac{\partial}{\partial t} \left( \rho_s \frac{1}{r^2} \right) = -\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_s Y_{s,i} \right) + \omega_{s,i}
\]

Droplet Surface:
- Surface regression
- Evaporation of fuel
- Condensation/Dissolution of products
- Radiative heat exchange

Energy Conservation:
\[
\frac{\partial (\rho_s C_{ps} T_s)}{\partial t} + \nu_r \frac{\partial (\rho_s C_{ps} T_s)}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \lambda_s \frac{\partial T_s}{\partial r} - q_r \right) - \sum_{i=1}^n \frac{\partial p_s \left( Y_{s,i} \nu_r C_{ps} \right) T_s}{\partial r}
\]

Net Radiative Heat Flux

Droplet Interior:
\[
\frac{\partial (\rho_s C_{pi} T_i)}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \lambda_i \frac{\partial T_i}{\partial r} \right)
\]
\[
\frac{\partial Y_{i,j}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \nu_{i,j} \frac{\partial Y_{i,j}}{\partial r} \right)
\]
Model: further details

- detailed reaction mechanism of \( \text{C}_2\text{H}_5\text{OH} \) oxidation (Norton&Dryer, 1992)
  - 33 species
  - 142 reversible elementary reactions
- molecular transport parameters
  (CHEMKIN database & estimates)
- ethanol/water vapor pressure correlations
  (Kurimara et al. 1995)
- ethanol/water liquid density correlations
  (Bai et al. 1998)

Improved non-luminous Plank-mean radiation model:
- derived from the "rediscovered" exact analytical solution for spherically-symmetric system (Kuznetsov, 1951)
- allows for arbitrary radial distribution of the Plank-mean coefficient (i.e., free from the commonly-used approximation of \( \kappa_p = \text{const} \))
- takes advantage of the spherical symmetry (numerical efficiency)

No empirical model parameter adjustments were applied
Results: small droplets

Hara & Kumagai (1991), \( d_0 = 0.93 \text{ mm} \)

- model flame position is defined at the location of \( T_{\text{max}} \)
- the level of agreement for the flame standoff is acceptable as the experimental values have large uncertainty (poor ethanol flame visibility)
Results: large droplets

FSDC-2 experiments, 100% ethanol droplets

$d_0 = 2.79$ mm

$d_0 = 3.41$ mm

$d_0 = 5.83$ mm

Note the scale!
Droplet Reburning (FSDC-2)

- some (large) initial droplets that underwent extinction followed by subsequent vaporization stage could be re-ignited (up to 5 re-ignitions)
- in the model, this procedure was simulated by restarting the previous run with the imposed temperature profile that imitated the effect of igniter wire

![Graphs showing model-predicted burning rate](image)

Model-predicted burning rate

Well-reproduced sequence of radiative extinction events!
Results: Flame Standoff

(FSDC-2, only limited data available)

100% ethanol droplet (reburn) case, $d_0 = 2.89$ mm

- model flame standoff is defined by the location of $T_{\text{max}}$
- reasonable agreement between the model and the experiment
Average Burning Rate

- excellent agreement with the FSDC-2 and Hara & Kumagai data
- model shows no significant differences between 100% ethanol and 96% ethanol/4% water droplet burning rates
- advantages of the present detailed model over simplified approaches

- simplified analytical model (Filho, 1999)
- simplified numerical model (Puri & Libby, 1992)

- present model

- FSDC-2 (100% C₂H₅OH droplets)
- FSDC-2 (96% C₂H₅OH - 4% H₂O droplets)
- Hara & Kumagai (1991)
- Okajima & Kumagai (1975)
Extinction diameter

- excellent agreement between the model predictions and the experimental data
- first experimental (and confirmed theoretically) value of ethanol droplet radiative extinction diameter
Water Condensation & Azeotropic Behavior Based on the Model Analysis

\[ d_0 = 1 \text{ mm, initially } 100\% \text{ C}_2\text{H}_5\text{OH} \]

Water mass fraction vs. Time (s)

Fractional gasification rate vs. Water mass fraction

Vapor pressure (atm) vs. Water mass fraction

Azeotrope
condensation of water occurs only during a short initial period of time until the droplet composition approaches the azeotropic point (about 4% of water by weight)

for the remainder (main part) of the burning history, droplet combustion proceeds primarily via preferential gasification of ethanol

the above phenomenon explains the observed similarities in the predicted burning behavior of pure ethanol and 96% ethanol/4% water (azeotropic composition) droplets
Summary

- first extensive experimental information on ethanol droplet burning in microgravity
  - burning rates
  - extinction diameters
  - radiative extinction diameter (~ 4 mm)
  - flame diameters

- the presented numerical model is capable of predicting in detail the ethanol droplet burning behavior for the broad range of initial droplet sizes

- ethanol droplet combustion is less influenced by water condensation (as compared to the previously studied methanol cases) due to azeotropic behavior of ethanol/water mixtures

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ABSTRACT

The microgravity ethanol droplet combustion experiments were performed aboard the STS-94/MSL-1 Shuttle mission within the Fiber–Supported Droplet Combustion–2 (FSDC–2) program. The burning histories and flame standoffs for pure ethanol and ethanol/water droplets were obtained from the images recorded with two 8 mm videocameras. The obtained results show that average gasification rate is related to the initial droplet size in a manner similar to n–alkanes and methanol and consistent with the results of Hara and Kumagai [1] and the data taken recently in the NASA–Lewis 2.2 s droptower [2].

A transient, moving finite–element chemically reacting flow model applied previously to spherically symmetric combustion of methanol, methanol/water, n–alkane, and n–alkane binary mixture droplets was adopted for the problem of ethanol droplet combustion. The model includes detailed description of gas–phase reaction chemistry and transport, a simplified description of liquid phase transport, and non–luminous radiative heat transfer. Gas–phase chemistry was described with the detailed reaction mechanism of Norton and Dryer [3], which consists of 142 reversible elementary reactions of 33 species. Another recently published reaction mechanism of high–temperature ethanol oxidation [4] was also considered.

The model predictions were found to compare favorably with the experimental data. The model analysis also indicates that water condensation in the case of ethanol has smaller effect on average droplet gasification rate as compared with previously studied methanol cases. This effect is explained by non–ideal (azeotropic) behavior of binary ethanol–water mixtures. Further analysis of computational results and ethanol droplet radiative extinction behavior will be discussed.

REFERENCES
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