Combustion Behavior of Sub-millimeter Sized Oxygenated and n-Alkane Fuel Droplets

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Abstract
Petroleum-derived liquid fuels have been widely used to power the aerospace and ground transportation vehicles. Despite their projected decrease in availability in the near future, forecasts suggest that demand for liquid transportation fuel will continue to grow. Liquid fuels are preferred over other energy sources due to their high energy content, matured applied technologies, and existing fuel manufacturing/distribution infrastructure. Therefore, understanding the combustion of liquid fuels is immensely important both for developing advanced engines and emission controls. The simplest configuration for a liquid fuel that is amenable to numerical simulation with detailed kinetics is an isolated droplet burning in an environment in which streamlines of the flow are radial and the mass and energy transport are one-dimensional entirely due to the evaporation process - a configuration that can be attained under ‘zero’ and/or ‘micro’ g condition. As simple as the one-dimensional droplet combustion configuration may appear, it can provide an understanding of phenomena that have relevance in real spray combustion environments. These include moving boundary effects, unsteady heat conduction and mass diffusion in the droplet and surrounding gas, variable properties (dependent on temperature and composition), phase equilibrium at the interface, radiation dynamics, and detailed kinetic processes.

Finite volume formulation based computational fluid dynamic analysis has been applied to understand the physicochemical processes of droplet combustion for sub-millimeter sized various oxygenated and n-alkane fuels. To resolve the flame dynamics and combustion-generated species, fuel specific detailed chemical kinetic models have been employed for all the analyses. The fuels under the ‘oxygenated fuel’ category include methanol (CH₃OH) and four butanol isomers (n-, sec-, iso- and tert-C₄H₉OH) whereas for ‘n-alkanes’ we considered n-heptane (n-C₇H₁₆) and n-decane (n-C₁₀H₂₂). The primary scientific explorations of this thesis work are to better understand (a) microgravity fire-suppression of an untested fire-suppressant, (b) combustion kinetic model refinement of butanol (C₄H₉OH) isomers, and (c) directly induced cool flame dynamics of higher n-alkane fuels. The chronological development of the research direction shifts from a relatively
small fuel like methanol (CH$_3$OH) to heavier straight paraffinic fuel e.g. n-decane (n-C$_{10}$H$_{22}$). The first installment of the thesis is directed towards answering the feasibility of then-newly considered fire-suppressant xenon (Xe) for microgravity space application by the National Aeronautics and Space Administration (NASA). Methanol was used as model fuel to assess the combustion behavior under xenon-rich environment. The comprehensive analysis revealed that xenon promotes longer burning time and higher flame temperature compared to existing other diluents/extinguishers and can support hot flame with much lesser oxygen content than its counterparts. The exceptionally low thermal diffusivity of xenon is identified to be responsible for the significantly higher peak gas temperature and prolonged burn time. This detailed analysis clearly debilitates the potential of xenon as a next-generation fire-suppressant for microgravity applications and helped NASA in safeguard financial investment for International Space Station (ISS) experiments using xenon.

The second installment of the thesis outlines the efforts directed towards improving the gas phase kinetic model of butanol isomers based on droplet combustion experiments and computations. This is a unique contribution where the traditional gas-phase experiment/theory-driven kinetic model is further refined in light of critical recommendations from the droplet combustion analysis. The comprehensive kinetic model of Sarathy et al. (Combust. Flame, 2012) is one of the two widely used model for butanol isomers which has been extensively validated against homogeneous gas phase experiments. The numerical simulation of the butanol droplet combustion experiments at atmospheric conditions predicted the faster burning rate and larger flame diameter using the above model. An exhaustive perturbation analysis is carried on chemical, thermodynamic and transport parameters influences (while simultaneously isolating their cross-influences) to pinpoint the root cause of faster burning tendency of the model. The synthesized results from this huge variable-matric perturbation revealed that the isomer-specific species transport parameters were responsible for the observed behavior, and recommendations were made to update relevant Lennard-Jones potential parameters.

The final segment of the thesis discusses the direct initiation of cool flame combustion for submillimeter-sized higher n-alkane droplets (n-heptane and n-decane) for possible terrestrial experiments without the necessity of radiative extinction as frequently encountered onboard the ISS experiments. It has been found that the dimensionality of the droplet ($D_o = 0.5$ mm) statistically reduces the possibility of achieving direct cool flame burn for the droplet by simply varying the ignition energy initiation. Therefore, it was conceptualized that a combination of a reduced ignition source and induction chemistry modulation may hold the possibility of direct initiation of cool flame for n-C$_7$H$_{16}$ and n-C$_{10}$H$_{22}$ even in ground-based drop tower experiments. To facilitate this idea, we numerically investigate the droplet combustion under selective ozone (O$_3$) augmented ambient where O$_3$ serves as an induction chemistry modulator through its liberation of atomic O via molecular decomposition. The available atomic O then reacts with the surrounding fuel producing OH radical, and eventually water and heat. This latter heat input acts as a secondary
thermal feedback to the droplet surface facilitating steady surface burning rate which then stabilizes the cool flame near the droplet surface. It was found that the fuel physical properties, especially flash point, play a decisive role in determining the nature of the initial cool flame dynamics and the ozone requirements. Higher flash point fuel (here, n-C\textsubscript{10}H\textsubscript{22}) is likely to undergo initial dumped cool flame oscillation than its lower value counterpart (n-C\textsubscript{7}H\textsubscript{16}) and will require higher O\textsubscript{3} loading under identical ambient. In the near-limit condition, such a directly introduced cool flame fails to attain a steady burn and enters into a continuously evolving oscillatory cool flame. Analyses further indicate that the dynamic interaction of degenerate chain branching and chain termination/propagation reaction classes of QOOH (Q=C\textsubscript{n}H\textsubscript{2n}, here n = 7) species associated with the low-temperature kinetic regimes, and continuous fuel leakage across the flame location contribute to the ever-increasing trends of the oscillation magnitude.