

Combustion characteristics of a single decane/ethanol emulsion droplet and a droplet group under puffing conditions

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Abstract

Combustion characteristics of an ethanol-in-decane emulsion droplet and a droplet group under puffing conditions have been investigated by direct numerical simulation (DNS). Before puffing, a quasi-steady flame is formed in the wake of the parent decane droplet. Due to superheating, boiling of ethanol sub-droplets is initiated. Following rapid growth of the vapor bubble, ethanol vapor is unsteadily ejected out and interacts with the downstream wake flame. The local gas mixture fraction is affected by this ejection. The gas-phase temperature and reaction rate also show different characteristics from those of a 1D steady flame. In the dual-fuel system, fuel/air mixing in combustion can be characterized by the scalar dissipation rates (SDRs) due to mixing of decane/air and ethanol/air and cross mixing of decane/ethanol. The transient interaction between the droplet wake flame and the ejected vapor by puffing is evident in the flame S-curves. The interaction is further quantified by the budget analysis in the mixture fraction – SDR space. The contribution of the cross SDR between decane and ethanol to the rate of change of the SDR of the primary fuel decane is initially negative, which is particular to puffing. Later the cross SDR can also become positive. As the mixing continues, the magnitude of the SDRs becomes smaller. When puffing occurs in the transverse direction, the ejected vapor may sweep a region within a few diameters away from the parent decane droplet. If other emulsion droplets are in this region of influence, inter-droplet interactions occur. A multiple-droplet case demonstrates this interaction and implies that such an interaction will occur in an emulsion fuel spray and should be considered in modeling a multi-component emulsion fuel spray in a combustor.

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1. Introduction

Reducing emissions of carbon dioxide (CO₂) and soot from liquid fuel combustion is significantly important due to increasing environmental concerns. Using biofuels such as bioethanol or biodiesel is one of the effective ways for reducing harmful emissions. Adding bioethanol to diesel is one possible solution for diesel engines [1,2]. Ethanol is oxygenated, i.e. an ethanol molecule contains an oxygen atom, which contributes to reducing particulate matter (PM). The miscibility of ethanol in diesel can be improved by adding biodiesel into the blend, which works as a surfactant agent. The blend forms ethanol-in-diesel emulsion, with ethanol dispersed as tiny sub-droplets in the continuous phase of diesel. Above a certain threshold of the ethanol-to-diesel ratio, puffing or microexplosion occurs due to the distinctly different boiling temperature of the two fuels. Following explosive boiling of superheated ethanol sub-droplets, puffing (partial microexplosion) causes partial droplet breakup and microexplosion violent breakup of the entire droplet [3–5]. When puffing or microexplosion occurs in a fuel spray, secondary atomization will be induced. Generally, secondary atomization enhances droplet evaporation and fuel/air mixing. Although with a great potential, our understanding on secondary atomization induced by puffing and microexplosion is still far from sufficient. It is therefore significantly important to understand the combustion characteristics of such fuel blends under puffing conditions for better and further utilization of biofuels. This is a complex physical problem on fluid and combustion dynamics, which is highly worth tackling.

In our previous DNS studies [5–7], physical mechanisms related to emulsion droplet puffing/microexplosion have been unveiled comprehensively, including vapor bubble growth and droplet breakup [5], convective heating of an emulsion droplet [6], and convective fuel-vapor/air mixing for a single emulsion droplet and a droplet group [7]. From these results, fuel-vapor/air mixing characteristics under puffing conditions have been unveiled for non-reacting emulsion fuel droplets. The objective of the present study is to investigate combustion dynamics of emulsion droplets, especially focusing on (1) interactions between puffing ethanol vapor and droplet combustion using scalar dissipation rates (SDRs) as a primary physical and modeling parameter and (2) change of droplet group combustion characteristics due to puffing. To simplify the combustion kinetics and the boiling temperature property, decane is used as a surrogate fuel, and decane/ethanol emulsion is considered. Our in-house experimental study has confirmed that the droplet combustion characteristics are similar using decane. Using an enlarged-scale

single emulsion droplet (diameter $D \sim 2$ mm) [7], it has been shown that the local flame luminosity increases transiently when puffing occurs, due to the modulated local equivalence ratio by the ejected ethanol vapor. Such a flame/vapor interaction is also expected to occur in a fuel spray. To directly relate the present results to droplets in a fuel spray, typical spray-scale droplets of $D \sim O(10 \mu\text{m})$ are considered, as in [5–7]. Both a single decane/ethanol emulsion droplet and a droplet group are considered. As pointed out in [8], the time of heating for spray-scale droplets in a combustor is generally short, and puffing is more likely to occur than complete microexplosion. Therefore puffing effects on combustion characteristics of an emulsion fuel droplet and a droplet group are investigated.

2. Mathematical formulations, numerical methods, and case setup

The governing equations are the conservation equations of mass, momentum, energy and species mass fractions [5–7]. The energy equation is transformed into the temperature equation. Compressibility is included to account for explosive boiling and thermal expansion. Newton's viscosity law is used and heat conduction is modeled by Fourier's law. Mass diffusion is modeled by Fick's law with a unity Lewis number in the gas phase. Temperature-dependent physical properties to cover the necessary temperature range are retrieved from the database of NIST (National Institute of Standards and Technology) [9].

The rate of phase change $\dot{\omega}_p$ is formulated at an evaporating or boiling interface, which is resolved in the grid system, as [5–7,10]

$$h_l \dot{\omega}_p = [\lambda \nabla T \cdot \mathbf{n}], \quad (1)$$

$$\dot{\omega}_p (Y_{i,G} - Y_{i,L}) = [\rho D_{diff} \nabla Y_i \cdot \mathbf{n}], \quad (2)$$

where h_l is the latent heat of evaporation, λ the thermal conductivity, D_{diff} the diffusion coefficient and \mathbf{n} the surface-normal unit vector. The subscript L denotes the liquid phase and G the gas phase, respectively. The square brackets denote the difference of a variable f between the liquid and gas phases at the interface, i.e. $[f] = f_L - f_G$. For the evaporation on the surface of the parent decane droplet, the Clapeyron–Clausius relation is used [5–7,10]. For the boiling of ethanol, the superheat degree $\Delta T = T - T_b$, where T_b is the boiling temperature, determines the mass boiling rate in Eq. (1). Using the above rates of phase change, jump conditions for mass, momentum and heat transfer at the resolved interface are given [5–7,10].

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