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n-Butanol droplet combustion: Numerical modeling and reduced gravity experiments

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Abstract

Recent interest in alternative and bio-derived fuels has emphasized butanol over ethanol as a result of its higher energy density, lower vapor pressure and more favorable gasoline blending properties. Numerous efforts have examined the combustion of butanol from the perspective of low dimensional gas-phase transport configurations that facilitate modeling and validation of combustion kinetics. However, fewer studies have focused on multiphase butanol combustion, and none have appeared on isolated droplet combustion that couples experiments with robust modeling of the droplet burning process. This paper presents such an experimental/numerical modeling study of isolated droplet burning characteristics of *n*-butanol. The experiments are conducted in an environment that simplifies the transport process to one that is nearly one-dimensional as promoted by burning in a reduced gravity environment. Measurements of the evolution of droplet diameter ($D_o = 0.56$–0.57 mm), flame standoff ratio ($FSR \equiv D_f/D$) and burning rate (K) are made in the standard atmosphere under reduced gravity and the data are compared against numerical simulation. The detailed model is based on a comprehensive time-dependent, sphero-symmetric droplet combustion simulation that includes spectrally resolved radiative heat transfer, multi-component diffusive transport, full thermal property variations and detailed chemical kinetic. The simulations are carried out using both a large order kinetic mechanism (284 species, 1892 reactions) and a reduced order mechanism (44 species, 177 reactions). The results show that the predicted burning history and flame standoff ratios are in good agreement with the measurements for both the large and reduced order mechanisms. Additional simulations are conducted for varying oxygen concentration to determine the limiting oxygen index and to elucidate the kinetic processes that dictate the extinction of the flame at these low oxygen concentrations.

Keywords: *n*-Butanol; Biofuel; Droplet combustion; Microgravity; Modeling

1. Introduction

The growing interest in normal butanol (n-C_4H_9OH, boiling point of 391 K) as a non-petroleum fuel for internal combustion engines,

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either as a gasoline surrogate or an additive to increase performance of both gasoline and diesel fuels due to its favorable properties relative to ethanol [1–3], has stimulated fundamental research to understand its combustion kinetics. The experimental configurations used for this purpose typically incorporate a zero or one-dimensional transport dynamic (i.e., in shock tubes [4–6]), constant volume combustion chambers [7], jet stirred reactors [8–14], and opposed flow diffusion flames [15] with pre-vaporized butanol to facilitate *ab initio* modeling of the flow and combustion dynamics involved.

Few studies of *n*-butanol combustion have been carried out to evaluate kinetic mechanisms derived from spray or droplet dynamics, and none have done so incorporating detailed kinetic scheme. The work of Wang et al. [16] is noteworthy for using the environment of a direct injection diesel engine fueled with a mixture of diesel fuel and *n*-butanol to validate a reduced kinetic mechanism using the KIVA-3vr2 code [17], which requires certain spray model constants to be calibrated and adjusted to make the liquid and vapor penetrations match experimental measurement of these quantities, as well as submodel inputs for turbulence, gas jet/collision for spray, spray/droplet breakup, and droplet evaporation and wall collision dynamics.

The simplest configuration for a liquid fuel that is amenable to detailed simulation 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 due entirely to the evaporation process. As simple as the one-dimensional droplet flame may appear, it is relevant to the complex environment of a spray through elements that carry over to the spray environment [18]. 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 a detailed kinetic mechanism for the combustion process. Computer simulations based on assuming spherical symmetry recently been applied to a range of alkane, alcohol and methyl ester systems [19–22].

In this paper we present a comprehensive numerical simulation of the combustion of isolated *n*-butanol droplets that assumes spherical symmetry. The intent is to examine the potential of the combustion kinetics previously developed for butanol using targets from low dimensional gaseous configurations as noted previously, to predict droplet combustion targets. These include the evolutions of droplet and flame diameters (D and D_f, respectively), and the burning rate $K\left(\equiv\left|\frac{dD^2}{dt}\right|\right)$. The initial droplet diameters (D_o) are essentially constant in this study (between 0.56 mm and 0.57 mm) and the combustion process is examined in the standard atmosphere. The simulations presented here employ a detailed kinetic mechanism for *n*-butanol that incorporates 284 species and 1892 reactions [23]. The results are compared to experimental data as well as to predictions that employed a reduced order kinetic model [16] consisting of 44 species and 177 reactions.

2. Experimental setup and procedure

Individual *n*-butanol droplets are formed, deployed, and ignited under conditions that achieve nearly spherically symmetric burning. As with a number of prior studies (e.g., [22,24,25]) nearly spherical flames were achieved by burning the test droplets under free-fall conditions. Figure 1 illustrates the experimental procedures for the present study.

A piezoelectric droplet generator [26] propels fuel droplets (D_o on the order of between 0.5 mm and 0.6 mm) onto the intersection of two 14 μm SiC fibers crossed at approximately 60° [25,27] The fuel droplet is then ignited

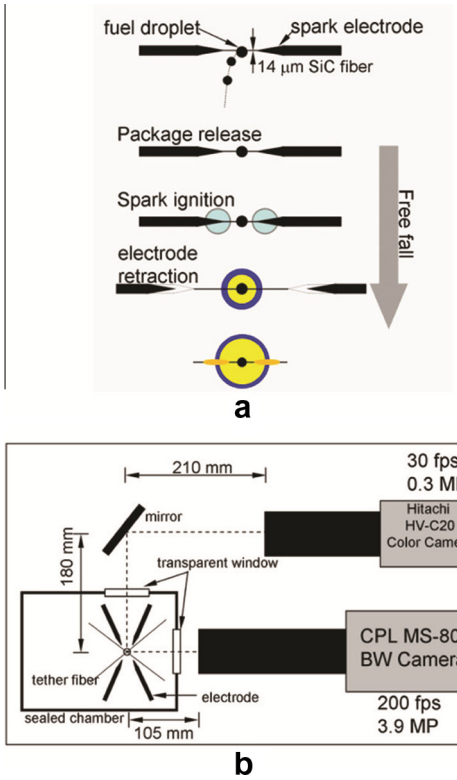

Fig. 1. (a) Schematic diagram of experimental procedure to deploy droplets onto SiC fiber. (b) Experimental setup (numbers in millimeters not to scale).