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Soot formation in non-premixed counterflow flames of butane and butanol isomers

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ABSTRACT

Soot formation processes for butane and butanol isomers have been experimentally investigated and compared in a counterflow non-premixed flame configuration at atmospheric pressure. Non-intrusive laser-based diagnostic techniques, including Laser Induced Incandescence and Light Extinction, have been adopted for soot volume fraction measurements. Experimental results of these C₄ fuels have been compared to illustrate the effects of hydroxyl (–OH) group and the isomeric structures on soot formation process. Under the investigated conditions, butane isomers were observed to form more soot than butanol isomers, thereby showing the effect of the hydroxyl group. The effects of isomeric structural differences on sooting propensity were also observed within the butane and butanol isomers. In addition, while soot volume fraction was seen to increase with increasing fuel mole fraction, the ranking of sooting propensity for these C₄ fuels remained unchanged. Effects of varying strain rate and oxygen mole fraction on soot formation were studied herein as well. For each isomeric class, two chemical kinetic models available in the literature were used to simulate and compare the spatially-resolved profiles of the soot precursors. The amount of soot precursors predicted by the models was different and the initial fuel breaking pathways were also found to differ significantly. Furthermore, no direct correlation between the computed mole fractions of soot precursors and the measured amount of soot formed in the present experimental conditions was observed.

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1. Introduction

Currently, 80% of world energy demand is met by using fossil fuels [1]. With the projected world energy demand expected to triple by the end of this century [1], alternative and renewable means of energy resources have huge potential in meeting the ever increasing world energy demand. Biofuels, amongst many other alternative sources of energy, offer multiple benefits in terms of providing energy security, economic advantages, and environmental protection [1].

Extensive research has been conducted on biofuels that are produced from the biomass [2]. The so-called second generation biofuels do not pose a threat to food security as these biofuels can be produced from inedible crops [2]. Butanols are second generation biofuels, which are considered as a substitute to currently used first generation ethanol as blend in gasoline. Butanol isomers are high in energy density (36 MJ/kg) compared to ethanol (27 MJ/kg) [3]. Additionally, butanol isomers except for *tert*-butanol are less miscible

in water than ethanol, and hence provide ease in fuel distribution through existing infrastructure [2]. Biochemical processes for butanol isomers production, except for *tert*-butanol, have been established and are less capital intensive [2,4]. *tert*-Butanol that is derived as a petroleum by-product from the propylene oxide, is often used as an octane enhancer in gasoline [5].

As biofuels are considered for practical applications, interest of the research community in fundamental research for butanol isomers has been increasing. The investigation of their fundamental properties assists in the design of advanced engines to control the combustion processes. This is evident as there have been numerous fundamental combustion studies of butanols conducted on laminar premixed and non-premixed flames e.g., [6–25], flow reactors e.g., [26–31], ignition delays in shock tubes e.g., [32–41] and rapid compression machines e.g., [42–45], fuel pyrolysis e.g., [46–50], and jet stirred reactors e.g., [7,13,19,51–56]. In addition, engine studies were conducted for butanol isomers to determine brake specific fuel consumption, exhaust gas temperature, and thermal efficiency e.g., [57–62].

Along with the aforementioned studies, it is also imperative to conduct studies related to carbonaceous emissions. Soot is combustion generated carbonaceous particulate matter which has been considered responsible for climate change and health problems. As soot


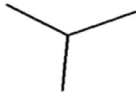

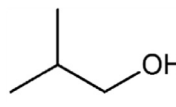
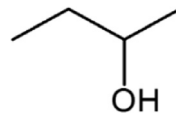
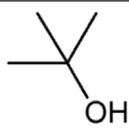
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Table 1
Chemical structures of butane and butanol isomers.

<i>n</i> -butane	<i>iso</i> -butane	<i>n</i> -butanol	<i>iso</i> -butanol	<i>sec</i> -butanol	<i>tert</i> -butanol
					

formation adversely affects the performance and lifetime of practical combustors and engines, understanding soot formation processes for different conventional and alternative fuels in flames is vitally important to rationalize their use as a potential source of energy [63]. The C_4 fuels investigated in this study are *n*- and *iso*-butanes, as well as *n*-, *iso*-, *sec*-, and *tert*-butanols. The structures of these fuels are shown in Table 1. By comparing butanol and butane isomers, it allowed us to investigate the effects of hydroxyl ($-OH$) group and the isomeric structures on sooting tendency.

Previously, Camacho et al. [63] studied the sooting characteristics of *n*-butane, *iso*-butane, *n*-butanol, and *iso*-butanol in a burner stabilized stagnation premixed flame configuration to investigate the impact of fuel bound hydroxyl group, as well as the effect of fuel structure. They found that under the same C/O ratio, butanol flames nucleate sooner than butane flames. It was concluded by Camacho et al. [63] that the sooting behavior in the premixed flames at the nucleation stage can be predicted by the soot precursors, while at the mass growth stage the relationship between the predicted benzene concentration and the sooting behavior becomes less clear, considering the complexity of soot formation process. McEnally and Pfefferle [64] studied the sooting behavior of butanol isomers by doping 3500 ppm of each of butane and butanol isomers in a coflow methane-air non-premixed flame. They found that benzene formation is directly linked to propargyl (C_3H_3) species concentration. It is noted that both the studies of Camacho et al. [63] and McEnally and Pfefferle [64] have focused on the incipient soot formation process.

To our knowledge, none of the literature studies have been conducted to investigate the soot formation of these butanol isomers in a non-premixed counterflow flame configuration, and all the butanol isomers have not been compared with the butane isomers in such a sooting flame configuration. Counterflow non-premixed flame is known to provide an aerodynamically-clean and well-characterized configuration for experiments and simulations. With judicious mixture compositions for the fuel and oxidizer streams, the resulting non-premixed flame can be situated at different locations relative to the stagnation surface so that it is possible to separate the processes of soot formation and oxidation for further characterization. In this study, the sooting behavior of each flame is characterized and determined by measuring its spatially-resolved soot volume fraction profile.

Various techniques of soot measurement, such as gravimetric sampling, condensation particle counters, differential mobility particle sizes, and transmission electron microscopy using thermophoretic sampling, have been developed [65]. These techniques rely on the collection of soot particles manually, examining them by their physical parameters, such as weight, particle mobility in an electric field, etc., and the use of a microscope. As such, these sampling techniques are time consuming and some of them are intrusive. Faster, non-intrusive optical techniques have been developed to characterize soot formation in combustion. Two such laser-based techniques of soot particle measurements, namely Laser Induced Incandescence (LII) and Light Extinction (LE), have been used in the present study. In particular, the use of planar LII imaging in conjunction with line-of-sight LE calibration technique provides very fast, quantitative, and spatially-resolved soot volume fraction measurements.

In the following, we will first specify the experimental details, including a counterflow burner facility, LII/LE setup, calibration procedure using the LE technique to determine a calibration factor to convert the LII signals into quantitative soot volume fraction measurements, and the current test matrix. Next, the computational methodology and the literature reaction mechanisms employed to simulate the counterflow flame structures at varying experimental conditions will be introduced. Subsequently, the experimental results of butane isomers and butanol isomers with variations of strain rate, fuel loading, and oxygen mole fraction will be presented and compared, followed by the discussion of computational results, including flame structure, concentrations of soot precursors, and chemical kinetic analyses based on gas-phase chemistry.

2. Experimental specifications

2.1. Counterflow burner facility

A counterflow burner facility was used to establish a non-premixed flame. The burner consisted of two aerodynamically converging opposing nozzles of 10 mm exit diameter with a separation distance of $L = 11$ mm. More details on this burner facility can be found in [66,67], and hence a brief description of the system setup is given below. Liquid fuels were injected using a high precision liquid fuel pump, and were vaporized by providing heated annular coflow of heated nitrogen in the vaporization chamber. The gaseous fuels, namely butane isomers, were introduced using a mass flow controller, capable of controlling flow rates as low as 20 standard cubic centimeters per minute. The fuel/nitrogen mixture was introduced from the bottom nozzle, while nitrogen and oxygen were mixed in a separate line and introduced from the top nozzle. Supply lines from the flow panel to the bottom nozzle were maintained at an appropriate temperature by using heating tapes to prevent condensation of liquid fuels.

2.2. Laser induced incandescence

Laser Induced Incandescence (LII) has been widely used technique for soot measurements e.g., [68–90]. In the LII technique, a Continuum Powerlite 8010 Nd:YAG laser was used to provide a laser output of 532 nm wavelength (the second harmonic) at 10 Hz repetition rate. This visible wavelength facilitates precise laser sheet alignment in the center of the burner, which is crucial in soot measurements as the soot volume fraction varies radially. Since the primary soot particle sizes are expected to be in the range of 2–90 nm, the wavelength of 532 nm also fulfills the Rayleigh absorption criterion of $\frac{\pi D}{\lambda} \ll 1$, where D is the diameter of the soot particle and λ is the laser wavelength. The laser beam has a Gaussian profile with the least square factor of 0.95, and the laser power used for the LII measurements was 220 mW. The short laser pulse width of 7 ns results in rapid heating of soot particles, as seen from a representative temporal profile of LII signal shown in Fig. 1. It is noted that the LII signal profile in Fig. 1 is normalized with the maximum LII signal. The laser beam was guided in the sooting zone using dichroic mirrors. The propagating laser beam has a uniform beam diameter of 8 mm, as the Gaussian

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