



NO_x formation and flame velocity profiles of *iso*- and *n*-isomers of butane and butanol

Gregory A. Chung, Benjamin Akih-Kumgeh, Graeme M.G. Watson, Jeffrey M. Bergthorson *

Department of Mechanical Engineering, McGill University, 817 Sherbrooke West, Montreal, Canada H3A 2K6

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Abstract

NO formation and flame propagation are studied in premixed flames of *iso*- and *n*-isomers of butane and butanol through experimental measurements and direct simulation of experimental profiles. The stabilized flame is realized through the impingement of a premixed combustible jet from a contraction nozzle against a temperature-controlled plate. The velocity field is obtained by means of Particle Image Velocimetry (PIV) and nitric oxide concentration profiles are measured using Planar Laser Induced Fluorescence (PLIF), calibrated using known NO seeding levels. It is found that NO formation in *n*- and *iso*-isomers is comparable under the conditions considered, except for rich butanol mixtures, whereby NO formation is higher for *iso*-butanol. Generally, less NO is formed in butanol flames than in the butane flames. The experiment is simulated by a 1D chemically reacting stagnation flow model, using literature models of C1–C4 hydrocarbons [Wang et al., 2010] and butanol combustion chemistry [Sarathy et al., 2009, 2012]. NO prediction is tested using two of these mechanisms with a previously-published NO_x submechanism added into the butane and butanol models. While a good level of agreement is observed in the velocity field prediction under lean and stoichiometric conditions, discrepancies exist under rich conditions. Greater discrepancies are observed in NO prediction, except for the C1–C4 mechanism which shows good agreement with the experiment under lean and stoichiometric conditions. The current study provides data for further development of mechanisms with NO_x prediction capabilities for the fuels considered here.

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1. Introduction

There is increased interest in using butanol isomers as alternative fuels for spark-ignition engines. These C4 alcohols are characterized by more favorable energy densities and physical properties compared to the more widely used

ethanol biofuel. The need for characterization of their combustion properties has led to various experimental and modeling studies.

Experimental investigations have focused on ignition behavior [1–5], flame propagation [6–10], detailed speciation in homogeneous reactors and flat flames [8,10,11], as well as system-level combustion in engines, as reviewed in [12]. Closely linked to these experimental studies are detailed chemical kinetic modeling efforts. Models have been proposed based on validation of homogeneous reactor experiments, such as shock tube

* Corresponding author.

E-mail address: jeff.bergthorson@mcgill.ca (J.M. Bergthorson).

and jet-stirred reactors [1,13,5], while others have extended validation targets to flames [8,14,15,10,16]. As reviewed by Kohse-Höinghaus et al. [17], these models and experiments have led to understanding of some key mechanistic pathways in butanols that differ from the oxidation of non-oxygenates, such as alkanes.

Comparative flame studies of alcohols have also been reported. Veloo and Egolfopoulos [7] investigated the laminar flame propagation of the four butanol isomers, observing the much slower propagation of *tert*-butanol flames compared to those of the other three isomers. Oßwald et al. [11] have studied the detailed chemical structure of rich, low-pressure, flat flames of the four butanol isomers. The authors conclude that macroscopic properties, such as temperature, major species, and equilibrium mole fractions, are similar for all isomers. Differences were found to arise in the pool of intermediate oxygenated species such as aldehydes and ketones, whose formation pathways can be linked to the structure of the fuel. The highly branched *tert*-butanol was found to exhibit higher hydrocarbon intermediates and fewer oxygenates. These observations are similar to those reached in an earlier study by Yang et al. [18] regarding oxygenated intermediates arising from these butanol isomers.

While progress has been made in relating combustion dynamic properties, such as flame propagation, to oxidation chemistry, the important question of NO_x emission and its relation to fuel structure has not been addressed in detail. There is a growing need to investigate NO_x emission and mitigation strategies during the combustion of all types of fuels. The quantitative determination of NO_x formation in flames continues to be a challenge. NO_x formation is considered to occur in a number of ways; one of which is the prompt or Fenimore mechanism [19] which implicates the fuel combustion intermediates leading to CH radical formation. Differences in NO_x formation propensity of fuels with comparable adiabatic flame temperatures would be expected to be closely linked to the prompt mechanisms. Various NO measurement approaches have been suggested, with Laser Induced Fluorescence (LIF) emerging as a favored technique with various excitation line options [20–22]. However, NO_x measurement by LIF has only been extensively applied to flames of lower carbon compounds, especially methane. Higher alkanes, such as butane isomers and other components of practical fuels, have received less attention in terms of NO_x experiments and modeling. There is also a need to evaluate the emission levels of alternative fuels, such as butanol, relative to conventional hydrocarbon fuels, such as butanes. In system-level tests, these evaluations are rendered difficult by the numerous physical and chemical processes involved. Furthermore, the hydrodynamics and propagation speeds of

butanol flames are only addressed in a limited number of studies [7]. For further mechanism validation, stagnation flame experiments enable the assessment of model performance under realistic, strained flow fields. These areas merit further attention in the process of detailed characterization and modeling of the combustion of butanol isomers.

This study is aimed at investigating the relative reactivity of *iso*- and *n*-isomers of butanol and butane by means of stagnation flame experiments. The butane isomers are chosen as surrogates for conventional gasoline due to their similar chemical structure to the butanol isomers. Velocity profiles are compared with predictions obtained using literature chemical kinetic models [8,16,23]. A key contribution in this work is the quantitative measurement of NO concentration profiles in these flames using Planar Laser Induced Fluorescence PLIF in order to identify the role of chemical structure and mixture composition on the overall NO_x formation. Though studies have been performed investigating NO formation in ethanol fuels [24], this is the first study to directly compare the NO formation of alcohol with alkane fuels. Since the chemical kinetic mechanisms used in this work do not yet have NO_x submodels, a NO_x submechanism developed for methane combustion, GDF-kin3.0 [25,26], has been incorporated into the mechanisms and used to simulate the experiments.

2. Stagnation flame experiments and 1D modeling

Experiments are carried out in a stagnation flame set-up, as shown in Fig. 1. The experiment is realized as a jet of premixed combustible gas impinging on a temperature controlled plate at a defined separation distance as in Bergthorson et al. [27]. The laminar jet issues from a contrac-

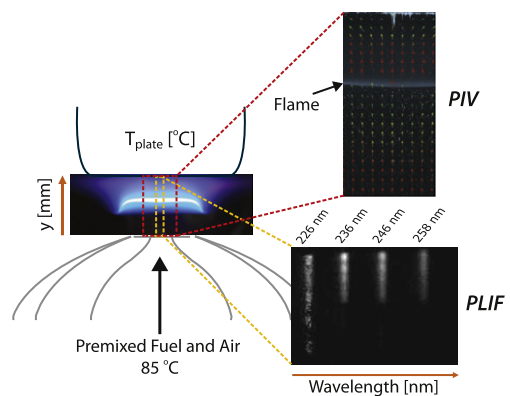


Fig. 1. Experimental set-up for velocity field and NO profile measurements.

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