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A comparative study of *n*-propanol, propanal, acetone, and propane combustion in laminar flames

Jing Gong, Shuang Zhang, Yu Cheng, Zuohua Huang *, Chenglong Tang, Jiaxiang Zhang

State Key Laboratory of Multiphase Flow in Power Engineering, School of Energy & Power Engineering, Xi'an Jiaotong University, Xi'an 710049, China

Abstract

The laminar flame speeds of C_3 oxygenated fuels (*n*-propanol, propanal and acetone) and hydrocarbon (propane) were measured in a combustion bomb to compare combustion characteristics of C_3 alcohol, aldehyde, ketone, and alkane. Propanal shows the highest flame speeds while acetone gives the lowest one. The experimental observations are further interpreted with chemical kinetic models. The effects of distinctive molecular structures on the fuel consumption pathways are clarified. Propanal generates a large H atom pool that enhances the oxidation, leading to the highest flame speeds. However, acetone forms methyl radical (CH_3) and has lower flame speeds as a consequence. The calculated maximum concentrations of H, OH, and CH_3 confirm this analysis. It is found that propanal yields the highest H and OH concentrations while acetone produces the lowest H and OH concentrations among all tested fuels. Moreover, acetone presents higher CH_3 concentration, especially for fuel rich condition. *n*-Propanol and propane show comparable flame speeds and similar radical concentrations, especially H and OH. The different kinetics among hydrocarbon species with the same carbon numbers can provide a horizontal view in the hierarchical hydrocarbon chemistry.

Keywords: Laminar combustion; Propanol; Propanal; Acetone; Propane

1. Introduction

Energy efficiency and emission reduction have become major topics of interest to the combustion community in the last few decades. Biofuels have been investigated as an alternative fuel to resolve these issues. Particularly, small alcohols have been commercialized and widely used in engines. Recently, the fermentation methods of alcohols have been well developed. This facilitates the application of alcohols and attracts more attention to the study of alcohol chemistry. Many works have been done on alcohols to clarify their combustion characteristic and chemical kinetic models were developed to predict experimental data and understand complex combustion phenomena [1–7]. The previous studies indicate that aldehydes, mainly produced from parent alcohols by the reactions at the α-carbon or hydroxyl (OH)

* Corresponding author. Fax: +86 29 82668789.
E-mail address: zhhuang@mail.xjtu.edu.cn (Z. Huang).

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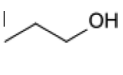
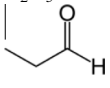
group, play an important role in the decomposition and oxidation of alcohols as key stable intermediate products [8–11]. Ketones are another important intermediate species in the combustion of hydrocarbons and oxygenates. Aside from being intermediates in combustion, aldehydes and ketones are also toxic emissions from engines that threaten environmental safety and human health. Many studies have been focused on the detection and formation of these toxic emissions [12–14]. An accurate detailed kinetic model is required not only for the control of these emissions, but also for understanding the combustion chemistry of other molecules that are formed from aldehydes and ketones in combustion systems. Most research focuses on single fuel chemistry, fuel isomers, and the hierarchical structure of fuels with the same functional group but varied carbon chain length [6,15–21]. It is found that the reactions related to the destruction of functional groups play an important role on the global reactivity of a specific fuel. In the present work, hydrocarbons with different functional groups and the same carbon number are studied to aid the development of a more accurate reaction model.

C_3 oxygenated fuels are the smallest hydrocarbons including alcohol isomers, aldehyde and acetone structures. Propanol isomers can be obtained through fermentation [22–25]. Acetone is one of the main products from the traditional ABE (Acetone–butanol–ethanol) fermentation method [26]. An early study by Norton and Dryer [11] concluded that higher concentrations of propanal enhanced the overall reactivity of *n*-propanol, while acetone, a product of *iso*-propanol oxidation, decreases overall reactivity. Li et al. [27] investigated acetone, *n*-propanol, and *iso*-propanol with tunable synchrotron photoionization and molecular beam mass spectrometry. Flame species including isomeric intermediates were identified. Veloo et al. [28] studied the flame propagation and extinction of *n*-propanol, *iso*-propanol, and propane in the counterflow configuration at atmospheric pressure. The effects of the presence and the location of hydroxyl radical were investigated. Benjamin et al. [29] investigated the ignition behavior of selected C_3 oxygenated hydrocarbons behind reflected shock waves, including propanal and acetone. Differences between isomer were revealed for ketone (acetone) and aldehyde (propanal). Burluka et al. [30] measured the laminar flame speed of propylene oxide, propanal, and acetone, but the calculated results had only qualitative agreement with the experimental results. Ranzi et al. [31] reviewed the kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels hierarchically and comparatively, including C_3 alcohol isomers, propanal and acetone. However, more experimental data and further kinetic studies are needed for more accurate predictions of the combustion characteristics of C_3 fuels. In the present study, the laminar flame speeds of *n*-propanol, propanal, acetone, and propane are investigated in this study using a constant volume bomb for the validation of chemical kinetic models, which are used for a comparative chemical kinetic study. The oxidation mechanisms of fuels with different functional groups are also investigated by comparing the intermediate species pools that are accumulated from the oxidation of specific molecules.

2. Experimental approach

Laminar flame speeds were measured in a cylindrical combustion bomb with a 180 mm of inner diameter and a length of 210 mm. 80 mm diameter optical windows are located on both sides of the chamber. The combustion chamber was heated up to the initial temperature of 343 K and 393 K by an electrical band heater and the temperature was monitored by a thermocouple installed in the chamber with an accuracy of ±3 K. The liquid fuels, *n*-propanol, acetone and propanal, were injected into the heated chamber using micro syringes through a valve. The purities of liquid fuels used in this study are more than 99.8%. The main properties of the fuels tested are tabulated in Table 1. To reduce the uncertainty of the amount of liquid fuel, different measuring ranges of micro syringes with microscopic scales were used for each target volume. The operation of the fuel injection valve was instantaneous to avoid the possible fuel loss

Table 1
Properties of the fuels tested in this study.

	n-Propanol	Propanal	Acetone	Propane
Molecular formula	C_3H_7OH	C_2H_5CHO	CH_3COCH_3	C_3H_8
Chemical structure				
Heat of combustion (kcal/mol)	−483.22	−455.78	−423.52	−530.52
Boiling point (K)	370	321	329	231
Density at 20 °C (kg/m^3)	803	810	791	1.83
Molecular weight (g/mol)	60.1	58.08	58.08	44.1

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