



A comprehensive experimental and modeling study of 2-methylbutanol combustion



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ARTICLE INFO

Article history:

Received 12 October 2014

Received in revised form 20 January 2015

Accepted 20 January 2015

Available online 20 February 2015

Keywords:

Chemical kinetic modeling

Shock tube

Constant volume combustion vessel

2-Methylbutanol

Ignition delay

Laminar flame speed

ABSTRACT

2-Methylbutanol (2-methyl-1-butanol) is one of several next-generation biofuels that can be used as an alternative fuel or blending component for combustion engines. This paper presents new experimental data for 2-methylbutanol, including ignition delay times in a high-pressure shock tube and premixed laminar flame speeds in a constant volume combustion vessel. Shock tube ignition delay times were measured for 2-methylbutanol/air mixtures at three equivalence ratios, temperatures ranging from 750 to 1250 K, and at nominal pressures near 20 and 40 bar. Laminar flame speed data were obtained using the spherically propagating premixed flame configuration at pressures of 1, 2, and 5 bar. A detailed chemical kinetic model for 2-methylbutanol oxidation was developed including high- and low-temperature chemistry based on previous modeling studies on butanol and pentanol isomers. The proposed model was tested against new and existing experimental data at pressures of 1–40 atm, temperatures of 740–1636 K, equivalence ratios of 0.25–2.0. Reaction path and sensitivity analyses were conducted for identifying key reactions at various combustion conditions, and to obtain better understanding of the combustion characteristics of larger alcohols.

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1. Introduction

In recent years, the interest in alternative fuels has increased due to more stringent emission regulations and health concerns related to combustion of traditional fuels. Oxygenated fuels have been considered as potentially attractive alternative fuels, or fuel additives, to fossil fuels in order to reduce NO_x and particulate emissions [1]. In addition, the production of oxygenated fuels from renewable sources can offset CO₂ emissions from combustion devices. However, the combustion characteristics of oxygenated fuels need to be evaluated to determine advantages and disadvantages in the context of practical applications. Some oxygenated fuels can be used directly, while others need to be blended with traditional fuels prior to entering the combustor [2]. Ethanol, a first generation biofuel, is an attractive alternative bio-based alcohol fuel and can be used as a fuel extender for petroleum fuels. However, disadvantages such as high O/C ratio, high hygroscopicity,

and low energy density can be problems with fuel storage, blending, and use in combustion engines. Therefore, the higher alcohol fuels, such as C₄ and C₅ alcohols, have been studied as next-generation biofuels. Recently, extensive combustion chemistry studies on butanol isomers [3–20] have been conducted and the focus of alcohol combustion research is shifting towards the C₅ family of alcohols, including *n*-pentanol [21–26], *iso*-pentanol (3-methyl-1-butanol) [27–31], and 2-methylbutanol (2-methyl-1-butanol) [32–35] because the longer chain alcohols are better suited for the use in combustion engines.

The interest for using 2-methylbutanol as a bio-derived fuel candidate has increased because it can be produced from various substrates by modified *Escherichia coli* bacteria [36] and photosynthesis by cyanobacteria [37]. However, there have been limited studies on 2-methylbutanol combustion. Tang et al. [24] measured the high temperature ignition behavior of C₅ alcohols (*n*-pentanol, *iso*-pentanol, and 2-methylbutanol) in the temperature ranging from 1100 to 1500 K and pressures of 1.0 and 2.6 atm. The ignition delay time and the global activation energy of the three isomers both decreased in the order of *iso*-pentanol, 2-methylbutanol, and *n*-pentanol. A high temperature chemical kinetic model for 2-methylbutanol was proposed and compared against their

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ignition data. Li and co-workers [32] measured laminar flame speeds of 2-methylbutanol/air mixtures at temperatures of 393, 433, and 473 K and pressures of 0.1, 0.25, 0.5, and 0.75 MPa using the spherically propagating flame. Experimental results showed that 2-methylbutanol has close laminar flame speeds with *n*-butanol. Zhao et al. [22] calculated pressure and temperature dependent rate constants for the thermal decomposition of *n*-pentanol and its isomers. Serinyel et al. [33] measured the concentrations of reactants, products, and intermediate species at a pressure of 10 atm, equivalence ratios of 0.5, 1, 2 and 4, and temperature ranging from 700 to 1200 K in a jet-stirred reactor (JSR) using GC and FTIR, and simulated their measurements using a detailed chemical kinetic mechanism. Recently, Zhang et al. [34] measured pyrolysis species of 2-methylbutanol in a flow reactor using synchrotron vacuum ultraviolet photoionization mass spectrometry at low and atmospheric pressures and tested a kinetic model against their measurements. The results indicate that the decomposition of 2-methylbutanol is similar to *iso*-butanol rather than *n*-butanol. Lucassen and co-workers [35] investigated the combustion chemistry of 2-methylbutanol in low-pressure premixed flames using flame-sampling molecular-beam mass spectrometry. Experimental data were compared with a detailed high-temperature chemistry to identify important fuel consumption pathways in the combustion of 2-methylbutanol.

The purpose of the present study is to expand experimental data available for 2-methylbutanol combustion at a broader range of conditions, in order to improve the mechanistic understanding of its combustion using a detailed chemical kinetic modeling. This study presents a comprehensive experimental dataset for 2-methylbutanol oxidation over a wide range of temperatures, pressures, and equivalence ratios. A comprehensive chemical kinetic model for 2-methylbutanol was developed using the rate rules established for modeling studies on other C₄ and C₅ alcohols. The model is compared against recently published experimental data, as well as new data presented herein. To our knowledge, this experimental and modeling study is the first to address the low-temperature and intermediate-temperature reactivity of 2-methylbutanol.

2. Chemical kinetic model

The detailed chemical kinetic model for 2-methylbutanol includes both low- and high-temperature chemistry. The proposed model is based on previous alcohol modeling studies [1] of the C₄-alcohols [13], *n*-pentanol [23], and *iso*-pentanol [31], and a similar methodology was used in this study to develop a detailed chemistry model for 2-methylbutanol. For this work, the *iso*-pentanol model [31] has been extended by adding 109 species and 429 reactions to represent the combustion chemistry of 2-methylbutanol and its various intermediate species. Only a brief description of the model development is discussed herein. Most reaction classes and rate parameters follow directly from previous butanol isomers modeling work, as described by Sarathy et al. [1,13] and in Supplementary Material of [13]. It should be noted that the methods utilized for kinetic modeling of larger alcohols are approximations due to the lack of fundamental kinetic data. Therefore, the proposed model is an initial attempt at comprehensively modeling combustion of a complex alcohol fuel, for which significant basic research is needed to improve the underlying chemical fidelity.

To illustrate the naming of the species for the 2-methylbutanol mechanism, 2-methylbutanol is denoted as c5h11oh-2 in the mechanism (see Fig. 1 for its molecular structure). The carbon sites are labeled alphabetically (i.e., a, b, c, d, and e) to denote radical sites in the molecule. In this way, the β -hydroxypentyl radical at the tertiary site is denoted as c5h10oh-2b, while the

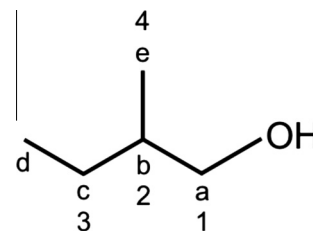


Fig. 1. Structure of 2-methylbutanol (c5h11oh-2) with carbon sites labeled.

α -hydroxypentyl radical is written as c5h10oh-2a. Additionally, the carbon chain is labeled numerically (i.e., 1, 2, 3, and 4) and the location of a double bond is identified by a hyphen followed by the number of the first carbon in the double bond (e.g., 2-methyl-1-butenol is c5h9oh21-1).

The major classes of elementary reactions considered for the oxidation of 2-methylbutanol are as follows:

High-temperature reaction classes

1. Unimolecular fuel decomposition.
2. H-atom abstraction from the fuel.
3. Fuel radical decomposition.
4. Fuel radical isomerization.
5. H-atom abstraction reactions from enols (i.e., unsaturated alcohols).
6. Enol-Keto tautomerizations and isomerizations catalyzed by H, HO₂, and formic acid.
7. Addition of H atoms to enols.
8. Enol radical decomposition.
9. Unimolecular decomposition of enols.
10. Reaction of O₂ with α -hydroxypentyl radicals to directly form an aldehyde + HO₂.

Low-temperature reaction classes (R refers to a 2-methylbutanol radical such as C₂H₅C(CH₃)CH₂OH and QOOH refers to a hydroxypentyl hydroperoxide radical such as C₂H₅C(OOH)(CH₃)C·HOH)

11. Addition of O₂ to fuel radicals (R + O₂ = ROO).
12. R + ROO = RO + RO.
13. R + HO₂ = RO + OH.
14. R + CH₃O₂ = RO + CH₃O.
15. ROO radical isomerization (ROO = QOOH) including Waddington type reaction mechanism.
16. Concerted eliminations (ROO = enol + HO₂).
17. ROO + HO₂ = ROOH + OH.
18. ROO + H₂O₂ = ROOH + HO₂.
19. ROO + CH₃O₂ = RO + CH₃O + O₂.
20. ROO + ROO = RO + RO + O₂.
21. ROOH = RO + OH.
22. RO decomposition.
23. Formation epoxy alcohols via cyclization.
24. QOOH = enol + HO₂ (radical site beta to OOH group).
25. QOOH = alkene/enol + carbonyl + OH (radical site gamma to OOH group) including unconventional water elimination reaction.
26. Addition of O₂ to QOOH (QOOH + O₂ = OOQOOH).
27. Reaction of O₂ with α -hydroxypentyl hydroperoxide radicals (e.g., C₂H₅C(OOH)(CH₃)C·HOH + O₂).
28. Isomerization of OOQOOH and formation of carbonyl hydroxypentyl hydroperoxide species and OH including Waddington type reactions mechanisms.
29. Decomposition of carbonyl hydroxypentyl hydroperoxide species to form oxygenated radical species and OH.

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