Detailed Chemical Kinetic Modeling Study of Isobutene Oxidation: Ignition Delay Time

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Abstract

A detailed chemical kinetic mechanism of isobutene oxidation has been developed to describe the combustion of isobutene. Ignition delay time (IDT) experiments have also been carried out to improve our understanding of the ignition characteristic of isobutene. A series of IDT experiments were performed in NUIG shock tubes and rapid compression machines (RCMs) under conditions not previously studied. The combination of shock tube and RCM data greatly expands the data available for validation of isobutene oxidation models to higher pressures (10–50 atm) and lower temperatures (700–1500 K). Important reactions highlighted via flux and sensitivity analyses include: hydrogen atom abstraction from isobutene by molecular oxygen, hydroxyl, and hydroperoxyl radicals; methyl allyl–methyl allyl radical recombination and the reaction between methyl allyl and hydroperoxyl radicals. The current mechanism accurately predicts the combustion characteristics of isobutene across the range of experimental conditions presented in this study.

Keywords: Isobutene oxidation, Shock tube, Rapid compression machine, Chemical kinetics, Ignition, Flame speed

I. INTRODUCTION

Understanding the combustion chemistry of the butene isomers is a prerequisite for a comprehensive description of the chemistry of C_1 to C_4 hydrocarbon and oxygenated fuels such as butanol. For the development and validation of combustion models, it is thus crucial to improve the knowledge about the C_4 combustion chemistry in detail. Isobutene, one of the butene isomers, is an important intermediate in the combustion of larger branched hydrocarbons, such as isobutene, iso-octane etc. Developing the comprehensive kinetic model of isobutene is part of our whole project in describing the C_1 to C_4 chemistry also an extending work based on propene [1-2].

Several studies have been devoted to the pyrolysis and oxidation of isobutene [3-5], there is a lack of experimental data available in the literature for isobutene at low temperatures (600–1000 K) and high pressures (>10 atm).

Experiments carried out in this work are shown in Table I.

TABLE I.
Ignition delay time data for isobutene oxidation obtained in this study.

Reactor Type	T–Range, K	P–Range, atm	ϕ Range	Dilution
Shock tube	940–1500	10–50	0.3–2.0	in “air”
RCM	700–996	10–50	0.3–2.0	in “air”

II. EXPERIMENTAL METHODS

Ignition delay time measurements for isobutene were obtained in at NUIG ST and NUIG RCM respectively. Detailed explanation for these two facilities can be found in [2].

III. PARTIAL RESULTS

As shown in Fig. 1, the current model predicts the combustion characteristic of isobutene accurately.

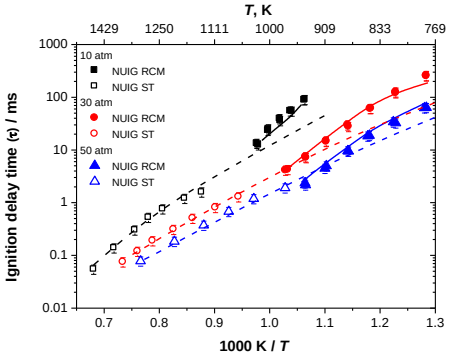

Fig. 1. IDT validation of the model (solid and dashed lines) against the experimental results at φ = 0.3 in air.

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