



The oxidation of 2-butene: A high pressure ignition delay, kinetic modeling study and reactivity comparison with isobutene and 1-butene

Yang Li, Chong-Wen Zhou, Kieran P. Somers, Kuiwen Zhang,
Henry J. Curran*

Combustion Chemistry Centre, National University of Ireland, Galway, Ireland

Received 3 December 2015; accepted 31 May 2016

Available online 16 June 2016

Abstract

Butenes are intermediates ubiquitously formed by decomposition and oxidation of larger hydrocarbons (e.g. alkanes) or alcohols present in conventional or reformulated fuels. In this study, a series of novel ignition delay time (IDT) experiments of trans-2-butene were performed in a high-pressure shock tube (HPST) and in a rapid compression machine (RCM) under conditions of relevance to practical combustors. This is the first IDT data of trans-2-butene taken at engine relevant conditions, and the combination of HPST and RCM results greatly expands the range of data available for the oxidation of trans-2-butene to higher pressures (10–50 atm), lower temperatures (670–1350 K) and a wide range of equivalence ratios (0.5–2.0). A comprehensive chemical kinetic mechanism has simultaneously been developed to describe the combustion of trans-2-butene. It has been validated using the IDT data measured here in addition to a large variety of literature data: jet-stirred reactor (JSR) speciation data, premixed flame speciation data, flow reactor speciation data and laminar flame speed data. Moreover, the reactivity of trans-2-butene is compared to that of the other two isomers, 1-butene and isobutene, and these comparisons are discussed. Important reactions are highlighted via flux and sensitivity analyses and help explain the differences in reactivity among the butene isomers.

© 2016 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

Keywords: Trans-2-butene; Shock tube; Rapid compression machine; Chemical kinetics; Ignition delay time

1. Introduction

Alkenes are important intermediates formed by the combustion of larger hydrocarbons, e.g., alka-

nes and alcohols. Moreover, liquefied petroleum gas (LPG) produced during oil refining contains significant amount of olefins, particularly propene and butenes [1], with gasoline fuel containing butenes, pentenes and hexenes in various amounts. Butene is the shortest alkene with structural isomers, namely 2-methylpropene (isobutene), which is a branched isomer, and 1-butene, cis-2-butene

* Corresponding author. Fax: +353 91525700.

E-mail address: henry.curran@nuigalway.ie
(H.J. Curran).

(*c*-2-C₄H₈) and *trans*-2-butene (*t*-2-C₄H₈), which are three linear isomers.

Recently, there have been some high-temperature and low-pressure experimental and kinetic modeling studies performed on *trans*-2-butene combustion, including pyrolysis and oxidation, speciation [2–4], flame speed [2,5], ignition temperature [5], etc., Table S1 of the Supplemental material. However, there is a lack of experimental data available in the literature at engine relevant, high-pressure and low-temperature, conditions. In addition, few studies have been specifically concerned with reactivity effects of the isomeric fuel structures.

In view of the above considerations, we have measured ignition delay times in a high-pressure shock tube (HPST) and in a rapid compression machine (RCM) under conditions of low temperatures (600–1000 K) and at high pressures (>10 atm), which are conditions of direct relevance with respect to gasoline, diesel, and low-temperature combustion (LTC) engine technologies. A comprehensive chemical kinetic mechanism to describe *trans*-2-butene oxidation has been developed including detailed low- and high-temperature reaction pathways specific to unsaturated fuel chemistry, and it is validated against the experimental results. An ignition reactivity comparison of three butene isomers (*trans*-2-butene, 1-butene and *isobutene*) has been performed, and a detailed chemical kinetic mechanism (AramcoMech 2.0) has been developed to explain the reactivity dif-

Table 1
Detailed mixture compositions (%).

	Fuel	O ₂	Diluent	ϕ
<i>t</i> -2-C ₄ H ₈	1.72	20.64	77.64	0.5
	3.38	20.29	76.33	1.0
	6.54	19.63	73.83	2.0
<i>c</i> -2-C ₄ H ₈	3.38	20.29	76.33	1.0

ferences which account for the isomeric structure effects on ignition/reactivity properties.

2. Experiment

Experiments were performed in the NUI Galway HPST and RCM facilities as described previously [6,7]. All fuels were acquired from Sigma Aldrich at 99.5% purity. Oxygen, nitrogen, argon and carbon dioxide were acquired from BOC Ireland at high purity ($\geq 99.5\%$).

Table 1 shows that identical experimental conditions at $\phi = 1.0$ for *cis*- and *trans*-2-butene were selected ($p = 10, 30$ and 50 atm), and Fig. 1 shows the IDT measurements for these two isomers and they are identical. Therefore, they will be named as 2-butene in the following text. Typical pressure-time traces and original experimental data are shown in the Supplemental material, Fig. S1 and Tables S3–S17.

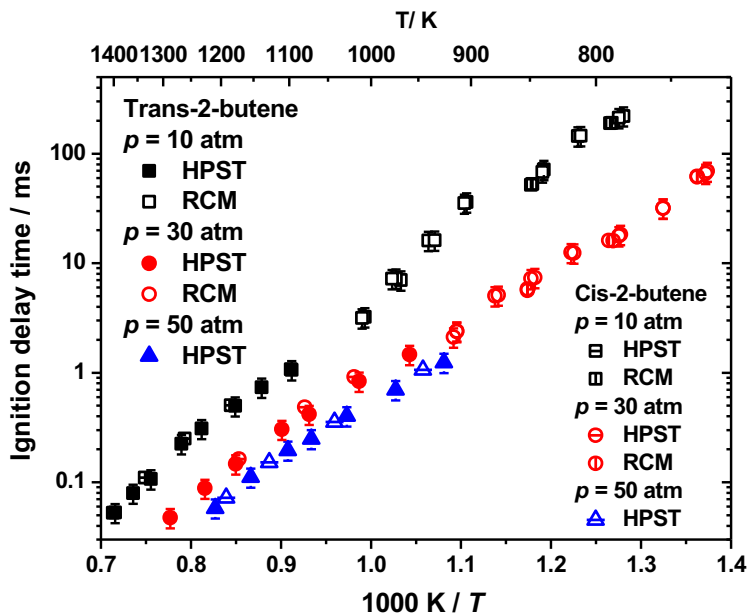


Fig. 1. IDT measurements for *trans*/*cis*-2-butene at $\phi = 1.0$ and $p = 10, 30, 50$ atm.

Download English Version:

<https://daneshyari.com/en/article/6477922>

Download Persian Version:

<https://daneshyari.com/article/6477922>

[Daneshyari.com](https://daneshyari.com)