



ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Proceedings of the Combustion Institute xxx (2014) xxx–xxx

Proceedings
of the
Combustion
Institutewww.elsevier.com/locate/proci

Experimental and kinetic modeling study of trans-2-butene oxidation in a jet-stirred reactor and a combustion bomb

Yann Fenard^a, Philippe Dagaut^{a,*}, Guillaume Dayma^a,
Fabien Halter^{a,b}, Fabrice Foucher^b

^a CNRS-INSIS, 1C Avenue de la Recherche Scientifique, 45071 Orléans cedex 2, France

^b University of Orléans, PRISME, 8 Rue Léonard de Vinci, 45072 Orléans cedex 2, France

Abstract

Butenes are intermediates ubiquitously formed by decomposition and oxidation of larger hydrocarbons (e.g. alkanes) or alcohols present in conventional or reformulated fuels. This study provides new complementary data for the oxidation of trans-2-butene. The oxidation of trans-2-butene was studied for measuring stable species concentration profiles during the oxidation of the fuel at atmospheric pressure, over a range of equivalence ratios ($0.5 \leq \varphi \leq 2$), and temperatures (900–1450 K). A combustion bomb apparatus was used to determine laminar flame velocities of trans-2-butene in air at 1 atm, 300 K, and for equivalence ratios of 0.8–1.4. The oxidation of trans-2-butene was simulated under these experimental conditions using an extended detail chemical kinetic reaction mechanism (201 species involved in 1788 reactions). This mechanism is based on a previously proposed scheme for the oxidation of hydrocarbons. Good agreement with experimental data presented in this article was obtained which significantly improves kinetic modeling ability. The structure of a trans-2-butene premixed low pressure flat flame recently published was also successfully modeled. Sensitivity and reaction pathways analyses were performed to get insights into the processes involved in the oxidation of trans-2-butene.

© 2014 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

Keywords: 2-Butene; Jet-stirred reactor; Flame speed; Kinetic model

1. Introduction

Alkenes are important intermediates formed by combustion of larger hydrocarbons, e.g., alkanes and alcohols. With 4 carbon atoms, butene is a good candidate for upgrading detailed

mechanisms of middle size species in combustion reaction schemes. Butene is the shortest alkene with isomers: a branched isomer, 2-methylpropene (iso-butene), and three linear isomers, i.e., 1-butene and the cis/trans 2-butene. The pyrolysis and oxidation of iso-butene has been extensively studied in the last decades in shock tubes [1–6], turbulent flow reactor [7], JSR [8], and premixed laminar flames [9]. Studies on 1-butene oxidation have been conducted in JSR [10,11] and shock

* Corresponding author. Fax: +33 238696004.

E-mail address: dagaut@cnrs-orleans.fr (P. Dagaut).

<http://dx.doi.org/10.1016/j.proci.2014.05.007>

1540-7489/© 2014 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

Please cite this article in press as: Y. Fenard et al., *Proc. Combust. Inst.* (2014), <http://dx.doi.org/10.1016/j.proci.2014.05.007>

tube [11]. For both iso-butene and 1-butene, laminar burning velocities have been measured [12]. Recently, the pyrolysis in a low-pressure flow reactor [13] and the oxidation in low-pressure premixed flames [14] have been performed on butene isomers.

The purpose of this work is to provide new experimental data on trans-2-butene oxidation using a JSR and a combustion bomb. The new data set and low pressure flat flames data [14] were used for validating the proposed kinetic reaction mechanism.

2. Experimental

2.1. Jet stirred reactor

The reactor [15,16] is made of a 4 cm diameter fused silica sphere (27.2 cm^3) connected at 4 nozzles of 1 mm i.d. opposed in pair, allowing admission and mixing of reactants diluted with nitrogen ($<100\text{ ppm H}_2\text{O}$, $<50\text{ ppm O}_2$, $<1000\text{ ppm Ar}$, $<5\text{ ppm H}_2$). A mixture of trans-2-butene 6.0027%mol and N_2 93.9973%mol (Air Liquide) was used. In the experiments, the fuel was highly diluted before entering the reactor. Oxygen was 99.995% pure. A thermocouple (0.1 mm Pt–Pt/Rh-10%, located inside a thin-wall silica tube) was used for measuring the temperature inside the reactor; it is movable along the JSR vertical axis. During the experiments, a good thermal homogeneity was obtained (gradients of ca. 1 K/cm). A movable fused silica low pressure sonic probe was used to sample reacting mixtures. The samples were transferred to the analyzers through a Teflon line heated at 200 °C. An online FTIR (Nicolet 6700 – 2 m path length, 500 mbar and resolution of 0.5 cm^{-1}) was used to measure CH_2O , H_2O , CO and CO_2 concentrations. Off-line analyses were also performed, after collection of the samples and storage in 1L Pyrex bulbs, by gas chromatographs (GC) equipped with capillary columns (DB-624, CP-Al2O3-KCl, and Carbo-plot-P7), a thermal conductivity detector (TCD), and a flame ionization detector (FID). O_2 and H_2 were quantified with a TCD whereas CH_4 , C_2H_6 , C_2H_4 , C_2H_2 , C_3H_6 , $\text{C}_3\text{H}_4\text{-A}$, $\text{C}_3\text{H}_4\text{-P}$, trans and cis-2- C_4H_8 , 1- C_4H_8 , 1,3- C_4H_6 , 1,2- C_4H_6 , 1- C_4H_6 , 2- C_4H_6 , isoprene, C_4H_4 , C_4H_2 , 1,3-cyclopentadiene, and C_6H_6 were quantified with a FID. A GC-MS (Varian V1200) operating with electron ionization (70 eV) was used for products identification. Other products were found: i- C_4H_8 , 2-methyl-2-butene, 2-methyl-1-butene, 3-methyl-1-butene, t2- C_5H_{10} , c2- C_5H_{10} , 1,3-cyclopentadiene, 1,3- C_5H_8 and toluene. The larger products were detected by GC/FID and GC/MS at trace concentrations. Toluene was the most abundant with a maximum detected concentration of 3 ppm. This is consistent with [14] ($[\text{toluene}]/[\text{benzene}] = 0.1$)

and with our modeling. The experiments were performed at atmospheric pressure and the reactor temperature was varied stepwise.

2.2. Laminar flame speed setup

The device used here [17] consists of a stainless steel spherical combustion chamber with an inner diameter of 200 mm for a total volume of 4.2 L. The sphere is surrounded by a resistance wire allowing heating up to 473 K. A vacuum pump reduces the residual pressure inside the device $<0.003\text{ mbar}$ before gases injection. We used the same fuel-nitrogen mixture as in Section 2.1. Due to that nitrogen dilution, oxygen and nitrogen were added to get the oxygen/nitrogen ratio in air (20.9%mol of $\text{O}_2/79.1\%$ mol of N_2) and match the desired equivalence ratio. Quantities of gases were introduced via thermal flow meters (Brooks 5850S). A fan installed inside the chamber ensured a perfectly homogeneous premixed mixture. The fan was stopped 5 s before ignition to avoid perturbations during the flame propagation. A piezo-electric pressure transducer and a type-K thermocouple were used to check respectively the pressure level and the initial temperature before ignition. The maximum deviation between the effective initial pressure inside the combustion chamber and the required initial pressure was about 1%. The initial temperature of the prepared mixture was known at 2 K. Two tungsten electrodes (diameter 1.5 mm), with a 1-mm gap, linked to a conventional capacitive discharge ignition system, were used for spark production at the center of the chamber. Two opposite and transparent windows (diameter 82 mm) provide optical access into the chamber. A LED illuminator (HardSoft DLR IL104G) equipped with an objective (HSO-PL-360) was used to provide continuous and incoherent light with a wavelength of 528 nm. A parallel light was created using a pinhole (diameter 3 mm), placed at the focal point of the objective, and a plano-convex lens (diameter 70 mm, focal length 1000 mm). After passing through the lens and the combustion chamber, the beam is displayed on a screen. The visualization of the flame was obtained using a classical shadowgraph method. Instantaneous images were recorded using a high-speed video camera (Photron Fastcam) operating at 6000 images per second. The temporal evolution of the expanding spherical flame was then analyzed. Measurements were limited to flames with diameters $<50\text{ mm}$, corresponding to a volume of burned gases less than 1.6% of the chamber volume. Under such conditions, the total chamber pressure can be considered constant during the initial stage of flame expansion. The laminar burning velocity extraction follows the procedure used before [17]. The measured flame radius (R_f) against time (t) determines the stretched spatial flame velocity:

Download English Version:

<https://daneshyari.com/en/article/6679260>

Download Persian Version:

<https://daneshyari.com/article/6679260>

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