



# An experimental and chemical kinetic modeling study of 1,3-butadiene combustion: Ignition delay time and laminar flame speed measurements



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## ABSTRACT

Ignition delay times for 1,3-butadiene oxidation were measured in five different shock tubes and in a rapid compression machine (RCM) at thermodynamic conditions relevant to practical combustors. The ignition delay times were measured at equivalence ratios of 0.5, 1.0, and 2.0 in 'air' at pressures of 10, 20 and 40 atm in both the shock tubes and in the RCM. Additional measurements were made at equivalence ratios of 0.3, 0.5, 1.0 and 2.0 in argon, at pressures of 1, 2 and 4 atm in a number of different shock tubes. Laminar flame speeds were measured at unburnt temperatures of 295 K, 359 K and 399 K at atmospheric pressure in the equivalence ratio range of 0.6–1.7, and at a pressure of 5 atm at equivalence ratios in the range 0.6–1.4. These experimental data were then used as validation targets for a newly developed detailed chemical kinetic mechanism for 1,3-butadiene oxidation.

A detailed chemical kinetic mechanism (AramcoMech 3.0) has been developed to describe the combustion of 1,3-butadiene and is validated by a comparison of simulation results to the new experimental measurements. Important reaction classes highlighted via sensitivity analyses at different temperatures include: (a) OH radical addition to the double bonds on 1,3-butadiene and their subsequent reactions. The branching ratio for addition to the terminal and central double bonds is important in determining the reactivity at low-temperatures. The alcohol-alkene radical adducts that are subsequently formed can either react with HO<sub>2</sub> radicals in the case of the resonantly stabilized radicals or O<sub>2</sub> for other radicals. (b) HO<sub>2</sub> radical addition to the double bonds in 1,3-butadiene and their subsequent reactions. This reaction class is very important in determining the fuel reactivity at low and intermediate temperatures (600–900 K). Four possible addition reactions have been considered. (c) <sup>3</sup>O atom addition to the double bonds in 1,3-butadiene is very important in determining fuel reactivity at intermediate to high temperatures (> 800 K). In this reaction class, the formation of two stable molecules, namely CH<sub>2</sub>O + allene, inhibits reactivity whereas the formation of two radicals, namely C<sub>2</sub>H<sub>3</sub> and C<sub>2</sub>HCHO, promotes reactivity. (d) H atom addition to the double bonds in 1,3-butadiene is very important in the prediction of laminar flame speeds. The formation of ethylene and a vinyl radical promotes reactivity and it is competitive with H-atom abstraction by H atoms from 1,3-butadiene to form the resonantly stabilized C<sub>4</sub>H<sub>5</sub>-i radical and H<sub>2</sub> which inhibits reactivity. *Ab initio* chemical kinetics calculations were carried out to determine the thermochemistry properties and rate constants for some of the important species and reactions involved

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in the model development. The present model is a decent first model that captures most of the high-temperature IDTs and flame speeds quite well, but there is room for considerable improvement especially for the lower temperature chemistry before a robust model is developed.

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## 1. Introduction

1,3-Butadiene is an important intermediate towards the formation of soot and poly-aromatic hydrocarbons (PAH) through the proposed “C<sub>2</sub> + C<sub>4</sub>” benzene formation pathways. Therefore, an accurate knowledge of 1,3-butadiene oxidation chemistry is essential to the further development of models for PAH and soot formation. Moreover, 1,3-butadiene is also an important intermediate in the pyrolysis and oxidation of higher-order hydrocarbons, and its oxidation kinetics are important to the hierarchical development of the kinetic mechanisms of hydrocarbon combustion. Thus, the development and validation of combustion models for 1,3-butadiene will help improve our knowledge of detailed C<sub>4</sub> combustion chemistry and is an extension of our previous studies of the butene isomers [1–3].

Ignition delay times for 1,3-butadiene oxidation were previously measured by Fournet et al. [4] and Libby et al. [5]. Fournet et al. [4] measured ignition delay times for 1,3-butadiene/O<sub>2</sub>/argon mixtures containing 85–95% argon diluent in the temperature range 1200–1700 K, at pressures of 8.5–10 atm. Libby et al. [5] measured ignition delay times in the temperature range 1390–1810 K at pressures in the range 1.5–3.8 atm at equivalence ratios from 0.25–1.0. Davis and Law [6] measured the laminar flame speeds for 1,3-butadiene/air mixtures by using the counter-flow twin flame configuration over an extensive range of equivalence ratios at standard conditions of temperature and pressure. Hansen et al. [7] used molecular-beam flame-sampling and time-of-flight mass spectrometry to measure the intermediate species to unravel important pathways leading to the formation of benzene in a premixed, laminar, low-pressure 1,3-butadiene flame. They concluded that the reactions C<sub>3</sub>H<sub>3</sub> + C<sub>3</sub>H<sub>3</sub> ↔ C<sub>6</sub>H<sub>6</sub> and C<sub>4</sub>H<sub>5</sub>-i + C<sub>2</sub>H<sub>2</sub> ↔ C<sub>6</sub>H<sub>6</sub> + H are roughly of equal importance in benzene formation.

There is a dearth of experimental ignition delay time data available in the literature for 1,3-butadiene at lower temperatures (650–1200 K) and at higher pressures (> 10 atm), which are conditions of direct relevance to gasoline, diesel and low-temperature combustion engine technologies. Moreover, further measurements of flame speeds and species concentration profiles in reactors will also contribute to an improved understanding of 1,3-butadiene pyrolysis and oxidation. In this work, ignition delay time measurements of 1,3-butadiene oxidation under engine conditions including both low to intermediate (600–1000 K) and higher temperatures (1000–1600 K) have been measured. Additionally, flame speed measurements at 1 and 5 atm at temperatures of 295 K, 359 K and 399 K and over a wide range of equivalence ratios have also been taken.

## 2. Experimental methods

In this study, ignition delay times for the oxidation of 1,3-butadiene were measured at fuel-lean, stoichiometric and fuel-rich equivalence ratios with various levels of argon dilution, or in air, as was the case for one of the mixtures. Additionally, pressure ranges examined in the study spanned the range of p<sub>5</sub> = 1–40 atm, where p<sub>5</sub> is the reflected-shock pressure. The mixture compositions as well as the facility used for each mixture are shown in Table 1. ‘Air’ in the case of the experiments presented in this study refers to nitrogen and oxygen in a 79/21 ratio. The shock tube (ST) experiments were carried out in the shock tubes at Texas A&M Univer-

sity (TAMU), King Abdullah University of Science and Technology (KAUST), Xi’an Jiaotong University (XJTU), the University of Central Florida (UCF), and at NUI Galway (NUIG). All RCM experiments were carried out in the twin-opposed piston RCM at NUIG. The mixture compositions (mole %) investigated in this study from different groups are shown in Table 2. The ignition delay times reported in this study along with associated pressure and temperature conditions are available as Supplementary material.

### 2.1. Ignition delay time measurements

Table 3 lists the details of each shock tube and measurement techniques described in this work. Even though the measurement technique or exact definition of ignition delay time adopted by each experimental group is slightly different, the simulation results for ignition delay time are consistent with the experimental definition. This similarity is primarily due to the fact that most markers for ignition delay time are similar when the mixtures are at least reasonably exothermic (< 96% dilution).

#### 2.1.1. NUI Galway rapid compression machine

Ignition delay times for 1,3-butadiene/‘air’ mixtures at φ = 0.5, 1.0 and 2.0 at pressures of approximately 10, 20 and 40 atm were measured at NUIG in the rapid compression machine which has been described in the recent propene study by Burke et al. [15]. Here the ‘air’ used in these experiments is a mixture of O<sub>2</sub> and N<sub>2</sub> in the molar ratio of 1:3.76. The ignition delay time definition in this work is shown in Fig. 1 and is taken from the time of peak pressure at the end of compression to the time of maximum rate of pressure rise due to ignition.

It is well known that the heat loss profiles generally garnered from experimental, nonreactive pressure profiles must be included to simulate rapid compression machine data accurately. To this end, a nonreactive profile, for which an experiment is performed by replacing oxygen with nitrogen in the fuel–‘air’ charge, has

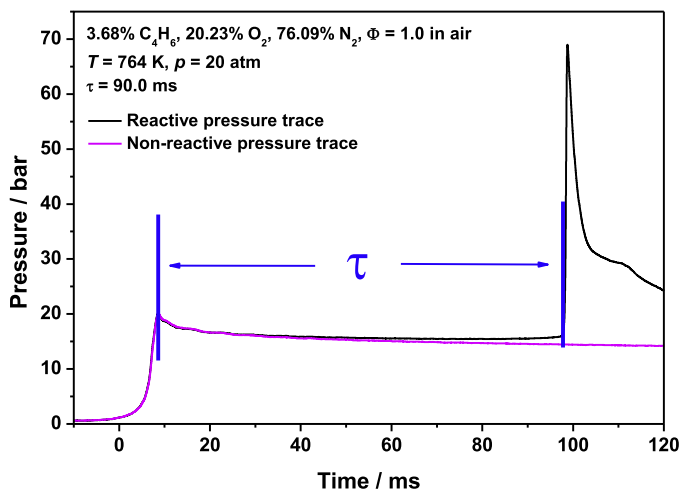


Fig. 1. Sample pressure trace from the NUI Galway RCM for 1,3-butadiene oxidation. (Pink line: nonreactive trace, black line: reactive trace). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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