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An experimental and modeling study of propene oxidation. Part 2: Ignition delay time and flame speed measurements

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ABSTRACT

Experimental data obtained in this study (Part II) complement the speciation data presented in Part I, but also offer a basis for extensive facility cross-comparisons for both experimental ignition delay time (IDT) and laminar flame speed (LFS) observables.

To improve our understanding of the ignition characteristics of propene, a series of IDT experiments were performed in six different shock tubes and two rapid compression machines (RCMs) under conditions not previously studied. This work is the first of its kind to directly compare ignition in several different shock tubes over a wide range of conditions. For common nominal reaction conditions among these facilities, cross-comparison of shock tube IDTs suggests 20–30% reproducibility (2σ) for the IDT observable. The combination of shock tube and RCM data greatly expands the data available for validation of propene oxidation models to higher pressures (2–40 atm) and lower temperatures (750–1750 K).

Propene flames were studied at pressures from 1 to 20 atm and unburned gas temperatures of 295–398 K for a range of equivalence ratios and dilutions in different facilities. The present propene–air LFS results at 1 atm were also compared to LFS measurements from the literature. With respect to initial reaction conditions, the present experimental LFS cross-comparison is not as comprehensive as the IDT comparison; however, it still suggests reproducibility limits for the LFS observable. For the LFS results, there was agreement between certain data sets and for certain equivalence ratios (mostly in the lean region), but the remaining discrepancies highlight the need to reduce uncertainties in laminar flame speed experiments amongst different groups and different methods. Moreover, this is the first study to investigate the burning rate characteristics of propene at elevated pressures (>5 atm).

IDT and LFS measurements are compared to predictions of the chemical kinetic mechanism presented in Part I and good agreement is observed.

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1. Introduction

As highlighted in Part I [1] of this study, propene is an important intermediate species in the combustion of larger hydrocarbons. In that paper speciation measurements were made in jet-stirred and flow reactors during propene oxidation and were presented along with a new detailed kinetic mechanism to describe propene oxidation. Here we present an investigation of the ignition and flame speed characteristics of propene across a wide range of conditions. Existing data in the literature are limited to relatively high-temperatures and low-pressures. The aim of this study is to expand the available experimental data for propene oxidation to lower temperatures and higher pressures. Table 1 is a compilation of ignition and flame speed measurements for propene reported in the literature compared with the present measurements.

Presented herein are the results of an unprecedented, comprehensive propene oxidation study conducted by several different groups using a wide assortment of experimental facilities and techniques, with the focus on ignition delay times and laminar flame speeds. First is a section detailing the different facilities, starting with the shock tubes and followed by the rapid compression machine and flame speed facilities. A brief summary of the chemical kinetic mechanism is then given, including the assumptions and routines used to model the various experiments. A results section forms the bulk of the second half of this paper; it provides comparisons and analyses both between model and experiment as well as between experiments from different groups at overlapping conditions.

Several studies have investigated propene pyrolysis and oxidation at high temperatures. Burcat and Radhakrishan [2] measured ignition delay times of 31–932 μs in the temperature range of 1274–1840 K and over a post-shock pressure range of 2.19–7.04 atm for propene/oxygen mixtures containing 84.0–96.7% argon diluent. Qin et al. [4] measured shock tube ignition delay times in the temperature range of 1270–1820 K over a post-shock pressure range of 0.95–4.7 atm with measured times of 10–1535 μs for propene/O_2/argon mixtures containing greater than 90% argon diluent. The measurements made in the Qin et al. study were observed to be shorter than those from the Burcat and Radhakrishan study under similar conditions; however, Qin et al. did not identify possible sources of the disagreement.

Hidaka et al. [3] investigated the thermal decomposition of propene behind reflected shock waves over a temperature range of 1200–1800 K, measuring the product distribution using infrared laser absorption spectroscopy and gas chromatography. The authors reported species profiles for C_3H_6, C_2H_2, C_4H_6, C_3H_4, and C_6H_6.

Law and co-workers [5,6] reported laminar flame speed measurements for propene in two studies. Davis et al. [5] reported laminar flame speeds for propene/air mixtures at room temperature and atmospheric pressure carried out using the counterflow twin flame configuration. Jomaas et al. [6] investigated the laminar flame speed of C_2–C_3 hydrocarbons, including propene, from a spherical flame in a constant-pressure chamber at pressures of 1, 2 and 5 atm. The laminar flame speed reported by Jomaas et al. at $\varphi = 1.0$ is $\approx$3 cm s^{-1} slower than that reported by Davis et al. Saaed and Stone [7] studied burning velocities of propene–air mixtures at various temperatures (293 and 425 K) and pressures (0.5, 1.0, 2.0 and 3.5 bar) in a constant-volume spherical vessel.

2. Experimental methods

Ignition delay time measurements for propene were obtained in six different shock tube facilities; at NUI Galway (NUIG ST), Texas A&M University (TAMU), Rensselaer Polytechnic Institute (RPI), Stanford University (SULP and SUHP), and King Abdullah University of Science and Technology (KAUST). Ignition delay time measurements were also obtained in two Rapid Compression Machines (RCMs) located at NUI Galway (NUIG RCM) and the University of Connecticut (UConn). Table 2 provides details of the important features of each facility.

Figure 1 shows a comparison of the conditions examined in this study and the previously published shock tube ignition delay times for propene oxidation. The present study covers a broader range of conditions particularly at higher pressures and lower temperatures than measurements previously found in the literature as shown in Table 1. Tabulated experimental data are included in the Supplementary Material.

An important feature of the present study is the direct comparison of ignition delay time measurements carried out at common experimental conditions in different shock tubes and rapid compression machines located at the co-author's respective institutions. Unambiguous comparisons of independent combustion kinetic target measurements, such as ignition delay time, are important because they provide cross-validation of facilities and experimental methods that have been used by the collaborator's research groups in numerous prior studies. Measurements made at common conditions in different facilities also provide a comparison of the collective scatter in the data from multiple facilities relative to the estimated uncertainty limits reported for each experiment, providing another assessment of the uncertainty estimates for kinetic targets, in this case ignition delay time.

Similarly, laminar flame speed measurements are compared from five different experimental installations. Princeton University

Table 1
Ignition delay time and flame speed data for propene.

Reactor type	T (K)	p (atm)	φ	Dilution	Ref.
Parameter range for propene oxidation evident in the literature					
Ignition delay time					
Shock tube	1274–1870	2.19–7.04	0.5–2.0	84–97%	[2]
Shock tube	1200–1800	≈2.65	–	>95%	[3]
Shock tube	1270–1820	0.95–4.7	0.5–2.0	>90%	[4]
Flame speed					
Counterflow	298	1	0.5–2.0	In 'air'	[5]
Spherical flame	298	1–5	0.5–2.0	In 'air'	[6]
Spherical flame	293 and 425	0.5–3.5	0.8–1.6	In 'air'	[7]
Parameter range for propene oxidation obtained in this study					
Ignition delay					
Shock tube	1100–1750	2–40	0.5–2.0	≈72–96%	
RCM	750–1100	10–40	0.5–2.0	≈75–95%	
Flame speed					
Heat flux method	298–398	1	0.5–2.0	≈70–80%	
Spherical flame	295–298	1–20	0.8–1.6	In 'air' – ≈80%	