



1-Butanol ignition delay times at low temperatures: An application of the constrained-reaction-volume strategy



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ABSTRACT

Ignition delay times behind reflected shock waves are strongly sensitive to variations in temperature and pressure, yet most current models of reaction kinetics do not properly account for the variations that are often present in shock tube experiments. Particularly at low reaction temperatures with relatively long ignition delay times, substantial increases in pressure and temperature can occur behind the reflected shock even before the main ignition event, and these changes in thermodynamic conditions of the ignition process have proved difficult to interpret and model. To obviate such pressure increases, we applied a new driven-gas loading method that constrains the volume of reactive gases, thereby producing near-constant-pressure test conditions for reflected shock measurements. Using both conventional operation and this new constrained-reaction-volume (CRV) method, we have collected ignition delay times for 1-butanol/O₂/N₂ mixtures over temperatures between 716 and 1121 K and nominal pressures of 20 and 40 atm for equivalence ratios of 0.5, 1.0, and 2.0. The equivalence ratio dependence of 1-butanol ignition delay time was found to be negative when the oxygen concentration was fixed, but positive when the fuel concentration was held constant. Ignition delay times with strong pre-ignition pressure increases in conventional-filling experiments were found to be significantly shorter than those where these pressure increases were mitigated using the CRV strategy. The near-constant-pressure ignition delay times provide a new database for low-temperature 1-butanol mechanism development independent of non-idealities caused by either shock attenuation or pre-ignition perturbations. Comparisons of these near-constant-pressure measurements with predictions using several reaction mechanisms available in the literature were performed. To our knowledge this work is first of its kind that systematically provides accurate near-constant-enthalpy and -pressure target data for chemical kinetic modeling of undiluted fuel/air mixtures at engine relevant conditions.

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1. Introduction

Recently, there has been strong interest in the combustion of 1-butanol and other butanol isomers due to their potential as biofuel candidates for next-generation green transportation fuels [1,2]. Butanol ignition data at high pressures and low temperatures are particularly needed due to their relevance to practical engine combustion environments and significance in the validation of detailed chemical reaction mechanisms at these conditions. Many experimental studies of the oxidation of one of the isomers, 1-butanol, have been performed by researchers using various facilities and techniques [3–11]. However, there still appears to be a lack of consensus among the ignition delay time measurements found in these studies (see Fig. 1), especially at low temperatures. In addition, while the pressure dependence of ignition delay time of 1-butanol/air mixture has been studied extensively to yield a

consistent result [3,6,11], few investigations exist for the equivalence ratio or oxygen concentration dependence except that reported in [6].

Computational studies of 1-butanol ignition are also abundant. Although detailed chemical kinetic reaction mechanisms for 1-butanol and the other isomers have been proliferating rapidly in recent years [11–15], Fig. 1 shows that there are significant discrepancies between the different mechanism predictions, particularly at relatively low temperatures ($T < 1000$ K). While it is true that some of these mechanisms were not optimized for low temperature chemistry, these discrepancies still imply that more high-quality data at low temperatures are of critical importance for improvement of these mechanisms.

This wide variation in model prediction thus motivates further measurements of high-pressure and low-temperature 1-butanol ignition delay times. In some of the previous 1-butanol oxidation studies behind reflected shocks, the mixtures utilized were highly diluted in argon and thus the energy release during reaction was small [4,5,7]. However, in many other cases, undiluted

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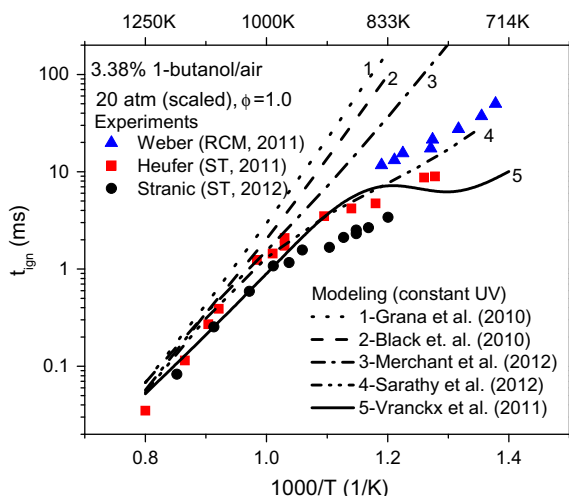


Fig. 1. Previous ignition delay time measurements for 1-butanol oxidation in air at $\phi = 1.0$. The constant-energy (U), constant-volume (V) model calculations utilize five recent mechanisms [11–15].

high-concentration mixtures (fuel/air) at elevated pressures and low temperatures were employed and these data were found to exhibit pre-ignition pressure ramps and/or steps prior to the primary ignition event [5,16–25]. The reasons for these rises are difficult to confirm as both real fuel chemistry inside the measurement volume and non-localized ignition outside of the reaction volume can contribute to the pressure increases observed inside the measurement volume [5]. Similar phenomena were also observed in rapid compression machines (RCM) [26–28] and research engines [29]. Such dramatic pressure effects are different from the normal, though undesired, gradual pressure increase (dp_2/dt) observed behind reflected shocks in dilute mixtures [30], and these effects may be temperature-dependent [11,31], pressure-dependent [11,31], and even fuel-dependent [32]. Generally these effects cannot be simply reproduced by a detailed kinetic mechanism under constant-energy (U), constant-volume (V) constraints. These complications are further motivation to seek strategies for interpreting data exhibiting pre-ignition pressure change, as well as to establish new techniques for generating databases without these thermodynamic complications.

In the current study, we measured ignition delay times of 1-butanol/ O_2/N_2 behind reflected shock waves at various temperatures, pressures and equivalence ratios, using two methods. First, data were collected using a conventional shock-tube test-gas-loading method. These data were simulated with both a constant-volume model and a specified-pressure model incorporating the measured pressure profiles into the chemical kinetic model calculations. The measurements were then repeated employing a new shock-tube test-gas-loading method, called constrained reaction volume (CRV) [33], that limits the volume of reacting gases and creates near-constant-pressure test conditions. These CRV measurements can be compared to mechanism predictions with a simple and appropriate gasdynamic model using constant or specified pressure (P) and enthalpy (H), thereby avoiding the complications and errors associated with constant U , V or constant P , H modeling of conventional (full shock tube filling) reflected shock experiments.

2. Experimental methods

2.1. High-pressure shock tube

All ignition delay time experiments were performed using the Stanford high-purity, high-pressure shock tube (HPST). The driver

section is 3 m long with a 7.5-cm internal diameter. The stainless steel driven section has a length of 5 m and an internal diameter of 5 cm and was heated to 91 °C to prevent condensation of the test gas mixture. A tailored gas mixture (40% N_2/He) was used as the driver gas for experiments to achieve test times up to 10 ms. Driver inserts were implemented in all shock tube experiments to eliminate the non-ideal pressure rise typically seen in the reflected shock region at long test times [30,34]. Five axially-spaced PCB pressure transducers (PCB 113A), at locations 1.1 cm, 31.6 cm, 69.7 cm, 92.5 cm and 123.0 cm away from the endwall of the driven section, were employed to record pressure during the ignition experiments and connected to four Philips time-interval counters (model PM6666) for measurement of the incident shock speed. The initial reflected shock temperature and pressure were calculated from the incident shock speed at the endwall, using one-dimensional shock-jump relations and assuming vibrational equilibrium and frozen chemistry, with uncertainties in initial post-shock temperature and pressure of less than $\pm 1.5\%$. The driven section was evacuated to an ultimate pressure of less than 10^{-5} torr, with a combined leak and outgassing rate of less than 10^{-4} torr/min before each shock. Liquid fuel was introduced by direct injection using a gas-tight syringe (model 1010 TLL SYR) into a 12.8-liter stainless-steel mixing tank maintained at 120 °C. Oxygen and nitrogen were from Praxair (research grade) and Sigma Aldrich anhydrous 1-butanol (99.8%) was used as the fuel source without further preparation. A test gas mixture of 1-butanol/ O_2/N_2 was prepared manometrically and stirred using a magnetically-driven vane assembly for at least 30 min prior to the experiments. Further details on the shock tube facility can be found in [35].

2.2. Shock tube diagnostics

Three diagnostics were used during the experiments: laser absorption at 3.39 μm , OH^* emission near 306 nm and sidewall pressure (see Fig. 2). Initial fuel concentration was measured by laser absorption using a 3.39 μm Spectra-Physics He–Ne laser. Liquid-nitrogen-cooled IR photovoltaic InSb detectors (Infrared Associates, IS-2.0) with a large linear dynamic range were used for measurements of incident and transmitted laser intensities. Ignition was indicated by emission near 306 nm from the $A^2\Sigma^+ - X^2\Pi(0,0)$ band of excited OH radical (OH^*) that was detected using a modified UV-enhanced PDA36A Si detector and Schott UG5 filter (not shown) with an optical arrangement that provided a temporal resolution of better than 10 μs . A flip mirror placed between shock tube windows and PDA36A detector was used to switch between laser absorption measurements in Regions 1, 2, and 5 and detection of OH^* chemiluminescence. Pressure time-history in the test section was monitored using a Kistler pressure transducer (603B1) coated with a thin 0.5 mm layer of RTV silicone, which provided an alternative definition of ignition delay time. The measurement location of all diagnostics was 1.1 cm from the endwall.

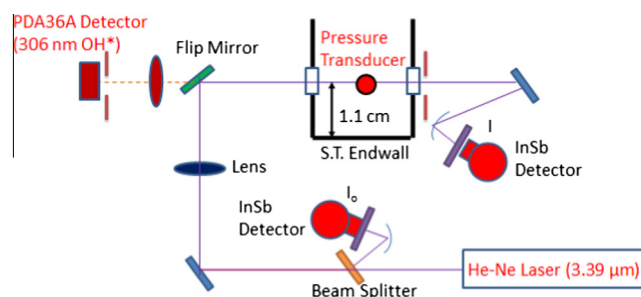


Fig. 2. Schematic of experimental set-up for ignition delay time measurements.

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