



# OH and C<sub>2</sub>H<sub>4</sub> species time-histories during hexadecane and diesel ignition behind reflected shock waves

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## Abstract

The first simultaneous multi-species laser absorption time-history measurements for OH and C<sub>2</sub>H<sub>4</sub> were acquired during the oxidation of *n*-hexadecane and commercial diesel fuel (DF-2). The experiments were performed behind reflected shock waves in a new second-generation aerosol shock tube over a temperature range of 1120K to 1373 K and a pressure range of 4–7 atm. Initial fuel concentrations varied between 150 and 1800 ppm with equivalence ratios between 0.4 and 2, and were determined using 3.39 μm He–Ne laser absorption. OH concentration time-histories were measured using absorption of frequency-doubled ring-dye laser radiation near 306.7 nm. Ethylene time-histories were measured using absorption of CO<sub>2</sub> gas-laser radiation near 10.5 μm. Comparisons are given of these species concentration time-histories with two current large *n*-alkane mechanisms: the LLNL-C-16 mechanism of Westbrook et al. [13] and the Jet-SurF C-12 mechanism of Sirjean et al. [14]. Fair agreement between model and experiment is seen in the peak ethylene yields for both fuels; however, modeled early time-histories of OH, an important chain-branching species, differ significantly from current measurements.

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## 1. Introduction

Detailed species time-history measurements during reaction of gas-phase diesel fuel and diesel fuel surrogates are needed to test and refine the large reaction mechanisms used to model the ignition of these fuels. Such measurements are difficult to achieve. Gas-phase studies of these fuels in conventional shock tubes typically require extreme

heating of both the shock tube and mixing assembly, because of the low fuel vapor pressure. As well, in the case of multi-component fuels such as diesel, normal loading techniques that use the vapor-pressure above the liquid fuel tend to fractionally distill the fuel, and again extreme heating is necessary to avoid these effects [1,2]. High-quality gas-phase experiments are, however, necessary in order to be able to separate the physical processes, such as evaporation, that occur during burning, from the chemical processes, such as oxidation, which are described by the large reaction mechanisms. An alternative strategy to study the gas-phase chemistry of low-vapor-pressure fuels is thus required.

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The recent development of an aerosol shock tube [3,4] provides a new approach for gas-phase studies of low-vapor-pressure fuels. Using this method, low fuel loading and fractional distillation can be avoided, as the fuel is introduced into the shock tube at room temperature as a spatially-uniform aerosol. This fuel aerosol is then completely evaporated into the gas-phase by the intermediate high temperatures (500–700 K) that momentarily exist behind the incident-shock wave. Gas-phase low-vapor-pressure fuels can then be studied at high temperatures (1000–1500 K) and pressures behind the subsequent reflected shock wave. Using this aerosol shock tube method, we have previously measured ignition delay times in gas-phase *n*-dodecane and diesel [3–5]. Critical to the temperature and mixture accuracy of these measurements is the requirement that the initial test gas mixture be spatially uniform in the shock tube. The second-generation aerosol shock tube used in this present study has been demonstrated to provide even higher spatial uniformity than our first-generation facility [4].

In our laboratory, we have developed sensitive, species-specific, and quantitative UV and visible laser absorption diagnostics for an array of important combustion species including OH, CH<sub>3</sub>, CH, NH<sub>2</sub>, and NO [6]. Recently, we have extended our suite of laser absorption diagnostics into the infrared. Using commercially available IR gas and diode lasers we have developed quantitative measurement capabilities for C<sub>2</sub>H<sub>4</sub>, H<sub>2</sub>O, CO<sub>2</sub>, CH<sub>4</sub> and selected *n*-alkanes [7–9]. Use of these laser absorption diagnostics in shock tubes has allowed the generation of multi-species time-histories under near-constant-volume conditions intended as targets for chemical kinetic modeling.

To elucidate the inner workings of the large reaction mechanisms describing diesel and diesel-surrogate ignition chemistry, we have applied this multi-species strategy to two important transient species that appear during diesel and *n*-hexadecane oxidation: OH, and C<sub>2</sub>H<sub>4</sub>. Time-history measurements of OH are extremely useful in quantifying ignition processes, as they provide critical information about the radical-pool population. OH profiles in these systems typically show an immediate rapid rise (that is dependent on fuel decomposition kinetics) to a relatively long-lived pre-ignition plateau (that is dependent on the slower oxidation kinetics of the stable alkene intermediate species), and a final strong exponential rise during ignition. Time-history measurements of ethylene, C<sub>2</sub>H<sub>4</sub>, provide quantitative information on the main high-temperature decomposition product and pathways of alkanes. Other groups have examined multiple species during hexadecane and diesel combustion in a jet-stirred reactor (JSR) [10–12], but these studies do not provide the detailed information on the short, transient time scales available in shock tubes.

Here we present measurements of OH and C<sub>2</sub>H<sub>4</sub> during the oxidation of diesel fuel (DF-2) and a single-component large-alkane surrogate for diesel fuel, *n*-hexadecane. Comparisons are given of these species concentration time-histories with two current large *n*-alkane mechanisms: the LLNL-C-16 mechanism of Westbrook et al. [13] and the JetSurF C-12 mechanism of Sirjean et al. [14].

## 2. Experimental setup

### 2.1. Aerosol shock tube

The experiments were performed in a new second-generation aerosol shock tube (AST II). This facility is shown schematically in Fig. 1. The shock tube consists of a driver and driven section. At the downstream end of the driven section is a 1.2 m long square test section (10 × 10 cm) that is contained between two gate valves. This is the portion of the shock tube that is initially filled with aerosol. Just before the incident-shock wave is initiated, the gate valves are set to the configuration shown in Fig. 1 where the driven gate valve is open and the endwall gate valve is closed. As the incident-shock wave travels through the aerosol, the small droplets are quickly evaporated, leaving behind a purely gas-phase mixture. Thus behind the reflected shock the test gas mixture can be considered fully evaporated and fully mixed. The measured spatial variations in concentrations of the resulting mixture are typically less than 1% [4]. Species concentration time-history measurements are then made using laser absorption behind the reflected shock wave through sidewall windows located at 4 cm from the endwall. In Fig. 1, the reflected shock has propagated nearly all the way through the aerosol mixture (labeled C).

### 2.2. Laser absorption

Three CW laser systems are used in these experiments: an IR He–Ne laser to measure initial

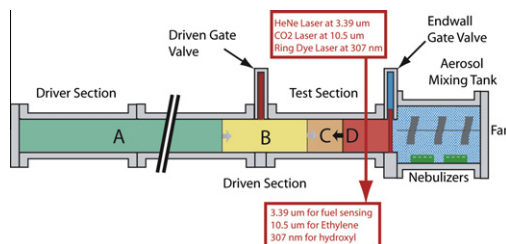


Fig. 1. Schematic of aerosol shock tube (AST II) setup. The different regions in the tube are (from left to right): (A) driver gas, (B) incident-shock heated driven gas with no fuel, (C) incident-shock heated test mixture with fuel, and (D) reflected shock heated test mixture.

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