



# Shock tube/laser absorption measurements of the pyrolysis of a bimodal test fuel

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## Abstract

A novel three-color, three-species laser absorption sensor for measurement of small (C<sub>2</sub>–C<sub>4</sub>) alkenes is introduced. This scheme, combined with an existing two-color CH<sub>4</sub> ICL laser sensor and an existing one-color HeNe laser fuel sensor, was applied to the study of the decomposition of a bio-derived, highly-branched alcohol-to-jet (ATJ) test fuel in a shock tube, yielding multiple species (methane, ethylene, propene, and isobutene) time-history measurements for temperatures between 1070 K and 1320 K and pressures between 1.3 atm and 1.5 atm. Simulations of the decomposition product yields for this fuel using a recent detailed reaction mechanism for highly-branched alkanes from Oehlschlaeger et al. (2009) compare favorably with these results. © 2016 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

*Keywords:* Shock tubes; Lasers; Alkenes; Isobutene

## 1. Introduction

Due to concerns about environmental impact, energy security, and resource scarcity, much interest has developed recently concerning replacing conventional, petroleum-derived jet fuels with synthetic jet fuels derived from alternative fossil sources such as shale and renewable sources such as biomass to various liquids [1]. In particular, synthetic jet fuels, as opposed to strictly alcohols or alternative fuels such as hydrogen or methane are attractive as blend components for conventional jet

fuels due to their similarities in energy density and physical and chemical properties.

Conventional distillate jet fuels contain thousands of different compounds, and can typically have significant fractions of iso-paraffins (~40%), n-paraffins (~27%), cyclo-paraffins (~17%), and aromatics (~13%) [2–4]. This spread of chemical components has an averaging effect on the chemical reaction kinetics of these fuels, allowing fuels with significantly different composition to have similar ignition and combustion behavior needed for commercial aviation [5]. However, when a synthetic fuel component is blended with a distillate fuel, a bimodal distribution of major components may occur and the assumption and consequences of an average fuel behavior may fail. This disparity in composition presents an array of challenges to the

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commercial use of this test fuel component; a common example cited is the failure of fuel line seals because of the lack of a significant aromatic content in the fuel [6].

Anomalously high concentrations of *n*- or iso-paraffins can also have a substantial impact on the chemistry of the test fuels, as may be anticipated from the differences reported by Li et al. in the ignition delay times of branched and normal paraffins [7]. Support for these results may be found in the pyrolysis measurements of neat *n*-paraffins, such as *n*-heptane and *n*-dodecane, that show the formation of significant amounts of ethylene as the major decomposition product [8,9], while iso-paraffins, such as iso-octane and iso-cetane, predominantly form the highly branched alkene isobutene [10]. Importantly, ethylene and isobutene are known to display different ignition delay times and different ignition delay time trends. Thus, we believe that, as hypothesized recently by Wang et al. [11], knowledge of the detailed kinetics behavior during pyrolysis will help elucidate the differences in global reaction parameters, such as ignition delay times, for test fuels formed of different components.

Species time-histories of methane and ethylene as the decomposition products of single jet fuel archetypal components have been measured previously behind reflected shock waves using laser absorption [8]. As well, ethylene yields for distillate rocket propellants have been measured using this method [9]. In the current study, a new laser strategy to measure ethylene, propene and iso-butene using three different IR wavelengths was developed to monitor the time-histories of these three species simultaneously. This approach was then used to examine the decomposition products of a bimodal test fuel composed almost entirely of two highly branched iso-alkanes derived from the linkage and dehydrogenation of multiple tert-butyl alcohols. This test fuel, known as C1 in current studies supported by the U.S. Federal Aviation Administration, contains greater than 99.5% iso-paraffins and has two primary components 75% iso-C<sub>12</sub>H<sub>26</sub> and 25% iso-C<sub>16</sub>H<sub>34</sub>. The high presence of iso-paraffins and near-zero presence of other classes of hydrocarbons, including aromatics and *n*-paraffins, has a substantial impact on the decomposition products of the test fuel.

## 2. Experimental setup

### 2.1. Shock tube

The experiments in this work were performed in a heated, helium-driven, stainless-steel, high-purity shock tube at Stanford University. The driven section of the shock tube is 8.54 m long and the driver section is 3.35 m long. Each section is 14.13 cm in diameter [12]. The shock speed was calculated by recording the time differences of the passage of the

incident shock wave over five pressure transducers located axially along the length of the tube near the end wall. These four speed measurements were used to calculate the attenuation of the shock wave, which was extrapolated to yield the shock speed incident on the end wall of the shock tube. The reflected shock speed and post-incident shock and post-reflected shock conditions were then calculated with an uncertainty of less than  $\pm 1\%$  in pressure and less than  $\pm 1\%$  in temperature [12] using standard shock jump equations. Pressure transducers and ports for optical access were located 2 cm from the end wall of the shock tube to allow monitoring of reaction progress.

Mixtures were prepared in a heated stainless steel mixing tank. To generate vapor from the test fuel, a known amount of test fuel was introduced into an evacuated borosilicate glass bulb heated above 120 °C. After allowing the fuel to heat and vaporize for 5 min, the fuel vapor was then introduced into the mixing tank, which was heated to 130 °C. Test fuel was diluted with argon to provide the correct fuel mole fraction. The test fuel and argon were then allowed to mix for 30 min before experiments were performed. The argon used in these experiments was research grade ( $\geq 99.999\%$ ) supplied by Praxair. The bimodal test fuel and its thermochemical properties, necessary for determining post-reflected shock conditions, were provided from GCxGC composition measurements [2,3].

### 2.2. Lasers

Three laser sensors were used in these experiments. First, a one-color (i.e., one wavelength) sensor using an infrared HeNe gas laser operating at 3.392  $\mu\text{m}$  was used to measure the initial test fuel concentration in the shock tube. Due to high-frequency variations in output of the HeNe, a common-mode rejection scheme using a reference detector to monitor the laser intensity prior to its passage through the shock tube, was implemented. Second, a two-color sensor using a fiber-coupled ICL supplied by Nanoplus GMBH<sup>TM</sup> was operated at 3148.81 and 3148.66  $\text{cm}^{-1}$  and was used to measure CH<sub>4</sub> time-varying concentration using the two-color online absorption minus offline absorption scheme described by Sur et al. [13]. Third, a three-color sensor using Access Laser<sup>TM</sup> CO<sub>2</sub> gas laser operating at 10.532 and 10.675  $\mu\text{m}$  and a Daylight Solutions<sup>TM</sup> ECQCL operated at 881.4  $\text{cm}^{-1}$  was used to measure C<sub>2</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, and iC<sub>4</sub>H<sub>8</sub> concentrations. For the tunable lasers (ICL, CO<sub>2</sub> laser, ECQCL), the wavelength was verified before and after each shock wave experiment using a Bristol Instruments<sup>TM</sup> 721B-MIR wavemeter.

The initial fuel and time-varying species mole fractions were calculated using Beer's Law

$$\text{Absorbance} = -\ln \frac{I}{I_0} = kxPL = nx\sigma L$$

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