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Ignition delay time and CO time-history measurements in a shock tube during high performance jet fuel surrogate combustion

Andrew R. Laich[1], Erik Ninnemann[1], Sneha Neupane[1], and Subith S. Vasu[2]

Center for Advanced Turbomachinery and Energy Research (CATER), Department of Mechanical and Aerospace Engineering, University of Central Florida, Orlando, FL 32816

The chemical kinetics of diisobutylene, a proposed biofuel, has been studied behind reflected shock waves near 10 atm over a temperature range of 1186 – 1414 K. A stoichiometric mixture consisting of 0.15% diisobutylene was used to investigate ignition behavior and speciation during oxidation experiments performed in a shock tube. Time resolved measurements of carbon monoxide were measured behind reflected shock waves with a continuous wave quantum cascade laser centered at a frequency of 2046.20 cm^{-1} using a fixed-wavelength spectroscopy scheme.

I. Nomenclature

DIB-1 = 2,4,4-trimethyl-1-pentene
DIB-2 = 2,4,4-trimethyl-2-pentene
RCM = rapid compression machine
CO = carbon monoxide
T_5 = temperature behind reflected shock wave
P_5 = pressure behind reflected shock wave
R = universal gas constant
σ = absorption cross-section of the absorbing species
L = path length of the absorbing species
α = absorbance
I or I_{trans} = transmitted laser intensity
I_0 or I_{ref} = reference incident laser intensity
X_{CO} = mole fraction of carbon monoxide
CWQCL = continuous wave quantum cascade laser
IDT = ignition delay time

II. Introduction

Real fuels, such as gasoline, diesel, and refined kerosene (jet fuels) are composed of many constituents that can have different compositions based on many factors including variance in the refining process, and place of origin of crude oil. This adds much difficulty in creating chemical kinetic models for real-fuels and calls for the need of a surrogate to minimize the complexity while maintaining important characteristics and kinetic information. Representing primary chemical classes of a particular fuel is paramount in surrogate model development. Diisobutylene-1 (DIB-1) or 2,4,4-trimethyl-1-pentene is one such compound that can be used to represent olefins in real-fuels, and is the focus of the current study.

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[1] Graduate Student, University of Central Florida, Orlando, Fl 32816, Student Member
[2] Associate Professor, CATER, University of Central Florida, Orlando, FL 32816, Associate Fellow, subith@ucf.edu

Previous experimental studies of diisobutylene include both of its isomers 2,4,4-trimethyl-1-(and -2-) pentene, DIB-1 and DIB-2 respectively, in shock tubes and a rapid compression machine (RCM) in neat mixtures, or blends with other compounds such as isooctane, toluene and ethanol [1-3]. Most recently Li et al. [1] studied ignition delay times in a high pressure shock tube of two quaternary and one quinary surrogates containing diisobutylene at pressures of 10, 15, and 20 bar between 950 – 1300 K at lean, stoichiometric and rich conditions. The authors compose a reaction mechanism to predict ignition of gasoline surrogates and through much analysis it is revealed that ignition delay times are highly dependent on temperature over other parameters. Mittal et al. [2] investigates neat (DIB, toluene and isooctane) and blended diisobutylene ignition delay times in a RCM at 15 to 45 bar. Metcalfe et al. [3] studied ignition of both isomers of diisobutylene (individually and blended) at 1 and 4 atm between 1200 and 1550 K. The authors found that DIB-2 reacted faster than DIB-1 and the ignition of the mixture relied on the relative proportion of each isomer. The ignition characteristics were well captured through predictions of a detailed kinetic mechanism. This work presents not only ignition delay times, but time-resolved carbon monoxide (CO) time-histories of DIB-1 during oxidation experiments in a shock tube

III. Experimental Procedure

Carbon monoxide time-histories were measured in the stainless, double-diaphragm, and heated shock tube facility at the University of Central Florida (UCF), specific details of which can be found in refs. [4-12]. Both driver and driven sections have an inner diameter of 14.17 cm, with these experiments utilizing a single polycarbonate diaphragm separating driver/driven sections. A normal shock wave was initiated via pressurizing the driver section to burst the diaphragm, with either helium or some composition of helium and nitrogen. Approximately 2.00 cm from the end-wall are machined ports placed circumferentially, several of which house windows that allow optical access for an emission detector, laser diagnostics, and pressure probes. The incident shock velocity was measured using four Agilent 53220A timer counter boxes linked to five equally spaced PCB 113B26 piezoelectric pressure transducers along the last 1.5 m of the driven section. From the velocity, temperature (T_5) and pressure (P_5) behind reflected shock waves was calculated using the quasi 1-D normal shock relations

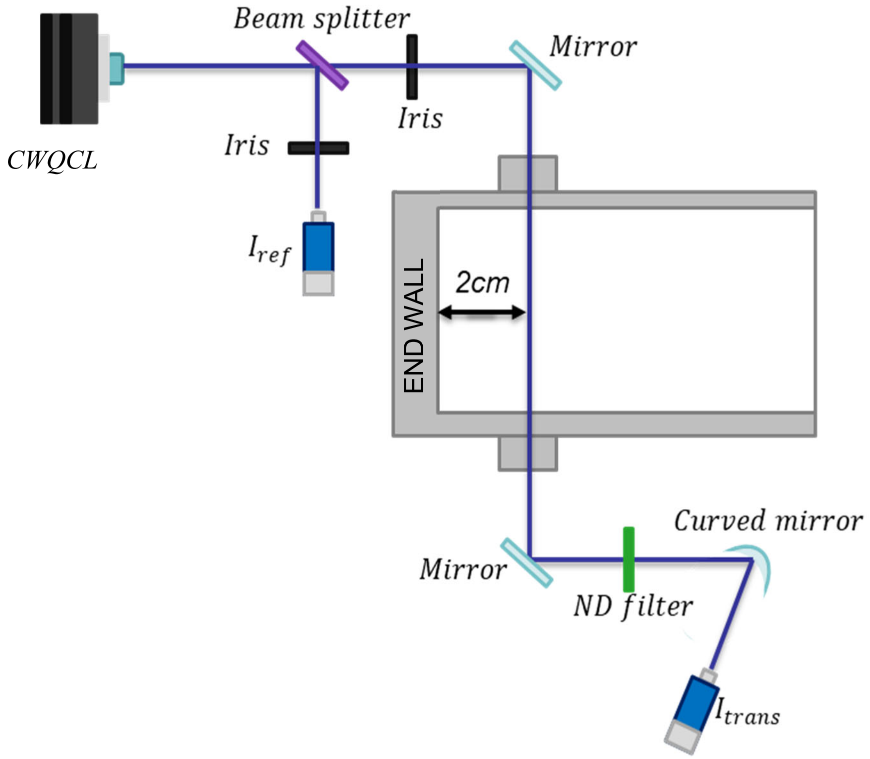

Fig. 1 Schematic of the laser absorption setup used at the 2.00 cm location of the shock tube.

Time-resolved measurements of carbon monoxide were measured using a continuous wave quantum cascade laser (Alpes QCL) with a fixed-wavelength direct absorption measurement technique at 2046.20 cm^{-1}, as shown in Fig. 1. This particular wavelength was chosen for these measurements in an effort to mitigate interference from other forming species. With preliminary simulations, the interference was found to be negligible. Experimental mole fractions of carbon monoxide were obtained by using the Beer-Lambert Law,

$$X_{CO} = \frac{\alpha RT}{\sigma PL}$$

where

$$\alpha = -\ln\left(\frac{I}{I_0}\right)$$

is the absorbance, R is the universal gas constant (cm^3*atm/K*mole), T is the temperature of the gas (K), σ is the absorption cross-section of the absorbing species (cm^2/molecule), P is the total pressure of the gas (atm), and L is the path length (cm). In the absorbance expression, I and I_0 are the transmitted and reference laser signals, respectively. These signals were obtained by focusing laser light onto thermoelectrically cooled HgCdTe (MCT) detectors (Vigo Systems, PVI-2TE-5). The absorption cross-section for carbon monoxide was determined experimentally by shock heating a mixture of 1% CO/12% He in argon, where an empirical relation was developed for validity within targeted experimental conditions. The absorption cross-section obeys a power law fit for both temperature and pressure at the chosen line.

IV. Results and Discussion

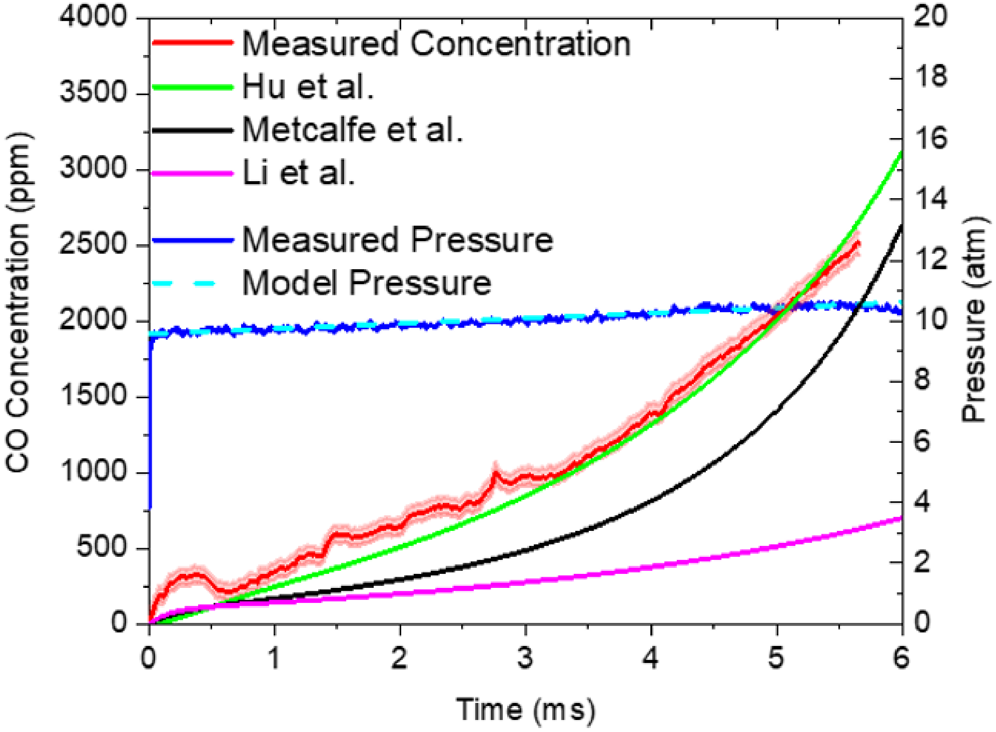

Fig. 2 Pressure and CO time-history measurements during the oxidation of 0.15% DIB-1 at 1186 K and 9.57 atm.

Pressure, CO time-history, and ignition delay time (IDT) measurements of 0.15%DIB-1/1.8%O2/Ar were carried out behind reflected shock waves from 1186 – 1414 K and 8.5 – 10.9 atm. Chemical kinetic mechanisms from Hu et al. [13], Metcalfe et al. [3], and Li et al. [1] were used in Chemkin-Pro using a 0-D homogeneous batch reactor with a constant internal energy, constant volume model assumption. Though some of the pressure traces exhibit a slight first order linear rise, the models accurately predict this without the need to seed in a dP/dt trend; however, do not capture the heat release due to the ignition event. Carbon monoxide time-histories show truncation due to an arrival of a compression/expansion wave, or rise in pressure from ignition event, though useful insight is still gained. The model of Hu et al. captures the measured CO profile, as shown in Fig. 2, with very good agreement in rate and concentration level throughout. Both models of Metcalfe et al. and Li et al. underpredict concentration level throughout showing a slower rate of CO formation when compared to gathered data. This difference is more pronounced with the Li et al. mechanism as the slower rate persists throughout the shown test time, which ultimately results in an overprediction in IDT as well.

V. Conclusions

In summary, CO time-history and ignition delay time measurements were carried out behind reflected shock waves in the UCF shock tube facility. A fixed wavelength direct absorption laser setup was implemented using a continuous wave QCL to temporally resolve CO concentrations throughout test times. Gathered data were compared to three literature mechanisms, with great agreement realized with the mechanism of Hu et al., with large discrepancies observed with comparison to the Li et al. mechanism. Future work will include chemical kinetic analyses to better understand the significant differences between the Li et al. and other models, including rate of production, pathway, and sensitivity analyses.

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References

1. Li, H., Qiu, Y., Wu, Z., Wang, S., Lu, X., and Huang, Z. "Ignition delay of diisobutylene-containing multicomponent gasoline surrogates: Shock tube measurements and modeling study," *Fuel* Vol. 235, 2019, pp. 1387-1399.
doi: https://doi.org/10.1016/j.fuel.2018.08.132
2. Mittal, G., and Sung, C.-J. "Homogeneous charge compression ignition of binary fuel blends," *Combustion and Flame* Vol. 155, No. 3, 2008, pp. 431-439.
doi: https://doi.org/10.1016/j.combustflame.2008.05.003
3. Metcalfe, W. K., Pitz, W. J., Curran, H. J., Simmie, J. M., and Westbrook, C. K. "The development of a detailed chemical kinetic mechanism for diisobutylene and comparison to shock tube ignition times," *Proceedings of the Combustion Institute* Vol. 31, No. 1, 2007, pp. 377-384.
doi: https://doi.org/10.1016/j.proci.2006.07.207
4. Koroglu, B., Pryor, O. M., Lopez, J., Nash, L., and Vasu, S. S. "Shock tube ignition delay times and methane time-histories measurements during excess CO2 diluted oxy-methane combustion," *Combustion and Flame* Vol. 164, 2016, pp. 152-163.
doi: https://doi.org/10.1016/j.combustflame.2015.11.011

5. Ninnemann, E., Kim, G., Laich, A., Almansour, B., Terracciano, A. C., Park, S., Thurmond, K., Neupane, S., Wagnon, S., Pitz, W. J., and Vasu, S. S. "Co-optima fuels combustion: A comprehensive experimental investigation of prenol isomers," *Fuel* Vol. 254, 2019, p. 115630.

doi: https://doi.org/10.1016/j.fuel.2019.115630

6. Loparo, Z. E., Ninnemann, E., Thurmond, K., Laich, A., Azim, A., Lyakh, A., and Vasu, S. S. "Acousto-optically modulated quantum cascade laser for high-temperature reacting systems thermometry," *Optics Letters* Vol. 44, No. 6, 2019, pp. 1435-1438.

doi: 10.1364/OL.44.001435

7. Zhang, K., Lokachari, N., Ninnemann, E., Khanniche, S., Green, W. H., Curran, H. J., Vasu, S. S., and Pitz, W. J. "An experimental, theoretical, and modeling study of the ignition behavior of cyclopentanone," *Proc. of the Combust. Inst.* Vol. in press, 2018.

8. Ninnemann, E. M., Barak, S., Pryor, O., and Vasu, S. "Is Ignition in a Shock Tube Homogeneous? An Experimental Study Behind Reflected Shock Waves," *2018 AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, 2018.

9. Ninnemann, E., Koroglu, B., Pryor, O., Barak, S., Nash, L., Loparo, Z., Sosa, J., Ahmed, K., and Vasu, S. "New insights into the shock tube ignition of H2/O2 at low to moderate temperatures using high-speed end-wall imaging," *Combustion and Flame* Vol. 187, No. Supplement C, 2018, pp. 11-21.

doi: https://doi.org/10.1016/j.combustflame.2017.08.021

10. Neupane, S., Barnes, F., Barak, S., Ninnemann, E., Loparo, Z., Masunov, A. E., and Vasu, S. S. "Shock Tube/Laser Absorption and Kinetic Modeling Study of Triethyl Phosphate Combustion," *The Journal of Physical Chemistry A* Vol. 122, No. 15, 2018, pp. 3829-3836.

doi: 10.1021/acs.jpca.8b00800

11. Barak, S., Ninnemann, E., Neupane, S., Barnes, F., Kapat, J., and Vasu, S. "High-Pressure Oxy-Syngas Ignition Delay Times With CO2 Dilution: Shock Tube Measurements and Comparison of the Performance of Kinetic Mechanisms," *Journal of Engineering for Gas Turbines and Power* Vol. 141, No. 2, 2018, pp. 021011-021011-7.

doi: 10.1115/1.4040904

12. Pryor, O., Barak, S., Lopez, J., Ninnemann, E., Koroglu, B., Nash, L., and Vasu, S. "High Pressure Shock Tube Ignition Delay Time Measurements During Oxy-Methane Combustion With High Levels of CO2 Dilution," *Journal of Energy Resources Technology* Vol. 139, No. 4, 2017, pp. 042208-042208-6.

doi: 10.1115/1.4036254

13. Hu, E., Yin, G., Gao, Z., Liu, Y., and Jinfeng, K. "Experimental and kinetic modeling study on 2,4,4-trimethy1-1-pentene ignition behind reflected shock waves," *Fuel* Vol. 195, 2017, pp. 97-104.

doi: 10.1016/j.fuel.2017.01.055