Contents lists available at ScienceDirect





Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Fuel-rich n-heptane oxidation: A shock tube and laser absorption study



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ARTICLE INFO

Article history: Received 22 March 2017 Revised 23 June 2017 Accepted 14 July 2017 Available online 29 July 2017

Keywords: Shock tube n-Heptane Laser absorption Fuel rich Chemical kinetics

ABSTRACT

The chemical kinetics of n-heptane (n-C₇H₁₆) – an important reference compound for real fuels – oxidation are well studied at stoichiometric and lean conditions. However, there is only limited information on the n-heptane chemical kinetics in fuel-rich combustion. In order to verify the accuracy of chemical kinetic models at these conditions, the oxidation of rich n-heptane mixtures has been investigated. Combustion of n-C₇H₁₆/O₂/Ar mixtures at equivalence ratios, φ , of 2.0 and 3.0 behind reflected shock waves has been studied at temperatures ranging from 1066 to 1502 K and at pressures ranging from 1.4 to 6.2 atm. Reaction progress was monitored by recording pressure and absorption time-histories of ethylene (C₂H₄) and n-heptane at a location 2 cm from the endwall of a 14-cm inner diameter shock tube. Ethylene and n-heptane absorption time-histories were measured, respectively, using absorption spectroscopy at 10.532 μ m from a tunable CO₂ laser and at around 3.4 μ m from a continuous wave distributed feedback interband cascade laser (ICL). The measured absorption time-histories were compared with modeled predictions from the Lawrence Livermore National Lab (LLNL) detailed n-heptane reaction mechanism. To the best of our knowledge, current data are the first time-resolved n-heptane and ethylene concentration measurements conducted in a shock tube at these conditions.

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1. Introduction

Recent research has pursued the combustion and performance advantages of in-cylinder reforming processes where fuel is injected into O₂-deficient engine operating conditions, to convert a portion of the fuel into products containing significant levels of small-chained partially-oxidized hydrocarbons. The presence of reformate can extend knock limit and dilution tolerance of SI combustion [1,2]. By exploiting the properties of reformate with well-understood engine technologies, such as dilute SI combustion and compression ratio, light-duty vehicle fuel economy can be increased towards legislated fuel economy mandates (e.g., CAFE 2025 [3]). One such method is fuel injection in the negative valve overlap (NVO) period in order to convert a portion of the fuel into short-chain hydrocarbons (e.g., ethylene) by partial oxidation and thermal cracking. These products may then be used to control the combustion properties of the fuel and air mixture introduced

* Corresponding author. E-mail address: subith@ucf.edu (S.S. Vasu). into the other cylinders [4]. In an NVO environment, the mixture within the cylinder is often fuel-rich [2]. Other strategies known as spark-assisted HCCI (SA-HCCI) and spark assisted compression ignition (SACI) have been pursued as well [5]. In this case, HCCI heat release is obtained after a stoichiometric NVO assisted by spark initiation. The recent dedicated exhaust gas recirculation strategy (D-EGR) [6] uses one of cylinders to produce a reformate and can result in fuel savings of up to 10%. Fuel rich conditions also exist in other common combustion environments, such as diesel engine sprays and in aircraft gas turbines.

It has been found that the concentration of reformate species is strongly dependent on the injected fuel type and the time available for reactions [7,8]. Surprisingly, a comparison of species concentrations obtained during NVO reformate experiments including hydrogen (H₂), acetylene (C_2H_2), and ethylene (C_2H_4) and those predicted with recent Lawrence Livermore National Labs (LLNL) mechanisms [9–11] did not match [4]. The model predictions failed to capture the experimental trend of increased reformate concentrations with advanced fuel injection timings. Thus, a detailed understanding of the fuel chemistry that occurs during engine relevant oxygen deficient conditions is warranted.

http://dx.doi.org/10.1016/j.combustflame.2017.07.016

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f able 1 Summary of experimental conditions and species diagnostics used in n-heptane oxidation studies in shock tubes.						
Study	Year	Pressure (atm)	Temperature (K)	Fuel loading	Equivalence ratio (φ)	Species Diagnostics
This work	2017	1.4-1.9, 4.8-6.2	1066-1502	2%	2.0, 3.0	n-heptane: 3.403 µm ethylene: 10.532 µm
Tekawade et al. [34]	2016	10	686-1290	0.05-0.5%	1.0	CO: 4.59 µm
Campbell et al. [33]	2015	6.1-7.4	651-823	1%	0.75	n-heptane: 3.93 µm OH, CH ₂ O: 306.7 nm CO ₂
						4.2 μm H ₂ O:2.5 μm OH*: emission
Zhang et al. [13]	2013	2, 10	1200-1500	0.38%	1.0	CH*: emission
Pyun et al. [14]	2013	1.5	1200-1600	1%	Pyrolysis	CH ₄ : 3.43 μm ethylene: 10.532 μm
Pilla et al. [40]	2011	1.3-3.3	1350-1950	300 ppm	Pyrolysis	ethylene: 10.532 µm
Davidson et al. [20]	2010	2	1300-1600	300 ppm	1.0	n-heptane: 3.39 µm ethylene: 10.532 µm OH:
						306.5 nm CO ₂ : 2.7 μm H ₂ O: 2.5 μm
Shen et al. [41]	2009	9–58	786-1396	0.5-1.8%	0.25, 0.5, 1.0	OH*: emission
Vasu et al. [21]	2009	15	1121-1332	750–1000 ppm	0.5	OH: 306.5 nm
Davidson et al [29]	2007	16-20	1100-1560	100_500 nnm	1 pyrolysis	CH ₂ : 216 nm

0.40%

1.87%

02-07%

300 ppm

0.9-5.5%

0.5, 1.0, 2.0

0.5, 1.0, 2.0

01 - 04

0.8-1.2

0.5 - 3.0

S

1500-1650

720-1100

850-1280

1357-1784

660-1350

n-Heptane is a component of primary reference fuel for both diesel and gasoline, and is one of the most well studied fuels especially at stoichiometric and lean conditions [12-26]. However, there is a lack of rich n-heptane combustion studies in the literature, and those that do investigate rich mixtures do not provide concentration time-histories of intermediate species [20,21,25,27-34]. Ethylene has been shown to be produced in significant guantities during fuel-rich n-heptane combustion and is therefore of high importance for mechanism development [12,21,35]. The use of non-intrusive, laser-based diagnostics in shock tubes enables in-situ measurements of species concentration time-histories and reaction rates with high temporal resolution. Concentration timehistory data from shock tubes offers rich targets for chemical kinetic model development and validation when compared to ignition delay time data or endpoint species measurements provided by gas chromatograph (GC/MS) techniques [17,36–38].

In this work, time-histories of ethylene and n-heptane absorbances were measured at pressure ranges from 1.4 to 6.2 atm over a temperature range of 1066 to 1502 K with mixtures of nheptane and oxygen in an argon bath at equivalence ratios (φ) of 2.0 and 3.0 and with initial n-heptane concentration of 2% behind reflected shock waves. This work is an extension of previous experiments, detailed in [39]. Results were compared to the predictions of LLNL detailed heptane chemical kinetic mechanism, which has not been validated at equivalence ratios of above 1.0 [11]. A summary of the conditions and diagnostics used in this and previous work performed in shock tubes is provided in Table 1.

To the best of our knowledge, current data are the first timeresolved n-heptane and ethylene concentration measurements conducted in a shock tube at these conditions of high fuel loading, rich mixtures, and over a wider pressure range than previously investigated.

2. Experimental procedure

2.1. Shock tube facility

Smith et al. [32]

Herzler et al. [42]

Gauthier et al. [30]

Davidson et al. [28] Ciezki et al. [25]

2005

2005

2004

2001

1993

2

50

2.0-3.8

3.2 - 41

12-25, 45-60

Experiments were performed in a stainless steel, heated shock tube located at the University of Central Florida (UCF) with an inner diameter of 14 cm. The details of the shock tube facility are in Refs. [43-46] and only a brief description is provided here. The shock tube facility with double diaphragm configuration is designed for producing pressures ranging from 1 to 90 atm and temperatures ranging from 600 to 4000K. In the current work, a single diaphragm configuration was utilized; the diaphragms were



CH*, OH*: emission

CH*, OH*: emission

CH*: emission

OH: 306.5 nm

CH*: emission

Fig. 1. Measured absorbance at $3.4 \,\mu\text{m}$ versus initial mixture pressure in the shock tube across multiple tests.

0.127 mm and 0.381 mm thick in order to achieve test pressures (P_5) ranging from 1.4 to 1.9 atm and 4.8 to 6.2 atm, respectively.

All measurements were performed at a test section located 2 cm away from the endwall of the driven section, which has eight optical access ports. A Kistler 603B1 piezoelectric pressure transducer with Room Temperature Vulcanization (RTV) silicone coating was installed in one access port to measure pressure in the reflected shock region. A pair of sapphire windows, 3 mm thick Download English Version:

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