Combustion and Flame 166 (2016) 45–54

Contents lists available at ScienceDirect

Combustion and Flame

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

Autoignition study of ULSD#2 and FD9A diesel blends

Goutham Kukkadapu*, Chih-Jen Sung

Department of Mechanical Engineering, University of Connecticut, Storrs, CT 06269, USA

ARTICLE INFO

Article history:
Received 20 November 2015
Revised 22 December 2015
Accepted 22 December 2015
Available online 19 January 2016

Keywords:
Diesel
ULSD#2 diesel
FD9A diesel
Rapid compression machine
Ignition delay time
Low temperature combustion

ABSTRACT

Autoignition study of two well-characterized reference diesel fuels with similar cetane ratings but different compositional characteristics has been conducted using a heated rapid compression machine (RCM). The two diesel blends used in the current study were a commercial grade ultra-low-sulfur diesel (ULSD) #2 reference fuel, ULSD#2, and Fuels for Advanced Combustion Engines (FACE) research diesel, FD9A. Ignition delay time measurements were conducted at compressed pressures of 10 bar, 15 bar, and 20 bar covering low-to-intermediate temperatures between 678 K and 938 K. In addition, experiments were carried out with diesel/O_2/N_2 mixtures at varying equivalence ratios of $\phi = 0.5$, 0.69, and 1.02. Equivalence ratio was varied by changing the oxygen mole percentage while keeping the fuel mole percentage fixed at 0.514%. Therefore, the present ignition delay time measurements illustrate the effect of oxygen concentration on diesel autoignition. The experimental results showed that diesel blends with similar cetane ratings and different compositional makeups exhibited varying ignition propensities in different temperature regimes, thereby demonstrating the effect of molecular composition on autoignition characteristics. In particular, the difference in ignition propensities was observed at temperatures at which the low temperature branching reactions are active. Furthermore, the ignition delay time measurements from the current RCM study were found to complement well with the existing shock tube data in the literature, and hence this investigation provides additional experimental database of diesel blends needed for development and validation of diesel surrogate models.

1. Introduction

Cetane ratings determined using the American Society for Testing and Materials (ASTM) standard test procedures, such as cetane number (CN) [1] and derived cetane number (DCN) [2], are widely used to quantify the ignition quality of a fuel. In the ASTM standard test procedures, liquid fuel is injected into hot oxidizer gases and the induction time for the mixture to ignite is measured. The induction time or the ignition delay time is then used to determine the cetane rating of a fuel. It is noted that this measured ignition delay time includes both physical and chemical induction times. The physical induction time is related to spray processes during which the liquid fuel breaks down into droplets, vaporizes, and mixes with hot oxidizer to form a combustible mixture. On the other hand, the chemical induction time relates to the time taken by the combustible mixture to ignite. The processes prevalent in the ASTM standard test procedures that are used to determine the cetane ratings are similar to those encountered in conventional compression ignition (CI) engines. Thus, the cetane rating of a fuel is a good metric to understand how a fuel would perform in a conventional CI engine. A recent computational study [3] has shown that for the induction times relevant to diesel fuels in the ASTM test vessels, the physical induction times are more dominating in controlling the ignition delays. Since the cetane rating is heavily influenced by physical processes, it may not be a good indicator of fuel ignition propensity under homogeneous ignition conditions.

Because of increasingly stringent engine emission standards, there is an urgent need to develop next-generation combustion technology with a focus on higher efficiency and reduced emissions. Advanced combustion technologies, such as low temperature combustion (LTC), are currently being pursued to develop such cutting-edge engines. The engines operating on LTC modes, such as partially premixed compression ignition (PPCI), are designed to operate at lower in-cylinder charge temperatures, greater degree of premixing, and higher dilution levels, which slow down the overall reactivity leading to ignition. Delaying the ignition timing results in increasing dominance of fuel chemistry and also leads to flame structure, heat release rate (HRR) profile, and temperature stratification that are different from those observed in conventional CI engines [4]. This increase in influence of ignition chemistry on the performance of LTC engines underscores the importance of understanding the autoignition characteristics of diesel fuels under LTC-relevant conditions, namely high pressures and low-to-intermediate temperatures.

* Corresponding author. fax: +1 860 486 5088.
E-mail address: goutham.kukkadapu@uconn.edu, goutham.4238@gmail.com (G. Kukkadapu).

http://dx.doi.org/10.1016/j.combustflame.2015.12.022
0010-2180/

Table 1
List of literature studies on autoignition of diesel blends.

Study	Facility	Pressure (atm)	Temperature (K)	ϕ	Oxidizer
Spadaccini and Tevelde [5]	Flow reactor	10–30	625–1000	0.3–1	Air
Penyazkov et al. [6]	Shock tube	4.7–10.4	1065–1838	0.5–2	Air
Haylett et al. [8]	Shock tube	1.7–8.6	947–1261	0.2–1	Varying O_2/Ar ratios
Gowdagiri et al. [9]	Shock tube	10, 20	671–1266	0.5, 1	Air

Very few studies in the literature have focused on autoignition characteristics of diesel fuels. The literature studies that focused on ignition delay times of diesel fuels are listed in Table 1, including the facilities and the conditions of pressure, temperature, equivalence ratio, and dilution used in the experiments. Spadacinni and Tevelde [5] conducted ignition delay time measurements of diesel type fuels in a continuous flow reactor. The fuels studied in [5] included Jet-A, JP-4, *n*-cetane, No. 2 diesel, and a research grade diesel. The ignition delay time correlations deduced from their measurements showed that Jet-A was more reactive than No. 2 diesel [5]. Penyazkov et al. [6] measured ignition delay times of American commercial diesel (DF-2) using a pre-heated shock tube and compared the ignition delay times of DF-2 with those of Jet-A taken from Dean et al. [7]. The comparison of [6] showed that the ignition delay times of DF-2 were higher than those of Jet-A, with a factor of 2–6 difference depending on the conditions. Haylett et al. [8] conducted ignition delay time measurements of four different diesel blends, including a European grade diesel with CN ~ 55 and three American grade diesels with DCN ~ 42–46, in an aerosol shock tube to understand the effects of cetane rating and aromatic content percentage on ignition propensities. Haylett et al. [8] found that the differences in ignition delay times of the different diesel fuels tested to be small and that the ignition delay times generally decreased with increasing cetane rating. In addition, the measured ignition delay times of the American grade diesel fuel of CN ~ 43 by Penyazkov et al. [6] and those by Haylett et al. [8] were seen to show a good agreement. Gowdagiri et al. [9] recently reported the ignition delay times of petroleum (F-76) and algae (HRJ-76) derived diesel blends. The two diesel blends used in [9] exhibited big differences in DCN values and compositions. Specifically, the DCN of F-76 was reported to be 48.8, while that of HRJ-76 was reported to be 76 [9]. Despite the differences in DCN values and fuel compositions, Gowdagiri et al. [9] noticed that the ignition delay times of the two diesel blends were indistinguishable for temperatures greater than 1000 K. Gowdagiri et al. [9] also observed that the petroleum derived diesel (F-76) and Jet-A exhibited identical ignition delay times across a wide range of temperatures they investigated.

Clearly, more ignition delay datasets of diesel reference fuels are needed in order to fully understand the effects of cetane rating and fuel composition on ignition propensities. Therefore, the objectives of the current study are two-fold. First, using a heated rapid compression machine, two fully-characterized diesel reference fuels with similar cetane rating but different compositional characteristics have been studied to explore the effect of fuel composition on ignition propensities by measuring and comparing their ignition delay times over a wide range of pressures and temperatures. The two diesel reference fuels used herein were a commercial grade ultra-low-sulfur diesel (ULSD) #2 reference fuel, ULSD#2, and Fuels for Advanced Combustion Engines (FACE) research diesel, FD9A. These two diesel blends have been chosen as their cetane ratings are similar to those of the diesel fuels used in conventional diesel engines and they have received special attention from the engine community, especially the Coordinating Research Council (CRC). In addition, there are ongoing, concerted efforts in developing surrogates for these well-characterized diesel reference fuels and the associated chemical kinetic models. Hence, the second objective of this investigation is to provide benchmark ignition delay database of the two diesel fuels at varying pressures, oxygen concentrations, and temperatures needed for development and validation of surrogate models.

In the following, a detailed comparison of the properties and compositions of the two diesel blends used in the current study and those studied in the literature shall be first discussed. The experimental facility, its characterization, and the test matrix will be introduced and specified next, followed by the presentation and discussion of the present experimental results.

Table 2
Comparison of properties and compositions of the diesel blends used in the current study and in Gowdagiri et al. [9].

Property/composition	ULSD#2	FD9A	F-76
H/C ratio [9,12]	1.80	1.80	1.80
DCN [9,12]	43.7	44.2	48.8
CN [12]	43.3	43.9	–
Density (kg/m^3) [12]	848	846.2	–
Heat of combustion (MJ/kg) [12]	42.90	42.86	–
Saturates (wt%) [9,13]	**69.85**	**62.60**	**82**
iso-Alkanes	18.44	23.40	20
n-Alkanes	16.38	10.26	56
Cycloalkanes	35.03	28.94	6
Aromatics (wt%) [9,13]	**30.05**	**36.43**	**16**
Alkylbenzenes	9.83	25.10	–
Indanes/tetralins	8.13	7.93	–
>2 aromatic rings	12.09	3.41	2
Others [9,13]	**0.10**	**0.94**	**2**

2. Properties and compositions of diesel blends

ULSD#2 was obtained from Chevron Philips, while FD9A was acquired from the CRC. Table 2 shows and compares the properties and compositions of the two diesels used in the current study and F-76 used in [9]. It is noted that different types of analyses were conducted by the CRC to determine the compositions of the diesel blends, and the compositional characteristics of ULSD#2 and FD9A from these different types of analyses documented in the CRC reports [10–13] show noticeable differences in fuel composition for the given blend. Considering the differences in the reported compositions, the average values of the compositional characteristics from the latest report, determined using 2D GCMS [13], are listed in Table 2. The interested reader is referred to the original reports [10–13] for further details.

As seen from Table 2, while both ULSD#2 and FD9A exhibit similar CN and DCN values, H/C ratio, density, and heats of combustion, their compositions are different. In particular, FD9A contains higher amounts of aromatics accompanied by lower amounts of saturates when compared to ULSD#2. However, in terms of weight percentage of paraffins (*n*-alkanes + *iso*-alkanes), both the blends constitute similar amounts –34.82% in ULSD#2 and 33.66% in FD9A. Comparison of the weight percentages of the aromatic components shows that FD9A contains higher amounts of alkylbenzenes – more than double of that in ULSD#2. In addition, 2D GCMS analysis of [13] showed that FD9A has high amounts of C_8–C_{10} alkylbenzenes which constitute to about 75% of the total alkylbenzenes. It is also observed that ULSD#2 consists of higher