



Full Length Article

Ignition delay times for jet and diesel fuels: Constant volume spray and gas-phase shock tube measurements



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ABSTRACT

Ignition delay times for conventional and alternative jet and diesel fuels were measured in a constant volume spray combustion chamber and a shock tube in homogenous gas-phase reflected shock experiments. Experiments were performed in the spray environment for injection of liquid fuel sprays into hot air at 1.0, 2.14, and 4.0 MPa and 620–830 K. Shock tube experiments were performed for homogenous stoichiometric fuel/air mixtures at pressures around 2, 4, and 8 MPa and for 660–1310 K. These experiments characterize relative fuel reactivity, the dependence of reactivity on temperature and pressure, and allow for correlation of reactivity under spray and homogenous gas-phase conditions. Important results include the observation of three temperature regimes for reactivity in the shock tube experiments: high- and low-temperature regimes with positive overall activation energy connected by a negative-temperature-coefficient (NTC) regime. While increasing pressure was shown to result in decreasing ignition delay in all regimes, pressure was shown to have an appreciably larger influence in the NTC regime. Spray ignition experiments exhibited decreasing temperature dependence with increasing temperature from the low-temperature regime towards the entrance to the NTC. Fuel reactivity trends from spray ignition experiments, quantified using the derived cetane number (DCN), were found to correlate via a power law relationship with ignition delay times measured in the shock tube at NTC conditions, suggesting that DCN is primarily sensitive to NTC gas-phase chemical kinetic reactivity. The extensive experimental database reported here for jet and diesel fuels at high-pressure engine-like combustion conditions should be valuable for the future development of real fuel chemical kinetic modeling.

1. Introduction

Approximately 80–85% of the world's energy is generated (or transformed) in combustion-based systems [1] and the transportation sector is predominantly powered by the combustion of liquid fuels. Transportation engines are mostly either reciprocating internal combustion engines (ICEs) or gas turbines that today operate with either increasing compression or pressure ratios to maximize thermal efficiency. Many new high-efficiency concepts for both gas turbines and ICEs rely on some operation within the low temperature combustion (LTC) regime, placing an increased importance on low-temperature fuel reactivity, known to be highly dependent on fuel composition [2,3]. One global chemical kinetic fuel property of importance for ICEs and gas turbine operation is the propensity for fuels to autoignite under both premixed and non-premixed conditions. Global reactivity measurements, such as measures of ignition delay time, allow for both fuel screening and fuel design (new fuels or blends) and provide modeling targets for chemical kinetics models and computational fluid dynamics

(CFD) combustion simulations ultimately used for engine design optimization.

The ignition delay time, a time delay between the initiation of a combustion process and the first energy release, is a classic measure of fuel reactivity. The ignition delay time can be measured in a number of systems, including homogenous systems where chemical reaction is initiated by a change in temperature (e.g., shock tube), spray systems where chemical reaction is initiated by injection of a fuel spray into an oxidizer, or directly in engines where chemical reaction is initiated by piston compression. Measurements of ignition delay times have been used to define reactivity metrics, such as research and motor octane numbers (RON and MON), cetane number (CN), and derived cetane number (DCN).

The reactivity of diesel fuels is generally described using the cetane number (CN) and/or derived cetane number (DCN), where the ignition quality of the fuel directly influences the time or crank-angle dependent pressure within the chamber of a compression ignition engine and can strongly influence performance (efficiency, emissions, knocking, engine

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wear, etc.) [4]. The CN is determined through measurements made in a Cooperative Fuel Research (CFR) engine [5], a single-cylinder engine with variable compression ratio, where CN is defined by the critical compression ratio for autoignition. DCN is determined through measurements performed in either an Ignition Quality Tester (IQT) [6] or a Fuel Ignition Tester (FIT) [6]. Both the IQT and FIT are compact combustion spray chambers. They consist of a constant volume combustion chamber (CVCC) with an injection nozzle embedded at one wall. Fuel is injected into the heated and compressed gas within the chamber. Pressure sensors provide ignition delay determination. Both IQT and FIT are conceptually the same with different geometries and injectors. The IQT has shorter testing times, higher repeatability and sensitivity, as well as allows DCN measurement with smaller volumes of fuel. Here we describe DCN measurements made in a custom constant volume spray combustion chamber at Rensselaer. This device is similar to the IQT and FIT but has the advantage of by having a larger chamber volume and, therefore, minimizes wall effects.

Petroleum jet and diesel fuels are generally similar in terms of the distribution of organic classes, containing mostly *n*-, *iso*-, and *cyclo*-alkanes and aromatics. They are also similar in terms of overall reactivity but with diesel fuels containing on average heavier hydrocarbons and, therefore, having slightly different physical properties (e.g., higher density and viscosity). Jet fuels have standards established by the U.S. Air Force and Federal Aviation Administration (FAA) that require jet fuels to exhibit traits that maximize performance of the jet engines in which they are designed to operate within [7]. For example, there are several different types of jet fuel (e.g., Jet A, JP-8, JP-5, JP-10) depending on application, be it operating in cold climates or low flammability for fueling on aircraft carriers. The most important performance characteristics of a jet fuel are its heat of combustion, volatility, lubricity, stability, and corrosivity [7,8]. Of note however, is that jet fuel specifications do not include a reactivity metric (e.g., CN or DCN) and chemical reactivity is known to vary between jet fuel types and even batch-to-batch within a given jet fuel type. Diesel fuels on the other hand are rated for reactivity, through CN and/or DCN.

Due to the environmental impact of petroleum fuels and a desire for diversified fuel sources, non-petroleum alternatives have been researched extensively. Those fuels have been classified according to their source, synthesis method, and chemical composition. Many alternative fuels that have been developed in recent decades are oxygenated hydrocarbons that are unsuitable for aviation and military use due to their reduced energy density (e.g., alcohols or esters). However, pure hydrocarbon alternative fuels have been generated using a number of methods, including Fischer Tropsch [9], hydroprocessing [10], alcohol-hydrocarbon, and synthetic biological [11] pathways.

In the present study, the ignition quality of a range of six petroleum and four alternative (Fischer Tropsch and hydroprocessed) jet and diesel fuels has been experimentally studied. Experiments have been completed in spray and homogenous ignition environments under ICE and gas turbine conditions for the determination of ignition delay and DCN. Finally, relationships between DCN and ignition delay under various conditions are examined. These data provide a deep database for the consideration of fuel reactivity variability and for future modeling efforts and builds on prior work on the ignition of petroleum and alternative jet and diesel fuel ignition reported in recent years.

Important previous experimental works on the autoignition of real jet fuels include shock tube studies of Dean et al. [12], the first to report homogenous shock tube ignition delay times for Jet A with measurements at modest pressures (0.85 MPa) and high temperature conditions (1000–1700 K), and Vasu et al. [13] who next reported shock tube measurements for Jet A and JP-8 at higher pressure (1.7–5 MPa) and conditions that span low- to high-temperature regimes (715–1229 K). Kahandawala et al. [14] measured ignition delay times for mixtures of JP-8/O₂ dilute in argon baths near 2 MPa and at high temperatures (1100–1600 K). Our group followed with a number of shock tube studies [15–19] greatly extending the range of fuels considered to new

conventional and alternative jet and diesel fuels with the focus on quantifying the influence of fuel composition, fuel/oxidizer mixture composition, and thermodynamic conditions from high- to low-temperature combustion conditions and at high pressures.

Most recently, Valco et al. [20] has reported ignition delay time measurements carried out in a rapid compression machine for Category A U.S. Air Force jet fuels at low temperature conditions: 625–735 K and 2 MPa. Similarly, Davidson et al. [21] reported shock tube ignition measures for the same fuels at 700–1250 K and 1.2 MPa. The Category A jet fuels [7] are controlled and well characterized petroleum jet fuel samples that represent low, average, and high reactivity jet fuels. Here we expand on the previous work for both jet and diesel fuels by considering a broad range of fuels with reactivity differences, including the Category A jet fuels. We consider extreme pressure conditions (up to 8 MPa) and also compare and correlate ignition measurements made in multiphase spray and homogenous gas-phase environments to examine the potential of using DCN to describe the gas-phase reactivity as measured in shock tube ignition experiments.

2. Experimental methods

Spray ignition experiments were performed in the Rensselaer constant volume spray combustion chamber (CVSCC) previously described by Tekawade and Oehlschlaeger [22–24]. In prior studies the CVSCC has been shown to agree well with IQT measurements for temperature-dependent spray ignition delay times [22] and also provide determinations of DCN [23,24] within the repeatability limits of both the IQT and FIT.

The CVSCC is an enclosed cylindrical chamber with an internal volume of 500 mL (7.6 cm in diameter and 11 cm in height) that allows the measurement of spray ignition delay times at ambient pressures from 0.1 to 5 MPa and ambient temperatures up to 850 K. Spray ignition delay experiments are carried out by electrically heating the chamber to a desired temperature and pressurizing the chamber with medical grade air (dry air: 21% O₂ and 79% N₂). A mechanical pintle-style fuel injector actuated with an electric solenoid valve provides a controlled fuel spray injected with specified duration into the chamber. The liquid fuel spray evaporates, mixes with the heated air, and ignites, allowing for the observation of a spray ignition delay time, defined as the time interval between start of injection and start of combustion. The fuel injection and chamber pressure are monitored using high-speed pressure transducers (Kistler Model 6041A) providing determination of the start of injection (SOI), end of injection (EOI), and start of combustion (SOC). Fig. 1 illustrates an example experiment.

In the present study the duration of fuel injection was held constant at 6.5 ± 0.5 ms for an injection pressure of 15.2 MPa. The SOI and EOI are determined from characteristic features of the fuel injection pressure that have been previously determined to coincide with injector needle lift and closure based on correlation of the measured injection pressure with high-speed images of the spray injection [22]. The SOI is defined by an inflection in the injection pressure that corresponds to needle lift (i.e., needle lift relieves upstream fuel pressure) and the EOI is defined via a minimum in injection pressure that corresponds with needle return/closure (i.e., closure stops injector pressure drop). After a time delay following SOI, the measured chamber pressure rises due to the onset of ignition and combustion. The time of SOC is defined using the first peak in the rate of heat release (RHR), based on the first derivative in chamber pressure (dP/dt):

$$RHR = \frac{V_{chamber}}{\gamma - 1} \frac{dP}{dt}$$

where $V_{chamber}$ is the volume of the chamber and γ the specific heat ratio. The oscillation in pressure following ignition in Fig. 1 is caused by the reflection of a pressure wave within the cylindrical CVSCC following local ignition, similar to pressure oscillations associated with knock in internal combustion engines.

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