



Full Length Article

An experimental study of the spray ignition of alkanes



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ABSTRACT

Spray ignition experiments were carried out in a constant volume spray combustion chamber (CVSCC) for determination of first-stage and total ignition delay times for pure alkane fuel components in air at 650–825 K and 1–4 MPa, providing insight into their oxidative reactivity under spray combustion conditions. Experiments for *n*-alkanes (heptane, decane, dodecane, and hexadecane) illustrate strong single-stage ignition at pressures of 2.14 and 4.0 MPa and two-stage ignition at pressures of 1.0 MPa. The total ignition delay for *n*-alkanes was found to decrease with increasing chain length according to $\tau \propto \text{carbon number}^{-0.7}$. Highly branched alkanes, iso-octane and iso-cetane, were found to have very distinct two stage ignition where the ratio of the time scales of total ignition to first-stage ignition delay ranges from approximately two to three. The lightly branched 2,6,10-trimethyldodecane was found to behave similarly to *n*-alkanes with reactivity between *n*-heptane and *n*-decane, indicating that *n*-alkanes suitably emulate the spray ignition behavior of lightly branched alkanes for engineering experiments or predictions. Cycloalkanes, cyclohexane and methylcyclohexane, were found to have long total ignition delay times, of the order of the highly branched alkanes, but to ignite in a single stage. All ignition delay times were found to decrease with increasing temperature and pressure, with reduction in overall activation energy at temperatures around 750–825 K indicative of the influence of competition between chain branching and propagation that occurs at the low-temperature onset to the negative-temperature-coefficient regime. Comparisons between the results from the CVSCC and those from the Ignition Quality Tester (IQT) show good correlation for fuels with nearly single-stage ignition. However, this is not the case for fuels with strong two-stage ignition behavior, where ignition delay determinations are shown to be sensitive to the definition of ignition delay and experimental parameters.

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1. Introduction

Fuel reactivity is a key consideration in the design and analysis of combustion engines as it influences the rate of heat release and thereby engine efficiency, power density, and emissions. A number of fundamental experimental configurations have been historically used to probe gas-phase fuel reactivity including shock tubes, rapid compression machines (RCM), laminar flames, jet-stirred reactors, and flow reactors. Results from these experiments have provided insight into fuel oxidation kinetics and validation targets for kinetic models. Spray ignition experiments have also been used for characterizing the reactivity of fuels at low-temperature conditions important in advanced internal combustion engine strategies [1–3] and have been carried out in constant volume enclosures [4–14], pressurized steady-flow devices [15,16], RCMs [17,18], shock tubes [19], and engines [20,21] with varying heating, fuel injection, and

other experimental strategies. Externally-heated constant volume enclosures, electrically heated or otherwise, have the advantage of purely quiescent ambient conditions not obtainable in flow devices, RCMs, shock tubes, or engines. Additionally, externally-heated and constant volume enclosure avoid the added complication of the pre-combustion of a high-oxygen-concentration charge to provide the desired high temperature and pressure ambient conditions [12,14]. For these reasons and their simple operation, commercialized externally-heated constant volume devices have been developed for the measurement of the Derived Cetane Number (DCN), a reference parameter for comparing fuel reactivity, that can be measured using standardized ASTM methods in the Ignition Quality Tester (IQT) [3–7] and Fuel Ignition Tester (FIT) [8] devices. The establishment of fuel reactivity specifications for Low Temperature Combustion (LTC) strategies has been somewhat addressed by experiments performed in constant volume spray experiments [9–11]; however, while the IQT and FIT devices provide precise DCN measurements for moderate- to high-reactivity fuels (e.g., diesel and jet fuel), the established DCN measurements can deviate for

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low reactivity fuels [22,23] where slow and often two-stage spray ignition processes creates a challenges for appropriately defining ignition delay.

In addition to the definition of the DCN reference for fuel reactivity, constant volume spray combustion experiments have allowed for the exploration of fuel reactivity under a range of thermodynamic conditions of interest within the low-temperature chemistry regime [24–27]. These experiments have been modeled with computational fluid dynamics (CFD) simulations containing reduced chemical kinetic models and have been used to explore the importance of spray physics, evaporation, mixing, and chemistry in spray ignition and combustion [24,26]. In some cases, where ignition delay times are very long and spray breakup, evaporation, and mixing phenomena are fast relative to chemistry, results from spray ignition experiments show reasonable correlation with ignition in homogenous systems [24–26].

The objective of the present work is to: (1) provide a wide-ranging database for spray ignition delay times for alkanes; (2) characterize the influence of alkane structure and thermodynamic conditions on spray ignition; (3) investigate the relative magnitude of first-stage heat release during spray combustion, not captured by DCN measurements, for a variety of pure alkanes; and (4) to provide targets for CFD-based studies of fuel spray reactivity. Spray ignition experiments are reported for the ignition of alkane compounds found in transportation fuels following their injection into air at temperatures from 650 to 825 K and elevated pressures (1–4 MPa). First-stage and total ignition delays, typically with $\pm 5\%$ precision, were measured in a constant volume spray combustion chamber (CVSCC). The fuels chosen for this study are pure normal, branched, and cyclic alkanes providing a variety of molecular structures that exist in real fuels [28] and exhibiting a range of reactivity and two-stage ignition behavior. Comparisons are also made with results from the IQT device and kinetic modeling calculations performed under homogenous constant volume conditions.

2. Experimental method

2.1. Constant volume spray combustion chamber

Experiments were carried out in a constant volume spray combustion chamber (CVSCC), see Fig. 1 for a schematic. The CVSCC is a cylindrical chamber with an internal diameter of 7.6 cm and internal length of 11 cm (volume of 500 mL). It can operate at initial conditions of up to 850 K and 5 MPa. A fuel injector is mounted in the top wall of the chamber such that the tip is flush with the inner wall. The bottom wall has an inlet and exhaust port for supplying a pressurized oxidizing mixture (air in this study) and discharging exhaust products from the chamber after combustion via high pressure tubing and valves. The bottom wall of the CVSCC also has a mounted pressure transducer and thermocouple. The CVSCC is externally heated using electrical resistance heaters.

The injector is a mechanical pintle-style diesel injector manufactured by Bosch (model W0133-1827210, shown in Fig. 2). When sufficient pressure is supplied to the injector, the injector pintle (needle) lifts and fuel is injected through an annulus formed by the nozzle orifice (1 mm in diameter) and pintle (0.5 mm in diameter at the tip). The injector provides lower pressure injection typical of gasoline direct injection systems but much lower than modern common-rail diesel engine injection systems. The present systems allows the use of much smaller fuel samples, as little as 50 mL, than common-rail systems, where samples of the order of a liter are required for circulation within the high-pressure fuel delivery systems. Additionally, longer ignition delay times (in excess of 2–3 ms), as mostly observed here, are typically chemistry limited with physical effects, dependent on injection pressure, less of controlling factor.

The stock injector has two leak-off ports designed to release extra fuel from the injector after it closes. The injector was modified to minimize the backflow of fuel and these ports were connected to

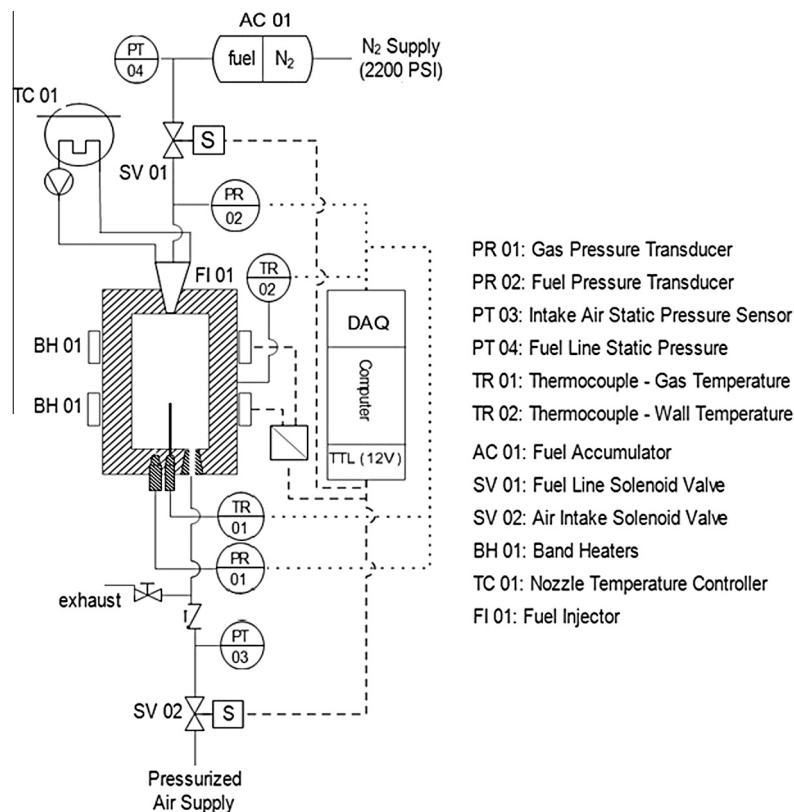


Fig. 1. Schematic of CVSCC. The injector (FI 01), located on the top of the chamber, injects fuel vertically downward.

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