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Laminar burning velocities at elevated pressures for gasoline and gasoline surrogates associated with RON

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ABSTRACT

The development and validation of a new gasoline surrogate using laminar flame speed as a target parameter is presented. Laminar burning velocities were measured using a constant-volume spherical vessel with ignition at the center of the vessel. Tested fuels included *iso*-octane, *n*-heptane, toluene, various mixtures of primary reference fuels (PRFs) and toluene reference fuels (TRFs) and three gasoline fuels of 70, 85 and 95 RON (FACE J, C and F) at the initial temperature of 358 K and pressures up to 0.6 MPa in the equivalence ratio ranging from 0.8 to 1.6. Normalized laminar burning velocity data were mapped into a tri-component mixture space at different experimental conditions to allocate different gasoline surrogates for different gasoline fuels, having RON of 70, 85 and 95. The surrogates of TRF-70-4 (17.94% *iso*-C_8H_{18} + 42.06% *n*-C_7H_{16} + 40% C_7H_8), TRF-85-1 (77.4% *iso*-C_8H_{18} + 17.6% *n*-C_7H_{16} + 5% C_7H_8), and TRF-95-1 (88.47% *iso*-C_8H_{18} + 6.53% *n*-C_7H_{16} + 5% C_7H_8) of RON 70, 85 and 95, respectively, are shown to successfully emulate the burning rate characteristics of the gasoline fuels associated with these RONs under the various experimental conditions investigated. An empirical correlation was derived to obtain laminar burning velocities at pressures that are experimentally unattainable as high as 3.0 MPa. Laminar burning velocities were comparable to the simulated values for lean and stoichiometric flames but they were relatively higher than the simulated values for rich flames. A flame instability assessment was conducted by determining Markstein length, critical Pecklet number, and critical Karlovitz number at the onset of flame instability.

1. Introduction

The production of efficient and less polluting internal combustion engines (ICEs) necessitates an understanding of the influence of fuel properties in ICEs. Typical refinery gasoline consists of hundreds of hydrocarbons that complicate its experimental and numerical investigation. It is often desirable to formulate a surrogate fuel to reduce the chemical and/or physical complexity of a real fuel to gain more insight and understanding of the underlying fundamental physics and chemistry [1]. Recent progress in formulating appropriate gasoline surrogate compositions has been reported in [2].

These surrogates, ranging from single to multi-components, are intended for specific targets. Single-component surrogates may be adequate for simple applications such as assessing combustion efficiency [3]; *e.g.*, *iso*-octane represents the simplest surrogate for gasoline fuel. Binary blends of primary reference fuels (PRFs) (*e.g.*, mixtures of *iso*-octane and *n*-heptane) have been widely adopted as convenient surrogates in investigating the role of research octane number (RON) [2–4]. However, multi-component surrogate mixtures are required for applications dependent upon fuel chemistry such as emission and soot formation [2], applications involving special types of flames such as lean premixed flames [5], or for building robust chemistry models of gasoline fuels. In this regard, developing a surrogate mixture with a small number of fuel components to represent full blend gasoline in terms of laminar combustion characteristics is a major challenge.

With the increasing range of possible suitable fuels and their blends for ICEs, it is necessary to specify associated laminar combustion characteristics, over the full range of equivalence ratios and initial pressure and temperature [6]. Many experimental and numerical studies have been conducted to determine the flame propagation characteristics of the individual components of gasoline surrogates [7–11]. Laminar burning velocities of *n*-heptane, *iso*-octane and toluene and various PRF mixtures have been measured at atmospheric pressure [7–12]. Bradley et al. [13] reported laminar burning velocities and Markstein lengths for *iso*-octane/air and *n*-heptane/*iso*-octane/air mixtures up to 1.0 MPa.

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Jerzembeck et al. [14] presented experimentally similar laminar flame characteristics at engine-relevant conditions for PRF (RON 84) and gasoline. Van Lipzig et al. [15] using a perforated plate burner reported measurements of the adiabatic laminar burning velocities of *n*-heptane, *iso*-octane, ethanol and blends of their binary and tertiary mixtures. Also, using the heat flux method, atmospheric measurements of un-stretched laminar burning velocities of a tertiary mixture of TRF fuel in an attempt to capture a commercial gasoline characteristics in terms of matching the flame speed were reported in [16]. Toluene reference fuels (TRFs)-ternary mixtures of toluene, *n*-heptane and *iso*-octane are proposed as surrogates to emulate refinery gasoline fuels [17,18]. However, there still scarcity in terms of reporting laminar burning velocity particularly at elevated pressure for appropriate tertiary gasoline surrogate fuels.

Morgan et al. [17] presented a second order model to map ternary compositions of toluene, *n*-heptane and *iso*-octane into RON space. They found that a TRF fuel, blended according to this model to match the same RON of the refinery gasoline, yielded a similar heat release event and pressure profile to the gasoline. In the present study, Morgan's model was used as a cornerstone to specify different TRFs that match the same RON of three different refinery gasoline fuels.

The objective of the present study is: first, to provide experimental laminar burning velocity data for neat fuels, various blends of PRFs and TRFs, and fuels for advanced combustion engines (FACE) gasolines; second, based on formulating different TRF mixtures, surrogate mixtures were tested to capture reasonable laminar combustion characteristics and matching the same RON of real gasoline fuels over a wide range of equivalence ratios and relatively high initial pressures. These characteristics determined by employing spherical flame configuration include flame speed, unstretched laminar burning velocity, Markstein number, and stretch rates at the onset of flame instabilities.

2. Experimental apparatus

A spherical stainless steel combustion vessel with 330 mm inner diameter (≈20 l) was designed and commissioned for laminar flame speed measurements. It has two orthogonal pairs of quartz windows with 120 mm in diameter and 50 mm in thickness, as schematically shown in Fig. 1, and is capable of withstanding the temperatures and pressures generated from deflagrations at initial pressures, P_0, of up to 0.7 MPa and initial temperatures, T_0, of up to 400 K. The vessel can accommodate both liquid and gaseous fuels and/or their blends.

An electric heater (1 kW) located inside on the bottom flange was used to heat the vessel and mixtures up to 400 K. The initial gas temperature was measured by two Chromel–Alumel thermocouples (sheathed with 1.5 mm diameter stainless steel tube) at two locations inside the vessel to assure thermal homogeneity of the mixture. One of the thermocouples was located near the optical central region to minimize the thermal effect from the vessel wall. The initial temperature of the mixture was monitored during a mixture preparation by a temperature controller. To improve the homogeneity of the mixture, a rotating fan was located inside the vessel at the top flange, which was driven by a magnet-electric motor. The convective heat transfer process was enhanced by the turbulence generated from this fan which assured temperature uniformity throughout the vessel as well as improving the liquid fuel evaporation rate.

Reactants were prepared in the combustion vessel using the partial pressure method, assuming an ideal gas model. The amount of injected liquid fuel was calculated from the partial pressure and fuel density. A liquid fuel was injected with calibrated gas-tight micro-syringes (5, 10 and 50 cm^3) using a needle valve under vacuum pressure of approximately 0.001 MPa then dry air composed of 20.947% O_2 and 78.084% N_2, 0.9% argon and the remaining 0.1% made up of carbon dioxide, helium, neon, and hydrogen on a molar basis was introduced according to initial conditions (ϕ, P_0, T_0), where ϕ is the equivalence ratio. Prior to filling the vessel, it was evacuated up to 0.001 MPa and purged with nitrogen to remove combustion products.

A pressure transducer (Keller; PAA-33X) monitored the partial pressure of reactants during mixture preparation as well as initial pressure before ignition. A second pressure transducer (Kistler; 6045A) captured pressure variations during flame propagation. A spark plug with two electrodes arranged in V-shape configuration to form a 1 mm gap was located at the center of the vessel. Ignition energy was supplied by a high voltage power supply (TREK; 40/15-H-CE), which was controlled by a function generator (Tektronix; AFG3021B). It was approximately 24 mJ based on the current and voltage measurement and integrated over spark duration.

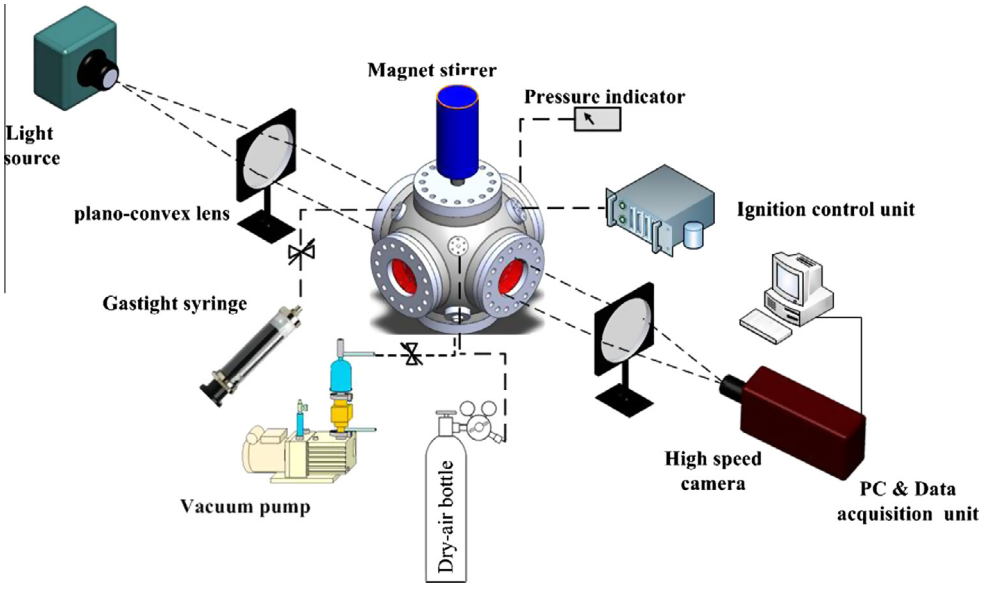

Fig. 1. Schematic of the experimental setup for the optical spherical combustion vessel.