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Experimental investigations of the influence of pressure on critical extinction conditions of laminar nonpremixed flames burning condensed hydrocarbon fuels, jet fuels, and surrogates

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Abstract

Critical conditions of extinction are measured for high molecular weight hydrocarbon fuels, jet fuels and surrogates at pressures up to 0.4 MPa. The hydrocarbon fuels tested are *n*-heptane, cyclohexane, *n*-octane, iso-octane, and *n*-decane. Jet fuels tested include JP-8 and Jet-A. The surrogates tested are the Aachen surrogate, consisting of 80% *n*-decane and 20% 1,3,5-trimethylbenzene by mass, and the 2nd generation POSF 4658 Princeton surrogate consisting of 49.6% *n*-dodecane, 24.3% iso-octane, 19.8% *n*-propylbenzene, and 6.3% 1,3,5-trimethylbenzene by mass. The counterflow, condensed-fuel configuration is employed. Air diluted with nitrogen at 298 K is injected onto the surface of a pool of heptane. The mass fraction of oxygen in the oxidizer stream is represented by $Y_{O_2,2}$. A flame is stabilized in the stagnation point boundary layer that is established above the liquid–gas interface. At a selected value of pressure p, and at a selected value of $Y_{O_2,2}$, the flow velocity of the oxidizer stream is increased until extinction takes place. The strain rate at extinction is calculated. The experiment is repeated for a range of pressures. The general ordering of extinction strain rates of hydrocarbon fuels was observed and found to be in general agreement with the predictions of kinetic models and experiments conducted at atmospheric pressure in earlier experiments and computations. An initial linear increase of extinction strain rate with pressure is observed at pressures up to 0.175 MPa, followed by a general flattening of the curves up to 0.35 MPa. At pressures above 0.35 MPa, extinction strain rates of some fuels begin to decrease with increased pressures. These general trends are consistent with results previously measured for *n*-heptane, *n*-hexane, and *n*-decane flames in a similar configuration.

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1. Introduction

Numerous experimental, computational and analytical studies have addressed combustion of

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various hydrocarbon fuels, hydrogen, and carbon monoxide at elevated pressures [1–11]. These studies include combustion in shock tubes and flow reactors [5–7,12,13] and counterflow nonpremixed flames [1,2,7,10,11], and have illuminated the influence of pressure on combustion. Some studies have provided critical conditions of extinction of methane and ethane flames [8–11]. There are, however, very few studies of extinction of high molecular weight hydrocarbon fuels in nonuniform flows at high pressure, with the exception of the early pioneering studies described in [1,2]. In the present work critical conditions of extinction are measured for nonpremixed combustion of various condensed hydrocarbon fuels, jet fuels, and surrogates at moderate pressure. The counterflow configuration is employed.

Two types of counterflow configurations—the vaporized fuel configuration and the condensed fuel configuration have been employed in previous studies on hydrocarbon fuels that are liquids at room temperature and pressure [14–17]. In the vaporized fuel configuration, liquid fuel is first vaporized and then introduced into the counterflow burner. In the condensed fuel configuration a gaseous oxidizing stream flows over the vaporizing surface of a liquid fuel. This configuration was employed in many previous studies at 1 atm [18–22], and at moderate pressures [1,2]. This configuration is employed in the present work. The condensed fuel configuration is particularly useful for experimental studies on those fuels that have high boiling temperatures where vaporization with negligible thermal breakdown is difficult to achieve. For *n*-decane, for example, the normal boiling point is greater than 500 K at a pressure of 5 bar. As a consequence, there is an increased risk of thermal breakdown of *n*-decane if the pressure exceeds 5 bar. Therefore the condensed fuel configuration is desirable for studies on high molecular hydrocarbon fuels at elevated pressures. Studies in the condensed fuel configuration closely resemble combustion of single fuel droplets. This is another reason for the selection of this configuration for the present study.

Niioka et al. [1] and Hiraiwa [2] measured critical conditions of extinction for *n*-heptane employing the condensed fuel configuration. In their experiments the liquid fuel was introduced into a cup. The surface of the fuel was maintained at the top of a porous plate placed on the cup to prevent liquid fuel from overflowing. Fuels tested include *n*-hexane, *n*-heptane, and *n*-decane. Air with different levels of dilution with nitrogen were considered. The strain rate at extinction was measured as a function of the pressure up to 3 MPa. A key finding of their studies is that at values of pressure close to atmospheric pressure, there is at first a linear increase in extinction strain rate with increasing pressure. At higher pressures and at high levels of dilution of air with nitrogen, the strain rate at extinction changes very little with increasing pressure [1,2]. If the air is not diluted, the strain rate at extinction first increases and then decreases [2]. A noteworthy feature of the work of Niioka et al. [1] is that by use of rigorous activation energy asymptotic analysis, a clear relation is made between the extinction strain rate measured in the condensed fuel configuration and extinction diameter of burning droplets, thus establishing the practical relevance of their studies. In the present study, critical conditions of extinction are measured for *n*-heptane, *n*-octane, iso-octane, *n*-decane, and cyclohexane.

The present study will also include measurements of critical conditions of extinction for jet fuels and surrogates of jet fuels. The motivation for this arises from a need to model combustion of practical fuels at high pressures. Commercial fuels, including jet fuels, kerosene, gasoline, and diesel, are composed of hundreds of aliphatic and aromatic hydrocarbon compounds. The major components of real jet fuels are straight-chain alkanes, branched-chain alkanes, cycloalkanes, aromatics, and alkenes [3,23–26]. On average, the composition by volume is approximately 60% alkanes, 20% cycloalkanes, 18% aromatics, and 2% alkenes [26]. Efforts to develop chemical-kinetic models that accurately describe the combustion of these practical fuels are critical to the development and the advancement of next-generation engines and power plants. However, due to the hundreds of chemical species found in practical fuels and the significant variation in the chemical composition between batches of fuel, the task of quantitatively studying and modeling them is both numerically and experimentally challenging. For this reason, studies on the combustion of jet fuels are often carried out using surrogates. Surrogate mixtures have only a handful of components, but are designed to simulate the most essential characteristics of real fuels. The fuels tested in the present work have been identified as possible components of surrogates [3,27,23,28].

The surrogates to be tested in the present work are the Aachen surrogate made up of *n*-decane (80 %) and trimethylbenzene (20 %) by weight, and the 2nd generation POSF 4658 surrogate developed by Dooley, et al. [29]. In a previous study [17], several batches of JP-8 and Jet-A, and fifteen possible surrogates of jet fuels were tested in nonpremixed systems at pressure of 1 atm. In this study [17] and other studies at 1 atm [14,15,30] the Aachen surrogate and a surrogate made up of *n*-dodecane (57 %), methylcyclohexane (21 %), and *o*-xylene (22 %), by weight, called Surrogate C were found to reproduce key aspects of nonpremixed [14,15,17] and premixed [30] combustion of JP-8. The Aachen Surrogate was found to be the best in reproducing critical conditions of autoignition of jet fuels, but not necessarily extinction, where a slightly

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