Low Temperature Oxidation of Hexane with In-Situ Fuel and Oxygen Concentration Measurements

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1 Introduction and Experimental Setup

The autoignition temperature is an important characteristic of fuels for safety concerns. While a standard test for the autoignition temperature the ASTME659-78 exists, only the minimum temperature for ignition at atmospheric pressure is investigated. The specific mixture composition is not being controlled since the liquid test fuel is injected into an open vessel, which has been heated to a test temperature. The fuel air mixture is not actively mixed, but it is expected that "a considerable range of compositions exit within pockets of gas in the vessel as evaporation of liquid fuel, or mixing of the injected gaseous fuel, occurs" [2].

The main concern for the commercial aviation industry is the ignition of fuel in the fuel tank or surrounding flammable leakage zones due to heated elements such as pipes carrying hot gas. Ignition may occur at any altitude and therefore a range of pressure and compositions needs to be investigated. Additionally, a better understanding of the applicability of the 225°C auto-ignition temperature for kerosene is sought.



Figure 1: Constant volume combustion vessel with a total volume of 400 mL and an optical path of 3.5 in.

nature of the ignition event. While other research groups have taken the appearance of any flame as a criterion for ignition [1], in this study the fuel and oxidizer concentration time history during the combustion event is obtained.
Past experiments have taken small samples

Time-resolved concentration measurements of

the fuel and oxidizer will provide insight into the

throughout the combustion event, which were then analyzed by a gas chromatograph. While this technique allows for a more comprehensive study of the composition, the techniques presented here are non-instrusive and have a measurement rate

of up to 300 Hz. In experiments performed by Wilk et al. [4] samples were taken every 10 to 30 seconds. They investigated propane [4] and propene [5].

In the present study the concentration of fuel was obtained using laser absorption at 3.39 microns. The wavelength, which corresponds to the C-H bond resonance was provided by a He-Ne laser. The ratio of the observed intensity to the intensity without any fuel present is related to the fuel concentration by Beers law, where the absorption cross-section is calibrated before heating the vessel.

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The oxygen concentration is measured by using 2f detection across an electronic transition spectral line near 763 nm. The tunable diode laser is modulated and swept across the absorption feature so that the peak of the second harmonic, which is related to the partial pressure of oxygen, is measured [3].

In the next series of experiment the light emission from the combustion will be recorded using a photodiode between 400nm to 600nm, to avoid the light emitted from the lasers. The main goal is to identify the appearance of cool flames and correlate the composition changes to these cool flames.

The experimental configuration used includes a closed glass vessel encased in an aluminum shell that is heated to the desired temperature, measured inside the glass vessel with a thermocouple covered in an inert coating. The test cell is a cylindrical vessel with windows mounted on the sides as shown in Figure 1 (diameter 2 in., length 8.3 in., and volume 400 mL). This vessel is embedded in a heating block driven by 800W heaters given temperature ramp of up to 15° C/min. The vessel is filled using the method of partial pressure and temperature data is taken with a K-type thermocouple coated in silica.

2 Autoginition Experiments

The initial tests performed used a stoichiometric mixture of hexane and air at pressures 200, 500, and 760 Torr. Hexane was chosen as a surrogate fuel for kerosene, because both fuels have an autoignition temperature of 225°C [1]. Using hexane gives a more controllable experiment than a commodity multi-component fuel like kerosene.

The following tests are done with a stoichiometric (2.16%) hexane-air mixture. The heater gives a linear ramp from room temperature to 300°C over 20 minutes. The low pressure experiment at 200 Torr (see Figure 2) shows slow reaction without any pressure rise, while the high pressure case (see Figure 3) shows an explosive reaction with a rapid drop in the fuel concentration present. Additionally, all of the fuel is consumed in the high pressure case, while some residual fuel remains in the low-pressure case (the heating is terminated once the ignition transient occurs).



Figure 2: Stoichiometric hexane-air mixture at 200 Torr total pressure reacting over 150 seconds without any detectable ignition-related pressure rise.



Figure 3: Stoichiometric hexane-air mixture at 760 Torr total pressure explosively reacting with a rapid pressure rise to a peak value of 2100 Torr.

In the auto-ignition process, significant reaction does not take place until the autoignition temperature is reached and explosive reaction occurs only at high pressure and fast heating rates. Future test will be performed over a range of test pressures, equivalence ratios, and heating rates.

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