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Low-temperature ignition behavior of iso-octane

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HIGHLIGHTS

- Auto-ignition properties of air-dilute iso-octane investigated at low temperatures.
- Homogeneous and inhomogeneous behaviors observed, strong ignition limits identified.
- Sankaran Criterion accurately predicts location of strong ignition limit *a priori*.
- Measured ignition delay times compared to zero-dimensional model predictions.
- Accuracy of predictions affected by ignition behavior for $\varphi = 1.0$, but not $\varphi = 0.25$.

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ABSTRACT

Auto-ignition properties of iso-octane mixtures were systematically investigated at conditions relevant to practical combustion devices using the University of Michigan Rapid Compression Facility and the Tsinghua University Rapid Compression Machine. Pressure time history measurements and high-speed imaging of the ignition process were used in both facilities to determine auto-ignition delay times and directly observe physical ignition behaviors. Test mixtures used fuel-to-O_2 equivalence ratios of $\varphi = 0.25$ and 1.0, and were air-dilute, i.e. molar O_2 to diluent gas (N_2, Ar) ratio of 1:3.76. The pressures and temperatures after compression ranged from 3 to 30 atm and 740–1125 K respectively. The comprehensive results of the present work combined with those from previous shocktube studies clearly illustrate the existence of both inhomogeneous and homogeneous auto-ignition behaviors at these conditions. Analysis of patterns in the ignition behaviors revealed a dependence on initial unburned temperature and pressure, as well as equivalence ratio, with distinct regions of thermodynamic state in which the behavior is consistent and repeatable. The strong ignition limits were identified for both φ using the experimental results and compared to predicted locations made using the Sankaran Criterion (the ratio of the laminar flame speed to the thermal gradient driven spontaneous propagation speed). Predictions made using an assumed thermal gradient of 5–10 K/mm were in excellent agreement with measurements at all conditions, clearly indicating that use of this criterion is an effective method for *a priori* prediction of auto-ignition behaviors for iso-octane. This validation of the Sankaran Criterion for iso-octane, an important reference hydrocarbon fuel, importantly broadens the use of this tool and is an indication that ignition processes in hydrocarbon and high hydrogen content fuels are fundamentally similar. Additionally, a comparison of the measured auto-ignition delay times to predictions made using zero-dimensional homogeneous reactor modeling revealed that for experiments with inhomogeneous ignition behaviors, agreement was dependent on φ and the auto-ignition delay time. The presence of inhomogeneous ignition behavior did not significantly affect the accuracy of auto-ignition delay time predictions for mixtures with $\varphi = 0.25$; whereas, for mixtures with $\varphi = 1.0$ the presence of inhomogeneous ignition behavior significantly reduced the accuracy of predictions if the auto-ignition delay time was greater than ~1 ms. These results indicate that while lowering φ may not eliminate inhomogeneous ignition behaviors, the subsequent effect of these behaviors on the predictive accuracy of typical zero-dimensional ignition modeling can be reduced or eliminated.

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1. Introduction

Low-temperature combustion strategies are used in both transportation and stationary power devices to decrease NO_x emissions and improve efficiency. Reductions in combustion temperature can be achieved using lean, pre-mixed, and/or dilute conditions, which present challenging stability, safety, and control issues. These difficulties stem in part from uncertainties in low-temperature chemistry as well as an increased instance and influence of abnormal ignition behaviors such as knock and misfiring in reciprocating engine systems or flashback and early ignition in gas turbine systems [1]. Therefore, successful application of low-temperature combustion strategies requires improved understanding of both low-temperature oxidation chemistry *and* chemically controlled ignition (auto-ignition) behaviors.

While the oxidation chemistry of iso-octane has been well studied, as indicated in Mehl et al. [2] and the references therein, only Fieweger et al. [3] and Vermeer and Oppenheim [4] have directly investigated the auto-ignition behaviors of iso-octane in a controlled and quiescent experimental apparatus. Vermeer and Oppenheim [4] employed optical techniques during auto-ignition measurements in a shocktube for air-dilute stoichiometric iso-octane, which revealed diverse auto-ignition characteristics at thermodynamic and mixture conditions relevant to practical combustion devices. These behaviors included homogeneous (spatially uniform emission or detonation wave) and inhomogeneous (localized reaction sites and deflagration) phenomena. Vermeer and Oppenheim further observed a clear transition between these auto-ignition behaviors at varying initial thermodynamic conditions, which they defined as the *strong ignition limit*. Fieweger et al. [3] expanded greatly on this work, classifying the auto-ignition behaviors of air-dilute stoichiometric iso-octane in a shocktube over a much broader range of initial temperatures, using pressure and CH emission time history characteristics. Consistent with the previous findings, Fieweger et al. [3] observed both homogeneous and inhomogeneous ignition behaviors and discovered a clearly defined strong ignition limit. The results of these studies are an important illustration that various auto-ignition behaviors are expected at conditions relevant to practical combustion devices using iso-octane, and that these generally repeatable behaviors are strongly related to initial unburned thermodynamic state.

The occurrence of similar auto-ignition behaviors and indeed a strong ignition limit at comparable thermodynamic conditions was reported previously by Meyer and Oppenheim [5] and Mansfield and Wooldridge [6] for air-dilute mixtures of hydrogen and syngas (hydrogen and carbon monoxide), respectively. Importantly, Mansfield and Wooldridge [6] discovered that a criterion first derived by Sankaran et al. [7] (Sankaran Criterion) could accurately predict the location of the strong ignition limit *a priori* using only basic flame and homogeneous reactor modeling. Remarkably, the criterion is a simple comparison of a thermal gradient driven propagation speed to the laminar flame speed. This predictive capability provided a new and unique tool that can be used in the design of combustion devices with high hydrogen content fuels, where auto-ignition behavior prediction and control is critical to performance and safety. Likewise, this ignition behavior criterion would be a valuable tool in the design of low-temperature combustion systems using iso-octane or other higher hydrocarbon fuels. Though its validity has not been evaluated for hydrocarbon fuels previous to the present work, the theoretical foundation of the ignition behavior criterion is not inherently fuel specific and a successful extension to non-hydrogen-based fuels is conceivable. Also highlighted in Mansfield and Wooldridge [6] were equivalence ratio dependent effects of ignition behavior on the accuracy of auto-ignition delay time predictions for syngas fuels made using typical zero-dimensional homogeneous modeling techniques. As auto-ignition delay time measurements were up to several orders of magnitude faster than predictions in cases with inhomogeneous ignition for syngas fuel, identifying and quantifying any effects for iso-octane is vital to its safe and effective use. This is especially important at low-temperature conditions where inhomogeneous behaviors are considerably more prevalent [3,4].

The objectives of the current study were first to evaluate the hypothesis that the Sankaran Criterion could be accurately applied to iso-octane fuel, and second to investigate the effects of auto-ignition behaviors on the predictive accuracy of basic auto-ignition delay time modeling for this fuel. These objectives were accomplished in part through new experimental studies of iso-octane auto-ignition behavior and auto-ignition delay times using the University of Michigan Rapid Compression Facility (UM-RCF) and the Tsinghua University Rapid Compression Machine (TU-RCM). The auto-ignition behavior results were combined with those from the shock tube studies of Fieweger et al. [3] and Vermeer and Oppenheim [4] to map auto-ignition behavior as a function of initial thermodynamic state and equivalence ratio. Using these maps, the strong ignition limit was identified for various equivalence ratios and the location of each limit was compared to predictions made using the Sankaran Criterion. Then the auto-ignition delay time measurements for all experiments were compared to predictions made using typical zero-dimensional homogeneous reactor modeling and the iso-octane oxidation mechanism of Mehl et al. [2] (referred to as the Mehl 2011 mechanism in the remainder of this paper).

2. Methods

2.1. Experimental

Ignition experiments were conducted using mixtures of iso-octane/air with molar fuel-to-O_2 equivalence ratios of $\varphi = 0.25$ and 1.0, at air levels of dilution, i.e. molar O_2-to-diluent gas ratio of 1:3.76. In the UM-RCF N_2 was the primary diluent, with small volumes of Ar and/or CO_2 added to modify the test temperature, and in the TU-RCM Ar was the primary diluent, with small volumes of N_2 added to modify the test temperature. In the UM-RCF, ignition experiments for $\varphi = 0.25$ were conducted between 3 and 20 atm for temperatures ~900–1125 K and experiments for $\varphi = 1.0$ were conducted at ~8 and 18 atm for temperatures ~830–975 K. In the TU-RCM, ignition experiments were conducted between at $\varphi = 0.25$ for 5–30 atm and temperatures ~740–1050 K. The reactant composition and initial state conditions for each auto-ignition experiment are provided in the Supplemental Material.

A detailed description and characterization of the UM-RCF can be found in Donovan et al. [8]. Briefly, the UM-RCF consists of the Driven Section, in which a gas mixture is rapidly compressed by the motion of a free piston (Sabot). Prior to compression, the test volume is evacuated and then filled with the test gas mixture. Upon firing, the Sabot travels the length of the Driven Section compressing the test gas mixture into the Test Section – a small cylindrical volume located at the end of the Driven Section. As the Sabot reaches its final position near the Test Section, the Sabot achieves an annular interference fit, sealing the test gas mixture in the Test Section. At this point, the Test Section is filled with a uniform and isentropically compressed test gas mixture at the desired initial thermodynamic condition. For this study, the Test Section was instrumented with a piezoelectric transducer (6125B Kistler, Amherst, NY) and charge amplifier (5010, Kistler, Amherst, NY) for pressure measurements at 100 kHz sampling frequency, and a transparent polycarbonate end-wall to permit high-speed imaging