Ph.D. Defense of

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High Pressure Ignition Chemistry of Alternative Fuels

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Using the Rapid Compression Machine at the University of Connecticut, studies of the autoignition behavior of alternative fuels are conducted in the temperature range 650 K to 900 K and the pressure range 15 bar to 50 bar with a focus on developing a fundamental understanding of the chemistry controlling the autoignition of alternative fuels at engine relevant—high-pressure and low-to-intermediate temperature—conditions. The alternative fuels studied here include five bio-alcohol fuels—*n*-butanol, *s*-butanol, *t*-butanol, *i*-butanol, and *i*-pentanol—that are studied to investigate the effect of the alcohol group and molecular structures on autoignition behavior. In addition, methylcyclohexane—an important component of fuels derived from alternative petroleum sources and a component in surrogate transportation fuel formulations—is studied.

The ignition delay of the alcohols shows no evidence of phenomena such as two-stage ignition and negative temperature coefficient (NTC) of the ignition delay. However, the relative reactivity shows a complicated dependence on the molecular structure and the pressure and temperature conditions. Moreover, *i*-pentanol and *t*-butanol show similar heat release behavior prior to the main ignition event. These results are explained through detailed chemical kinetic analysis in terms of the unique chemistry possible in each alcohol because of their unique structures.

The ignition behavior of methylcyclohexane is similar to alkanes and other cycloalkanes, in that methylcyclohexane shows strong two-stage ignition and NTC behavior. Analysis of a detailed kinetic model shows that the prominent reaction pathways causing this behavior are also similar between methylcyclohexane and similar molecules, indicating that the reaction types controlling the autoignition behavior of hydrocarbons are common among many fuel structures. In addition, gas samples extracted from the reaction chamber during the induction period are used to identify and quantify important intermediate species during the autoignition of methylcyclohexane.

The experimental data developed in this work provide a comprehensive set of archival ignition data that can be used to benchmark and validate chemical kinetic models for the combustion of alternative fuels. These data also indicate the remaining gaps in the understanding of the high-pressure ignition chemistry of alternative fuels and provide preliminary directions for future research to close the gaps.