High pressure combustion kinetics –

from elementary reaction steps to global models

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Abstract

Hydrocarbon fuels are quite certain to remain the energy storage medium of choice for the foreseeable future. And as the global interests in sustainable and renewable energy sources continues, research efforts are also underway in developing highly efficient engine concepts such HCCI and PCCI with a promise to simultaneously reduce emissions.

In order to assess the potential of novel fuels in advanced combustion systems, a detailed understanding of the extremely complex chemistry of combustion at engine relevant conditions is desired. A detailed chemical kinetic mechanism for combustion of comparatively small hydrocarbons requires hundreds of species and thousands of elementary reactions. Our research aims to elucidate the complex chemistry of combustion by combining various computational methods with experimental techniques to develop and validate kinetic mechanisms.

This presentation will discuss diverse lab scale measurements at elevated pressures to probe a single elementary reaction step (e.g. H + O2(+ M) → HO2 (+M)) up to validation of global mechanisms using Shock tubes, Rapid Compression Machine and Flow reactors. Both optical and mass spectrometric diagnostics are employed to interrogate the chemistry of interest and in separate experiments, synchrotron photo-ionization molecular beam mass-spectrometry is used to study isomer resolved kinetics. Finally, predictive models are developed based on a fundamental understanding of the elementary reaction kinetics, which are then verified using these experimental targets.