Use of biofuels, especially in automotive applications, is a growing trend due to their potential to lower greenhouse gas emissions from combustion. Ketones are a class of biofuel candidates which are produced from cellulose. However, ketones received rather scarce attention from the combustion community compared to other classes such as, alcohols, esters, and ethers. There is little knowledge on their combustion performance and pollutant generation. Hence their combustion chemistry needs to be investigated in detail. Diisopropyl ketone (DIPK) is a promising biofuel candidate, which is produced using endophytic fungal conversion. A detailed understanding of the combustion kinetics of the oxidation of DIPK in advanced engines such as, the homogeneous charge compression ignition (HCCI) engine is warranted. This dissertation concentrates on the combustion kinetics of DIPK over a wide range of temperature and pressure with a focus on HCCI engine application.

An existing DIPK kinetic mechanism has been reviewed and a single zone HCCI engine model has been modeled and validated against recent experimental data from Sandia National Lab. Therefore different HCCI modeling assumptions were tested and the DIPK reaction mechanism was modified with missing reactions and the required thermochemical data. As a result, the HCCI pressure trace, heat release rate and reactivity have been improved. In order to improve the ignition delay time simulation results, the low temperature oxidation of DIPK was studied as the fuel chemistry effects on the autoignition behavior becomes important in low temperature. Therefore DIPK low temperature oxidation experimental data was obtained from the synchrotron photoionization experiments conducted at the Advanced Light Source (ALS) so that the primary products as well as the dominant oxidation pathways are identified. Furthermore, the aldehydes oxidation, as a result of partial or incomplete combustion and as the primary stable intermediate products in oxidation and pyrolysis of biofuel were studied at low temperature in ALS.

A high temperature reaction mechanism was created using the reaction class approach. The reaction mechanism for DIPK was improved using the experimental data along with quantum chemical calculation of activation energies and barriers as well as vibrational modes for the important reactions identified in ALS experiment. The rate constants for important reactions were calculated based on modified Arrhenius equation. DIPK oxidation and pyrolysis were studied at high temperature and pressure using UCF shock tube. The ignition delay times as well as the product (methane) time histories were investigated and used as validation targets for the new model.

Major: Mechanical Engineering

Educational Career:
Bachelor’s of Mechanical Engineering, BS, 2006, Iran University of Science and Technology
Master’s of Mechanical Engineering, MS, 2010, Iran University of Science and Technology

Committee in Charge:
Subith Vasu Sumathi, Chair, MAE
Alain Kassab, MAE faculty
Jayanta Kapat, MAE faculty
Artem E. Masunov, Nanoscience Technology Center and Department of Chemistry

Approved for distribution by Subith Vasu Sumathi, Committee Chair, on December 5, 2014.

The public is welcome to attend.