Biodiesel Ignition Experiments and Chemical-Kinetic Modeling

Jeffrey M. Bergthorson, Department of Mechanical Engineering
McGill University, Montreal, QC H3A 2K6

McGill

The auto-ignition of methyl butanoate (MB), a surrogate for biodiesel, is investigated using the shock tube technique. The results will be used to optimize and validate detailed chemical kinetic mechanisms for MB combustion. Preliminary experiments have been performed at 1 - 5 atm using MB/air and MB/O_2/Ar mixtures. It has been found that MB ignition is similar to non-oxygenated hydrocarbons with respect to the influence of temperature, pressure and composition (Fig. 1).

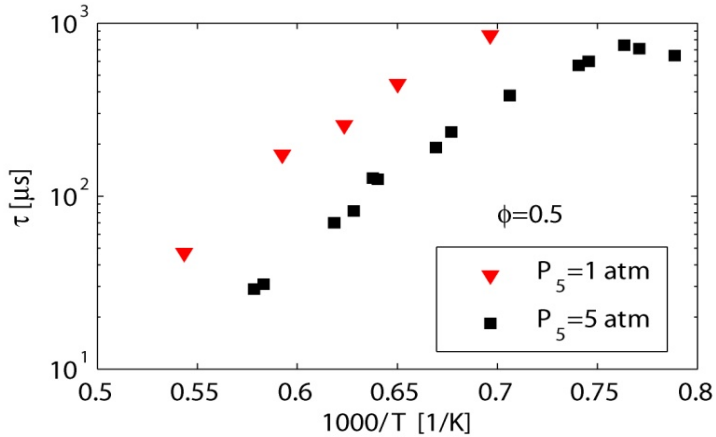

Fig. 1: Effect of temperature and pressure on methyl butanoate/air ignition

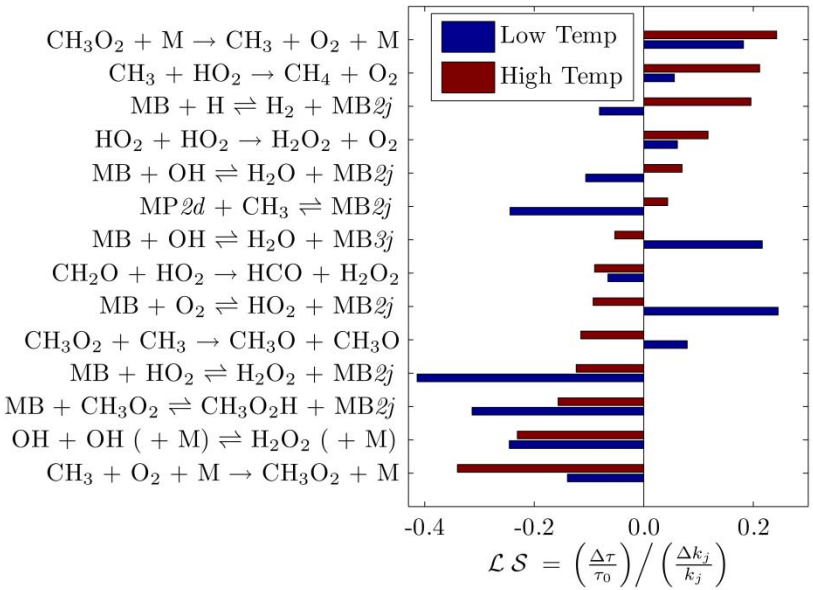

Fig. 2: Normalized sensitivity of ignition delays to reaction rates. Comparison of important reactions common to low and high temperature regimes.

It is known that the proposed methyl butanoate mechanism by Fisher et al. (2000) predicts ignition delays shorter than experimental measurement. Sensitivity analysis reveals the key reactions whose rates could be optimized. Figure 2 shows that in different temperature regimes, the same reactions may alter ignition delays to different extents (species names as in mechanism). Rates of fuel-specific reactions are compared to those of similar alkane reactions found in kinetic databases. A variation of the reaction rates of the most sensitive reactions, based on the results of the findings, is planned to optimize the model.