SAND2013-7292C

Predicting the combustion chemistry of biofuels: The high-temperature oxidation chemistry of butanol isomers

N. Hansen, S. S. Merchant, M.R. Harper, and W.H. Green

Combustion Research Facility, Sandia National Laboratories, Livermore, CA 94551
Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

Abstract: Concerns over energy security and environmental degradation have motivated many societies to move away from conventional, petroleum-derived fuels and to promote the use of alternative, bio-derived fuels. In particular, there has been a considerable amount of interest in utilizing alcohols as an alternative and/or additive to gasoline. Efficient technologies to convert biomass into butanol have stimulated enormous interest in the combustion community to characterize the combustion chemistry of its four different isomers. In this presentation we will summarize the experimental work we have been doing on understanding the high-temperature oxidation chemistry of *n*- and *iso*-butanol. In the experiments we used flame-sampling molecular-beam mass spectrometry to determine the detailed chemical structure of laminar, premixed flames at low-pressure. For each of the flames studied, the experimental data consists of isomer-resolved mole fraction profiles for about 40 different species and the entire set provides a comprehensive benchmark for testing of any combustion chemistry model for *n*- and *iso*-butanol. Being able to provide isomer-resolved data for the C_2H_4O, C_3H_6O, and C_4H_8O aldehyde, enol, and ketone intermediates was crucial for the development of a truly predictive model. The highlights of the latest model will be discussed as will be some significant differences to previously published models and ideas for further refinements/improvements.