Chemical Kinetic Modeling for Cleaner Energy Utilization

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Due to global warming concerns associated with energy utilization technologies, mankind is looking for cleaner more sustainable ways to utilize energy. Currently, a large part (~84%) of our energy is produced from oil, coal and natural gas using combustion technologies. Alternative energy sources do exist for power generation including solar, wind, nuclear, hydroelectricity, etc., but these are not suited to heavy duty road, sea and air transportation, among others, where high energy density liquid fuels are needed. It is likely that future low carbon fuels (LCFs) will be synthesized from biomass or captured CO2 via biodiesel, biomass to liquid (BTL) or gas to liquid (GTL) diesel processes. Moreover, ever decreasing emissions targets for greenhouse gases, NOx and particulate matter (PM10/PM2.5) requires the optimization of combustors via fundamental studies of fuels in controlled experiments. One can consider that there are four levels of research associated with combustor design and development; (i) quantum chemistry calculations of the thermodynamic parameters and rate constants associated with the species involved in elementary chemical reactions; (ii) detailed chemical kinetic mechanism development to describe fuel combustion chemistry in well controlled environments; (iii) mechanism reduction so that accurate chemistry can be combined with computational fluid dynamic (CFD) models; (iv) simulations of real combustor (engine, gas turbine, etc.) operating conditions. Chemical kinetic mechanisms are needed to predict important combustion parameters including ignition delay times, flame speeds, lean blow-out limits etc., in addition to intermediate and product species formation. These mechanisms can be very complex, comprising sometimes thousands of species and tens of thousands of reactions. In this seminar an overview of how detailed chemical kinetic mechanisms are formulated will be presented. Comparisons are made between the chemical mechanisms generated for conventional fossil fuels and those generated from biomass. It is observed that much of our understanding gained from the study of conventional fossil fuels can also be successfully applied to bio-derived fuels. These chemical mechanisms can also inform fuel design leading to optimal fuel efficiency with minimal emissions.

Prof. Henry Curran received his PhD degree in experimental and numerical studies of combustion kinetics from the National University of Ireland, Galway (NUIG) in 1994 and a DSc degree by research from the National University of Ireland in October 2011. He worked as a postdoctoral researcher and research scientist in Combustion Modeling at Lawrence Livermore National Laboratory (LLNL) with Drs Charles Westbrook and William Pitz from 1994 to 1999. Thereafter, he returned to Ireland to take an appointment as a lecturer in Physical Chemistry at Galway-Mayo Institute of Technology and was appointed Lecturer at the National University of Ireland Galway (NUIG) in 2005. He is currently director of the Combustion Chemistry Centre and Priority Research Area leader in Energy at NUIG. He is a member of the editorial boards of "Progress in Energy and Combustion Science" and "Combustion Theory and Modeling". He is a founder member of the Irish Section of the Combustion Institute, a fellow of both the Institute of Chemistry of Ireland and the Royal Society of Chemistry. He is a member of the Institution of Engineers Ireland, the American Society of Automotive Engineers and the Society of Automotive Engineers. He became a member of the Royal Irish Academy in March 2015. He was awarded the Boyle-Higgins gold medal in Chemistry by the Institute of Chemistry of Ireland in April 2017. He has been named by Clarivate Analytics as being among the top 1% of researchers cited in his field every year since 2014. He began consulting with Convergent Science in 2017.

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