COMBUSTION WEBINAR

The Computational Chemistry Consortium: Surrogate Fuel Mechanism Development, Pollutants Sub-Mechanisms and Components Library

Speaker: Prof. Henry Curran, National University of Ireland Galway (NUIG)

Time: *Sept. 26, 2020*
10 am EST; 4 pm Paris; 10 pm Beijing.

Meeting: *Zoom*

Registration (required):
Check https://sun.ae.gatech.edu/combustion-webinar/
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Biography: Prof. 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 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 (formerly Thomson Reuters) as among the top 1% of researchers cited in his field every year since 2014. He began consulting with Convergent Science in 2017.

Abstract: The Computational Chemistry Consortium (C3) is dedicated to leading the advancement of combustion and emissions modeling. The C3 cluster currently combines the expertise of six different technical groups led by Prof Henry Curran at NUI Galway and includes Prof. Heinz Pitsch at RWTH Aachen University, Prof. Tiziano Faravelli at the Politechnico di Milano, Dr. William Pitz at Lawrence Livermore National Laboratory, Drs Raju Mandhapati and Kuiwen Zhang at Convergent Science, and Dr. Stephen Klippenstein at Argonne National Laboratory has recently added his expertise in quantum chemistry calculations. The consortium is involved in combustion research aiming to refine existing chemistry models and to develop more efficient tools for the generation of surrogate and multi-fuel mechanisms, and suitable mechanisms for CFD applications.

This work gives an overview of the work that we have been doing and analyzing the results from the model, obtained by comparing with experimental targets typically used for model validation (i.e. ignition delay times, laminar flame speed, species measurements in ideal reactors and flames). Examples of model predictions, obtained by merging the kinetic modules of the disparate chemistry including hydrocarbon (alkene, alkane, aromatic and PAH species) and NOx chemistry, are presented. In addition, this work also describes the effort towards the generation of reduced mechanisms developed from our detailed mechanism to be used for practical CFD simulations.