COMBUSTION WEBINAR

Automatic Creation of Highly Reduced Combustion Kinetic Models

Speaker: Dr. Stephen Dooley, Trinity College Dublin

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Biography: Dr. Stephen Dooley is Associate Professor of Energy Science in the School of Physics, Trinity College Dublin and an interdisciplinary engineering scientist of a chemical bias dedicated to fundamental research in clean energy technologies. Prior to this he held independent academic appointments in Chemical & Environmental Sciences at the University of Limerick, held postdoctoral and professional research staff appointments at Princeton University, and worked as a Thermal Fluids Technical Specialist at Cummins Engine Company, UK. Prior to all of that, Stephen obtained his BSc (Chemistry) and PhD (Physical Chemistry) at National University of Ireland, Galway. Stephen's principle contributions have been in interpreting and exploiting the mechanisms of chemical reactions occurring in fuel and feedstock conversion devices to improve the clean and efficient operation, techno-economic viability, and/or fundamental comprehension of issues limiting to same. His research has been widely supported by Government (Science Foundation Ireland, European Research Council, Sustainable Energy Authority of Ireland) and Industry (Siemens Gas Turbines, TOTAL SA)

Abstract: Accurate low dimension chemical kinetic models for fuel combustion are now an essential component in the design of efficient gas turbine combustors. Even with increasing computational power, processing time stemming from model complexity will always be a factor desirable to minimize. In this regard, detailed chemical kinetic models are too computationally expensive for use. We proposed a novel data orientated automatic methodology (MLOCK) to produce "Compact Kinetic Models" that replicate a target set of detailed model properties to a high fidelity, but at fractions of the detailed model cost. For this purpose, an automatic computational algorithm is constructed to perform the reaction network simplification, and optimisation of reaction kinetic parameters to allow the resulting model to replicate a series of combustion phenomena of typical importance in gas turbine combustion. In this seminar, we describe the MLOCK algorithm, and account its performance in "compacting" two similar state-of-art detailed chemical kinetic models for methane combustion. It is shown that MLOCK readily condenses these models from 52 & 904 species respectively, to models of 15 species in an automated manner without great expense in operator time, while retaining high fidelity to the performance of the calculations of the parent detailed model.

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