OpenFOAM & Combustion Simulation

HyChem Modeling of Real-Fuel Combustion Chemistry

Prof. Hai Wang

Stanford University

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Host: Prof. Huangwei Zhang (National University of Singapore)

Register: https://nus-sg.zoom.us/webinar/register/WN_M3MNAQqUQa-Q6j6_xEptow

Abstract

The HyChem approach provides a viable path to rapidly developing physics-based combustion chemistry models for conventional and alternative fuels. The approach relies on rate-limiting reaction-pathway identification and laser diagnostics of time histories of key intermediates during thermal and oxidative fuel pyrolysis. The measurements typically yield lumped reaction steps and kinetics that are broadly applicable under a wide range of thermodynamic conditions. Coupled with a foundational fuel chemistry model, the resulting HyChem model is shown to make reliable predictions of the combustion behaviors, from heat release to flame ignition and extinction, of all multicomponent liquid fuels tested thus far. HyChem models thus developed are already compact in size and often directly amendable for computational fluid dynamics (CFD). Available models have been used for a wide range of CFD studies, including combustors of relevance to gas-turbine engines. The fundamental bases and assumptions of the HyChem approach will be discussed. The combustion properties of conventional jet fuels will also be overviewed and contrasted with a sample alternative fuel.

About the Speaker

Hai Wang is Professor of Mechanical Engineering at Stanford University. Prior to his appointment at Stanford, he was the Northrop Chair in Engineering and Professor of Aerospace and Mechanical Engineering at USC. He received his Ph.D. in Fuel Science from Penn State in 1992. He was a Professional Research Staff at Princeton University from 1994 to 1996 before starting his faculty career at the University of Delaware. He is best known for his work on the mechanisms and models of PAH and soot formation in combustion and development of chemical kinetic models for fuel combustion. He has made contributions in the application of ab initio quantum chemistry and reaction rate theory in chemical kinetics. He was involved in the early stage of GRI Mech development. He developed several widely used combustion reaction models, from USC Mech II, JetSurF to HyChem. He advanced stochastic methods for detailed modeling and uncertainty quantification. He contributed to the transport theories of nanoparticles and large molecules, atmospheric heterogeneous chemistry, nanomaterials synthesis, characterization and applications in solar cells and lithium ion batteries. He was the recipient of the AIAA Propellant and Combustion Award in 2018, and the Humboldt Research Award in 2019. He is a Fellow of ASME and an inaugural Fellow the Combustion Institute. He currently serves as the Co-Editor-in-Chief of Progress in Energy and Combustion Science and the Vice President (President-Elect) of the Combustion Institute.