COMBUSTION WEBINAR

Rising Star Lecture: Creating complex reaction models that can extrapolate with quantified uncertainty

Speaker: Prof. Michael Burke, Columbia University

Time: *Nov. 14, 2020*
10 am EST; 4 pm Paris; 11 pm Beijing.

Meeting: *Zoom*

Registration (required):
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Biography: Michael Burke is an Associate Professor of Mechanical Engineering at Columbia University, where he also holds affiliate appointments in Chemical Engineering and the Data Science Institute. Burke also serves as a colloquium co-chair for Gas Phase Chemical Kinetics at the 38th International Symposium on Combustion, awards committee chair and executive board member of the Eastern States Section of the Combustion Institute, and advisory board member for the CANTERA code. Prior to joining Columbia in 2014, Burke earned his Ph.D. in Mechanical and Aerospace Engineering in 2011 at Princeton University, where he was a Wallace Memorial Honorific Fellow, and worked as a Director's Postdoctoral Fellow in the Chemical Sciences and Engineering Division at Argonne National Laboratory. Burke is a recipient of the Combustion Institute's Research Excellence Award, the National Science Foundation's CAREER award, and the American Chemical Society's PRF Doctoral New Investigator Award. His publications have been featured in the "News and Views" section of Nature Chemistry, selected as the Feature Article in Combustion and Flame, and chosen for the Distinguished Paper Award at the 31st International Symposium on Combustion.

Abstract: Being able to predict the outcomes of complex reactions would be invaluable to various scientific and engineering disciplines, ranging from combustion to the Earth's atmosphere and beyond. However, doing so is no simple task – given that complex reactions often proceed through 100s of intermediate species undergoing 1000s of reactions, each occurring with rates that depend on temperature, pressure, and mixture composition. Given the vastness of thermodynamic space relevant to many systems, the ability to extrapolate is a common need for complex reaction models across varied domains. Yet, extrapolating knowledge of complex reactions to new environments is notoriously challenging due to the (1) rich temperature, pressure, and composition dependence of reaction rates; (2) difficulties in extrapolating limited data to new conditions with quantified accuracy; and (3) potential existence of "blind spots" in even the most comprehensive datasets. After outlining these challenges, I describe how recent advances in theoretical chemistry, multiscale modeling, and uncertainty quantification can be exploited to overcome these challenges. To this end, I describe (1) theoretical studies of kinetics in mixtures of reactive and energy-transferring colliders (and associated non-equilibrium phenomena) to achieve an understanding of composition dependence to match current understanding of temperature and pressure dependence; (2) uncertainty quantification that combines *ab initio* and experimental data across multiple scales to extrapolate data at limited conditions; and (3) high-throughput/automated experimentation designed to maximize the information generation rate and fill experimental blind spots. I will then close with a discussion of how these and other techniques can be combined into a cohesive strategy for creating complex reaction models that can *extrapolate* with quantified uncertainty.