DFD17-2017-002622
Abstract for an Invited Paper
for the DFD17 Meeting of
the American Physical Society

Direct Numerical Simulation of Turbulent Multi-Stage Autoignition Relevant to Engine Conditions[1]

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Due to the unrivaled energy density of liquid hydrocarbon fuels combustion will continue to provide over 80% of the world's energy for at least the next fifty years. Hence, combustion needs to be understood and controlled to optimize combustion systems for efficiency to prevent further climate change, to reduce emissions and to ensure U.S. energy security. In this talk I will discuss recent progress in direct numerical simulations of turbulent combustion focused on providing fundamental insights into key 'turbulence-chemistry' interactions that underpin the development of next generation fuel efficient, fuel flexible engines for transportation and power generation. Petascale direct numerical simulation (DNS) of multi-stage mixed-mode turbulent combustion in canonical configurations have elucidated key physics that govern autoignition and flame stabilization in engines and provide benchmark data for combustion model development under the conditions of advanced engines which operate near combustion limits to maximize efficiency and minimize emissions. Mixed-mode combustion refers to premixed or partially-premixed flames propagating into stratified autoignitive mixtures. Multi-stage ignition refers to hydrocarbon fuels with negative temperature coefficient behavior that undergo sequential low- and high-temperature autoignition. Key issues that will be discussed include: 1) the role of mixing in shear driven turbulence on the dynamics of multi-stage autoignition and cool flame propagation in diesel environments, 2) the role of thermal and composition stratification on the evolution of the balance of mixed combustion modes - flame propagation versus spontaneous ignition – which determines the overall combustion rate in autoignition processes, and 3) the role of cool flames on lifted flame stabilization. Finally prospects for DNS of turbulent combustion at the exascale will be discussed in the context of anticipated heterogeneous machine architectures.

[1]sponsored by DOE Office of Basic Energy Sciences and computing resources provided by the Oakridge Leadership Computing Facility through the DOE INCITE Program