

Insights from direct numerical simulation of multi-stage autoignition and flame propagation in intense shear-driven turbulence

Jacqueline H. Chen

Sandia National Laboratories
Livermore, CA 94550

* Corresponding author: jhchen@sandia.gov

Direct numerical simulation (DNS) of turbulent combustion on petascale supercomputers has transformed our ability to interrogate fine-grained gas-phase ‘turbulence-chemistry’ interactions in simple laboratory configurations. In particular, three-dimensional DNS, performed at moderate Reynolds numbers, at ambient and elevated pressure and with complex chemistry has provided an unprecedented level of detail used to isolate and understand mechanistic causality between turbulence, mixing and reaction in combustion regimes dominated by finite-rate chemical kinetics. DNS has provided new physical insights and statistics to assist in the development and assessment of models under different reacting flow scenarios. Insights from recent DNS of turbulent spontaneous multi-stage ignition relevant to diesel combustion and flame propagation in intense shear-driven turbulence relevant to lean premixed gas turbine combustion will be presented.

In the former problem, spatial inhomogeneities in mixture composition induced by sheared turbulence strongly affect low-temperature chemical reactions in turbulent mixtures of air and diesel fuel undergoing spontaneous ignition. Controlling the ignition delay of the system provides a means to improve the engine performance while reducing pollutant emissions. Autoignition in stratified mixtures has been the subject of many numerical and experimental studies. Several key findings on this subject have emerged, first that spontaneous ignition is favored in flow regions where the mixture has a composition close to an optimal, most reactive one, and where scalar fluctuations remain low during the ignition transient. Second, an equally important finding is that ignition in turbulent flows occurs no earlier than the corresponding minimum homogeneous ignition delay time; that is, it is thought that turbulence impedes the accumulation of radicals and heat in developing ignition kernels through dissipative effects.

Modern diesel engines traverse broad thermo-chemical regimes where low-temperature ignition chemistry coupled with interaction with the underlying turbulence is important. Recent DNS results will be presented which challenge these earlier findings, and in particular, show that for multi-stage ignition, the initiation of low-temperature ignition at fuel-lean conditions results in cool flames and spontaneous ignition fronts that form and propagate into unburnt fuel-rich mixtures prior to hot ignition occurring in those mixtures. Thus the turbulent transport of enthalpy and radicals leads to ignition occurring at locations with a different composition than the ‘most reactive’ one, and at a time comparable with if not shorter than the minimum ignition delay time. Doubly conditional statistics for temperature and key low-temperature scalars are presented to elucidate the role of scalar dissipation rate in modulating the spatial inhomogeneities in the mixture composition. Moreover, the effect of turbulent mixing on the dynamics of multi-stage spontaneous ignition and the eventual establishment of a high-temperature flame will be discussed.

In the latter problem, the effect of intense shear driven turbulence on the turbulent burning velocity and flame structure of a lean premixed methane/air flame is presented from DNS of an experimental lean premixed piloted jet flame at high Karlovitz number. In the so-called broken or distributed reaction zones regime turbulence-chemistry interactions are strong and the shear layer and the pilot can have a significant impact on the flame structure and its stabilization. Statistics will be presented from an analysis of flame stretch and flame thickness and their rates of change in iso-surface following reference frames showing these quantities are intimately connected. The effect of the pilot and shear-induced strain rate on flame stabilization will be discussed in terms of flame displacement speed and flame stretch factor statistics coupled with a chemical analysis of the flame structure.