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The know unknowns: Detailed simulations and low-order modeling to characterize facility-induced non-idealities in chemical-kinetics experiments

MATTHIAS IHME, Stanford University

Experimental investigations to study chemical-kinetics processes, reaction-rates or ignition properties are frequently accompanied by facility-induced non-idealities. Examples are turbulence and thermo-viscous boundary layers in rapid compression machines, temperature fluctuations and mixture inhomogeneities in flow-reactors, or shock-bifurcations and pressure drifts in shock-tubes. Although experimental investigations are carefully conducted to mitigate these effects, they are difficult to quantify experimentally. Simulations can assist in identifying these non-idealities and in guiding experimental instrumentation to improve measurement accuracies. This presentation discusses three different modeling approaches to characterize facility-effects in rapid compression machines, flow reactors, and shock-tubes. After providing an overview about these facilities and describing the underlying models, examples are presented to illustrate effects of turbulence, mixture-inhomogeneities, heat-losses, and thermal stratification on the ignition dynamics in these facilities. Diagnostics is developed to assess the sensitivity of the induction chemistry and to quantify reliable operating regimes that are not contaminated by these non-ideal processes.