Multiscale Kinetic Knowledge Propagation - Combustion Chemistry of Small Hydrocarbons

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Chemical kinetic models have become indispensable to the design of low-emission, highly efficient engines using both conventional and bio fuels. At this time, the predictive uncertainties of these models remain large. While the validity of a reaction model can be checked usually against a set of fundamental combustion data, the underlying problem of model uncertainty is nonetheless ill-defined mathematically. The accuracy of the reaction rate parameters can be assessed, in principle, by examining the scatter in the experimental data and/or the results obtained in ab initio quantum chemistry methods at different levels of theory. In this talk, the rate parameter uncertainty will be illustrated using a recent theoretical study as an example. It will be shown that the best theory available still leaves a rate uncertainty as large as a factor of 3. To address the above problem, we introduce the spectral uncertainty method, and more specifically the method of Polynomial Chaos Expansions and its application in examining the effects of kinetic model uncertainty on combustion predictions. An extension of this method, termed the Method of Uncertainty Minimization, has been developed to allow for forward and backward projections of uncertainties in both the reaction model and fundamental combustion experiments. The application of this method in the development of a recent CEFRC foundational fuel chemistry model and in designing better combustion experiments will be discussed.