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Predicting Combustion Chemistry & Focusing on the Important Aspects

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Because combustion chemistry is so complex, it is seldom possible to unambiguously determine all the important parameters experimentally. Instead, we usually need to predict the values of most or all of the parameters in the chemical kinetic models. In the past this was done primarily by analogy to rate coefficients and thermochemical parameters that had been measured previously, but because of gaps in the data many of these parameter values were little more than guesses. We know in principle how to compute most types of parameters from first principles, but it is usually impossible to solve the true quantum mechanical equations, so many different approximations have been introduced by quantum chemists and computational kineticists, introducing errors. Also the calculations are very computationally intensive, even for light fuels like gasoline. Making predictions before experiment is of course very challenging: Which species and reactions belong in the model? How can we compute the values of so many parameters efficiently? How can we quantitate the error bars on these parameter values? But on the other hand, working in predictive mode enables computer-aided design of new fuels and combustors, and facilitates design of good experiments to test the accuracy of model predictions. In this talk, we first summarize the state of the art of predictive chemical kinetics, showing some examples. Then we discuss how to focus our efforts on the most important aspects of combustion chemistry, e.g. how the details of the fuel chemistry affects/controls important fuel performance metrics such as ignition delay, extinction strain rate, and the formation of pollutants.