Modeling Complex Combustion Chemistry

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\[ \text{O} + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3 \]
\[ \text{OH} + \text{CH}_3 \rightarrow \text{CH}_2 + \text{H}_2 \text{O} \]
\[ \text{CH}_3 + \text{O}_2 \rightarrow \text{OH} + \text{CH}_2 \text{O} \]
\[ \text{CH}_2 + \text{N}_2 \rightarrow \text{HCN} + \text{NH} \]
\[ \text{O}_2 + \text{CO} \rightarrow \text{O} + \text{CO}_2 \]

Simulating the Entire Combustion System: Among the physical phenomena present in combustion systems are convection, radiation, buoyancy, turbulence, chemical reactions, and diffusion. To accurately model each of these phenomena in a combustion simulation requires large computer resources. The simulation is made more difficult by the range of length and time scales over which these processes occur.

Accurately Predicting Combustion Reactions: Combustion reaction mechanisms can involve large numbers of species and reactions. For example, the GRI methane combustion mechanism includes 49 chemical species and 279 reactions. It is impossible to include this full mechanism in a large combustion simulation. How can the degrees of freedom in the system be reduced without eliminating important reaction pathways?

Reducing the Reactions - ILDM: Chemical reactions occur over a wide range of time scales. In combustion, the reactions with fast time scales quickly converge to a low dimensional manifold. This manifold represents the progress of the slow reaction processes toward equilibrium. This manifold is computed using the methane combustion mechanism in a batch reactor. Manifolds are generated for a range of fuel/air ratios. Information from the manifold, including all species concentrations and temperature, is tabulated as a function of two parameters: fuel/air ratio and CO2 + H2O concentration. In this way, the large methane mechanism is reduced to a system which requires only two parameters.

Automation: The goal of my undergraduate thesis is to automate the process of creating and tabulating manifolds for different chemical mechanisms. The manifolds are computed in a batch reactor using CHEMKIN, a computer code that provides tools for the manipulation of complex chemical kinetics. A combustion simulation program can then utilize these tabulated manifolds by computing values for the two parameters at every location on the grid and then looking up the associated data (species concentrations and temperatures) in the table.