

ME DEPARTMENTAL SEMINAR

Friday, September 22, 2006

2:00pm – 3:00pm

2211 GG BROWN

**Professor Anthony M. Dean
Chemical Engineering Department
Colorado School of Mines**

“Engineering Applications of Detailed Chemical Kinetics”

Abstract:

This talk will outline how the combination of improved understanding of elementary chemical reactions and subsequent incorporation into realistic flow models has markedly improved our ability to describe “real-world” systems. Such approaches require development of accurate, detailed chemical mechanisms, which in turn require careful analysis of different types of elementary reactions. This talk will describe our approach to the characterization of elementary reactions, the construction of detailed mechanisms, and the combination of these mechanisms with the appropriate transport models to model the behavior of solid-oxide fuel cells.

In terms of elementary reactions, the $C_2H_5 + O_2$ reaction system will be used to illustrate the complexities of chemical activation. Here the initially formed adduct contains the energy of the newly formed C–O bond. The subsequent reactions of this energized adduct reflect the competition between its unimolecular reactions and its bimolecular collisional stabilization. As a result, multiple reaction pathways are available, and the rate coefficients for the various pathways depend on both temperature and pressure.

We illustrate kinetics/transport coupling by considering solid-oxide fuel cells. SOFCs are currently in development for use in a number of applications, including distributed power generation. These systems offer the potential for direct electrochemical oxidation of hydrocarbons without the requirement for upstream fuel reforming. However, at nominal operating temperatures of 600-1000°C, fuel stability and carbonaceous deposits within the fuel channels and porous anode structures present potential limitations to cell performance. Several illustrations of the application of detailed kinetics to SOFC operation will be considered.

One such example is the description of experimental and modeling investigations of methane reforming chemistry in a porous Ni-YSZ cermet anode. Using specially designed experiments and computational models, our objective is to develop and validate models that quantitatively describe chemical kinetics and gas transport within the anode structure of a solid-oxide fuel cell (SOFC). Another topic will be a description of the approach used to develop gas-phase molecular weight growth kinetics to characterize deposit formation within SOFCs. The ability of the model to quantitatively describe the differences in both conversion and deposit formation between butane and ethanol fuels will be described. We will then illustrate how these chemical mechanisms can be combined into a larger model that includes both transport and electrochemistry to predict SOFC behavior under a variety of operating conditions (e.g., upstream steam reforming of JP-8).