# 2009 Mechanical Engineering Lecture Series

## Challenges and Recent Progress in Development of Chemical Kinetic Models for Engineering Applications

**Harsha K. Chelliah**
Mechanical and Aerospace Engineering
University of Virginia

**Abstract:**
In computational simulations of reacting flows involving critical phenomena, finite-rate kinetics and the transport of reactants play an important role. Some examples include explosion limits, detonation limits, flammability limits, sooting limits, as well as flame ignition and extinction. The typical chemical kinetic models that describe these phenomena can include 100's of species (scalar variables) in 1000's of elementary reactions. Even with the highly parallelized computational architectures available today, the number of scalar variables that can be solved accurately depends on the spatial scale and the complexity of the problem. For engineering applications, however, by carefully considering characteristic time scales of the problem, systematically developed reduced reaction models can be implemented without any loss of accuracy and is the focus of this presentation. The approach is based on the concept of applying quasi steady-state approximation for species, as originally proposed by Borderstein for hydrogen-halogen system (1913) and Langmuir for heterogeneous oxidation of char (1915). It will be shown that the mathematical analysis tools developed as part of this work can be readily applied to a wide range of challenging reacting flow problems, ranging from thermo-acoustics instabilities in power generation systems to flame holding conditions in hypersonic engines. A live demonstration of the thermo-acoustics phenomenon will be part of the presentation!

**Biography:**
Professor Chelliah's general research interests are focused on better understanding the fundamental coupling between finite-rate chemistry and fluid flow with well coordinated theoretical and experimental investigations. His research work has covered a wide range of topics which includes droplets/particles interaction in flames, porous carbon particle combustion, thermo-acoustics interactions, and optimal reduced reaction models for hypersonic combustion. He received his PhD degree from Princeton University in 1989 and is currently a professor at the University of Virginia, where he teaches graduate level courses on Thermo-mechanics (Physics of Gases), Non-equilibrium Gas Dynamics, Combustion, and Advanced Combustion, and numerous undergraduate level courses. He is an associate fellow of AIAA and is a member of the Executive Committee of the Combustion Institute Eastern States Section.

***Date*: Friday, April 24 at 2:00 pm**
***Place*: 1202 EGR (Glenn L. Martin Hall)**

***Host*: Dr. Chelliah will be hosted by Prof. Michael Zachariah of Mechanical Engineering**