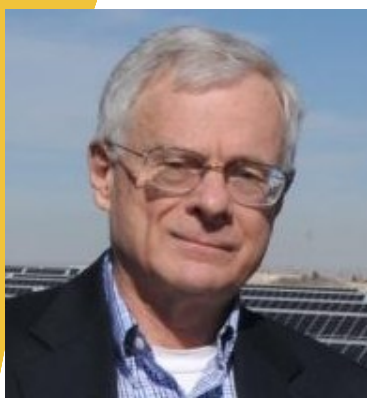
College of Engineering
Department of
Mechanical & Industrial Engineering

The Sidney E. Fuchs Seminar Series

3:30-4:30pm, Friday, March 1, 2013
Frank Walk Room



The effects of microstructure on transport and chemistry within porous composite electrodes for fuel cells and batteries

by Robert Kee, Ph.D.*

Mechanical Engineering; Colorado School of Mines

The performance of electrochemical devices (e.g., fuel cells and batteries) depends greatly upon the structure and microstructure of porous composite electrodes. It is well known that transport of ions and electrons, and in some cases multicomponent gas transport, can be very different from the intrinsic transport within the component phases. Because of great scale disparities between the complete electrode and its microstructure, effective transport properties (e.g., electronic and ionic conductivity) are required to model at the larger cell and system scales. A number of alternative approaches have been developed to model transport within porous electrode structures and to derive effective properties. Experimental techniques (e.g., focused ion beam—scanning electron microscopy, FIB-SEM and X-ray tomography) can deliver geometrically accurate three-dimensional representations of actual electrodes. Actual electrode microstructures can be discretized with finite-volume representations and conservation equations solved to predict transport within complex three-dimensional microstructures. In addition to advancing fundamental understanding and insight, such models provide the means to evaluate the validity of more-approximate models that may be derived from synthesized microstructures.

* Professor Kee holds the George R. Brown Distinguished chair at the Colorado School of Mines. Dr. Kee's research interests are primarily in modeling and simulation of chemically reacting fluid flow. Applications are generally in the area of clean energy, including fuel cells, photovoltaics, and advanced combustion. Dr. Kee's sponsored-research efforts are primarily in the modeling and simulation of thermal and chemically reacting flow processes, with applications to combustion, electrochemistry, and materials manufacturing. His fuel-cell research concentrates on elementary chemistry and electrochemistry formulations and their coupling with reactive fluid flow. Primary applications are to solid-oxide fuel cells operating on hydrocarbon fuels. His combustion research emphasizes the use of elementary chemical kinetics to understand fundamental flame structure. Recent research includes efforts on catalytic-combustion and water-mist flame suppression. The materials-processing efforts emphasize the design, optimization, and control of chemical-vapor-deposition processes, with applications ranging from thin-film photovoltaics to CMOS semiconductor devices. The work includes development of computational methods and software to solve systems of stiff differential equations. It also includes development of an extensive system of general-purpose chemical-kinetics and molecular-transport software. Dr. Kee is the principal architect and developer of the CHEMKIN software, which is the leading software package used worldwide for simulating chemically reacting flow.