Dr. Kee’s research efforts are primarily in the modeling and simulation of thermal and chemically reacting flow processes, with applications to combustion, electrochemistry, and materials processing. 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. Research on hydrocarbon reforming and microchannel reactors is closely tied to the fuel-cell research. In addition to research on the microstructural electrode behavior in Li-ion batteries, recent research is also concerned with large-scale sodium-based batteries. Other electrochemistry research is concerned with mixed- and proton-conducting ceramics for application in fuel cells and membrane reactors. The combustion research emphasizes the use of elementary chemical kinetics to understand fundamental flame structure. Recent efforts concentrate on flame-droplet interactions in strained flames with multicomponent hydrocarbon fuels. The materials-processing efforts focus on the development of chemical-vapor-deposition processes, with current applications in thin-film photovoltaics. All the research includes development of computational methods and software to solve systems of stiff differential equations. Prof. Kee has published nearly 200 archival papers documenting his research.

**Microstructural behavior of Li-ion battery electrode**

Because performance of Li-ion batteries depends greatly upon physics and chemistry at the electrode microscale, fundamental understanding at this scale is important. The microstructural geometry can be reconstructed from full batteries using focused-ion-beam—scanning-electron-microscopy (FIB-SEM) techniques or X-ray tomography. Using a combination of finite-volume and finite-element methods, three-dimensional computational models are developed to solve conservation equations representing electrochemical, thermal, and mechanical behavior. The models are valuable in helping to understand performance under ordinary operating conditions, and in predicting behavior in abnormal circumstances such as the heating associated with accident scenarios. By coupling the electrochemistry models with mechanical models, mechanical damage such as electrode fracture can be predicted. Because of great scale disparities between a complete electrode and its microstructure, effective physical and chemical properties are required to model at the larger cell and system scales. In addition to advancing fundamental understanding and insight at the microscale, the models provide the quantitative means to evaluate and validate the effective properties needed in upscaling.