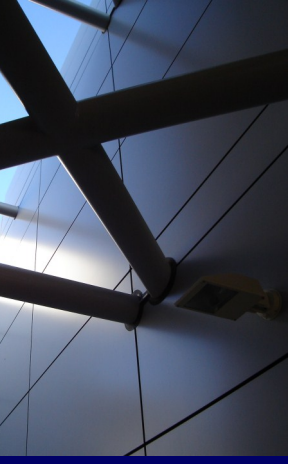

COLLOQUIUM
MECHANICAL ENGINEERING

The Department of Mechanical Engineering presents:

Dr. Van P. Carey

Mechanical Engineering Department
University of California at Berkeley

Friday, October 22
11:10AM-12:00PM
Bourns Hall A265

Hybrid Molecular Dynamics Modeling of Interfacial Phenomena in Boiling Processes

Abstract: The thermophysics of liquid-vapor interfaces has long been recognized as playing a key role in the physical mechanisms of boiling processes. This seminar will describe results of recent molecular dynamics (MD) simulation studies that explore the structure and stability of liquid-vapor interfacial regions using a hybrid analysis scheme that combines new formulations of capillarity theory with MD simulations that use similar interaction potentials. Two forms of this type of hybrid scheme have been developed: one for nonpolar fluids based on a Lennard-Jones interaction potential, and a second specifically for water using a modified treatment of the SPC/E interaction potential that accounts for water dipole interactions. The hybrid model has the advantage that the capillarity theory provides theoretical relationships among parameters that govern interfacial region structure and thermophysical behavior, while the companion MD simulations allow more detailed molecular level exploration of the interfacial region thermophysics. Predictions of interfacial region structure indicated by this kind of hybrid modeling will be described for pure non-polar and water liquid-vapor interfaces, and for water with dissolved ionic solutes (i.e., salts). Extension of the methodology to thin liquid films will also be described. Rupture of a free liquid film dictates merging of adjacent bubbles, which is particularly important in nucleate boiling heat transfer, bubbly two-phase flow in small tubes, and the mechanisms that dictate the Leidenfrost transition. To understand the mechanisms of bubble merging in nanostructured boiling surfaces and in nanotubes, it is useful to explore film stability and onset of rupture at the molecular level. Results obtained with the hybrid model indicate that wave instability predominates as an onset of rupture mechanism for free liquid films of macroscopic extent, but for free liquid films with nanoscale lateral extent (in, for example, nanostructured boiling surfaces), lack of film core stability is more likely to be the mechanism. Predictions of the hybrid models will be compared to results of experimental studies of the effects of ionic solutes on interfacial tension and bubble merging. The implications of the molecular dynamics model predictions for boiling processes in microchannels and boiling in nanostructured surfaces will also be discussed.

Bio: Professor Carey is widely recognized for his research on near-interface micro-scale phenomena, thermophysics and transport in liquid-vapor systems, and computational modeling and simulation of energy conversion and transport processes. Since joining the Berkeley faculty in 1982, Professor Carey's research has spanned a variety of applications areas, including high heat flux cooling of electronics, heat transfer in porous burners, data center energy efficiency, energy sustainability of information processing, fuel cell thermal management, building and vehicle air conditioning, forging and casting of aluminum, phase change thermal energy storage, Rankine cycle power for manned space missions, heat pipes for aerospace applications, advanced concentrating solar absorber designs, and turbomachinery technologies for green energy conversion applications.