Department of Chemical Engineering Seminar Series

"Where are we going and when will we get there? Using computer simulations to help chemical engineers understand thermodynamics and kinetics of complex systems"

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Lecture: 4:00-5:00 p.m.
Physics Astronomy Building (PAA) A110
Reception at 3:30 p.m. PAA A110

Abstract

Modeling tools like molecular dynamics, Monte Carlo or computational chemistry have long been hailed as panacea for connecting the atomic scale to the mesoscale for many problems of interest to chemical engineers including reaction engineering, self-assembly of nanomaterials and controlling biomolecule structure and function. Unfortunately, severe computational restrictions often limit wide-ranging use of these tools to their full potential. However, emerging multiscale modeling algorithms that are based on MD can overcome these challenges, dramatically increasing the computer's viability as a tool for scientific and engineering discovery.

The first part of this talk focuses on how we use computer simulations to determine equilibrium behavior of systems (i.e., *where we are going?*). I will briefly discuss the overarching way that modern molecular simulation theory addresses the challenge of determining equilibrium states when there are strong driving forces. Next, I will discuss to brief examples of how simulations help us predict equilibrium behavior in biological systems: enzyme inhibition in ionic liquids and protein/structure templating on nano-rough surfaces.

The second part of this talk focuses on how use computer simulations to determine kinetic features of systems (i.e, *when will we get there?*) Using a kinetic model for lignin pyrolysis as a starting point, I will discuss how our work addresses two major challenges in understanding and modeling complex reacting systems: prediction of reaction networks and prediction of reaction rates. Examples from a wide range of systems studied in our group including combustion, low temperature chemistry, and protein unfolding will demonstrate progress in this area.

Biography

Jim Pfaendtner works at the University of Washington. Research interests include Old English Sheepdogs and Crossfit.