Department of Aerospace and Mechanical Engineering

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Fluid Mechanics of Electrochemical Interfaces: Electrokinetic Instability and Hydrodynamic Chaos Near Ion-Selective Surfaces

**Tuesday,
April 15, 2014,
3:30P.M.**

**Lower Level
Auditorium,
Geddes Hall**

Refreshments served
at 3:00 p.m. in the
Geddes Hall
Coffee House

Electrochemical interfaces, e.g., the interface of an aqueous electrolyte with a charge selective surface such as an electrode or a membrane, are characterized by ion-transport, electrostatic interactions, and fluid flow. The equations governing these disciplines are the Nernst-Plank, Poisson, and Navier-Stokes, which are well established for more than a century. These equations have contributed understanding of various interfacial phenomena such as diffusion boundary layers, electric double layers, and electro-osmotic flows. However, the mainstream models for electrochemical interfaces in engineering practice use over-simplified assumptions about these equations. Most notably, fluid flow is often assumed prescribed or uncoupled to the equations describing charge transport. In recent years some insights about fluid coupling have been revealed owing to the method of matched asymptotic expansions, but these methods are limited due to their inherent assumptions including bulk electroneutrality and quasi-steadiness.

In this presentation, we will demonstrate the need for the development of specialized algorithms for simulation of electrochemical boundary layers, similar to the tools that have been traditionally used for simulation of turbulent flows. At the core of our investigation we consider ion transport through an ion-selective surface as a model problem with broad applications including water purification, chemical production, and microfluidic-based lab-on-a- chip systems. We will present results from our research and show that direct calculations, without asymptotic simplifications, can predict electrokinetic chaos with multi-scale vortices similar to turbulent boundary layer phenomena. These structures are shown to impact mixing and enhance system-level transport by an order of magnitude and to be consistent with experimental measurements. These calculations require resolving a wide range of spatio- temporal scales using unsteady solvers and often need massively parallel computational resources. We will discuss how development of such high-fidelity tools can lead to fundamental understanding of complex effects in electrochemical interfaces and facilitate their design and optimization.

Dr. Ali Mani
Department of Mechanical Engineering
Stanford University
Stanford, California

If you are interested in meeting individually with Dr. Mani, please contact Linda at 631-5431.