Chemical & Biomolecular Seminar Series

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Chemical & Biomolecular Engineering

University of Tennessee - Knoxville

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102 Colburn Lab

Brian Edwards received a B.S. degree in chemical engineering from the University of Illinois in 1986, and a Ph.D. in chemical engineering from the University of Delaware in 1991. He joined the faculty of the Chemical and Biomolecular Engineering Department at the University of Tennessee-Knoxville as an associate professor in 2001. He was promoted to the rank of full professor in 2008, and has served as the associate department head since 2006. His areas of expertise lie in the theoretical modeling and atomistic simulation of polymeric fluids, and has also recently worked on modeling self-assembly and transport in nanoporous membranes and applications of graphenic materials. In 2015, he cofounded Celtig LLC, an international producer of graphene, and currently serves as the company's CEO. He is the co-author of the textbook *Thermodynamics of Flowing Systems* and has published over 100 papers in journals and delivered approximately 200 technical presentations on these topics.

Steady Shearing Flow of an Entangled Polymeric Liquid

The polymer industries comprise a major component of the US manufacturing economy. These industries produce a variety of products ranging from household commodities to electronic components. Hence the flow of polymeric liquids is of fundamental and practical interest as most materials are processed in the liquid state. The intricate coupling between fluid motion and microstructure evolution greatly complicates analysis and control of processes used for fabrication of polymeric materials. Consequently, quantifying the response of polymeric fluids to the hydrodynamic forces typical of processing operations has posed great challenges. The description of these processes is hindered at high strain rates by a lack of clear understanding of the essential features of the inherent physical processes that occur at the atomistic scale under high strain rates, which ultimately affect the bulk-scale rheological behavior.

Many theories have been proposed to explain the microstructural responses of these complex liquids under flow, but each invariably diverged from experiment at high strain rates. Recent evidence suggests that part of the reason for these divergences is that most flow models track bulk-average properties that have effectively discarded the short-timescale dynamical phenomena of the individual molecules. In recent studies, we have observed via nonequilibrium molecular dynamics simulations of entangled polyethylene liquids that a remarkable dynamical response occurs at high strain rates in both shear and elongational flows: the polymeric liquid experiences a dramatic decrease in the number of chain entanglements, which leads to a network of highly-stretched chains that form effective tube-like structures through which neighboring chains experience anisotropic diffusion. In shear dominated flows, this ultimately leads to chain rotation and retraction cycles, which give rise to characteristic timescales that are much shorter than the reptation time of the quiescent liquid.

In this presentation, I will summarize our recent simulation work on shear flow of entangled polymeric liquids with the aim of presenting a coherent picture of the rich dynamical behavior of these fascinating fluids over the entire range of flow timescales. Emphasis will be placed on understanding the essential physical responses of the individual macromolecules to imposed flows of varying strength, and how the dynamical responses of the individual chain-like molecules contribute to the fluids' overall rheological and morphological responses.