Texas Tech University
Department of Chemical Engineering
Seminar Schedule

Deduction of Transport Properties from Molecular Characteristics

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Transport properties of complex matter are governed by molecular topology and interactions. Molecular simulations have the unique ability to explicitly account for the molecular characteristics and elucidate the structure-property relationships of these systems. Two examples of the use of simulations for investigating the transport properties of practical interest will be discussed.

The first example focuses on the separation of a dilute ethanol-water mixture. Separation of this mixture by distillation is expensive while chemistry based separation is difficult given that both water and ethanol are hydrophilic. Pervaporation based separation of the mixture using polyacrylate membranes was studied in this work. Results will be presented for the effects of polyacrylate chemistry on the solvent structure and mobility in these membranes. The results show that water molecules are dynamically coupled with the polyacrylate chains suggesting a mechanism which can be exploited to affect separation of the alcohol-water mixtures.

The second example focuses on the development of a simulation analogue of the experimental bead microrheology technique. The bead nanorheology simulation approach quantifies the connection between the probe particle motion in a soft material and the material viscoelastic properties. The results show that simulation results can be quantitatively analyzed using continuum mechanics theory to yield the storage and loss moduli of different materials. The suitability of the probe rheology approach for predicting nanoparticle motion in soft matter will be discussed, an ability that is important for applications such as nanoparticle based drug delivery.

Bio

Rajesh Khare has 25 years of experience working in the field of molecular simulations spanning both academia and industry. Following his Ph.D. (University of Delaware) and post-doctoral (University of Wisconsin-Madison) research, he worked in various scientific and managerial capacities in the R&D group at Accelrys, Inc. He joined the Chemical Engineering Department at Texas Tech University in 2005, where he is currently Professor and the Associate Department Chair. The primary underlying theme of Prof. Khare's research is the innovative use of molecular simulations for studying nanoscale transport phenomena, structure-property relationships in soft matter systems, and thermodynamics of mixtures. An important thrust of Prof. Khare's work is to make quantitative connections between the results of molecular simulations and laboratory experiments. Prof. Khare is an active member of the American Institute of Chemical Engineers (AIChE), where he has been involved in conference programming and the committees of the institute.

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