

Abstract Submitted
for the DFD06 Meeting of
The American Physical Society

Molecular Modeling of Transport across Surfactant Covered Oil-Water Interface¹ DMITRY KOPELEVICH, ANUJ CHAUHAN, ASHISH GUPTA, University of Florida — Mass transport across densely packed surfactant covered oil-water interfaces in microemulsions plays a key role in numerous applications such as separations, reactions, drug delivery, and detoxification. In this talk we present results of molecular modeling of transport of solute molecules across hexadecane-water interfaces covered by Brij surfactants and development of a theoretical model for the transport mechanism. We discuss effects of such parameters as solute sizes and degrees of hydrophobicity, as well as the length of surfactant molecules on the transport properties. We obtain a generalized Langevin equation for the solute transport using molecular dynamics simulations with the solute center of mass constrained in the direction normal to the interface. We observe non-trivial behavior of the stochastic force acting on the solute: the autocorrelation time of this force is extremely sensitive to the solute position within the interface and the force relaxation times differ by two orders of magnitude within a narrow region of the interface. This phenomenon is related to the density fluctuations of the surfactant as well as water and oil molecules around the solute. We further discuss implications of this phenomenon on the transport properties.

¹This research is supported by a grant from NSF CTS.

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Date submitted: 06 Aug 2006

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