

Abstract Submitted  
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**Mesoscopic simulations of binary mixtures and microemulsions using a stochastic, particle-based algorithm** ERKAN TUZEL, School of Physics and Astronomy, University of Minnesota, GUOAI PAN, THOMAS IHLE, DANIEL KROLL, Department of Physics, North Dakota State University — Particle-based simulation techniques provide an attractive alternative to traditional methods for the coarse-grained modeling of a fluctuating solvent. A particularly appealing algorithm introduced by Malevanets and Kapral[1], called Stochastic Rotation Dynamics, describes a fluid with an ideal gas equation of state. The algorithm has been successfully applied to study polymers, colloids, and vesicles in shear flow. Recently, this algorithm has been generalized to model fluids with non-ideal equations of state[2]. We will discuss how this can be used to study binary mixtures with a miscibility gap. Results for the demixing such as the phase diagram and measurements of interface fluctuations and the surface tension of a droplet will be shown. By tuning the ratio of surface tension and viscosity both damped and overdamped capillary waves were obtained. The coarsening of domains during spinodal decomposition is also investigated. In order to describe microemulsions, the model is further extended to include surfactant molecules. Preliminary results for the onset of emulsification will be presented. [1] A. Malevanets, R. Kapral, J. Chem. Phys. 110, 8605 (1999). [2] T. Ihle, E. Tuzel, D. M. Kroll, cond-mat/0509631; cond-mat/0511312.

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