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Development of Simulation Methods in the Gibbs Ensemble to Predict Polymer-Solvent Phase Equilibria THOMAS GARTNER, University of Delaware, Dept. of Chemical and Biomolecular Engineering, THOMAS EPPS, ARTHI JAYARAMAN, University of Delaware, Dept. of Chemical and Biomolecular Engineering, Dept. of Materials Science and Engineering — Solvent vapor annealing (SVA) of polymer thin films is a promising method for post-deposition polymer film morphology control. The large number of important parameters relevant to SVA (polymer, solvent, and substrate chemistries, incoming film condition, annealing and solvent evaporation conditions) makes systematic experimental study of SVA a time-consuming endeavor, motivating the application of simulation and theory to the SVA system to provide both mechanistic insight and scans of this wide parameter space. However, to rigorously treat the phase equilibrium between polymer film and solvent vapor while still probing the dynamics of SVA, new simulation methods must be developed. In this presentation, we compare two methods to study polymer-solvent phase equilibrium–Gibbs Ensemble Molecular Dynamics (GEMD) and Hybrid Monte Carlo/Molecular Dynamics (Hybrid MC/MD). Liquid-vapor equilibrium results are presented for the Lennard Jones fluid and for coarse-grained polymer-solvent systems relevant to SVA. We found that the Hybrid MC/MD method is more stable and consistent than GEMD, but GEMD has significant advantages in computational efficiency. We propose that Hybrid MC/MD simulations be used for unfamiliar systems in certain choice conditions, followed by much faster GEMD simulations to map out the remainder of the phase window.

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