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**Disentangle Model Differences and Fluctuation Effects in DPD Simulations of Diblock Copolymers** DAVID (QIANG) WANG, PARAMVIR SANDHU, JING JONG, DELIAN YANG, Department of Chemical and Biological Engineering, Colorado State University, Fort Collins, CO — In the widely used dissipative particle dynamics (DPD) simulations [Hoogerbrugge and Koelman, **Europhys. Lett.** **19**, 155 (1992); Groot and Warren, **J. Chem. Phys.** **107**, 4423 (1997)], polymers are commonly modeled as discrete Gaussian chains interacting with soft, finite-range repulsions. In the original DPD simulations of microphase separation of diblock copolymer melts by Groot and Madden [**J. Chem. Phys.** **108**, 8713 (1998)], the simulation results were compared and found to be consistent with the phase diagram for the “standard model” of continuous Gaussian chains with Dirac  $\delta$ -function interactions obtained from self-consistent field (SCF) calculations. Since SCF theory is a mean-field theory neglecting system fluctuations/correlations while DPD simulations fully incorporate such effects, the model differences are mixed with the fluctuation/correlation effects in their comparison. Here we report the SCF phase diagram for exactly the same model system as used in DPD simulations. Comparing our phase diagram with that for the standard model highlights the effects of chain discretization and finite-range interactions, while comparing our phase diagram with DPD simulation results reveal without any parameter-fitting the effects of fluctuations/correlations neglected in the SCF theory.

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