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Direct Comparisons among Fast Off-Lattice Monte Carlo Simulations, Integral Equation Theories, and Gaussian Fluctuation Theory for Disordered Symmetric Diblock Copolymers DELIAN YANG, JING ZONG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Based on the same model system of symmetric diblock copolymers as discrete Gaussian chains with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations, we directly compare, without any parameter-fitting, the thermodynamic and structural properties of the disordered phase obtained from fast off-lattice Monte Carlo (FOMC) simulations[1], reference interaction site model (RISM) and polymer reference interaction site model (PRISM) theories, and Gaussian fluctuation theory. The disordered phase ranges from homopolymer melts (i.e., where the Flory-Huggins parameter $\chi = 0$) all the way to the order-disorder transition point determined in FOMC simulations, and the compared quantities include the internal energy, entropy, Helmholtz free energy, excess pressure, constant-volume heat capacity, chain/block dimensions, and various structure factors and correlation functions in the system. Our comparisons unambiguously and quantitatively reveal the consequences of various theoretical approximations and the validity of these theories in describing the fluctuations/correlations in disordered diblock copolymers. [1] *Q. Wang and Y. Yin*, **J. Chem. Phys., 130**, 104903 (2009).

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