

Intra- and Inter-chain Pair Correlation Functions of Polymeric Fluids: A Comparison of Self-Consistent Polymer Reference Interaction Site Model and Polymer Density-Functional Theories

Yan Wang^S

Chemical and Biology Engineering, Colorado State University, Fort Collins, Colorado, U.S.A.

Jiawei Zhang, Suyu Wang and Baohui Li

Physics, Nankai University, Nankai, Tianjing, China

Jianzhong Wu

Chemical Engineering, University of California, Riverside, California, U.S.A.

Qiang Wang^C

Chemical and Biology Engineering, Colorado State University, Fort Collins, Colorado, U.S.A.

Q.Wang@colostate.edu

The structure of a polymeric fluid is usually characterized by the intra- and inter-chain pair correlation functions (PCFs), which can be used to determine both the thermodynamic and dynamic properties. Few theories, however, are available to predict such microscopic structures, which require that the segment-segment correlation effects be explicitly taken into account. In the well-developed self-consistent polymer reference interaction site model (SC-PRISM) (Heine et al., *Adv. Polym. Sci.* **173**, 209, 2005), the inter-chain PCFs are approximated by an intra-chain solvation pair potential, thus allowing its prediction of the intra- and inter-chain PCFs. On the other hand, Yu and Wu proposed an extended test-particle method (*J. Chem. Phys.* **118**, 3835, 2003), enabling prediction of these quantities using polymer density-functional theories (PDFTs). Here we directly compare the intra- and inter-chain PCFs predicted by various versions of PDFTs and SC-PRISM calculations with those obtained from Monte Carlo simulations. A simple model system of tangent hard-sphere chains allows us to unambiguously quantify the accuracy of these predictions as a function of the chain length and hard-sphere packing density.