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Hybrid Two-Chain Simulation and Integral Equation Theory: Application to Polyethylene Liquids HUIMIN LI, Dept. of Chemical Engr., Colorado School of Mines, Golden, CO 80401, DAVID T. WU, Dept. of Chemical Engr. and Chemistry, Colorado School of Mines, Golden, CO 80401, JOHN G. CURRO, Sandia National Laboratories, Albuquerque, NM 87185, JOHN D. MCCOY, Dept. of Materials Engr., New Mexico Technology, Socorro, NM 87801 —
We present results from a hybrid simulation and integral equation approach to the calculation of polymer melt properties. The simulation consists of explicit Monte Carlo (MC) sampling of two polymer molecules, where the effect of the surrounding chains is accounted for by an HNC solvation potential. The solvation potential is determined from the Polymer Reference Interaction Site Model (PRISM) as a functional of the pair correlation function from simulation. This hybrid two-chain MC-PRISM approach was carried out on liquids of polyethylene chains of 24 and 66 CH_2 units. The results are compared with MD simulation and self-consistent PRISM-PY theory under the same conditions, revealing that the two-chain calculation is close to MD, and able to overcome the defects of the PRISM-PY closure and predict more accurate structures of the liquid at both short and long range. The direct correlation function, for instance, has a tail at longer range which is consistent with MD simulation and avoids the short-range assumptions in PRISM-PY theory. As a result, the self-consistent two-chain MC-PRISM calculation predicts an isothermal compressibility closer to the MD results.

Huimin Li
Dept. of Chemical Engr., Colorado School of Mines, Golden, CO 80401

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