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**Molecular mechanics modeling of compressible polymer solutions based on an isobaric-isothermal ensemble.** MOEED SHAHAMAT, ALEJANDRO REY, McGill University — Understanding the thermodynamics and physical properties of polyethylene (PE) in hydrocarbons is significant for its industrial production. Of recent interest are atomistic simulations which provide a detailed molecular level insight without experimental efforts. This paper reports on the density of solutions of PE in hexane using molecular dynamics (MD) simulations at high pressures. The computed densities increase monotonically with raising external pressure and compare quite favorably with experimental and theoretical data. Furthermore, the effect of cut-off distance to density is investigated and it is shown that the density increases with increasing the cut-off radius. It has been revealed that for pressures below 100 bar the mixture density displays a large dependence on cut-offs and for higher pressures solution density and non-bonded interactions demonstrate weak sensitivity to cut-off distance. Analysis of the pair distribution function versus pressure shows that the amplitude of the first peak increases and the radial distribution function shifts to shorter separations reflecting structural change of the condensed phase. The implemented MD-NPT approach in this research provides a good insight into the polymer-polymer, polymer-solvent, and solvent-solvent interactions.

Moeed Shahamat  
McGill University

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