Equilibrium and Transport Simulations with a Density-Dependent m-6-8 United Atom Force Field

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The simulation methods necessary to compute virtually any thermophysical property for any material are available in the literature, but the lack of accurate force models to use in such simulations limits their utility. The long-term objective of this research is the development of a universal, transferable potential for accurate equilibrium and transport simulations. Using a so-called "m-6-8" potential form (which includes two terms in the dispersion series and allows for small adjustments to the repulsive wall strength) with united atom parameters optimized to second virial coefficient data, a pair potential model has been developed for small to medium hydrocarbons (linear and branched alkanes, alkenes, alkynes, and simple aromatics). Extension to the condensed phase has been performed through an effective triple-dipole potential, which takes the form of a density-dependent multiplier on the pair potential. In this paper, we detail simulation results obtained with the pair-only and density-dependent potential models with comparisons to other simulation force fields. In addition, we present results illustrating the phase regions and properties where triple-dipole interactions may reasonably be omitted and where they are non-negligible.