Thermophysical Properties of Fluids: From Simple Models to Applications

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Recent systematic and extensive computer simulations on realistic models have shown that the long-range interactions have only a marginal effect on the properties of fluids. This finding justifies the use of short-range models upon which a perturbation theory may be developed. Moreover, such models are usually also amenable to a theoretical treatment. Extended primitive models for water, methanol, ethanol, and carbon dioxide have been developed and two types of their applications to fluids are exemplified: (i) expressions for the thermodynamic properties of real fluids in a perturbed form are derived, and (ii) the primitive models are used directly in simulation studies to investigate the origin of specific phenomena, as e.g. preferential solvation in the mixed water-methanol solvent.