Coarse-grained modelling of complex fluids and electrolytes: From parameterization to applications

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Aqueous organic systems and electrolyte solutions are among the most important constituents of complex solutions involved in many industrial systems[1]. There is a need for accurate models able to both reproduce thermodynamic and transport properties of these systems[2]. Dissipative Particle Dynamics (DPD) seems to be a good alternative to standard atomistic simulations when dealing with large and complex systems. One of the key points in the accuracy of DPD simulations to reproduce thermo-physical properties is the availability of a thermodynamically consistent methodology to parameterize fluid-fluid interactions for different type of systems. Although several approaches have been proposed (Flory-Huggins c-parameter, Hildebrand solubility, etc.), they are not suitable for electrolytes or systems containing partially miscible molecules. We explore in this work several parameterization workflows able to address this problem. The obtained model will be illustrated through two examples: 1) the liquid-liquid equilibrium and interfacial tension of complex hydrocarbon systems, and 2) the osmotic coefficient for electrolyte solutions as a function of the salinity.

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[2] Z. Mester, A.Z. Panagiotopoulos. *J. Chem. Phys*. **142**, 044507 (2015)