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# Coarse-Grained Molecular Simulations to Estimate Thermophysical Properties of Phase Equilibria

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**Abstract :** Coarse-Grained (CG) molecular simulations have shown to be an efficient way to estimate thermophysical (static and dynamic) properties of fluids. Several strategies have been developed and reported in the literature for defining CG molecular models. Among them, those based on a top-down strategy (i.e. CG molecular models related to macroscopic observables), despite being heuristic, have increasingly gained attention. This is probably due to its simplicity in implementation and its ability to provide reasonable results for not only simple but also complex systems. Regarding simple Force-Fields associated with these CG molecular models, it has been found that the four parameters Mie chain model is one of the best compromises to describe thermophysical static properties (e.g. phase diagram, saturation pressure). However, parameterization procedures of these Mie-chain GC molecular models given in literature are generally insufficient to simultaneously provide static and dynamic (e.g. viscosity) properties. To deal with such situations, we have extended the corresponding states by using a quantity associated with the liquid viscosity. Results obtained from molecular simulations have shown that our approach is able to yield good estimates for both static and dynamic thermophysical properties for various real non-associating fluids. In addition, we will show that on simple (e.g. phase diagram, saturation pressure) and complex (e.g. thermodynamic response functions, thermodynamic energy potentials) static properties, results of our scheme generally provides improved results compared to existing approaches.

**Keywords :** coarse-grained model, mie potential, molecular simulations, thermophysical properties, phase equilibria
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