Extending the Capability of the SAFT-y Mie Group Contribution Approach

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A popular platform to increase the predictive capability of a thermodynamic description is a formulation within a Group Contribution (GC) approach. The SAFT-y Mie equation of state (EoS) is cast as a GC approach of the statistical associating fluid theory based on intermolecular Mie (generalized Lennard-Jones) potentials with variable repulsive and attractive ranges [1]. In this GC model, one represents the molecules as associating heteronuclear chains of fused spherical segments of various functional or chemical groups. Since its formulation in 2014 [2], the SAFT-y Mie EoS has been applied for providing an accurate description of the thermodynamic properties and fluid phase equilibria for a broad range of engineering applications. Indeed, it has been employed in the oil and gas industry to study the phase behavior of systems containing typical reservoir fluids (*i.e.*, alkanes, aromatics, water) [3] and in carbon capture and storage processes for density calculations or CO₂ absorption with amines. Additionally, it has been used in the pharmaceutical industry to predict the solvation, solubility, and partition coefficients of active pharmaceutical ingredients (e.g., paracetamol and lovastatin) [4]. The theory has been extended to predict the thermodynamic properties of aqueous electrolyte solutions [5]. In this contribution, we highlight the current capabilities of the SAFT-y Mie approach with a focus on the groups developed for the description of new chemical families. Investigations cover the phase equilibria and thermophysical properties of mixtures of relevance for industrial applications (including pharmaceuticals and carbon capture solvents), with modelling results being validated by comparison against literature experimental data.

References:

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