

# Predictive Models for the Phase Behaviour and Solution Properties of Weak Electrolytes: Nitric, Sulfuric and Carbonic Acids

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Electrolyte solutions are important in many natural and industrial processes. A sound modelling of the thermodynamic properties of electrolyte solutions is needed in both fields. Equations of state (EOS) are a versatile tool to describe the thermodynamic properties fluids. To describe electrolyte solutions, EOS for mixtures of molecular species are usually augmented with additional terms accounting for the long-ranged coulombic interactions present in these solutions. There has been significant progress in EOS modelling of solutions of strong electrolytes recently [1-3]. By contrast, solutions of weak electrolytes have rarely been studied.

In this work, the SAFT-VRE Mie EOS is extended to model weak electrolytes. To incorporate the dissociation reactions, thermodynamic equilibrium constants from experiments are taken from the literature and are coupled with the SAFT-VRE Mie modelling. Exemplary, models for three important inorganic acids are developed: nitric acid, sulphuric acid and carbonic acid. The models for the solvent water and the hydronium ion ( $\text{H}_3\text{O}^+$ ) are taken from previous work [3]. New models for the molecular acids and their anions are developed based on a fit to experimental data only of the respective acids in water. It is found that this parameter estimation is best carried out using data on the degree of dissociation and either phase equilibrium or activity data. The obtained SAFT-VRE Mie models describe different thermodynamic properties of the aqueous acids, such as densities, osmotic coefficients, activity coefficients, and vapour pressures of the solutions reliably over a wide temperature range.

## References

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