Modeling thermodynamic properties of mixed-solvent electrolyte solutions using ePPC-SAFT

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Electrolyte solutions are important in many industrial processes, e.g., CO_2 capture and sequestration, flue gas treatment, desalination, scale formation, corrosion resistance enhancement, batteries, pharmaceutical processes, etc. Modeling of thermodynamic properties of mixed-solvent electrolyte solutions is challenging.

In this work, the thermodynamic properties of (water + alkali halide) and (water + alcohol + alkali halide) are modelled using the ePPC-SAFT model [1, 2], that includes hard-chain, dispersion, association, non-additive hard sphere, mean spherical approximation (MSA), and Born contributions. The model is parameterized based on mean ionic activity coefficient (MIAC), vapour liquid equilibria (VLE), and liquid density, using reference databases proposed in previous works [3, 4]. Physically consistent ionic parameters are obtained based on thermodynamic properties in the aqueous solutions in an ion-specific approach, and used as is in mixed-solvent electrolyte solutions. The impacts of the relative permittivity and ionic diameters are investigated. Ion-pairing is accounted for using the association term. Wertheim and Bjerrum association functionality are compared. Contributions of the model terms are analysed. The model is tested on properties that have not been used in the parameterization.

References

[1] S. Ahmed, N. Ferrando, J.C. de Hemptinne, J.P. Simonin, O. Bernard, O. Baudouin. *Fluid Phase Equilib.*, 459, 138-157 (2018).
[2] J.S. Roa Pinto, N. Ferrando, J.C. de Hemptinne, A. Galindo. *Fluid Phase Equilib.,* 560, 113486 (2022).
[3] F. Yang, T.D. Ngo, G.M. Kontogeorgis, J.D. de Hemptinne, *Ind. Eng. Chem. Res.*, *in press* (2022).
[2] F. Yang, J. Qu, G.M. Kontogeorgis, J.D. de Hemptinne, *J. Phys. Chem.Ref. Data*, *in press* (2022).