Comparisons of Equation of State for Electrolytes: e-CPA and e-PPC-SAFT

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Since many applications in chemical engineering, including the increasingly important fields of carbon capture and storage and biotechnology, includes electrolytes it is of great importance that electrolyte systems can be accurately modelled [1]. Due to the long-range nature of the ionic interactions, even small amounts of ions can have a great impact on the overall system. Several aspects of the ionic interactions makes the modeling of electrolyte systems difficult [2] and models for electrolytes have not kept up with their non-electrolyte counterparts. There is therefore a need for improved models for the description of electrolyte systems.

In this work two successful equations of states, e-CPA [3] and e-PPC-SAFT [4], are compared. Parameters are optimized from the same data set and the adjustable parameters of the models are selected so they describe similar physics. In this way, the models are compared on a fair basis. The tests of the models also includes using various models for the relative static permittivity, which plays a significant role in modelling electrolyte solutions. Finally, several different sets of adjustable parameters are considered that describes different physics of the models and comparisons among these sets allows several aspects of the models and model terms to be uncovered.

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