

عنوان مقاله:

Application of the Non-Primitive MSABased Models in Predicting the Activity and the Osmotic Coefficients of Aqueous Electrolyte Solutions

محل انتشار:

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خلاصه مقاله:

The Non-primitive MSA based models (NP-MSA) were used to correlate the individual and the mean ionic activity coefficients of the symmetric and asymmetric aqueous electrolyte solutions. The results of the models for the mean ionic activity coefficients were directly used to calculate the osmotic coefficient for the electrolyte solutions studied in this work. In the NP-MSA models, the Ghotbi-Vera and the Boublik- Mansoori-Carnahan-Starling-Leland hard sphere equation of state as the reference system coupled with the non-primitive mean spherical approximation model (NP-GVMSA and NP-BMCSL-MSA models respectively). In correlating the mean ionic activity coefficients of electrolyte solutions, while the hard sphere diameters for anion were treated as a concentration-independent adjustable parameter, the diameters for cation were assumed to be concentration dependent. In the use of the non-primitive MSA-based models in correlating the individual ionic activity coefficients of electrolyte solutions, both anion and cation diameters were considered to be concentration dependent. The results for the mean ionic activity coefficients obtained from the NP-GV-MSA model compared favorably with those of the NP-BMCSL-MSA model produced in this work and also with those of NP-BMCSL-MSA available in the literature. It was shown that the NP-GV-MSA model more accurately calculate the mean ionic activity and the osmotic coefficients than those obtained from the NP-BMCSL-MSA models.

کلمات کلیدی:

electrolyte solution, non-primitive model, means spherical approximation, hard sphere, ionic activity coefficient and osmotic coefficient

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