

New Mean Spherical Approximation Method for Prediction of Solid Liquid Equilibria in Mixed Aqueous Electrolyte Solution

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The mean spherical method is improved by introduction of the new hard sphere equation of state. Solid liquid equilibria of mixed electrolyte solution play an important role in separation operation for many industrial processes involving electrolyte solution and prediction of activity coefficients is key problem to perform the calculation of solid liquid equilibria. In this work a new hard sphere equation of state with tetrakaidakahedron used and expanded to mixed hard sphere solution according to Santos mixing rule. thermodynamic properties like helmholtz free energy, chemical potential and finally activity coefficient of hard sphere system calculated and used as short range contribution in MSA method. New MSA model used in solid-liquid equilibria of mixed electrolyte solutions to calculate mean ionic activity coefficients at saturation conditions. Solid-liquid equilibria of ten systems modeled fairly with root mean square deviation about 0.01. The result compared with original MSA method and it is shown that MSA model combined with new hard sphere EOS can correlate the result better than BMSCL EOS.