

Modeling Surface Tension of Aqueous and Mixed-Solvent Electrolyte Systems

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A model has been developed for calculating the surface tension of aqueous, non-aqueous, and mixed-solvent electrolyte systems ranging from dilute solutions to fused salts. The model consists of a correlation for computing the surface tension of solvent mixtures and an expression for the effect of electrolyte concentration. The effect of electrolyte concentration has been derived from the Gibbs equation, which relates the surface tension to the surface excess of species. The surface excess is expressed using a modified Langmuir adsorption isotherm. The model extends the Langmuir adsorption formalism by introducing the effects of binary interactions between solute species (ions or molecules) on the surface. This extension is especially important for high electrolyte concentrations and in strongly speciated systems. The combined model has been shown to reproduce experimental data for a variety of mixtures. In particular, it accurately predicts the surface tension of ternary solvent mixtures using parameters determined from only binary data. The surface tension model has been coupled with a previously developed thermodynamic equilibrium model to provide speciation and activity coefficients, which are necessary for electrolyte systems. This makes it possible to reproduce the effects of complexation or other reactions in solution. In all cases for which experimental data are available and have been tested, the new model has been shown to be accurate for reproducing surface tension over wide ranges of temperature and concentration.