



THE ORGANIZATION, EVALUATION AND MODELING OF EXPERIMENTAL DATA : DEVELOPMENT OF A THERMODYNAMIC DATABASE, EVALUATION OF ENTHALPY DATA, MODELING PHASE BEHAVIOR IN AQUEOUS ELECTROLYTE MIXTURES

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Enthalpy data are crucial for design and operation of efficient chemical processes. Available experimental enthalpy data accuracy may be questionable when taken from multiple sources, each perhaps with a unique reference state and experimental background. The accuracy of the enthalpy data in the GPA database is evaluated with the application of equations of state and statistical analysis. Electrolyte systems, particularly aqueous electrolyte mixtures, are an important component of both natural and industrial processes. A fundamental understanding of electrolyte mixtures is crucial for interpreting natural phenomenon and vital for effective design and operation of chemical process separations. Accurate thermodynamic models and better comprehension of the underlying chemistry and physics are needed to improve the design of separation equipment. This work describes an extension and improvement of a vapor-liquid equilibrium solution method for weak electrolyte solutions focusing on carbon dioxide (CO₂), hydrogen sulfide (H₂S), sulfur dioxide (SO₂) and ammonia (NH₃). Additional considerations include systems of strong electrolytes in solutions of mixed weak and strong electrolytes.

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