MEASUREMENTS AND MODELS FOR HAZARDOUS CHEMICAL AND MIXED WASTES

EMSP Project Number 60155

June 15, 2001

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PROGRESS REPORT

Research Objectives

Aqueous waste of various chemical compositions constitutes a significant fraction of the total waste produced by industry in the United States. A large quantity of the waste generated by the U.S. chemical process industry is waste water. In addition, the majority of the waste inventory at DoE sites previously used for nuclear weapons production is aqueous waste. Large quantities of additional aqueous waste are expected to be generated during the clean-up of those sites. In order to effectively treat, safely handle, and properly dispose of these wastes, accurate and comprehensive knowledge of basic thermophysical property information is paramount. This knowledge will lead to huge savings by aiding in the design and optimization of treatment and disposal processes. The main objectives of this project are:

- Develop and validate models that accurately predict the phase equilibria and thermodynamic properties of hazardous aqueous systems necessary for the safe handling and successful design of separation and treatment processes for hazardous chemical and mixed wastes.

- Accurately measure the phase equilibria and thermodynamic properties of a representative system (water + acetone + isopropyl alcohol + sodium nitrate) over the applicable ranges of temperature, pressure, and composition to provide the pure component, binary, ternary, and quaternary experimental data required for model development.

Research Progress and Implications

As of August, 2001, forty-two months into the a three year project, we have made significant progress in the database development, developed and tested the models, have completed the pure component measurements, and have measured selected binary and ternary mixtures.

Database Development: An extensive literature search has been completed and the data are being compiled in a database on the internet shared by NIST and MTU. The database includes the vapor pressures, densities, and permittivities of the pure solvents; and the VLE, densities, and activity coefficients of the mixtures. It also includes a literature search on liquid phase activity models used with these systems. The database has been extended to over 250 data publications and over 100 modeling publications. The database will continue to be updated. These data were used to determine what compositions and temperatures are needed to complete and validate the data for each binary mixture

Model Development: Two models were investigated by NIST and MTU. The NIST model concentrates on the phase equilibria and coexisting densities and the MTU model concentrates on the liquid phase activities. The model developed at NIST for the phase equilibria and the densities of the coexisting phases uses the Peng-Robinson-Stryjek-Vera cubic equation of state for both the liquid and vapor phases. The density correction of Mathias et al.[1] is applied to the liquid density. The Wong-Sandler mixing rule is employed, with the NRTL model used for activity coefficient contributions to the mixing rules. This allows the cubic equation of state to be used for mixtures containing ions and other nonvolatile species. The model has been tested with pure solvents, solvent mixtures and solvent mixtures with salt. The model performs well predicting the vapor pressure and vapor composition, given the temperature and liquid composition, for pure solvents and solvent mixtures.

The model under development at MTU for the liquid phase activities uses the UNIFAC or UNIQUAC parameters. The models are being evaluated with the preliminary database.

Experimental Measurements: The data for this project were measured on three different apparatus. The three apparatus required are an ebulliometer at MTU, a high temperature/high pressure phase equilibria apparatus at NIST for azeotropic aqueous-organic-salt mixtures, and a coexisting density and vapor-liquid equilibrium apparatus at NIST. The activity coefficients from the ebulliometer measurements will be validated with the activity coefficients calculated from the vapor-liquid equilibrium data.

The pure component measurements are completed. The new ebulliometer at MTU is complete. Solvent-solvent and solvent-water measurements at MTU and NIST are complete. Water-salt measurements at NIST are complete. MTU and NIST are currently measuring water-solvent-salt mixtures.

Planned Activities

Remaining tasks:

- Test the model with a complete set of data.

- Combine the MTU and NIST modeling and measurement results.
- Prepare a final report on the project

[1] P.M. Mathias, T. Naheiri, and E.M. Oh. 1989. "A Density Correction for the Peng-Robinson Equation of