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**TITLE: HIGH TEMPERATURE HIGH PRESSURE THERMODYNAMIC MEASUREMENTS FOR COAL MODEL COMPOUNDS**

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## I. ABSTRACT

**OBJECTIVE:** The overall objective of this project is to develop a better thermodynamic model for predicting properties of high-boiling coal derived liquids, especially the phase equilibria of different fractions at elevated temperatures and pressures. The development of such a model requires data on vapor-liquid equilibria (VLE), enthalpy, and heat capacity which would be experimentally determined for binary systems of coal model compounds and compiled into a database. The data will be used to refine existing models such as UNIQUAC and UNIFAC.

**WORK DONE AND CONCLUSIONS:**

The flow VLE apparatus designed and built for a previous project was upgraded and recalibrated for data measurements for this project. The modifications include better and more accurate sampling technique, addition of a digital recorder to monitor temperature and pressure inside the VLE cell, and a new technique for remote sensing of the liquid level in the cell. VLE data measurements for two binary systems, benzene – ethylbenzene and ethylbenzene –quinoline, have been completed. The temperature range of data measurements was 180 C to 300 C for the first system, and 225 C to 380 C for the second system. The smoothed data were found to be fairly well behaved when subjected to thermodynamic consistency tests.

SETARAM C-80 calorimeter has been used for excess enthalpy measurements for benzene – ethylbenzene and ethylbenzene – quinoline binary liquid mixtures. Data were measured from 30 C to 285 C for liquid mixtures covering the entire composition range.

An apparatus has been designed for excess volume measurements for liquid mixtures at temperatures from 30 C to 300 C. The apparatus is currently being tested with data measurements for the ethylbenzene – quinoline system.

The combined VLE and liquid enthalpy data have been used to regress temperature dependent binary interaction parameters in the Wilson, NRTL and UNIQUAC activity coefficient models, and the temperature dependent binary group interaction parameters in the UNIFAC model. As a result, the above activity coefficient models have been extended for thermodynamic property calculation of coal model compounds at high temperatures and pressures.

All the work completed so far was done by the two graduate students, Mr. Ahmad Al-Ghamdi who finished his M.S. thesis in March 1997, and Mr. Qingwen Zhao who is expected to graduate with M.S. in chemical engineering in December, 1998.

**HIGHLIGHTS OF ACCOMPLISHMENTS:**

1. VLE data measurements for benzene-ethylbenzene, and ethylbenzene-quinoline have been completed.
2. Excess enthalpy measurements for benzene-ethylbenzene liquid mixtures have been completed.
3. Excess enthalpy and excess volume data for ethylbenzene-quinoline liquid mixtures are being measured.
4. The measured experimental data together with data available in the literature are being used to regress temperature dependent binary interaction parameters in different activity coefficient models.

**SIGNIFICANCE TO FOSSIL ENERGY PROGRAM:** Thermodynamic properties of coal derived liquids are essential for efficient design of coal liquefaction processes. Generalized models for these properties are, therefore, very much needed. Experimental data, especially at advanced temperatures and pressures are necessary for development of accurate models.

**FUTURE PLANS:** In the remaining months of this project, the work will be completed and the overall result will be a generalized model for thermodynamic properties of coal model compounds at high temperatures and pressures. Temperature dependent binary interaction parameters will be presented for the specific activity coefficient models, such as, Wilson, NRTL and UNIQUAC correlations, as well as the generalized UNIFAC group contribution model.

## II. ARTICLES AND PRESENTATIONS

1. V. N. Kabadi, "Thermodynamics of Coal Derived Fluids 3. VLE and Heat Capacities of Coal Liquid Fractions", FUEL, 75, 363, 1996.
2. A. Al-Ghamdi, S. Mahmood, and V.N. Kabadi, "A Flow Apparatus for High Temperature VLE Measurements", J. Chem. Eng. Data, in review.
3. Q. Zhao, and V. N. Kabadi, "Excess Enthalpy Measurements for Benzene-Ethylbenzene Liquid Mixtures from 30 C to 285 C", to be submitted to J. Chem. Eng. Data.

## III. STUDENTS SUPPORTED

Ahmad Al-Ghamdi, M.S. Chemical Engineering (completed March, 1997)
Qingwen Zhao, M.S. Chemical Engineering (expected December, 1998)
Shani Francis, undergraduate (Junior) ChE student
Tesila Sexton. undergraduate (Junior) ChE student