**THERMODYNAMIC AND RHEOLOGICAL
PROPERTIES OF SOLID-LIQUID SYSTEMS
IN COAL PROCESSING**

**Topical Report
June 30, 1995**

Prepared by

**Vinayak N. Kabadi
Chemical Engineering Department
North Carolina A&T State University
Greensboro, North Carolina 27411**

Submitted to

**United States Department of Energy
Pittsburgh Energy Technology Center
Pittsburgh, Pennsylvania 15236**

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Under Grant Number : DE-FG22-91PC91300

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PROJECT OBJECTIVES AND SCOPE:

The objective of this project is to develop a model for solid-liquid equilibria and a model for viscosities of the products of coal liquefaction processes. The same characterization procedure and representation by continuous distributions as used in our previous work on vapor-liquid equilibria and excess enthalpies of coal liquids will be used. Models when fully developed will give the solid-liquid phase equilibrium properties and viscosities as functions of temperature and pressure for known molecular weight distribution and structural characterization of the coal liquid. To accomplish this well, the project requires three tasks:

- (1) Solid-Liquid phase equilibrium model development: This will require data compilations for vapor pressure of solids and available single and multi-component solid-liquid phase equilibrium data. Model development will include models for thermodynamics of solids such as in coal products, thermodynamics of defined solid-liquid systems and finally application to complex coal derived products.
- (2) Experimental Viscosity Measurements: A viscometer will be purchased to measure viscosities of coal liquids and slurries at different temperatures and pressures. The data will be used in conjunction with literature data for viscosity model development.
- (3) Viscosity Model Development: Viscosity model development will require collection of physical property data for model compounds to estimate the model parameters. Both group contribution and corresponding states methods will be used to account of the effect of pressure and temperature on the liquid viscosity. The model will then be extended to coal liquid fractions. The experimentally measured viscosity data will be used to evaluate the model and recommend modifications.

SUMMARY OF ACCOMPLISHMENTS:

This project consisted of two different tasks: 1. Development of a model to compute viscosities of coal derived liquids, and 2. Investigate new models for estimation of thermodynamic properties of solid and liquid compounds of the type that exist in coal, or are encountered during coal processing.

As for task 1, a model for viscosity computation of coal model compound liquids and coal derived liquids has been developed. Two papers, the first describing the pure liquid model and the second one discussing the application to coal derived liquids, are expected to be published in Energy & Fuels shortly.

Marginal progress is reported on task 2. Literature review for this work included compilation of a number of data sets, critical investigation of data measurement techniques available in the literature, and investigation of models for liquid and solid phase thermodynamic computations. During the preliminary stages it was discovered that for development of a liquid or solid state equation of state, accurate predictive models for a number of saturation properties, such as, liquid and solid vapor pressures, saturated liquid and solid volumes, heat capacities of liquids and solids at saturation, etc. Most of the remaining time on this task was spent in developing predictive correlations for vapor pressures and saturated liquid volumes of organic liquids in general and coal model liquids in particular. The vapor pressure model and the saturated liquid volume model are scheduled to appear in Fluid Phase Equilibria and AIChE Journal respectively.

PUBLICATIONS RESULTING FROM THE PROJECT:

The following manuscripts were prepared and submitted for publication as a result of the research conducted under this grant. No patents resulted from this grant.

1. M. Palakkal and V. N. Kabadi, "Viscosity of Coal Derived Liquids 1. A Group Contribution Method for Pure Model Compound Liquids, " accepted by Energy & Fuels.
2. V.N. Kabadi and M. Palakkal, "Viscosity of Coal Derived Liquids 2. Application of the Model to Coal Liquid Fractions," submitted to Energy & Fuels.
3. J. Wang and V. N. Kabadi, "A Predictive Vapor Pressure Correlation for Organic Liquids," Fluid Phase Equilibria, in Review.
4. J. Wang and V. N. Kabadi, "Generalized Method for Prediction of Saturated Liquid Volumes Using Modified Rackett Equation and Van der Waals Volumes," accepted by AIChE Journal.

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