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PHASE EQUILIBRIUM PROPERTIES OF COAL-DERIVED LIQUIDS

Technical Progress Report for the
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Abstract

On July 1, 1980, work was initiated on a program for experimental vapor liquid equilibrium measurements on coal derived liquids. The principal investigators on the program are Dr. V. F. Yesavage and Dr. A. J. Kidnay, Department of Chemical and Petroleum Refining Engineering, Colorado School of Mines, Golden, Colorado. During the first six months of the program the type of phase behavior apparatus was selected and detailed design on the system was initiated including selection and sizing of all major equipment. At present all major equipment are on order and it is anticipated that fabrication of the equipment will be performed during the next six months.

Objective and Scope of Work

Thermodynamic property research is justly recognized as invaluable by process and design engineers in the petroleum, chemical, and allied industries. Thermodynamic data for pure fluids or complex mixtures, are essential in the optimum design of both physical and chemical processing units.

Coal derived liquids are a new and vital class of industrial compounds for which there are limited thermodynamic data. The principle investigators have conducted a program in the measurement and correlation of the enthalpy of coal derived liquids. Programs have also been undertaken to measure volumetric properties and K values of light gas - model compound systems and to measure dew points, vapor pressures and hydrogen solubilities in model compound and coal derived liquid systems. The objective of the present study is to measure equilibrium K values of coal derived liquids and

model compounds representative of coal liquids, and to use the results in the development of engineering correlations.

The program is divided into three major areas:

- 1) Design, construction, and evaluation of an equilibrium flash vaporization system for temperatures between 70 and 700°F, at pressures up to 2000 psia.
- 2) Measurements on samples of both coal derived liquids and mixtures of model compounds.
- 3) Preparation of engineering correlations for the measured K values and vapor liquid equilibria.

SUMMARY OF PROGRESS TO DATE

PROJECT PLAN AND PROGRESS												
Task	Work Statement	1980		1981			1982					
		7	12	1	6	7	12	1	6	7	12	
1	Equipment Design
2	Construction and Evaluation of Equipment
3	Experimental Measurements
4	Characterization of Samples and Products
5	Testing of Correlations

Work in Progress

Scheduled Work

SCHEDULE OF EXPENDITURES

Detailed Description of Technical Progress

Design & Fabrication of Vapor Liquid Equilibrium Apparatus

A wide variety of different kinds of equipment have been used to study the phase behavior of mixtures. The methods that have been employed include:

- a) Measuring the phase boundary of binary mixtures.
- b) Observing property discontinuities from volumetric measurements and thermal measurements of mixtures.
- c) Measuring the composition of samples in batch systems.
- d) Measuring the composition of samples from continuous remixing and separation in recirculating systems.
- e) Gas-liquid chromatography.
- f) Measuring the composition of samples from a once-through flow systems.

A major difficulty associated with measuring phase behavior of complex mixtures is the need to characterize the vapor and liquid sample products. This generally requires the collection of considerable quantities of the liquid and vapor products. Of all the methods listed above, the only method which can generate significant quantities of both liquid and vapor products is the once-through flow method. This method has been used previously in determining the K values for petroleum fractions.

For these reasons, we have designed a flow equilibrium flash vaporization system similar to the ones previously used on petroleum liquids.

Our system flow diagram is illustrated in Figure 1. The liquid under study will be pumped from the feed tank into a fluidized sand bath. The pump which will be used is a Pulsafeeder positive displacement reciprocating pump. The fluidized sand bath will be used as a preheater.

The fluid will then enter the equilibrium cell which will be enclosed in an air bath. The air bath will be an oven manufactured by Hotpack. It will have a maximum operating temperature of 350°C and a window for observation of the cell. The equilibrium cell will be a Jerguson windowed gage. The window will allow the monitoring of the liquid level. Temperature within the oven will be measured with a platinum resistance thermometer using a Kiethly digital multimeter.

Vapor will exit from the top and liquid from the bottom of the cell. Both vapor and liquid products will flow through heat exchanger coolers and will be collected in atmospheric separators for characterization or returned to the feed tank. The system is designed for mixing and recirculating of the two products; however, recirculation may not be feasible

VAPOR LIQUID EQUILIBRIUM APPARATUS

if significant composition upsets occur in the feed. The vapor and liquid samples will be collected during steady state operation.

Pressure measurements will be made using a Ruska differential pressure indicator in connection with a series of Heise bourdon tube gauges.

All major equipment is on order and one item has been delivered. Construction should begin within the next several months.

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