DOE/PC/90302--T6

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DE93 012266

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PROJECT TITLE: "Equilibrium and Volumetric Data and Model Development for Coal Fluids"

PROJECT PERIOD: October 1, 1992 to December 31, 1992

SUMMARY

During the present reporting period, the solubilities of hydrogen in benzene were measured at temperatures from 323.2 to 423.2 K (122.0 to 302.0 °F) and pressures to 15.7 MPa (2281 psia). These data are described with root-mean-square errors typically less than 0.001 in mole fraction by the Soave-Redlich-Kwong and Peng-Robinson equations of state when a single interaction parameter, C_{ij}, is used for each isotherm.

DE-FG22-90PC90302

EQUILIBRIUM AND VOLUMETRIC DATA AND MODEL DEVELOPMENT FOR COAL FLUIDS

Report for the Period
October1, 1992 to December 31, 1992

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EQUILIBRIUM AND VOLUMETRIC DATA AND MODEL DEVELOPMENT FOR COAL FLUIDS

ABSTRACT

The proper design, operation, and optimization of coal conversion and utilization processes depend heavily on knowledge of the phase behavior of the mixtures encountered in these processes. Frequently quoted statistics suggest that in conventional chemical plants 70% of the capital and 90% of the operation expenses are associated with phase separations. Since multiple stages occur in almost all stages of coal conversion processes - from feed preparation through conversion reactions to product separation - the proper description of phase behavior is important in each step of these processes.

The long term goal of our efforts is to develop accurate predictive methods for description of equilibrium phase properties for a variety of types of mixtures and operating conditions. The specific objectives of the work specified herein include:

(1) development of an experimental facility having the capability to provide data on equilibrium phase compositions (solubilities) and liquid densities, and doing so with greater accuracy and speed than our previous facility,

(2) measurement of equilibrium phase properties for systematically selected mixtures - specifically those containing important solute gases (such as hydrogen, carbon dioxide, methane, ethane, carbonyl sulfide, ammonia) in a series of heavy paraffinic, naphthenic and aromatic solvents (e.g., n-decane, n-eicosane, n-octacosane, n-hexatriacontane, cyclohexane, decalin, perhydrophenanthrene, perhydropyrene, benzene, naphthalene, phenanthrene, pyrene),

(3) testing/development of correlation frameworks for representing the phase behavior of fluids of the type encountered in coal conversion processes, and

(4) generalization of parameters in the correlation frameworks to enable accurate predictions for systems of the type studied, permitting predictions to be made for

systems and conditions other than those for which experimental data are available.

During the present reporting period, the solubilities of hydrogen in benzene were measured at temperatures from 323.2 to 423.2 K (122.0 to 302.0 °F) and pressures to 15.7 MPa (2281 psia). These data are described with root-mean-square errors typically less than 0.001 in mole fraction by the Soave-Redlich-Kwong and Peng-Robinson equations of state when a single interaction parameter, C_{ij}, is used for each isotherm.

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