COAL LIQUEFACTION: INVESTIGATION OF REACTOR PERFORMANCE, ROLE OF CATALYSTS AND PCT PROPERTIES. QUARTERLY PROGRESS REPORT, OCTOBER 1, 1984-DECEMBER 31, 1984

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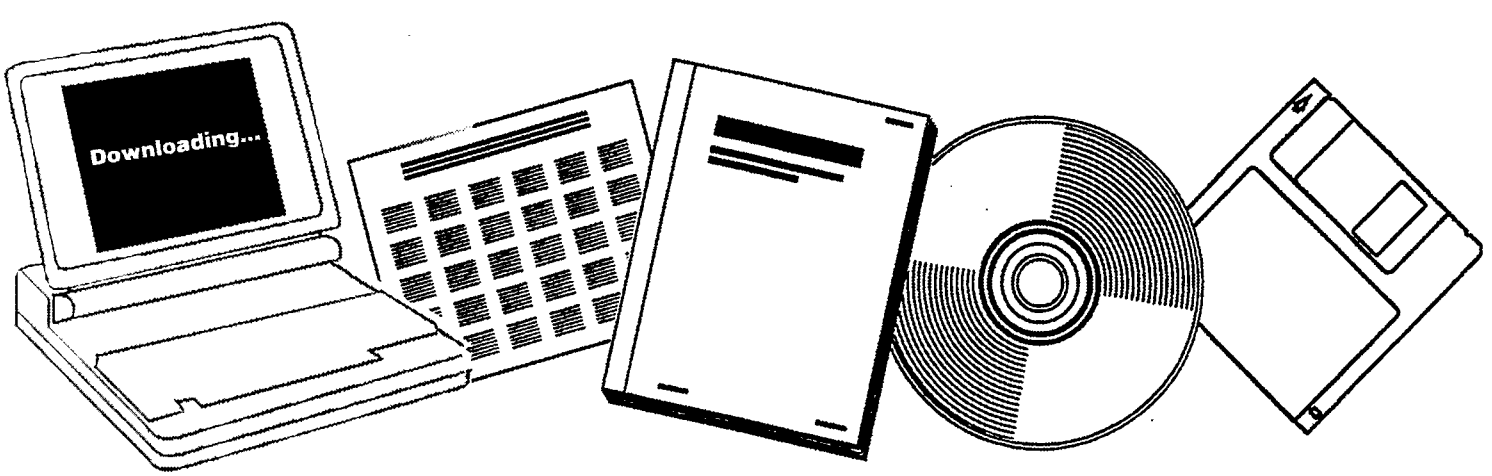

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Quarterly Progress Report

Coal Liquefaction - Investigation of Reactor Performance, Role of Catalysts and PCT Properties

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DISCLAIMER

1. Objective and Scope of Work

The objective of this work is to investigate areas of science and technology that have been defined as being of prime interest to coal processing technology development. These area include properties of coal liquids and slurries, reactor design, and performance in relation to reaction mechanisms. The work comprises investigations of the following high priority areas.

--Reaction kinetics and reactor performance in direct coal liquefaction

--Role of catalysts in indirect liquefaction and direct coal liquefaction

--Physical, chemical, and thermodynamic properties of coal liquefaction products.

Work done during the first year of work on this project is summarized in a Technical Progress Report submitted to the Department of Energy dated October 1984.

2. Progress During Quarter

This report summarizes work done during the period October 1, 1984 through December 31, 1984. A detailed description of work in each of the three tasks is given below.

Task 1. Reactor Kinetics and Reactor Performance in Direct Coal Liquefaction.

A computer simulation of a slurry reactor used in direct coal liquefaction was prepared during the first year of work on this project. The simulator is written in FORTRAN language and is general in the sense that by including different kinetic mechanisms a variety of direct coal liquefaction processes can be handled. Work during the second year of this project includes continued development and testing of the simulator for direct coal liquefaction processes and creation of new modules for other coal liquefaction

processes. The direct liquefaction processes being studied are the EDS (Exxon Donor Solvent) and the TSL (Two Stage Liquefaction). Other processes which are being incorporated into the simulator are the Fischer-Tropsch process, methanol synthesis, and the Mobil methanol-to-gasoline process. The computer modules are being developed in such a way that they can be used with the ASPEN simulator with a minimum of modification.

Task 2. Role of Catalysts in Indirect Liquefaction and Direct Coal Liquefaction.

A comprehensive report on indirect liquefaction was prepared during the first year on this project. This work is continuing, with attention being given to methanol synthesis via methyl formate, the role of CO_2 in methanol synthesis, and the various uses of CO_2 which is a by-product of coal conversion processes. The use of added catalysts in direct coal liquefaction will be studied as will novel methods for the liquefaction of coal.

The synthesis of methanol via methyl formate is of significant commercial interest because it permits carrying out the reaction at relatively low temperatures where the theoretical conversion per pass is much higher than at the higher temperatures used in direct methanol synthesis. The reaction takes place in two steps--the first being the conversion of methanol to methyl formate and the second the hydrogenolysis of methyl formate to methanol.

The role of CO_2 in methanol synthesis is not completely understood. There is evidence that supports the almost amazing finding that methanol, although made from CO, H_2, and 4-6% CO_2, may proceed entirely through CO_2 rather than through CO. The evidence for this will be examined.

Task 3. Physical, Chemical and Thermodynamic Properties of Coal Liquefaction Products.

Methods for estimating most of the important physical properties of coal liquids and products have been presented in the report prepared for the first year of work on the project. Work during the second year will be concentrated on incorporating these methods in the computer simulator which is being developed in Task 1.

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