COAL LIQUEFACTION: INVESTIGATION OF REACTOR PERFORMANCE, ROLE OF CATALYSTS, AND PCT PROPERTIES. TECHNICAL PROGRESS REPORT

PITTSBURGH UNIV., PA. DEPT. OF CHEMICAL AND PETROLEUM ENGINEERING

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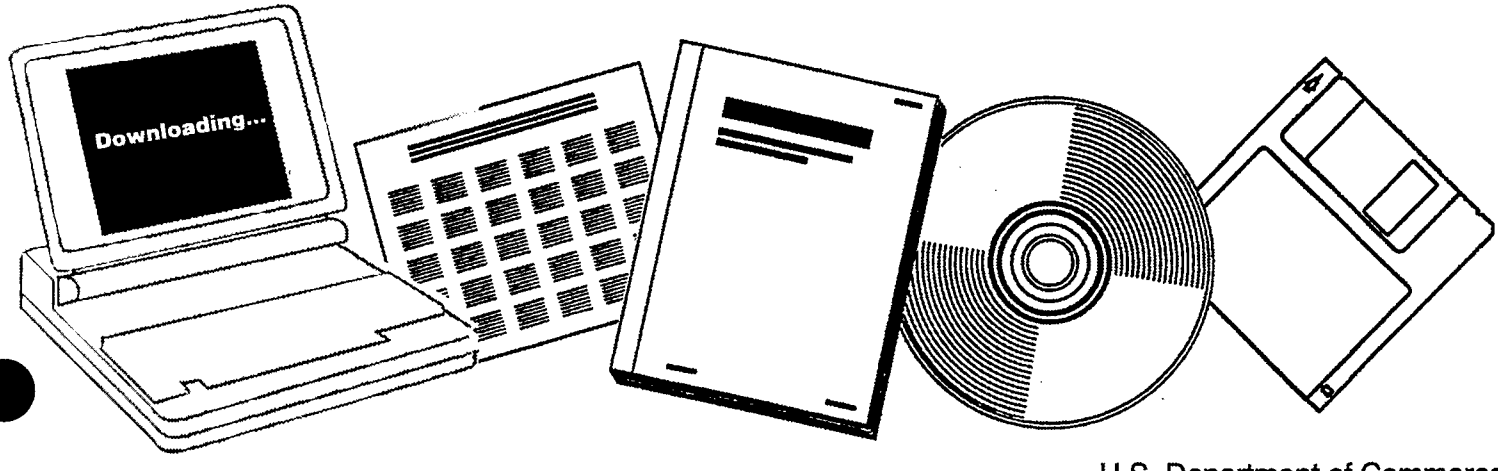

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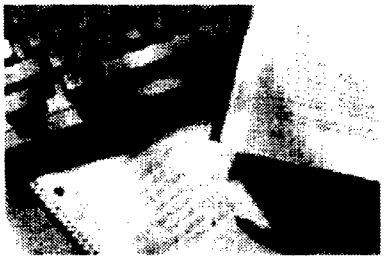

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TECHNICAL PROGRESS REPORT

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

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INTRODUCTION

The production of liquid fuels from coal is an important area of coal processing science and technology. Future demands for such liquids are expected to increase, and expected declining supplies of petroleum-based fuels will be unable to meet anticipated needs. Three areas of special interest to coal liquefaction are being studied in an on-going project at the University of Pittsburgh. They are reactor design and performance, the role of catalysts, and properties of coal liquids and slurries in direct and indirect coal liquefaction. This report presents the findings of the second year of work. The first year's work was submitted as a Technical Progress Report in October, 1984 to the Department of Energy.

The work was performed by faculty members, staff, post doctoral students, and graudate students in the Chemical and Petroleum Engineering Department, University of Pittsburgh in the period from October 1, 1984 through September 30, 1985.

The faculty members who participated were Alan Brainard, Yatish Shah, John Tierney, and Irving Wender, together with A. Sayari, a visiting research associate. Sebastian Joseph was the postdoctoral student, and Awdhoot Kerkar and Sadettin Ozturk were the graduate students.

SUMMARY

The report is divided into two sections plus an appendix. The first section reports on computer simulations which were developed for three important coal liquefaction processes -- the Mobil Methanol to Gasoline (MTG) process, the Fischer-Tropsch (F-T) process, and the synthesis of methanol. The models are designed to be general and information such as new kinetic equations or new physical property information can be readily added. Each of the models also provides for alternate reactor configurations. For the MTG process either a fixed bed or a fluidized bed can be used. The F-T model provides for a bubble column slurry reactor, a fluidized bed reactor or a fixed bed reactor. Either a fixed bed or a slurry bed can be used in the methanol synthesis model. A comparison of results obtained using the models and results reported in the literature is included to verify the model. Comparisons of alternate processing methods are also included to provide guidance in the selection of a reactor configuration for a specific process. Complete program listings are given in the Appendix, and sample problems with inputs and outputs are provided for the user. The programs are written in the FORTRAN language. It is ultimately desirable to make these models available in a form which can be used in ASPEN, the process simulator developed for DOE. As a first step, the use of ASPEN PLUS to predict thermodynamic and transport properties of systems of interest to coal liquefaction was studied.

In the second section, five areas of potential importance to indirect and direct coal liquefaction are reviewed. They are the synthesis of methanol via methyl formate, the role of carbon dioxide in methanol synthesis, the

synthesis of methanol using noble metal catalysts, the catalytic synthesis of higher alcohols from a new, high-yield sulfur-tolerant catalyst, and the direct liquefaction of coal mixed with heavy oils -- so-called coprocessing. Some unexpected but desirable synergistic effects are found when these two forms of fossil fuels, coal and heavy oil, are processed together. For each of these topics, a careful review of the literature was made and the reported findings evaluated. In certain cases, notably the role of carbon dioxide in methanol synthesis, conflicting experimental results and theories have been reported, although it does appear that the commercial synthesis of methanol proceeds through a carbon dioxide intermediate.

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