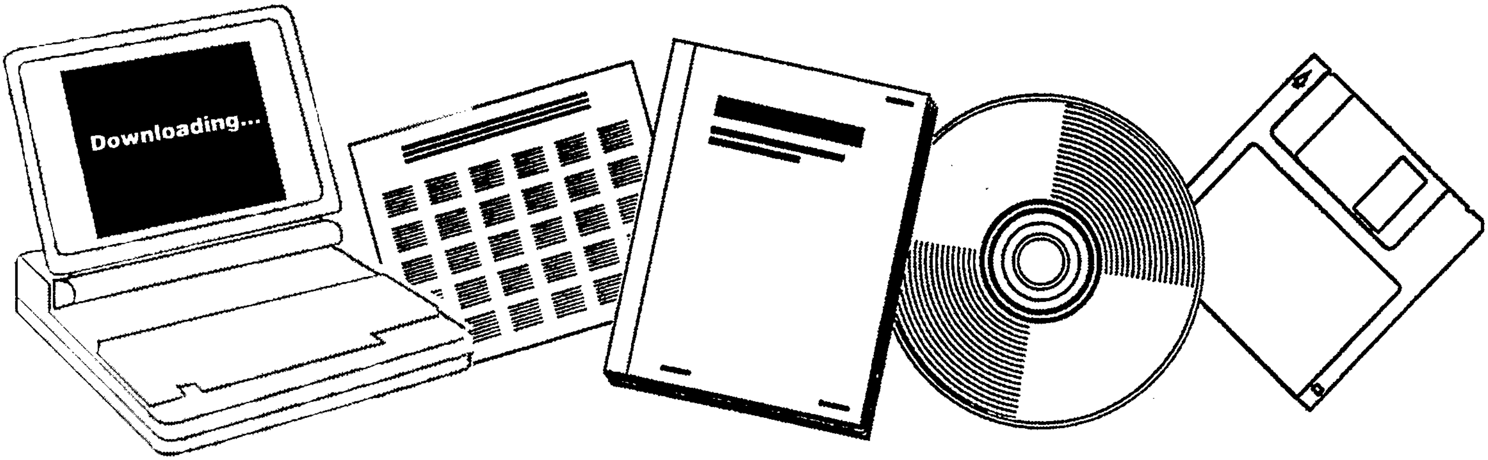
DE85015104

COAL LIQUEFACTION: INVESTIGATION OF REACTOR PERFORMANCE, ROLE OF CATALYSTS AND PCT PROPERTIES. QUARTERLY PROGRESS REPORT, APRIL 1-JUNE 30, 1985

PITTSBURGH UNIV., PA

1985



One Source. One Search. One Solution.

NTIS

Providing Permanent, Easy Access to U.S. Government Information

National Technical Information Service is the nation's largest repository and disseminator of government-initiated scientific, technical, engineering, and related business information. The NTIS collection includes almost 3,000,000 information products in a variety of formats: electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.

Search the NTIS Database from 1990 forward

NTIS has upgraded its bibliographic database system and has made all entries since 1990 searchable on **www.ntis.gov.** You now have access to information on more than 600,000 government research information products from this web site.

Link to Full Text Documents at Government Web Sites

Because many Government agencies have their most recent reports available on their own web site, we have added links directly to these reports. When available, you will see a link on the right side of the bibliographic screen.

Download Publications (1997 - Present)

NTIS can now provides the full text of reports as downloadable PDF files. This means that when an agency stops maintaining a report on the web, NTIS will offer a downloadable version. There is a nominal fee for each download for most publications.

For more information visit our website:

www.ntis.gov

U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161

DE85015104

DOE/PC/60054--T7

DE85 015104

Quarterly Progress Report

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

Alan J. Brainard
Yatish T. Shah
John W. Tierney
Irving Wender
Sebastian Joseph
Awdhoot Kerkar
Sadettin Ozturk
Abdelhamid Sayari

University of Pittsburgh
Pittsburgh, PA 15261

Prepared for the Department of Energy
Contract No. DE-FG22-83P PC60054

April 1, 1985 to June 30, 1985

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 areas 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 April 1, 1985 through June 30, 1985. 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.

Work continued on the development and testing of simulators for coal liquefaction processes. New 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.

Fischer-Tropsch Process

Two computer programs describing selectivity in Fischer-Tropsch synthesis carried out in slurry bubble column reactors have been developed. The first is a simplified plug flow model in which the liquid phase mass balance becomes an algebraic equation which is solved by trial and error while the gas phase mass balance is a set of first order differential equations which are solved using the Runge-Kutta fourth order technique. The program establishes the concentration of paraffins obtained due to the reaction up to carbon number 7 along with the concentration profiles of water which is a side product and H_2 and CO, the reactants. The conversion of synthesis gas along the reactor height and the variation of the gas velocity is also established. The results of the program indicate that the product slate closely follows the Schulz-Flory distribution.

The second is an axial dispersion model, developed with a view of overcoming the simplified assumptions made in the plug flow model and making the model equations more general. The resulting equations are second order differential equations. A set of 18 differential equations constituting a boundary value problem has been solved using the software package COLSYS (collocation techique). The program establishes the concentration profiles of hydrocarbons (up to C_6), water, H_2 and CO in both the gas and the liquid phases along with the variation of the syngas conversion and the variation of superficial gas velocity along the reactor.

Methanol-to-Gasoline Process

Modeling of the fluidized bed reactor for the MTG process is complete. The countercurrent backmixing model of Fryer and Potter (Ind. Eng. Chem. Fundam. 11, 338 (1972)) was used for modeling the fluidized bed. A lumped kinetic model developed by Chang et al. (J. Catal. 47, 249 (1977)) was used for modeling the MTG reaction. The heat balance was neglected since the bed operates in an essentially isothermal manner. Predictions from the model are in good agreement with experimental data.

Modeling of the fixed bed reactor is currently in progress. The fixed bed reactor is operated in an adiabatic manner and hence the lumped kinetic model used for modeling the reactions in the fluidized bed cannot be used here. A detailed kinetic model developed by Mihail et al. (Chem. Eng. Sci. 38, 1581 (1983)) is used for modeling the reactions in the fixed bed. A pseudo-homogeneous fixed bed reactor model is used since the reaction mechanism involves 37 species and 53 reactions steps.

ASPEN Compatibility

The direct coal liquefaction reactor model developed last year has been made compatible with the ASPEN simulator and now acts as a user-defined ASPEN unit operation model.

Methanol Synthesis

The simulation of an adiabatic fixed-bed reactor uses a one-dimensional plug-flow model to describe the actual reactor behavior. Besides methanol formation, the hydrogenation of carbon dioxide (shift reaction) is also considered. The effective reaction rates and the non-isothermal effectiveness factors are calculated by a separate package which can handle any type of kinetic expressions for these two reactions. The program is now ready to be executed in ASPEN format and provides concentration, temperature and conversion profiles together with effective reaction rates and effective factors.

A simulator has been developed for bubble-column slurry reactor for methanol synthesis. Plug-flow in the gas phase and axial dispersion in liquid and solid phases are assumed. The variation of gas flow rate, catalyst concentration and temperature along the reactor height are also considered. As in the case of fixed-bed reactor model, two reactions, formation of methanol and hydrogenation of carbon dioxide are taken into account. The program is now ready to be executed in ASPEN format.

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

A final draft of four subjects dealing with indirect liquefaction has been prepared. They are (a) the synthesis of methanol via methyl formate, (b) recent advances in understanding the mechanism of the synthesis of methanol, (c) methanol synthesis over transition metals and (d) some recent work on the catalytic production of higher alcohols from synthesis gas.

Literature on the coprocessing of coal has been collected. Coprocessing is defined as the hydrogenation of coal or coal-derived products with alternate feed materials such as residua, petroleum crudes, heavy oils, or various bitumens to produce liquids that would be suitable as transportation fuels or as refinery feedstocks. The area of coprocessing to be reviewed has the following constraints: it is a once-through processing of two feed materials, one of which, the heavy oils, will be the host or vehicle. Coal or a coal-derived material is the other constituent or feed.

The following combinations are not considered coprocessing: (a) coal plus coal-derived vehicles or hosts; this is essentially standard direct coal liquefaction, (b) combinations of synthetic fuels and (c) the upgrading of coal liquids.

Coprocessing, it is important to note, implies either once-through processing with no need for use of a recycle oil or, at worst, the use of only a small amount of recycle oil.

Coprocessing may well be the bridge that leads to a new process for the direct liquefaction of coal. The heavy, metal-laden oils, may be considered the "nearest thing" to coal and these oils and coals should be studied as a continuum, rather than as completely separate entities.

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

Work on this task was directed to becomming familiar with ASPEN Plus in order to apply it to the simulation of coal conversion processes. The pure component data bank of the ASPEN Plus simulator contains information on inorganic and hydrocarbon compounds up to $C_{21}H_{42}$. (This constitutes a total of 468 compounds.) There is no direct provision to utilize ASPEN Plus to handle complex mixtures such as are present in products of direct or indirect coal liquefaction processes, however, some work is in progress to see whether a pseudo-component approach might be adopted to utilize the compounds present in the ASPEN Plus data bank. To date, RESTOIC which is a routine used to simulate a chemical reactor has been successfully applied to the synthesis of methanol from carbon monoxide, carbon dioxide and hydrogen. This simulator has given the material and energy balances for these reactions for various feed ratios. In addition, various routines used to calculate the physical properties have been tried. These routines do not seem to affect the results to a great extent and, of course, have no effect on the material balance results.

Finally, ASPEN Plus has been utilized to predict the physical properties of the water-methanol system. Activity coefficients for this system have been determined from the Wilson equation and they have shown that the system is highly nonideal.

Reproduced by NTIS

National Technical Information Service
Springfield, VA 22161

This report was printed specifically for your order from nearly 3 million titles available in our collection.

For economy and efficiency, NTIS does not maintain stock of its vast collection of technical reports. Rather, most documents are custom reproduced for each order. Documents that are not in electronic format are reproduced from master archival copies and are the best possible reproductions available.

Occasionally, older master materials may reproduce portions of documents that are not fully legible. If you have questions concerning this document or any order you have placed with NTIS, please call our Customer Service Department at (703) 605-6050.

About NTIS

NTIS collects scientific, technical, engineering, and related business information – then organizes, maintains, and disseminates that information in a variety of formats – including electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.

The NTIS collection of nearly 3 million titles includes reports describing research conducted or sponsored by federal agencies and their contractors; statistical and business information; U.S. military publications; multimedia training products; computer software and electronic databases developed by federal agencies; and technical reports prepared by research organizations worldwide.

For more information about NTIS, visit our Web site at http://www.ntis.gov.

NTIS

Ensuring Permanent, Easy Access to U.S. Government Information Assets

SATISFACTION GUARANTEED

NTIS strives to provide quality products, reliable service, and fast delivery. Please contact us for a replacement within 30 days if the item you receive is defective or if we have made an error in filling your order.

▶ E-mail: info@ntis.gov
▶ Phone: 1-888-584-8332 or (703)605-6050

U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161   (703) 605-6000