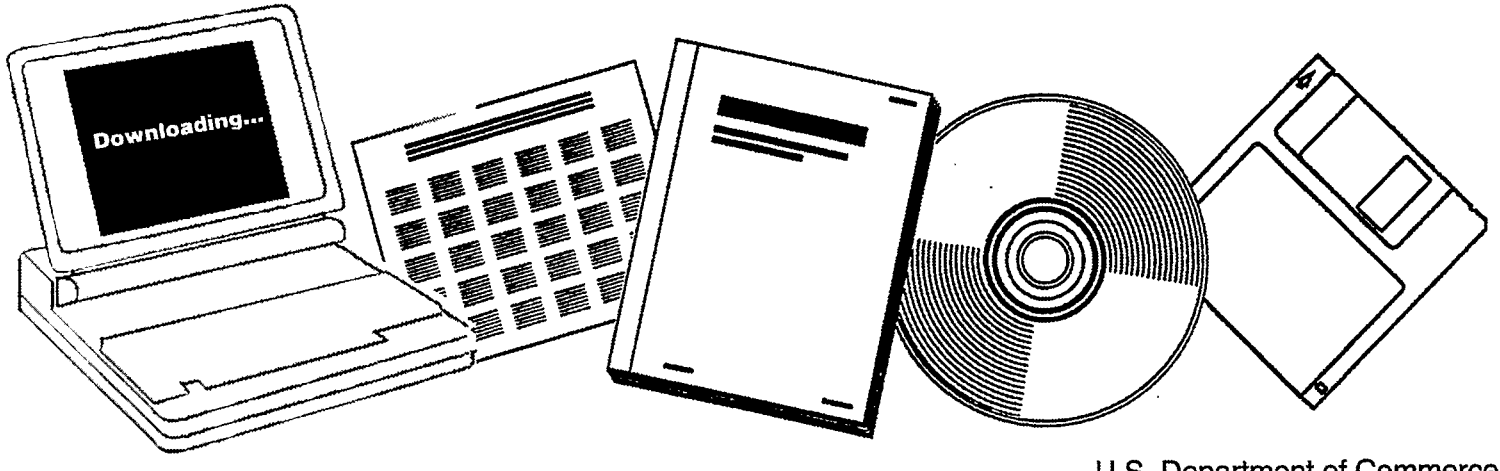
OPTIMIZATION OF COAL GASIFICATION PROCESSES. MONTHLY PROGRESS REPORTS FOR THE PERIOD JANUARY--DECEMBER 1968

WEST VIRGINIA UNIV., MORGANTOWN

1968



U.S. Department of Commerce
National Technical Information Service

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

OPTIMIZATION OF COAL GASIFICATION PROCESSES

Monthly Progress Reports for the
Period January - December 1968

C. Y. Wen

West Virginia University
College of Engineering
Morgantown, West Virginia 26506

Prepared for

Office of Coal Research
U. S. Department of the Interior

OCR Contract No. 14-01-0001-497

FE-497-T-2

CONTENTS

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 13 JANUARY 31, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

Optimization of methanation processes including the heat extraction system, the cold quench system, the recycle system and the combined system of heat extraction and cold quench has been completed. Since the cost of heat exchangers, particularly those of preheater and product cooler apreared to be the largest portion of the total equipment cost, detail heat exchanger optimization is being conducted. Together with the methanation reactor optimization, this phase of the study will be incorporated in the report.

The capacity data necessary for hot carbonate purification process have been obtained from the Bureau of Mines. These experimental mass transfer data were found to be quite different from the values calculated based theories, therefore further investigation is being conducted.

To start the optimization of steam-carbon reaction in a electrofluidized bed, it is necessary to obtain electric resistivity information. Some of these data are being sought from Iowa State University.

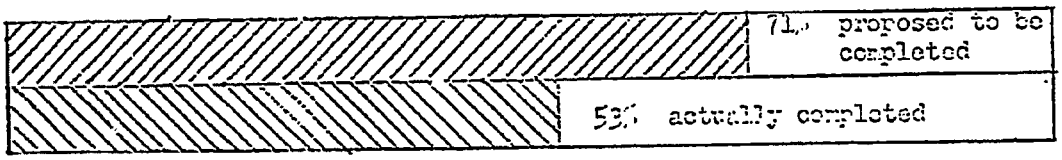
OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 13 JANUARY 31, 1968
(cont.)

Adiabatic equilibrium temperature and corresponding conversion of carbon-monoxide in water-gas shift reaction were obtained for different steam to gas ratios under various inlet temperature (250°C 900°C) using Institute of Gas Technology's data. Pressure effect on water-gas shift reaction has been found to be quite substantial, as much as four times, depending on the size of catalyst. A kinetic study indicates a rate equation based on pseudo first order with respect to carbon-monoxide is suitable for the pressure and temperature range under consideration.

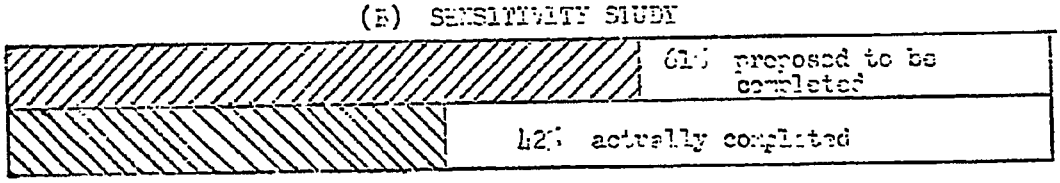
C. Y. Wen, Project Director

PROGRESS OF WORK FOR
OPTIMIZATION OF COAL GASIFICATION PROCESSES
FEBRUARY 29, 1968
OCR CONTRACT 14-01-0001-497

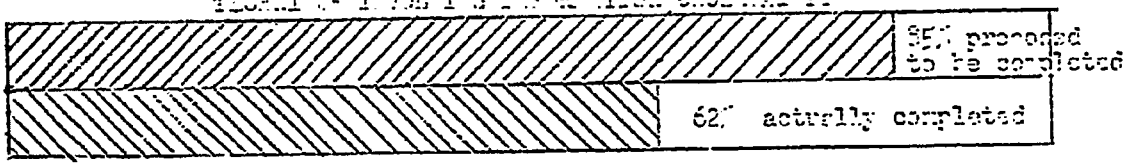
(A) INFORMATION GATHERING AND ASSIMILATION



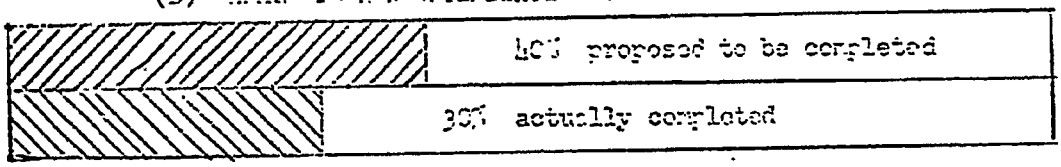
(B) SENSITIVITY STUDY



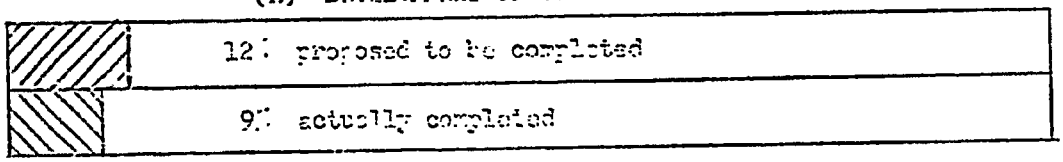
(C) DEVELOPMENT OF GENERAL OPTIMIZATION
TECHNIQUE INVOLVING ERROR AND UNCERTAINTY



(D) ANALYSIS AND OPTIMIZATION OF YIELDS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 15 MARCH 31, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

Equations necessary for the optimization and simulation of gas purification system have been established. The design equations for tower height, diameter, flow rates, temperature and concentration profiles are being programmed in IBM 7040. Shift reactor simulation is also progressing. The thermodynamic and kinetic information are now completed. They are being tested for various catalyst available commercially. Adiabatic reactor and cold quench system will be considered in view of the small amount of heat generated in the shift reaction.

The thermodynamic study of char steam reaction in fluidized bed system is now completed. Reactor model is tested to arrive at a model which is simple but closely resembling the actual reactor. Sensitivity analysis of subsystems is also being carried out.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 16 APRIL 30, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

The computer simulation of gas purification processes has been started. A few refinements of the performance equations are made. The simulation of the shift reactor is also started. Techniques useful for optimization of these processes are now being investigated.

The reactor models useful for simulation of fluidized bed gasifier are also being investigated. Of the many models available in literature, none can be directly adapted for solid-gas reaction systems. A fluidized bed reactor model capable of dealing with solid-gas reaction is being devised for simulation and optimization.

Sensitivity analysis of subsystems in methanation processes is now completed.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 17 MAY 31, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

Water-gas shift reactor was simulated on the computer. The study includes twelve cases of feed gas compositions containing various amounts of carbon monoxide and hydrogen. Allowable inlet temperatures for an adiabatic reactor were calculated for each case as a function of steam to carbon monoxide ratio.

Effect of H_2O/ CO ratio on the reaction rate was studied for high CO case, intermediate CO case and low CO case. The optimum ratio of steam to carbon monoxide was found to change with the amount of CO in the feed gas. Roughly, the composition of 50% steam and 50% dry gas was found to give high rates of reaction and consequently lower costs.

In choosing the proper rate equation for water-gas shift reaction, it was found that when the second order reaction rate equation is used, pressure effect becomes considerable. In this situation, high pressures are greatly advantageous. At pressure of 300 psig, the reaction rate becomes extremely slow, particularly when carbon monoxide content is very low and methane content is very high. For the range of carbon monoxide conversion studied, an optimum conversion exits in which by-passing of a portion of feed gas may become necessary.

In gas purification processes, the values of mass transfer coefficient, $K_G a$, for hot carbonate process has been checked and

recorrelated. The empirical correlation obtained based on 200 data points indicates

$$K_G a = 10^{-5} \, (PH - 8) \, L^{0.615} \, \text{Exp} \left(\frac{T - 460 - 2.92 \, P}{76} \right)$$

where

$$PH = 1.25 \, (8.20 - 1.75 \, x) \, y^{-0.015}$$

PH ranges between (9.2 and 10.6)

T is °R (519 ~ 723°R)

P is psi of CO_2 (0.67 ~ 75 psi)

L is lb./ft.^{2}hr. (166 ~ 9900 lb/hr.ft.^{2})

y is wt. ratio of K_2CO_3 to the solution (0.00605 ~ 0.545)

x is mole conversion (0.0091 ~ 0.40)

In addition a fluidized bed model based on discrete bubbles is being devised.

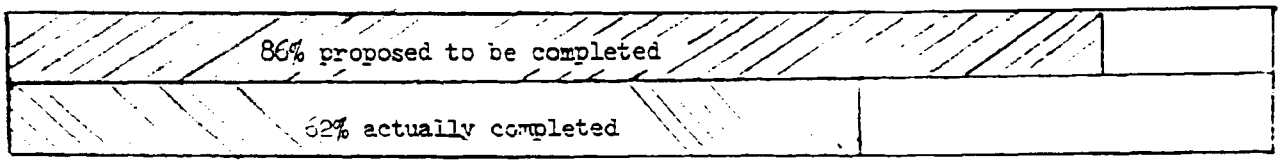
Steam carbon reaction in an electrofluidized bed is being investigated in order to obtain an economical feasibility of the process based on the future power cost.

C. Y. Wen

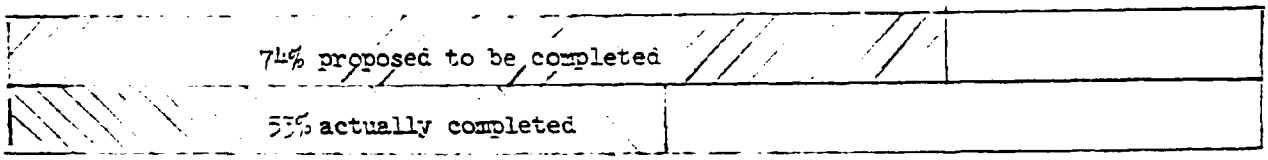
C. Y. Wen, Project Director

PROGRESS OF WORK FOR
OPTIMIZATION OF COAL GASIFICATION PROCESSES
MAY 31, 1968
OCR CONTRACT 14-01-0001-497

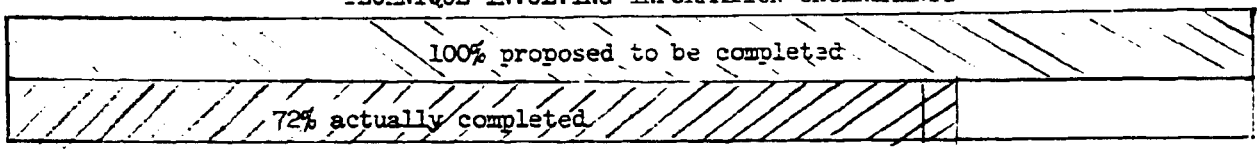
(A) INFORMATION GATHERING AND ASSIMILATION



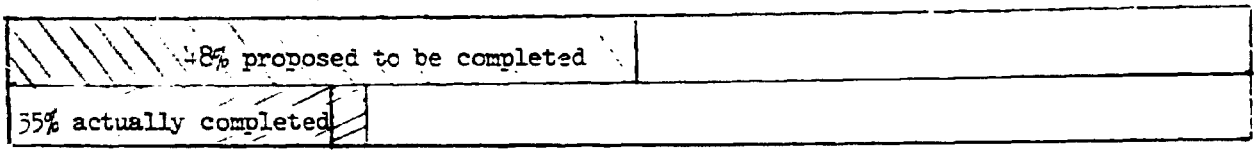
(B) SENSITIVITY STUDY



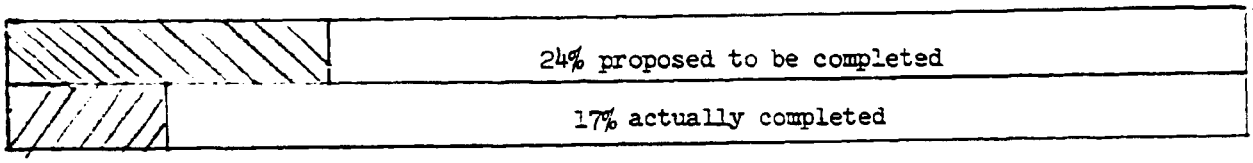
(C) DEVELOPMENT OF GENERAL OPTIMIZATION
TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 18 JUNE 30, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

A. Gasification Process

The study of selectivity for steam-hydrogen-carbon reactions was made. Other cases of selectivity are being studied.

For the equilibrium study of the gasification processes, the volatile material in coal is being taken into consideration particularly in the hydrogasification part.

The fluidized bed model has been formulated. The computer program on the model was completed. Some preliminary results for the test of the model based on experimental data were obtained. Refinement of the model is being made.

B. Water-Gas Shift Reaction Process

Based on the simulation accomplished so far, three decision variables; inlet temperature, diameter of the reactor, conversion of carbon monoxide, are selected for the optimization of water-gas shift process.

Optimum steam to gas ratio was proved to be largely dependent on the inlet feed gas composition, and their relationship was established. The optimum number of reactors will be determined after the optimization for a single reactor is achieved. For optimization, the dynamic programming approach will be used. An economic study of the shift reactor was also made.

C. Purification Process

Simulation of hot carbonate process is being made. Runge-Kutta method was selected for computer calculation.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 19 JULY 31, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

A. Gasification Process

The derivation of the equations for the study of the selectivities of the consecutive and parallel reactions without reducing particle size was completed. The concentration profiles and the selectivities in terms of reacting radius will be obtained by the computer. The case with reducing particle size will be studied. These studies will be applied to char-H_2O-H_2 reacting system.

Some effects on the new fluidized model were examined. The results are as follows:

1. The initial cell length has practically no effect on the final conversion.

2. For slow reaction, because of reaction control, the mass transfer coefficient is not important, but for the fast reactions (K = 0.7 1/sec., or 8.7 1/sec), the effect is very important. Both the Kunii and Davidson's equations for mass transfer coefficient were checked. Davidson's equation deviates more than Kunii's equation when experimental data are compared.

3. The effects of bubble size and reactor length are also important. The best expressions useful for scale-up still have to be found.

B. Water-Gas Shift Reaction

Economic study was made for the estimation of operating cost in water-gas shift process. The minimum total cost or objective function of optimization is related to the equipment cost and the approximated operating cost.

The problem of carbon deposition in water-gas shift reaction was studied. Possibility of carbon deposition under the outlet condition of reactor was investigated. The amount of steam which may prevent carbon

deposition was also calculated based on thermodynamic equilibrium constant. However, the amount of steam obtained from this approach was too large to be practical. Furthermore, many literature and experimental reports indicate that sufficient steam to gas ratio to prevent carbon deposition falls in the range between 5 to 1. Apparently this implies that the controlling factor in this problem is not the thermodynamic potential but the actual reaction rate of carbon production.

C. Purification Process

Simulation of hot carbonate process is being continued. The use of effective surface area of contacting is developed so that different size packing can be used for optimization study.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 20 AUGUST 31, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

A fluidized bed reactor model useful for computer simulation and optimization has been formulated. Report No. VIII entitled, "Bubble Assemblage Model for Fluidized Bed Catalytic Reactions," is enclosed

Another model for non-catalytic fluidized bed reactor is being formulated. Since the primary gasification phase and pretreatment phase involves fluidized bed operation, it is necessary to formulate workable reactor models before simulation and optimization can be performed. Gas purification and shift conversion phases are being simulated and optimized. Reports on these areas should become available soon.

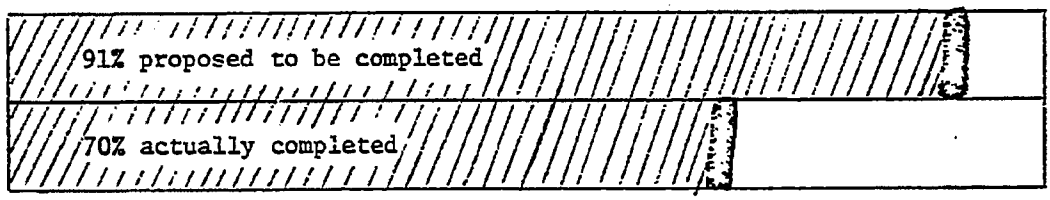
C. Y. Wen

C. Y. Wen, Project Director

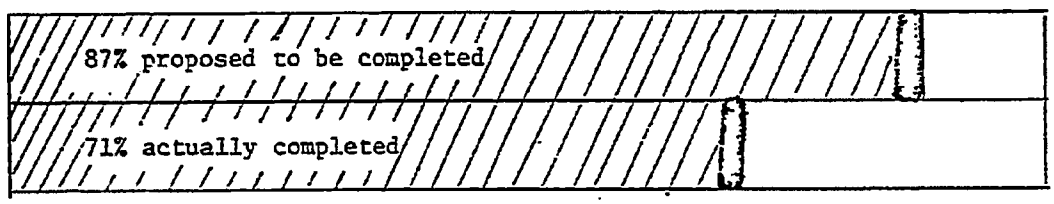
PROGRESS OF WORK FOR
OPTIMIZATION OF COAL GASIFICATION PROCESSES
AUGUST 31, 1968

OCR CONTRACT 14-01-0001-497

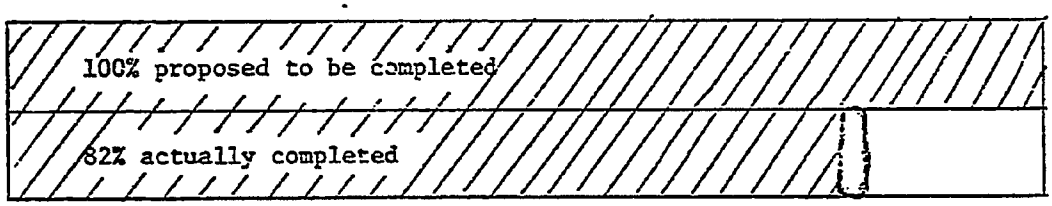
(A) INFORMATION GATHERING AND ASSIMILATION



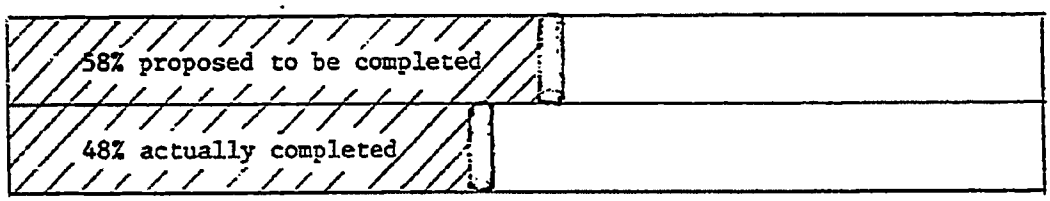
(B) SENSITIVITY STUDY



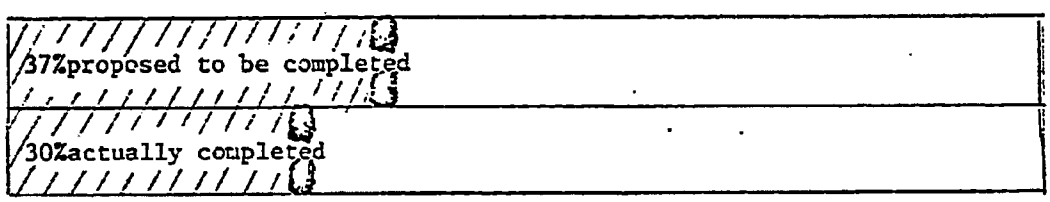
(C) DEVELOPMENT OF GENERAL OPTIMIZATION
TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 21 SEPTEMBER 30, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

(A) Water-Gas Shift Reaction

A computer program for the design of heat exchangers has been set up and its simulation is completed. Optimization of the water-gas reactor is being performed. However since a newly acquired rate equation, which is a first order with respect to carbon monoxide, demonstrates the catalyst pore-diffusion effect on reaction rate satisfactorily, it will be used for optimization instead of the previously chosen second order rate equation.

The overall optimization will be achieved by combining both the reactor and the heat exchanger.

(B) Gasification Phase

The report of the selectivity study for the simultaneous non-catalytic solid-fluid reaction will be furnished soon.

The application of the bubble assemblage model for fluidized catalytic reactors which is to be used for the non-catalytic solid-fluid reactions is being investigated.

(C) Purification Phase

Simulation of the gas purification by the hot carbonate process is completed. Economic evaluation and optimization of this phase is now being carried out.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 22 OCTOBER 31, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

During the last month the following progress was made on the optimization of coal gasification processes.

(A) Methanation Process

A modified kinetic equation was used for the optimization of methanation processes. A set of new cost information was obtained.

(B) Water-Gas Shift Reaction

Optimization of adiabatic water-gas shift reaction system was achieved for three different inlet compositions, thus the optimum values of equipment size, cost and operating conditions were obtained.

This optimization was based on first order rate equation which covers the effect of operating pressure and diffusion of carbon monoxide. These results, however, were compared with that obtained from second order rate equation, which proved there was only a small difference between them.

The simulation of water-quenching system for water-gas shift reaction is now being conducted.

(C) Gasification Phase

The selectivity study of the isothermal simultaneous non-catalytic solid-gas reactions has been completed. The non-isothermal case is now being studied. The equations for the first order independent reactions have been derived.

The computer programs were written in order to find the roots from the heat balance equations. For this, Newton's iteration method was used.

(D) Purification Process

Simulation of the absorber and the computer programming or the regenerator have been made. The effects of tower height, diameter, pressure, gas inlet conditions, packing, liquid rate and liquid concentration have been studied.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 23 NOVEMBER 30, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

(A) Shift Converter

Simulation of cold quenching system in water-gas shift reaction, particularly for the quenching part was made. Nozzle system for injection of water, behavior of droplet, and the pressure drop through the packings were studied. Dynamic programming is employed to search for the optimum conditions for the cold quenching system. A report on the optimization of the shift converter is being prepared.

(B) Coal Gasification Reaction

A computer program using Bolzano's method to find the roots was formulated. The effects of Nusselt number, Sherwood number and the ratio of heat of reactions on the selectivity and effectiveness factor were determined. More detailed studies pertaining to the criteria for optimum use still have to be made.

(C) Gas Purification

The computer simulation for the absorption of CO_2 by a hot carbonate process has been completed. The study now is being extended to the regenerator. A report on the optimization of gas purification phase is being prepared.

(D) Methanation Process

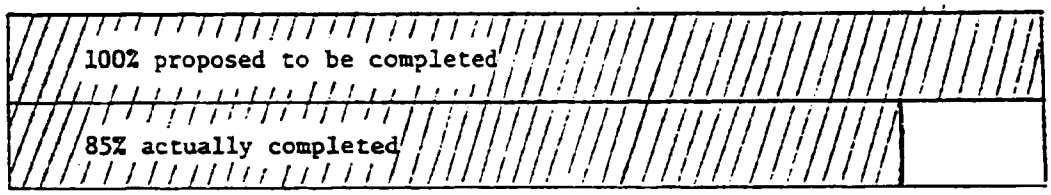
A new recycle system for the methanation of high CO case is being investigated. The method may provide a cheaper way to handle the high CO content gas.

C. Y. Wen, Project Director

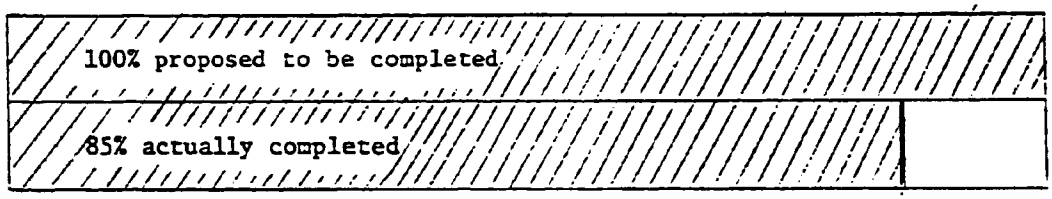
PROGRESS OF WORK FOR
OPTIMIZATION OF COAL GASIFICATION PROCESSES
NOVEMBER 30, 1968

OCR CONTRACT 14-01-0001-497

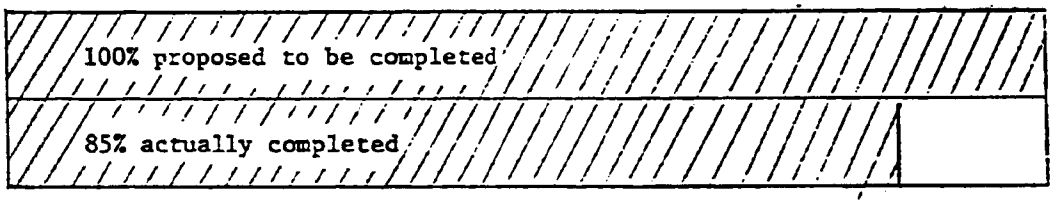
(A) INFORMATION GATHERING AND ASSIMILATION



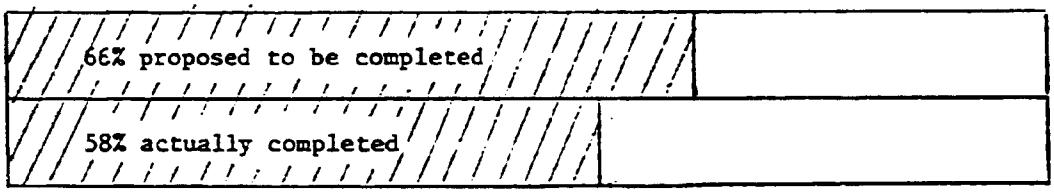
(B) SENSITIVITY STUDY



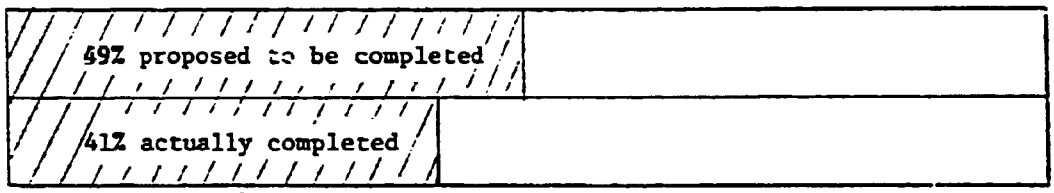
(C) DEVELOPMENT OF GENERAL OPTIMIZATION
TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 24 DECEMBER 31, 1968

to

Office of Coal Research
Contract No. 14-01-0001-497

(A) Gasification Phases

The theoretical study of non-catalytic, non-isothermal simultaneous first order reactions to find the best reacting conditions is nearly completed. The relation between effectiveness factor and Thiele modulus, selectivity and Thiele modulus will be plotted and the criteria will be found. A report is being prepared on this subject.

(B) Water-Gas Shift Reaction Phase

Results of optimization for adiabatic reactor in water-gas shift reaction are completely arranged and the annual report based on this will be finished soon. The computer program for the optimization of cold quenching system is being carried out.

(C) Gas Purification Phase

A comprehensive report on the optimization of gas purification phase using hot carbonate process is being prepared.

(D) Methanation Phase

A partial recycle system and combination of recycle and cold quench system are being investigated. The study shows a substantial savings by these new methods may be possible.

C. Y. Wen, Project Director

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