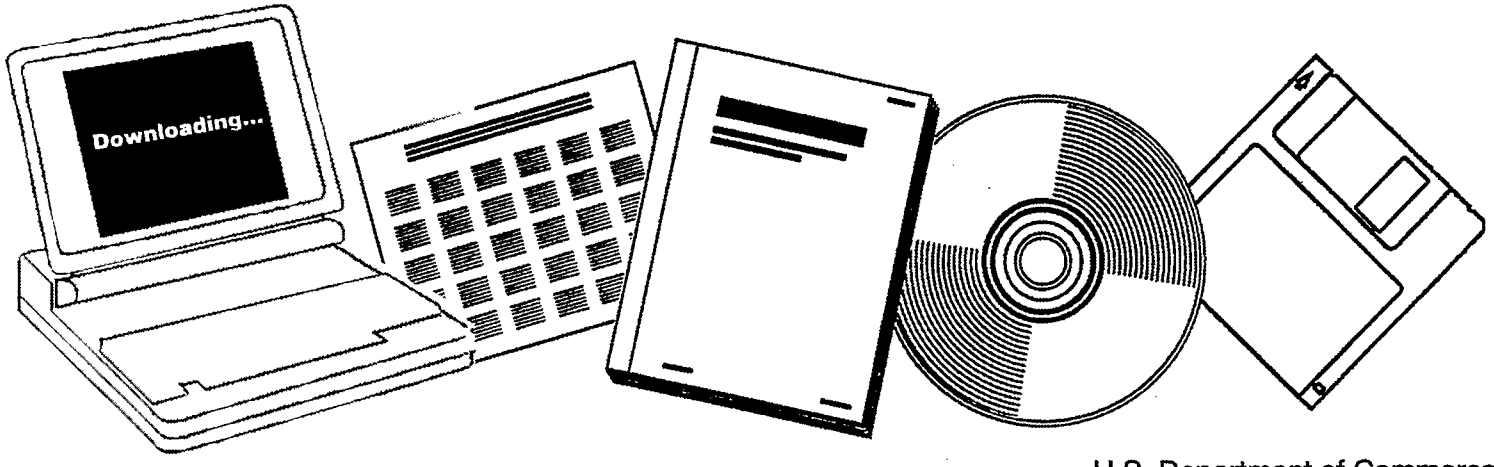
OPTIMIZATION OF COAL GASIFICATION PROCESSES. MONTHLY PROGRESS REPORTS FOR THE PERIODS JANUARY--MARCH AND MAY--DECEMBER 1969

WEST VIRGINIA UNIV., MORGANTOWN

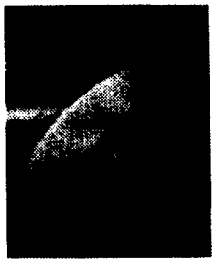
31 JAN 1969



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 periods
January - March and May - December 1969

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-3

CONTENTS

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 24 JANUARY 31, 1969

to

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

(A) Gasification Phase

The theoretical study of non-catalytic,non-isothermal simultaneous reaction is being completed. The model required for heat and mass transfer in fixed and fluidized bed reactions is being formulated.

(B) Water-Gas Shift Reaction Phase

Optimization of shift converters including heat exchangers, waste-heat boiler, reactors and compressors is being completed. Several problems associated with cost estimation such as steam cost, operating, labor and working capitals, etc. were discussed with personnel from I.G.T. The report on this phase is being prepared.

(C) Gas Purification Phase

A report on optimization of gas purification phase by hot carbonate process is being prepared. The study will show the cost of purification of gases generated by I.G.T. process, B.C.R. process, Pitts. Consol process and Kellogg process separately.

(D) Methanation Phase

Partial recycle systems and combination of recycle and cold quench system are being investigated.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 25 FEBRUARY 31, 1969

to

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

(a) Gasification Phase

The theoretical study of non-catalytic, non-isothermal heterogeneous reaction system is now being applied to fluidized bed reactor and reactor model needed for optimization of gasification phase is being formulated.

(b) Water-Gas Shift Reaction Phase

Result of optimization of adiabatic water-gas shift reaction system based on the cost accounting procedure provided by OCR is being compiled for a report.

Additional study on the temperature and concentration distribution within catalyst pellet has been made in order to ascertain the effect of heat and mass transfer on the overall conversion. Sensitivity analysis of pertinent parameters is also made to identify the important economic factors of this process.

(C) Gas Purification Phase

Capacity data reported by the Bureau of Mines and other investigators were taken at the pressure below 350 psia. Direct extrapolation of these data to the pressure of 1000 psia was found to give unreasonable result and more basic investigation on effect of pressure is being conducted so that more reliable extrapolation and subsequent optimization can be performed.

(D) Methanation Phase

Methanation of gas containing more than 10% of CO may be better achieved by combination of recycle and cold quench method. Approximately 15% saving can be realized with the combination of recycle and cold quench over the recycle method.

C. Y. Wen

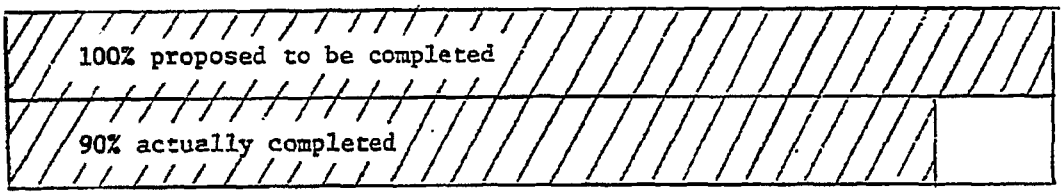
C. Y. Wen, Project Director

PROGRESS OF WORK FOR OPTIMIZATION OF COAL GASIFICATION PROCESSES

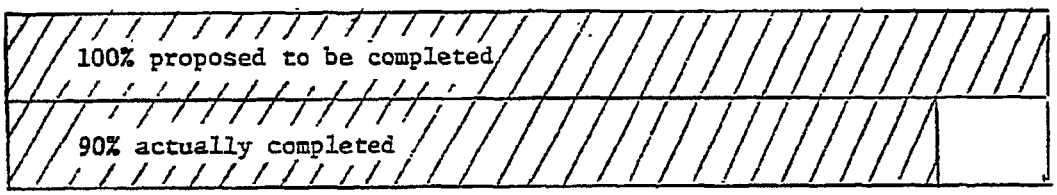
FEBRUARY 28, 1969

OCR CONTRACT 14-01-0001-497

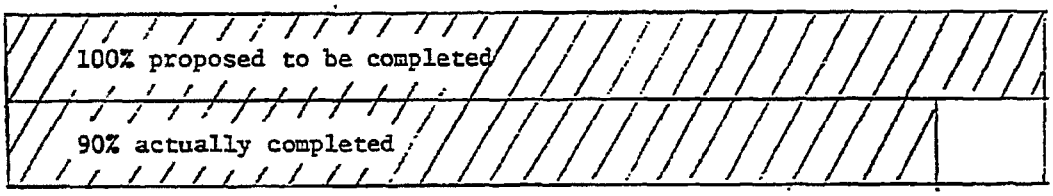
(A) INFORMATION GATHERING AND ASSIMILATION



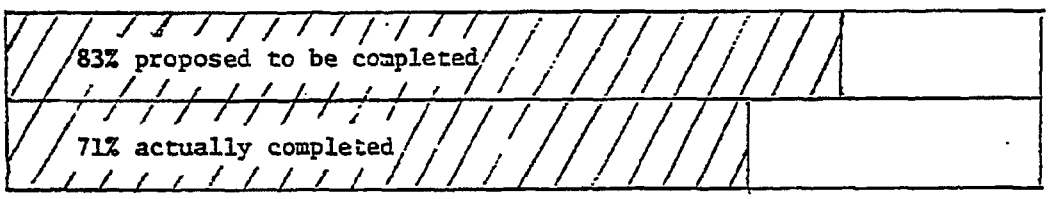
(B) SENSITIVITY STUDY



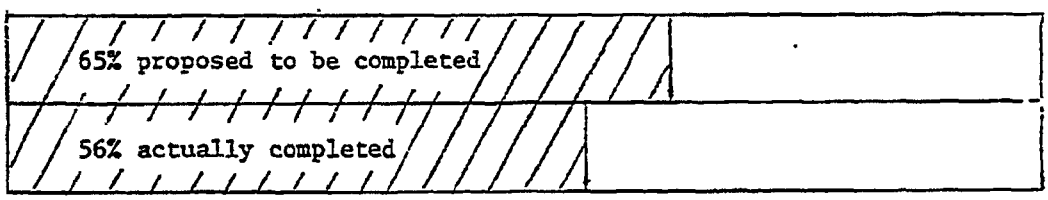
(C) DEVELOPMENT OF GENERAL OPTIMIZATION TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



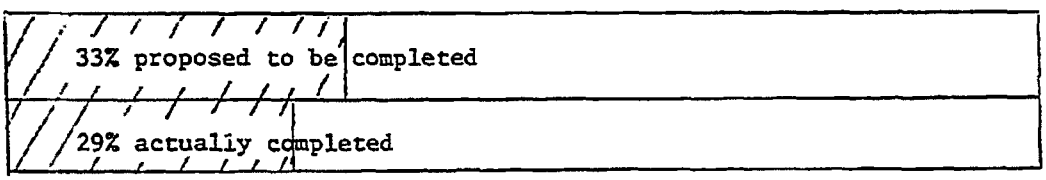
(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



(F) COMPARISON, EVALUATION AND RECOMMENDATION



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 28 MARCH 31, 1969

to

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

(A) Gasification Phase

A study on heat and mass transfer in fixed and fluidized beds under extremely low Reynold's number has been completed. In gasification operations very small particles are used for which no establish correlations on heat and mass transfer is available. New correlations of heat transfer and mass transfer coefficients were obtained which show good agreement with the reported literature values. These correlations are then used to construct mathematical models for fixed and fluidized bed contacting processes. Reports on these studies are nearly completed.

Theoretical study of non-siothermal simultaneous solid gas reactions is also completed and a report is being typed.

(B) Water-Gas Shift Reaction Phase

The report on the optimization of adiabatic water-gas shift reaction is being completed. Treatments of steam benefit in heat exchangers were discussed. Figures are being drawn for the completion of the report.

(C) Gas Purification Phase

Mass transfer coefficients for hot carbonate processes has been isolated from chemical reaction rate so that the model can be used for the scale-up of CO_2 and H_2S absorption process.

(D) Methanation Phase

Simulation of recycle with two cold-quench methanation has been completed. Results are compared with one quench methanation process and the recycle process. Savings in pumping cost and operating cost are indicated.

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. ~~30~~ 39 MAY 31, 1969

to

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

(A) Gasification Phase

Equilibrium composition calculation for coal gasification systems has been completed. The kinetic model suitable for optimization is being formulated. A report on simultaneous solid-gas reaction system is completed and attached with this report. Another report on mass transfer in fixed and fluidized bed is also completed and attached with this report.

(B) Water-gas Shift Reaction Phase

A report on optimization of adiabatic water-gas shift reaction is completed and copies are attached with this report.

(C) Gas Purification Phase

Simulation of absorption of CO_2 and H_2S is nearly completed.

C. Y. Wen

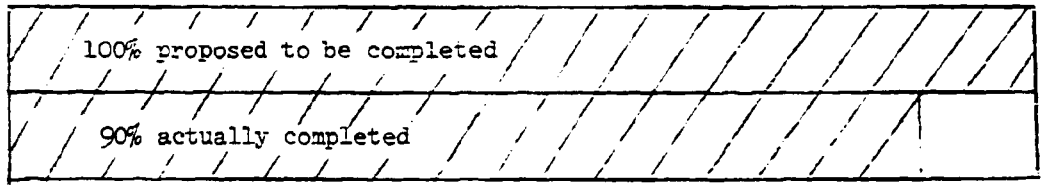
C. Y. Wen, Project Director

PROGRESS OF WORK FOR OPTIMIZATION OF COAL GASIFICATION PROCESSES

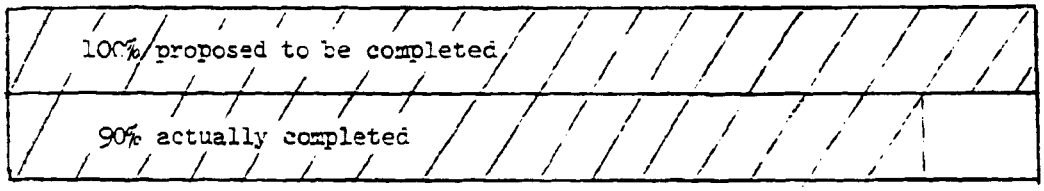
MAY 31, 1969

OCR CONTRACT 14-01-0001-497

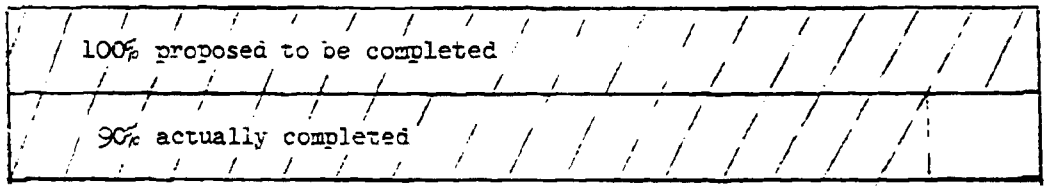
(A) INFORMATION GATHERING AND ASSIMILATION



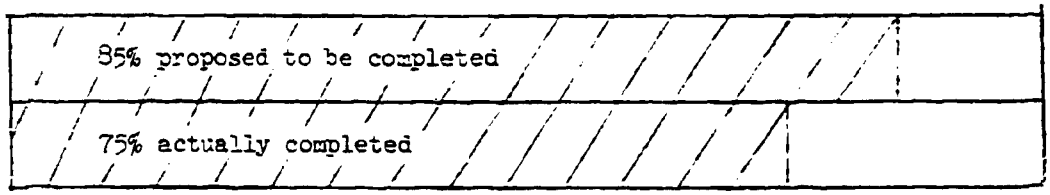
(B) SENSITIVITY STUDY



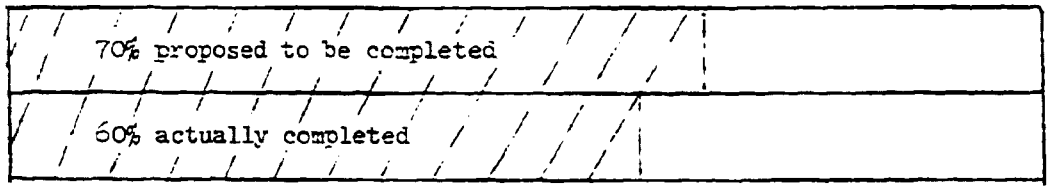
(C) DEVELOPMENT OF GENERAL OPTIMIZATION TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



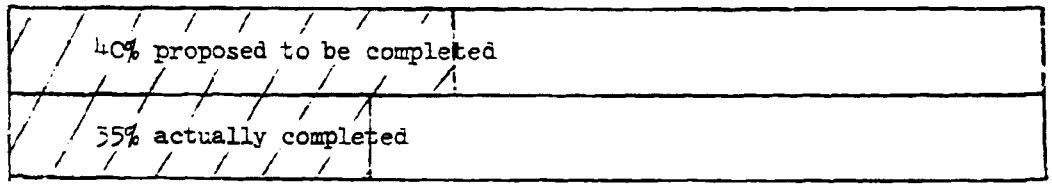
(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



(F) COMPARISON, EVALUATION AND RECOMMENDATION



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 31 JUNE 30, 1969

to

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

(A) Gasification Phase

A report on "Simultaneous Non-Isothermal Non-Catalytic Solid-Gas Reaction" is completed. Fluidized bed reactor model including heat and mass transfer is being developed.

(B) Water-Gas Shift Reaction Phase

The report on optimization of adiabatic water-gas shift reaction process has been completed. A computer program for the simulation of water-gas shift reaction using cold-quenching is set up. Dynamic programming approach will be applied since this system is regarded as a multi-stage process.

(C) Gas Purification Phase

Simulation of hot carbonate process is being completed.

(D) Methanation Phase

Optimization of a three-stage methanation reactor by dynamic programming method was studied. Some results, including reactor size, have been obtained. The final calculation for total equipment cost is doing now.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 32 July 31, 1969

to

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

(A) Gasification Phase

Examples from actual experimental data for multiple reactions such as carbon with various reacting gases are studied and compared with the theory developed.

(B) Water-Gas Shift Reaction Phase

The water-gas shift reaction employing cold-quenching system is simulated using computer-program. In order to apply the dynamic programming to present optimization, the appropriate decision and state variables are selected, and their admissible ranges of value are estimated under given conditions. Presently, the optimization of each stage for Case 3 is under progress. The super-CO content case will follow next.

(C) Gas Purification Phase

Simulation of hot carbonate purification process in a packed bed is completed. Various other contacting devices are now being investigated.

(D) Methanation Phase

Optimization of methanation process using dynamic programming techniques has been completed. The optimum reactor system was found to have 7 ft. diameter, 8.9 ft. high and consisting of four reactors in parallel. The total equipment cost for cold quench-recycle system is approximately $897,300, which is $76,310 less than the recycle system. A complete report of this study is sent under a separate cover.

C. Y. Wen

Dr. C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 32 August 31, 1969

to

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

(A) Gasification Phase

Solid-gas reaction in a fluidized bed is being modeled for simulation in computer.

(B) Water-gas Shift Reaction Phase

The computer program for the optimization of water-gas shift reaction employing cold quenching system is completed based on the simulation study achieved during the period. The amount of quenching water is fixed within the admissible range since the performance of reactor is not affected very much by the change of water quantity. The pressure drop through quenching port is shown to be negligibly small when compared to that through catalyst bed.

(C) Gas Purification Phase

Correlation of performance data and simulation of purification processes are now completed. Optimization of the process is being conducted.

(D) Methanation Phase

A complete report of "Optimization of Cold Quench-Recycle System in Fixed Bed Methanation Processes by Applying Dynamic Programming Techniques" has been submitted.

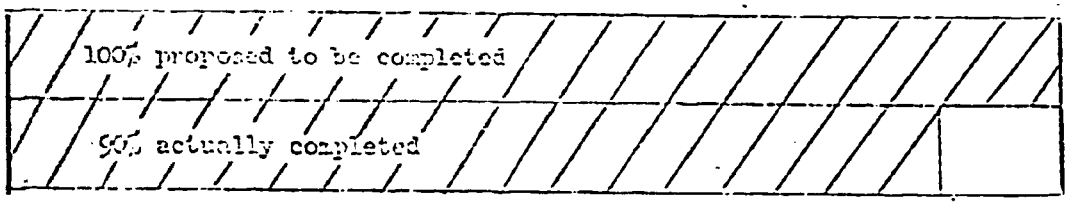
C. Y. Wen, Project Director

PROGRESS OF W[illegible]A FOR OPTIMIZATION OF COAL GASIFICATION PROCESSES

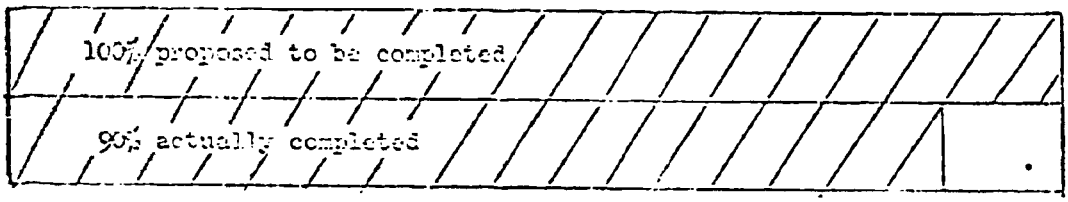
August 31, 1969

OCR CONTRACT 14-01-0001-497

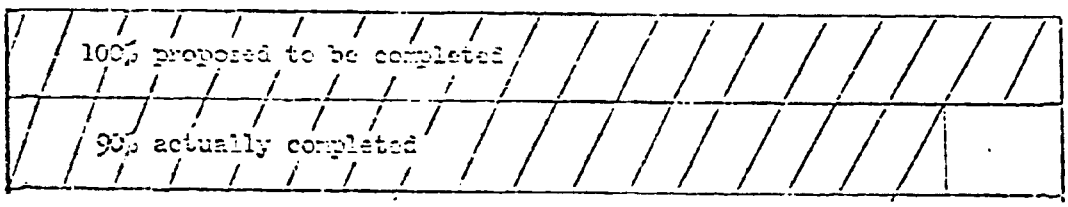
(A) INFORMATION GATHERING AND ASSIMILATION



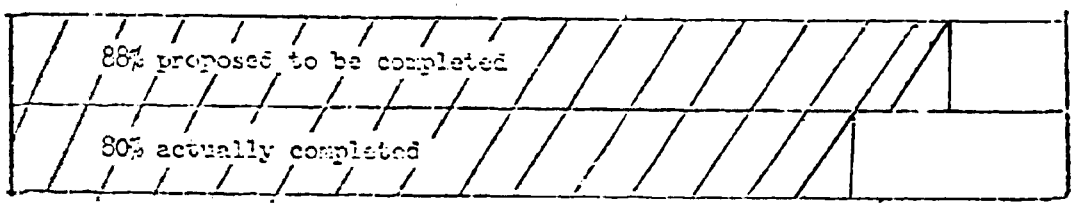
(B) SENSITIVITY STUDY



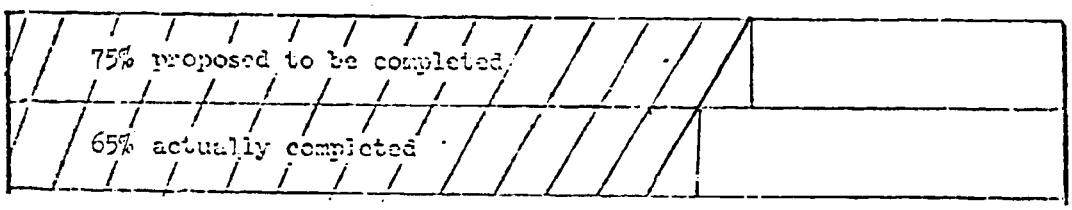
(C) DEVELOPMENT OF GENERAL OPTIMIZATION TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



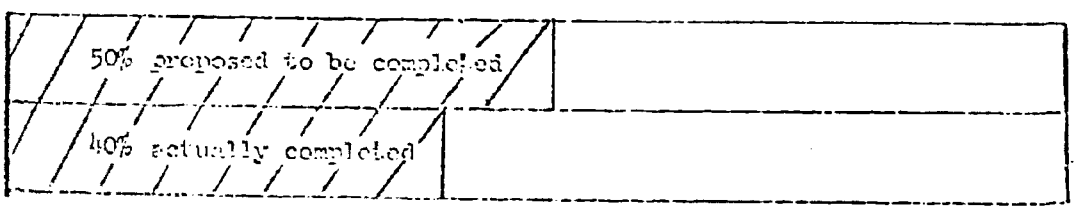
(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



(F) COMPARISON, EVALUATION AND RECOMMENDATION



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 32 September 30, 1969

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

(A) Gasification Phase

Kinetic data of gasification obtained recently from BCR and IGT are being examined. These data will be incorporated into mathematical model of fluidized bed reactor.

(B) Water-gas Shift Reaction Phase

The water-gas shift conversion process using cold-quenching system is optimized. Two cases including low CO content and high CO content are treated.

The number of stages is primarily fixed at three, and the forward dyanmic programming approach is applied for this multi-stage process optimization.

Comparing the adiabatic system, the result indicated that the overall cost can be reduced by the reduction in amount of steam and catalyst under current system. However, the reactor cost is not decreased because of the additional space required for quenching part in the reactor.

The optimization for the production of high H_2 content gas from synthesis gas by water-gas shift conversion is being performed.

A detailed report on this phase of study will be submitted as soon as the optimization of shift convector to produce hydrogen is completed.

(C) Gas Purification Phase

A satisfactory simulation of CO_2 and H_2S absorption in packed column using K_2CO_3 solution has been accomplished. The most important parameter in the design of the packed column is the mass transfer coefficient, K_Ga,

which have been correlated based on available literature data. The individual liquid film coefficient with chemical reaction is correlated as follows:

$$\frac{k_L\left(\frac{\mu^2}{g\rho^2}\right)^{1/3}}{D} = 0.0165\left(\frac{L}{a\mu}\right)^{2/3}\left(\frac{\mu}{\rho D}\right)^{1/3}\frac{\left(\frac{\mu^2}{g\rho^2}\right)^{1/3}\left(\frac{k_2C_R}{D}\right)^{1/2}}{\tanh\left[\left(\frac{\mu^2}{g\rho^2}\right)^{1/3}\left(\frac{k_2C_R}{D}\right)^{1/2}\right]}$$

where k_L = mass transfer coefficient in liquid side

μ = viscosity of liquid

g = gravitational acc.

ρ = desnity of liquid

D = diffusivity in liquid

L = liquid flow rate

a = effective surface area

k_2 = reaction rate constant in tower

C_R = concentration of OH^-

Optimization of the gas purification system is being carried out. The mixture of K_2CO_3 solution with mono-ethanol amine as absobent is also being considered.

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 33 OCTOBER 31, 1969

to

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

(A) Gasification Phase

Fluidized bed models for solid-gas reaction are being formulated for simulation and optimization of primary coal gasification processes.

(B) Purification Phase

A study on wet scrubbing in various scrubbers, including the turbulent bed contactor, venturi scrubber, spray tower scrubber, sieve plate scrubber, etc., is being conducted. Regeneration of hot carbonate solution from absorber is being simulated on computer and optimum conditions are being searched.

(C) Water-gas Shift Conversion Phase

The optimization study has been made for the production of process hydrogen from the effluent gas of gasifier by water-gas shift conversion. The unit cost of hydrogen will be approximated after the evaluation of purification cost. The report on the optimization results of water-gas shift conversion employing cold-quenching system is being prepared.

(D) Methanation Phase

Simulation of B.C.R. process with high CO methanation (with CO constant of 19%) is completed.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 3½ November 30, 1969

to

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

(A) Gasification Phase

Simulation models for moving bed and fluidized bed reactors are being formulated. Pyrolysis of coal is also studied.

(B) Water-gas Shift Reaction Phase

In connection with the gas purification and methanation processes, the flowsheet of water-gas shift conversion system including the optimum costs was prepared and submitted to the Office of Coal Research.

The final report on optimization of cold-quenching water-gas shift conversion and hydrogen production together with the various figures representing the results is almost completed.

(C) Gas Purification Phase

The simulation of absorber and regenerator is completed. The power cost required for recirculation of carbonate solution from regeneration may occupy a large fraction of the cost. Optimization of power recovery system is now being conducted.

(D) Methanation Phase

Subsystem optimization of various phases except primary gasification phase has been nearly completed. It is now necessary to combine each of the subsystems to an integral plant operation. This requires some adjustments of flow properties, heat exchange requirement, steam supply etc. to meet the overall plant need.

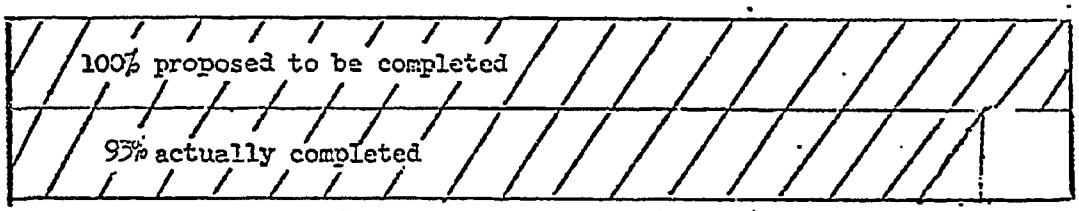
C. Y. Wen, Project Director

PROGRESS OF ORK FOR OPTIMIZATION OF COAL G FICATION PROCESSES

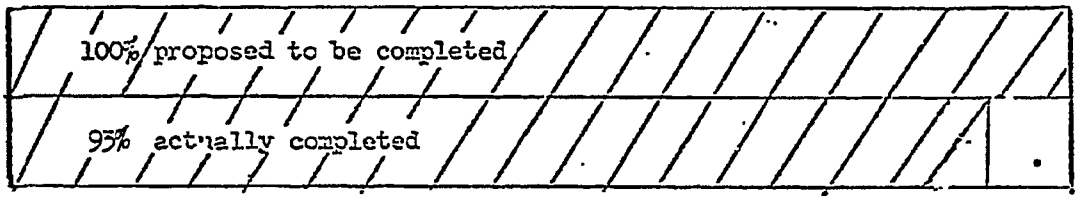
November 30, 1969

OCR CONTRACT 14-01-0001-497

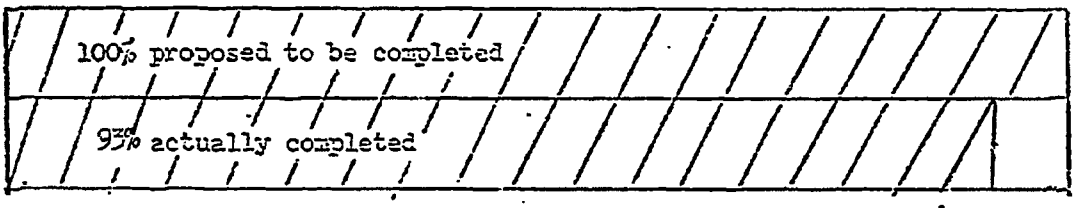
(A) INFORMATION GATHERING AND ASSIMILATION



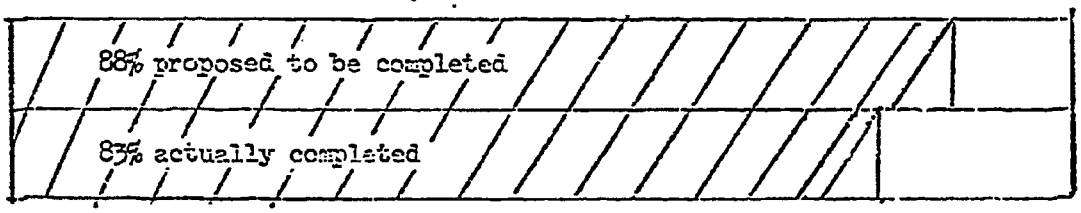
(B) SENSITIVITY STUDY



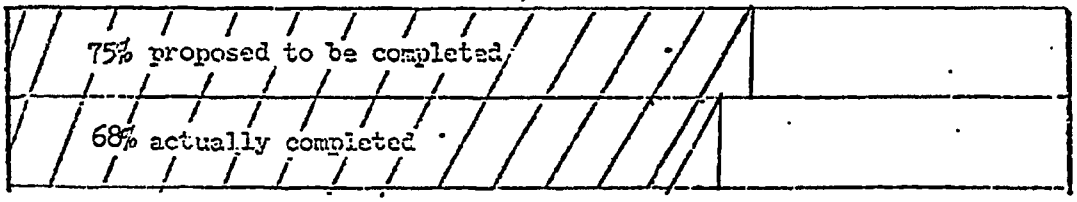
(C) DEVELOPMENT OF GENERAL OPTIMIZATION TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



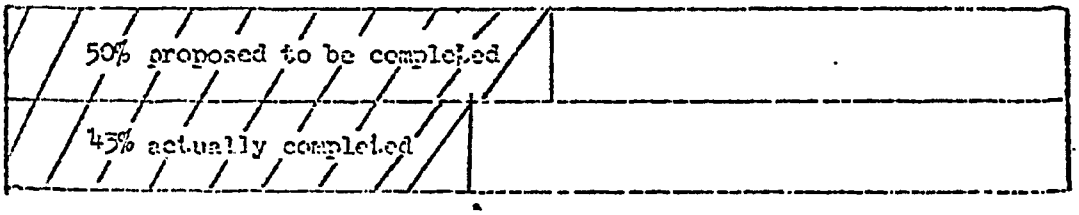
(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



(F) COMPARISON, EVALUATION AND RECOMMENDATION



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 35 December 31, 1969

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) Gasification Phase

Equations for material and heat balance for coal gasification processes in general form in dimensionless terms have been organized. The I.G.T. hydrogasification process will be simulated first on the computer.

(B) Water-Gas Shift Conversion Phase

In order to estimate the unit cost of hydrogen produced from coal by means of gasification, shift conversion and purification, the size and cost of purifier are being computed using the computer program of the U.S. Bureau of Mines.

All the calculations and drawings for quenching system water-gas shift conversion are completed.

(C) Gas Purification Phase

Heat transfer coefficients necessary to evaluate the temperature profile in hot carbonate gas absorber have been computed. The computer program developed can now deal with simulations of absorber and regenerator under non-isothermal conditions.

(D) Methanation Phase

The methanation computer program has been rewritten so that it can be used in the water gas shift-purification-methanation combined program.

In the old computer program all the heat capacities are based on pound mass. For the purpose of writing a more general program, it would be better to change the heat capacities based on pound mole. The product cooler design procedure should also be changed. The new program will be able to handle more complicated problems.

C. Y. Wen

C. Y. Wen, Project Director

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