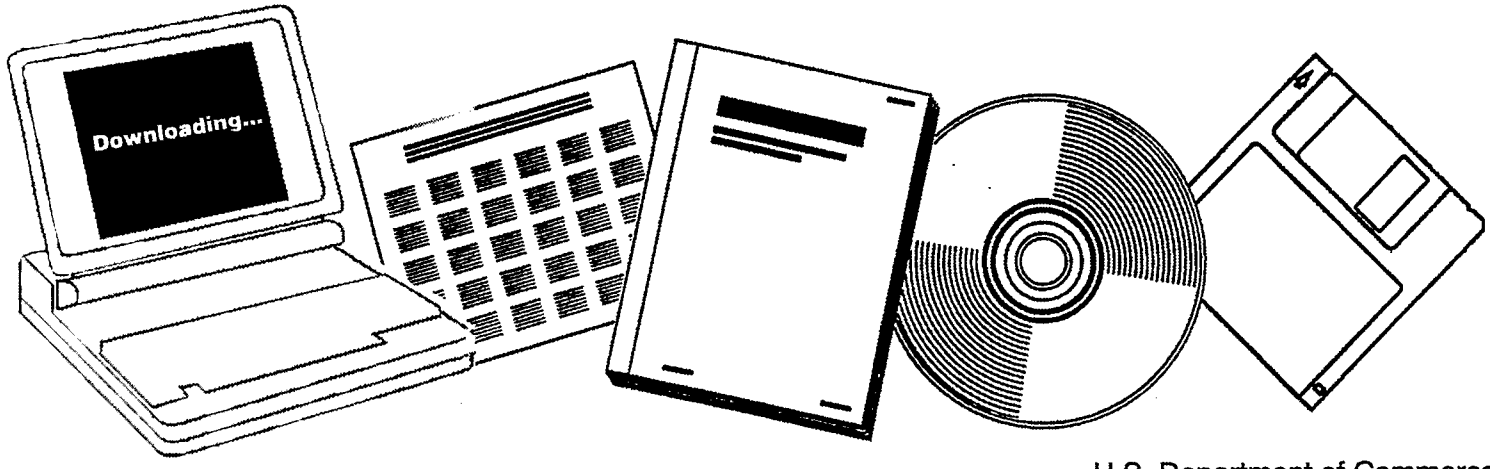
OPTIMIZATION OF COAL GASIFICATION PROCESSES. MONTHLY PROGRESS REPORT FOR THE PERIODS JANUARY--FEBRUARY, APRIL, AND JUNE--DECEMBER 1970

WEST VIRGINIA UNIV., MORGANTOWN

31 JAN 1970



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OPTIMIZATION OF COAL GASIFICATION PROCESSES

Monthly Progress Reports for the periods
January - February, April, and June - December 1970

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Prepared for

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

OCR Contract No. 14-01-0001-497

FE--497-T-4

CONTENTS

Monthly Progress Reports covering months
January, February, April, and June through
December 1970

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 36 January 31, 1970

to

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

(A) Gasification Phase

Computer program on fluidized bed reactors with solids gas reaction and mixing is being tested.

(B) Water-gas Shift Reaction Phase

A report on the optimization of water-gas shift conversion processes in fixed bed employing cold-quenching system is prepared.

(C) Gas Purification Phase

Computer simulation of gas purification processes using hot carbonate solution has been completed. Three cases of gas feeds (I.G.T. char hydrogasification, I.G.T. lignite hydrogasification and B.C.R. two stage processes) under isothermal conditions were treated. The computer simulation for gas purification processes under non-isothermal conditions has not been successful. The present method does not offer quick convergence when heat transfer calculation involving iteration is required. A better numerical technique which eliminates iteration is now being tested. The case involving absorption with pure water is being tested. The degree of removal of H_2S is also being examined. Pressure drop in the packed column is usually very small to present any problem.

(D) Methanation Phase

Revenue requirement for cold-quenching recycle system based on B.C.R. gasifyer effluent has been recalculated. The integration of subsystems, namely, gas purification, shift-conversion and methanation is conducted and readjustment of heat recovery system is made where required.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 3% February 28, 1970

to

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

(A) Gasification Phase

Computer simulation of solid-gas reactions in continuous moving bed and fluidized bed reactors are made taking into account reaction kinetics as well as heat and mass transfer phenomena. The models developed are satisfactory for describing the performance of the moving beds and fluidized bed reactors and are now used for scaling-up of coal gasification processes.

(B) Water-Gas Shift Reaction Phase

The optimization results of water-gas shift conversion using adiabatic reactor system and cold-quenching reactor system are combined together, and summarized in preparation for the presentation to ACS Symposium. The cost information is arranged for the prefinal report on coal gasification processes.

(C) Gas Purification Phase

Computer simulation of gas purification processes using the two different absorbents, hot potassium carbonate solution and pure water has been completed. Also three cases of gas feeds under isothermal and non-isothermal conditions were treated. Temperature differences affect very little on the final results. A better numerical technique without iteration was used. The results agreed well with those by calculation involving iteration. The degree of removal of H_2S with CO_2 is rather low so that new process is being taken into consideration. Optimal operating conditions were found by using the search technique. Prefinal report is being prepared.

(D) Methanation Phase

The prefinal report for OCR is being prepared.

1. Some information of the alternate methods of coal gasification have been collected.
2. Using new cost year index and cost factor the results of the methanation processes in old report were recalculated.
3. The costs of cooling water and process water have been investigated.

C. Y. Wen

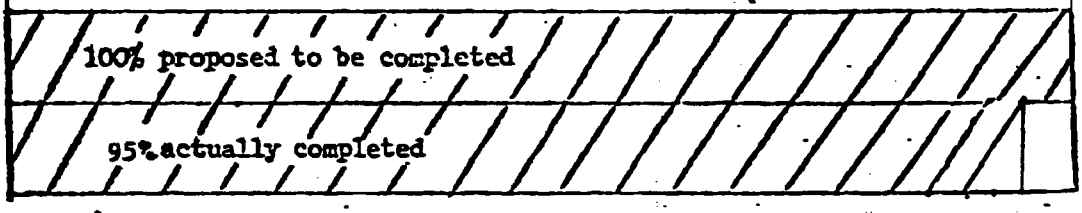
C. Y. Wen, Project Director

PROGRESS OF WORK FOR OPTIMIZATION OF COAL GASIFICATION PROCESSES

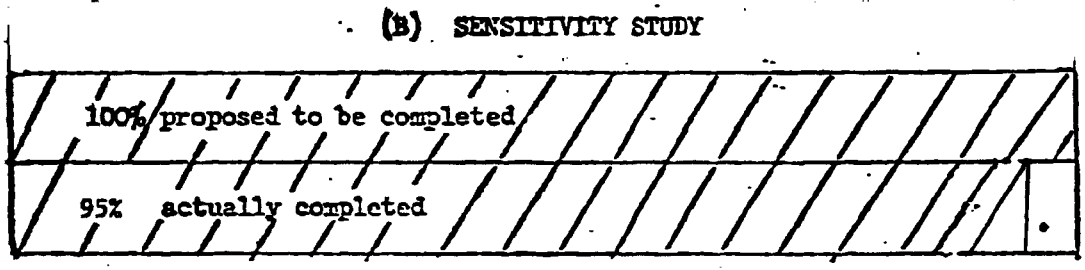
February 28, 1970

OCR CONTRACT 14-01-0001-497

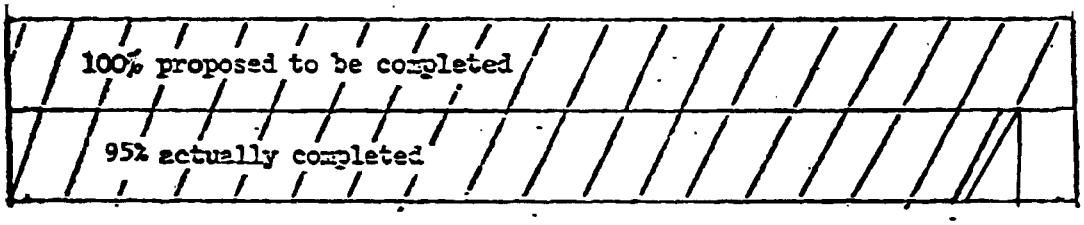
(A) INFORMATION GATHERING AND ASSIMILATION



(B) SENSITIVITY STUDY



(C) DEVELOPMENT OF GENERAL OPTIMIZATION TECHNIQUE INVOLVING INFORMATION UNCERTAINTY



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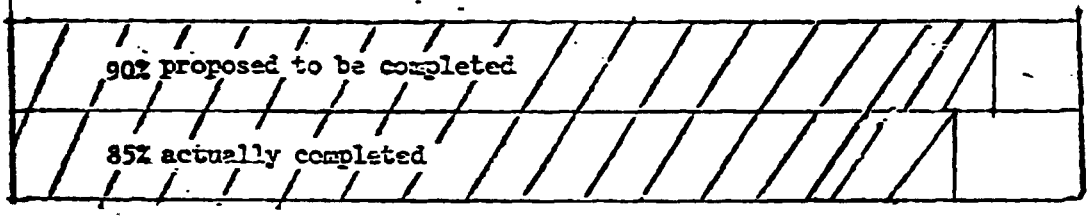

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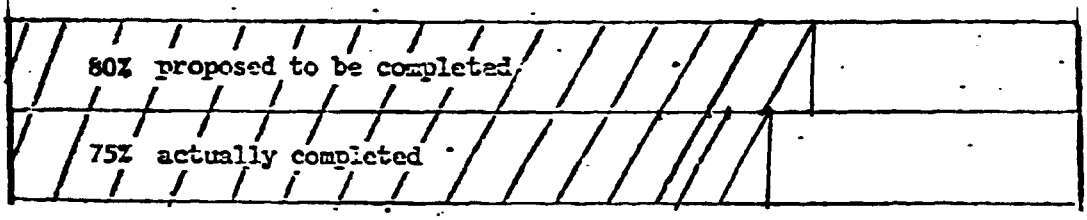

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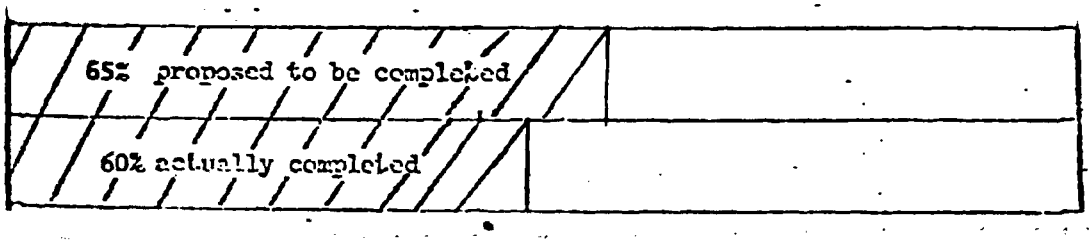


OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 38 April 30, 1970

to

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

(A) Gasification Phase

Office of Coal Research pre-final report is being prepared. Approximately 80% of "Gasification" part (Chapter 4 of the report) has been completed. Flow sheets of alternative methods of coal gasification are being prepared.

(B) Water-Gas Shift Reaction Phase

The pre-final report on the optimization of fixed-bed water-gas shift conversion processes is prepared. Cost information, a part to appear in the pre-final report, is being prepared.

(C) Gas Purification Phase

Pre-final report is being prepared. Simulation of H_2S and sulfur compounds removal is being performed in a computer. In normal operations activated carbon bed is used for removal of H_2S. The catalytic action of activated carbon promotes the oxidation of H_2S to elemental sulfur at room temperature.

Iron oxide bed is better for complete removal of H_2S. It is possible to reduce the concentration to less than 0.01 grain per hundred cubic feet.

(D) Methanation Phase

The pre-final report is completed.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 40 June 30, 1970

to

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

(A) Overall Plant Optimization

Branch and bound optimization techniques have been studied. These methods will be applied to the overall plant optimization.

(B) Gas Purification Phase

(1) The advantages of the improved hot potash process by the addition of certain organic or inorganic substance for acid gas removal were examined. The following findings were obtained:

(a) The use of amine promoted hot potash solutions may increase the liquid side mass transfer coefficient K_L by 1 to 5 times. This will greatly reduce the size of the absorber for CO_2 removal from low pressure gas stream but will not offer much advantage for CO_2 removal from high pressure gas stream.

(b) The greatest advantage of the Giammarco-Vetrocoke process, which uses arsenic - containing aqueous solutions for acid gas removal, is its capability of providing a treated gas containing less than 1 ppm H_2S even when absorption is carried out at elevated temperature and atmospheric pressure. However, the kinetics of this process is not clear. This process certainly deserves further investigation.

(2) The steam-to-CO_2 ratios required for the regenerator with and without the assumption of non-volatile solvent were compared. It was found that the ratio calculated for volatile solvent is more than twice of the ratio with non-volatile solvent. Therefore, this simplifying assumption should not be used in the design of the regenerator.

(3) Adsorption processes for removal of H_2S and C_6H_6 - the following points are clarified:

(i) Iron oxide processes can be used for removal of H_2S. This process can completely remove small to medium concentrations of H_2S without removing CO_2.

(ii) Activated carbon bed can be used for removal of organic compound, especially, for the recovery of C_6H_6, ether, CS_2, acetone etc. If the treated gas contains oxygen, this process is applicable to removal of H_2S, because carbon acts as catalysts for the reaction between H_2S and O_2.

Since the coating of the iron sponge with entrained oil or distillate will result in lowering of the activity of iron sponge the activated carbon bed should be used prior to the iron oxide process.

The designing procedure was established as follows:

(i) Activated carbon bed is used for removal of C_6H_6.

(ii) Iron oxide bed is used for removal of H_2S.

(iii) Concentration of C_6H_6 in the gas produced in gasifier is still unknown. 0.3% at inlet of adsorption process is assumed (this value may be changed in the future).

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 41 July 31, 1970

to

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

(A) Gasification Phase

The bubble assemblage model to simulate the fluidized bed reactor has already been proposed. It was found that the conversions predicted using this model agree well with the actual performance of both catalytic and non-catalytic reactions in the fluidized beds. The phenomena of solid dispersion in a fluidized bed was studied. Since the conversion of solids for non-catalytic reaction is dependent on the reaction rate of particles and the residence time of solid particles in the reactor, we must predict the length of stay of solid in the fluidized bed gasifier. It was shown that the bubble assemblage model can be used also well to simulate the solid dispersion in fluidized beds in the light of several reported experimental data. The results will be presented at the AIChE Meeting in Chicago. This may contribute to the optimization of fluidized bed gasifier.

(B) Water-Gas Shift Reaction Phase

The steam, gas ratio of the water gas shift conversion has been studied and the computer calculation has been completed. The result will be reported separately.

(C) Methanation

The waste heat recovery in the methanation system has been re-designed. The calculated amount of low pressure steam required in the purification system is larger than the expected amount set for the original design of the methanation system. Therefore the above change has to be done.

(D) Gas Purification

Optimization in the design of an absorber-regenerator system without the assumption of non-volatile solvent was performed. Optimization of the iron oxide process and the activated carbon process have been completed. The final report on the whole gas purification system is being written.

(E) Overall Plant Optimization

A simplified case with three reactors in series has been studied. In order to optimize this problem the discrete maximum principle has been applied. Due to some technical difficulties the result has not been obtained yet.

Kunio Yoshida for
C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 42 August 31, 1970

to

Office of Coal Research
Contract No. 14-01-001-497

(A) Gasification Phase

Simulation of primary gasification phase is being made. The complexity of reaction kinetics coupled with flow behavior of the reactor has been the major problem in arriving at realistic design procedure.

(B) Gas Purification Phase

Optimization of gas purification processes is completed. Hot carbonate process followed by monoethanol amine process seems to provide the best scheme for simultaneous removal of CO_2 and H_2S from the system. In this manner, hot carbonate process is primarily responsible for removal of CO_2 and the amine process is used for removal of H_2S without involving iron oxide process. Although iron-oxide process is optimized to reduce H_2S content to below 0.01 grain/100 SCF, it is not included as part of the optimum process. Removal of benzene and other organics can be achieved by the activated carbon towers. This process is also optimized. The final report on this phase is now complete.

(C) Coal Pretreatment Phase

Economic analysis of coal pretreatment phase has been started.

(D) Overall Plant Optimization

Subsystem optimizations are now near completion. This information are now combined to arrive at the overall plant optimization computer technique for this phase is now being developed.

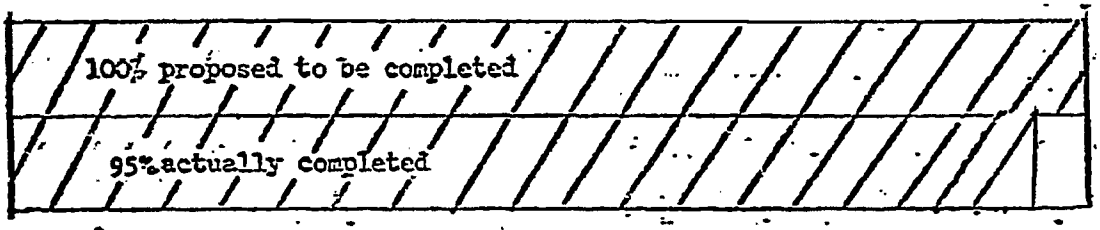
C. Y. Wen, Project Director

PROGRESS OF WORK FOR OPTIMIZATION OF COAL GASIFICATION PROCESSES

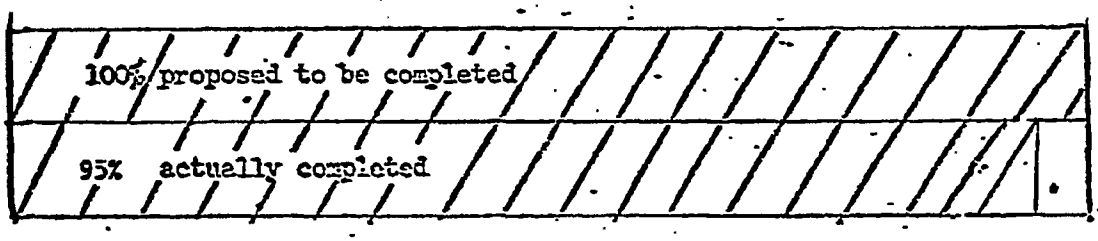
August 31, 1970

OCR CONTRACT 14-01-0001-497

(A) INFORMATION GATHERING AND ASSIMILATION



(B) SENSITIVITY STUDY



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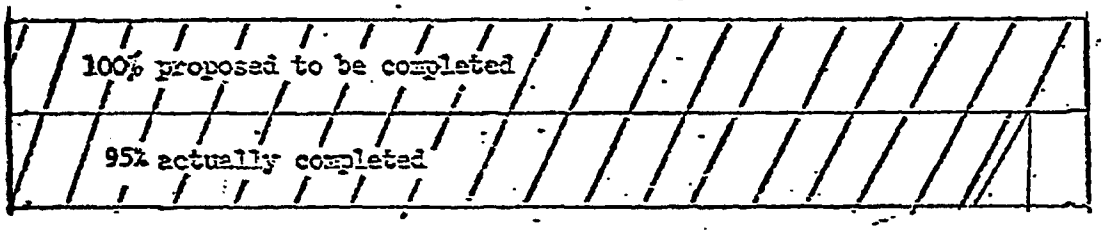
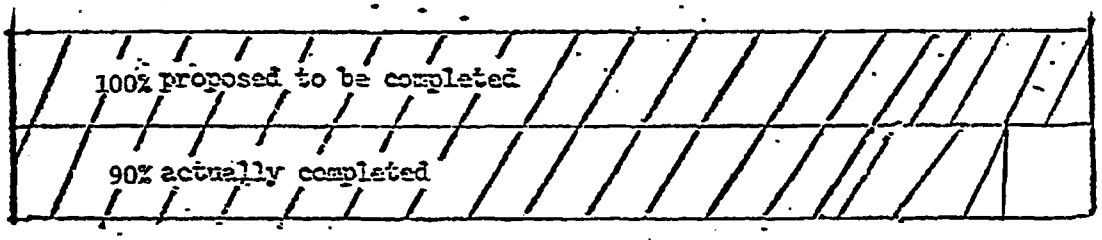
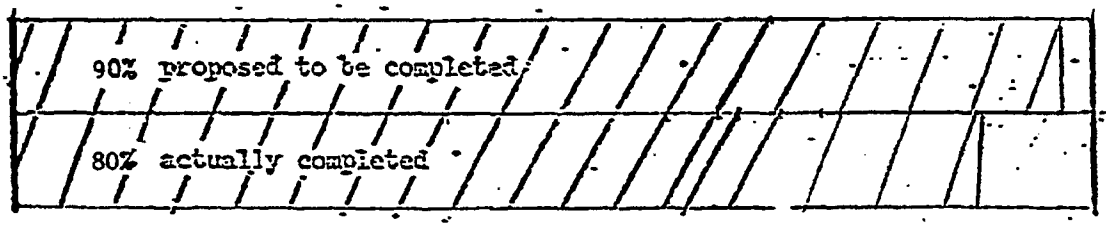


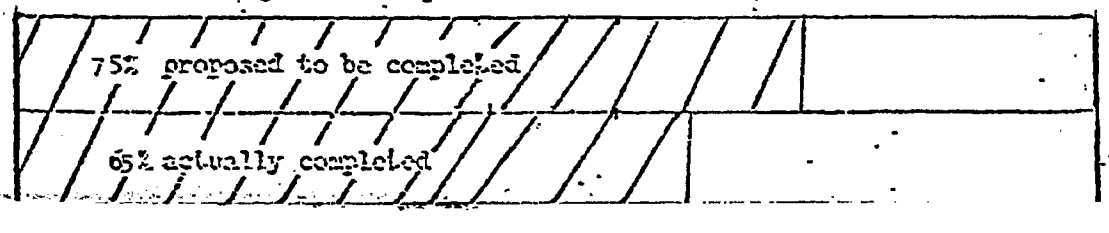
(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



(E) DEVELOPMENT OF COMPUTER PROGRAM



(F) COMPARISON, EVALUATION AND RECOMMENDATION



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 43 SEPTEMBER 30, 1970

to

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

(A) Coal Pretreatment

Various modes of coal pretreatment, feeding systems are studied. The types of coal to be fed and the methods of gasification to be employed will make considerable difference in the extent of coal pretreatment required.

(B) Gasification Phase

Computer programming of heat and material balance in a gasification reactor for various gas feed, solid feed and solid conversion is being prepared. Simulation of two-zone reactors in series is also under study.

(C) Gas Purification

A report on gas purification phase is completed and is attached with this report.

(D) Overall Plant Optimization

Feasibility of applying the multilevel technique to the overall plant optimization has been studied. The study included the methods of system simplification, the technique of reducing state variables and use of cut state variables in systems with a recycle.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 44 OCTOBER 31, 1970

to

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

Coal Pretreatment Phase

Heat and material balances for fluidized bed coal pretreatment operations have been formulated. Models necessary for simulation are being developed.

Coal Gasification Phase

Material balance, heat balance, carbon conversions, gas product distribution, and heat losses are being computed for a few of commercial gasifiers investigated. They are Winkler generators producing synthesis gas, Koppers Dust Gasification process, Lurgi Pressure Gasification Process and Leuna Slagging generators.

Overall Plant Optimization

Optimization techniques useful for a large complex system are mostly related to multilevel optimization methods. Among them, method of combining gradient technique and Lagrange multiplier technique is most promising. This method takes the advantages of its easiness in formulating equations and the iterations method of searching for optimal points along the gradient of Lagragian with respect to decision variables.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 45
FOR QUARTER ENDED NOVEMBER 30, 1970

to

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

Pretreatment Phase

Currently, work is being conducted on writing a computer program to give the composition of off-gas with its heating value for any composition of coal fed in the unit. This program would lead to sizing the unit and cost evaluation of this phase.

Gasification Phase

Carbon utilization for a coal gasification system was studied. The purpose of this study is to determine the minimum carbon requirement for producing 1 lb.-mole of methane in various coal gasification systems.

In order to simplify the calculation, only the material balance was considered for shift conversion, purification, and methanation phases. It was also assumed that regardless of the mode of heat addition to a gasifier, all the heat required for gasification comes from combustion of coal. Different efficiency factors were assigned for different methods of heat addition.

In order to identify problems associated with large scale units, material and heat balances of five industrial processes; Winkle generator, Lurgi Fixed Bed, Kopper's Injection process, Leuna Bed and Bureau of Mines process have been calculated.

C. Y. Wen, Project Director

PROGRESS OF WORK FOR OPTIMIZATION OF COAL GASIFICATION PROCESSES

November 30, 1970

OCR CONTRACT 14-01-0001-497

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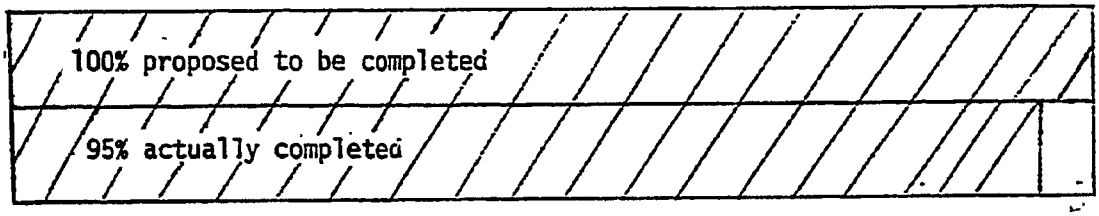

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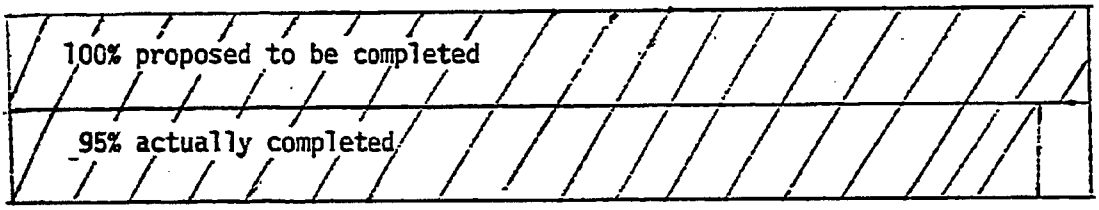

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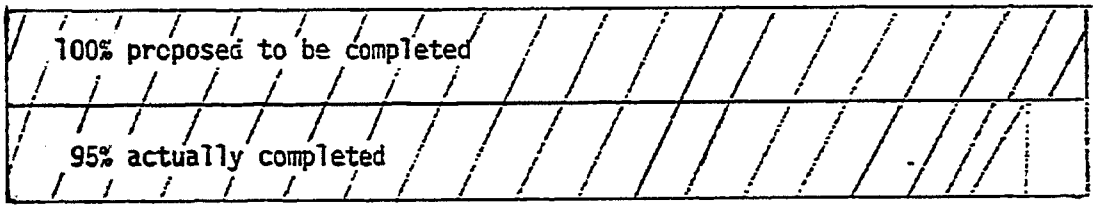
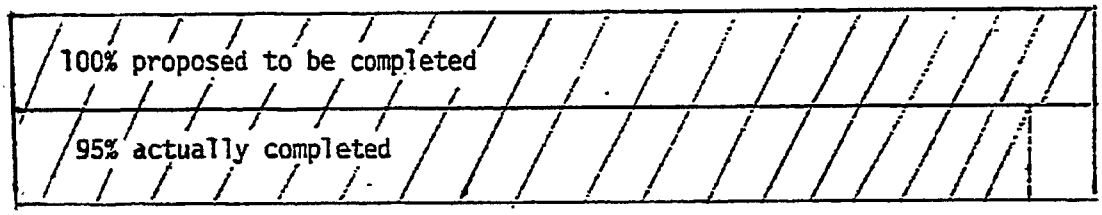


(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES



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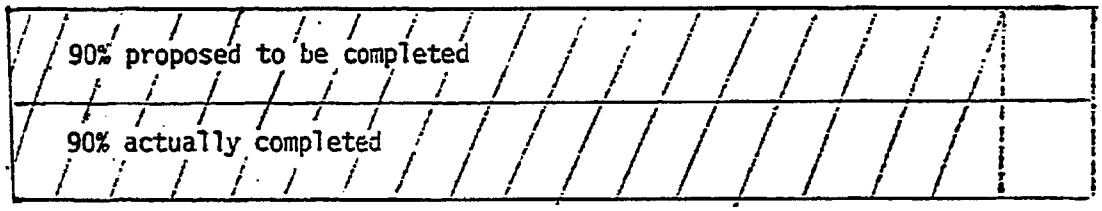
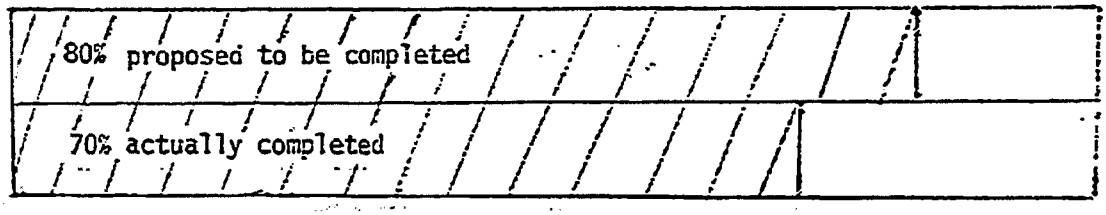


(F) COMPARISON, EVALUATION AND RECOMMENDATION



OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 46
DECEMBER 30, 1970

to

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

Gasification Phase

Simulation of secondary gasification phase to produce hydrogen rich gas suitable for hydrogasification has been performed. Based on material and heat balance, together with thermodynamic considerations, it was possible to select conditions favorable for production of H_2 and CO while lowering O_2 requirement.

Pretreatment Phase

Various coal pretreatment schemes and their advantages and disadvantages are studied quantitatively.

Overall Plant Optimization

Factors affecting the gas price based on OCR accounting procedure is being studied to examine if any possibility of modifying the accounting procedure exists in order to provide a reasonable standard for the computation of economic factors such as interest rate, return rate, tax, debt fraction, etc.

C. Y. Wen, Project Director

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