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OPTIMIZATION OF COAL GASIFICATION PROCESSES. MONTHLY PROGRESS REPORTS FOR THE PERIODS JANUARY--APRIL, JUNE, NOVEMBER, AND DECEMBER 1971

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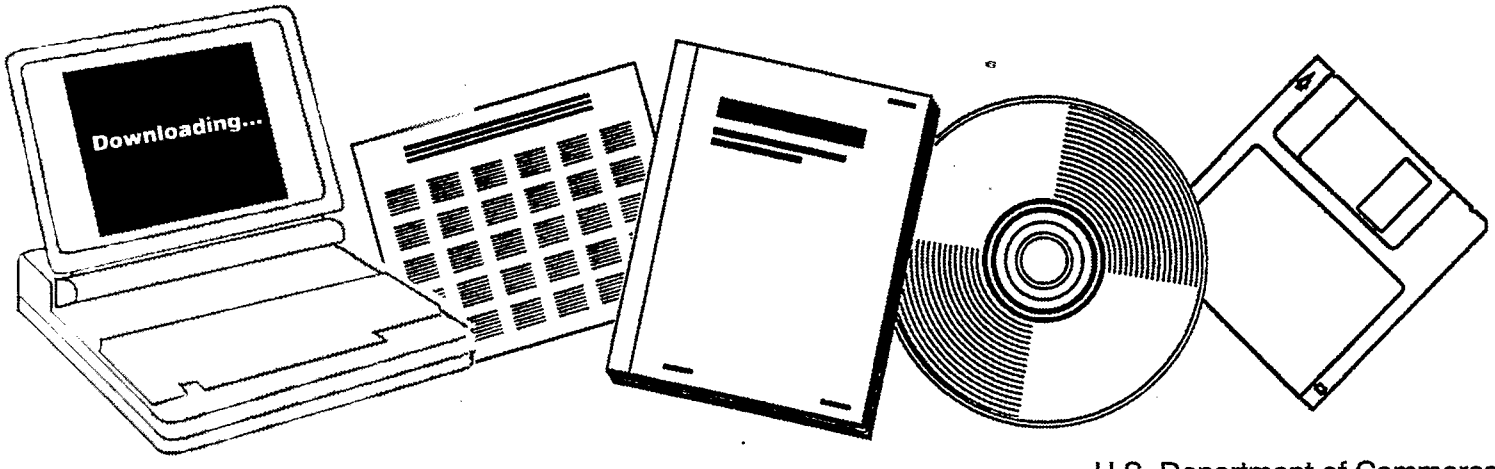

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OPTIMIZATION OF COAL GASIFICATION PROCESSES

Monthly Progress Reports for the periods
January - April, June, November, and December 1971

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MASTER

Prepared for

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

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FE--497-T-5

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Monthly Progress Reports covering January -
April, June, November, and December 1971

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OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 47
JANUARY 31, 1971

to

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

Gasification Phase

Calculations of carbon utilization without recycle in the gasification system are under study.

The computer programs simulating the following three cases have been completed.

(1) gasification → shift conversion → purification
→ methanation → pipeline gas

(2) gasification → shift conversion → purification
→ hydrogasification → pipeline gas

(3) gasification → shift conversion → purification
→ methanation → pipeline gas
→ hydrogasification → pipeline gas

The program is to evaluate the effect of variations of parameters on methane production.

Accounting Procedure

Procedure for computation of gas price is reviewed.

Overall Plant Optimization Phase

Carbon utilization for coal gasification processes has been studied.

The number of moles of carbon required to produce one mole of methane was tentatively set as the objective function to be optimized. Before the optimization can be done, computer simulations of gasification processes in terms of material and energy balances of each stage, have been prepared. The possible optimization technique to be used for this study is so called, "Multilevel Optimization Technique."

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 48
FEBRUARY 28, 1971

to

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

Computer simulations for a hydrogasification system has been made. The following assumptions were made for the simulation.

1. Char used for the secondary gasification is supplied by the primary gasification byproduct char. A complete carbon conversion in the secondary gasification is assumed.
2. Gas from the secondary gasification is shifted to a specified range of CO/H_2 ratio (1/4, 1/8 and 1/10).
3. Water gas-shift equilibrium and hydrogen-methane-carbon pseudo-equilibrium (with an approach factor of 2) were assumed in the primary gasification.
4. The heating value of pipeline gas is about 900 BTU/S.C.F.

Based on above assumptions, material balance and energy balance, equilibrium relations as well as heating value constraint were used for setting up the system equations. Eight equations for eight variables have been obtained.

A modified Newton-Raphson method subroutine from the computer center library has been used to solve these simultaneous equations.

From the attached figures, it can be seen that if no excess char is allowed to be produced from the gasification system, the optimum carbon utilization defined as lb-mole of carbon used/lb-mole of methane produced is at the range of 0.25 - 0.3 carbon conversion in the primary gasifier.

A report, "Study of Carbon Utilization in Coal Gasification Processes," is being prepared which will become available in a short time.

C. Y. Wen, Project Director

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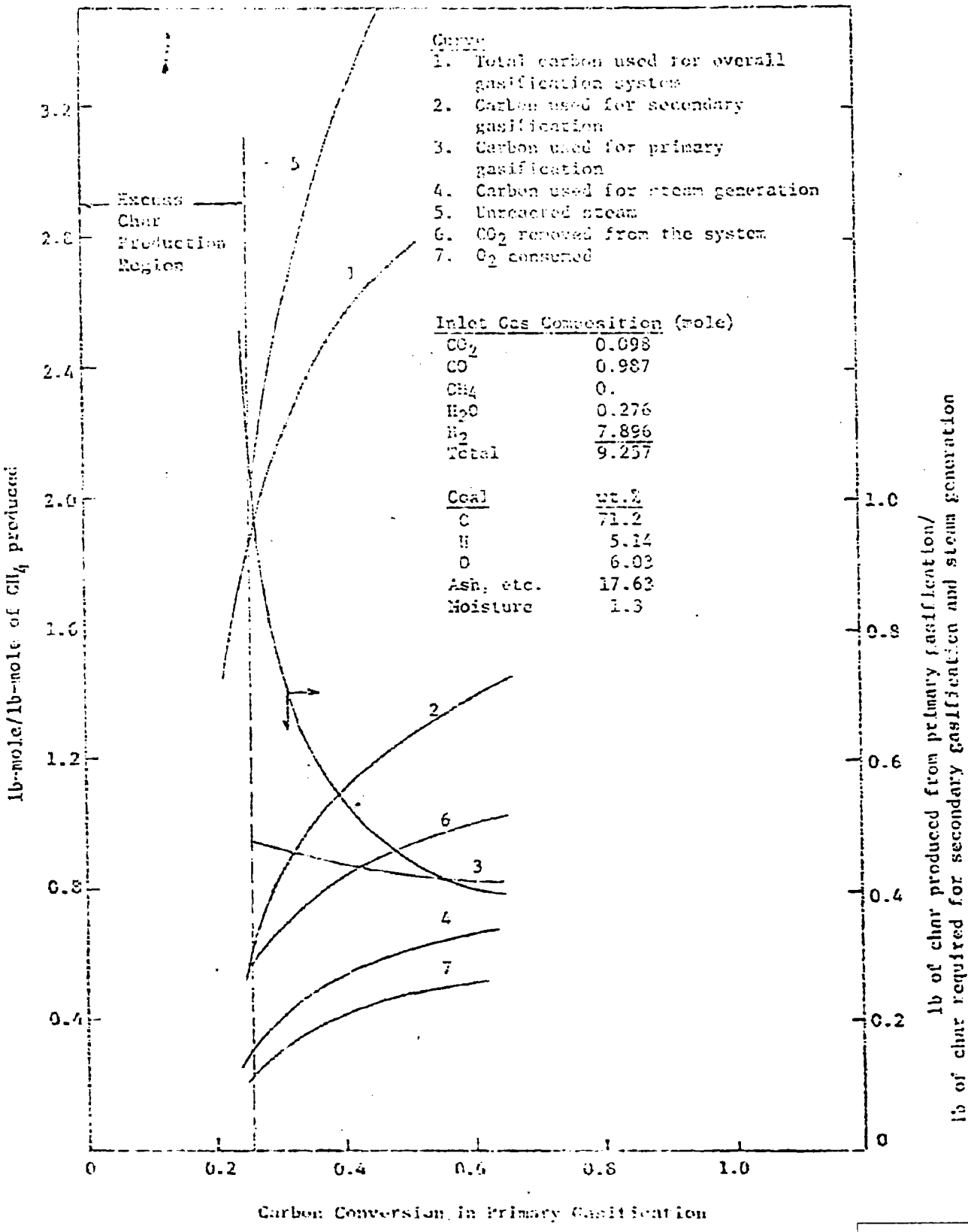

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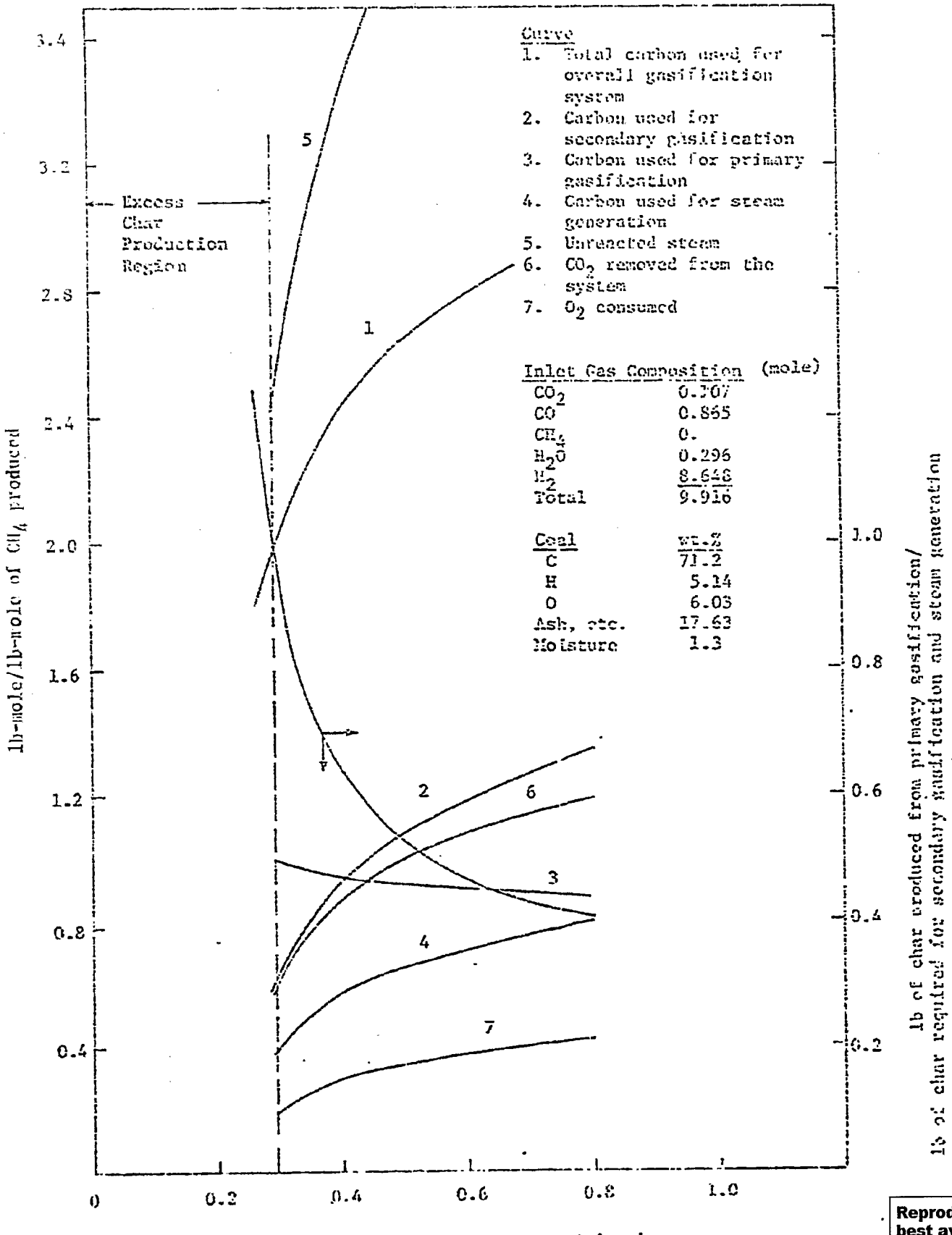

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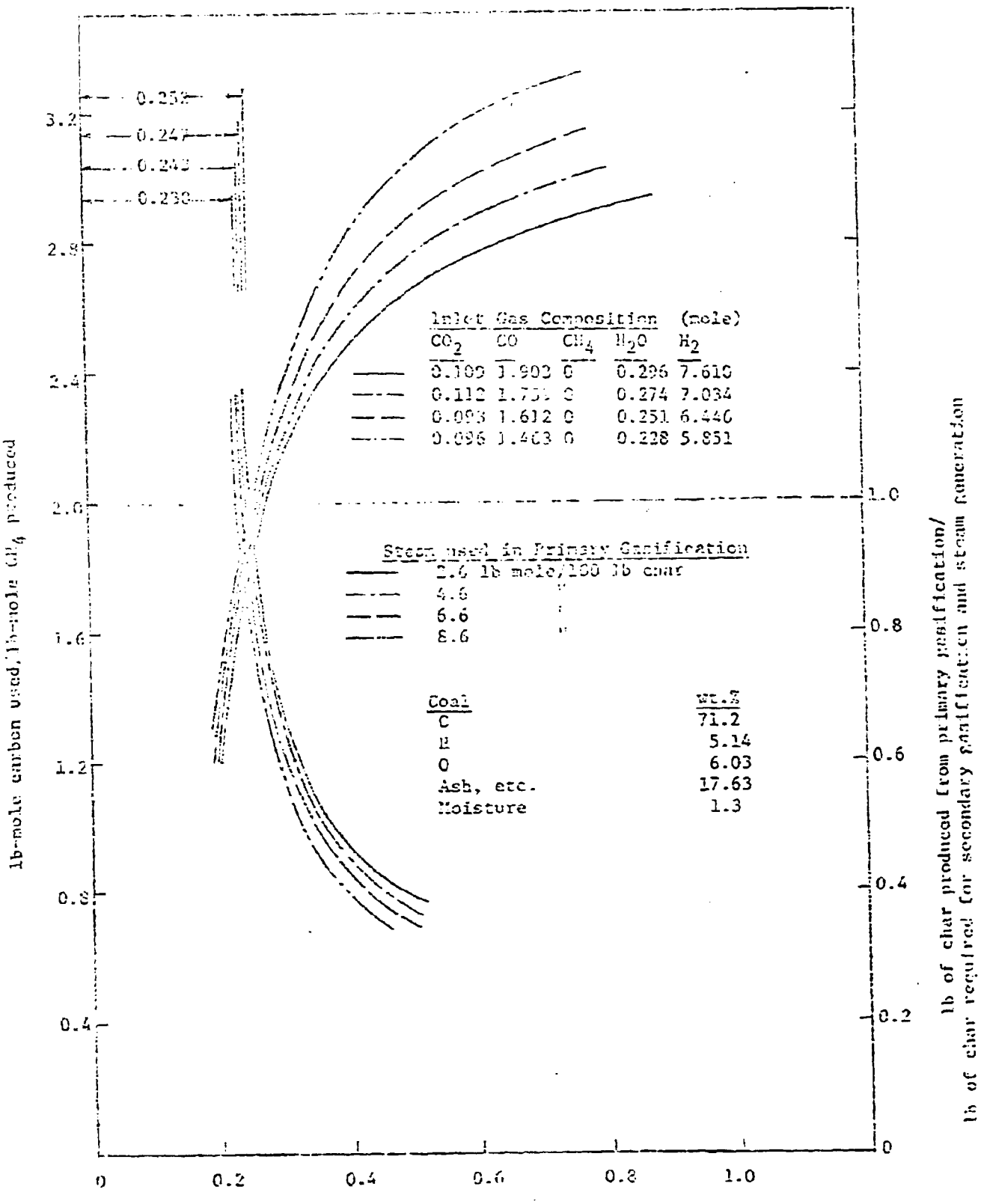

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PROGRESS OF WORK FOR OPTIMIZATION OF COAL GASIFICATION PROCESSES

February 28, 1971

OCR CONTRACT 14-01-0001-497

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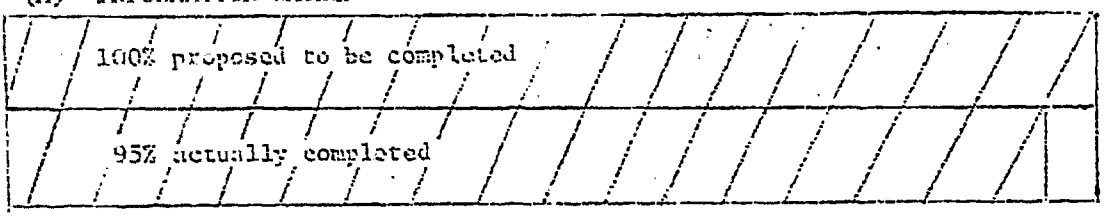

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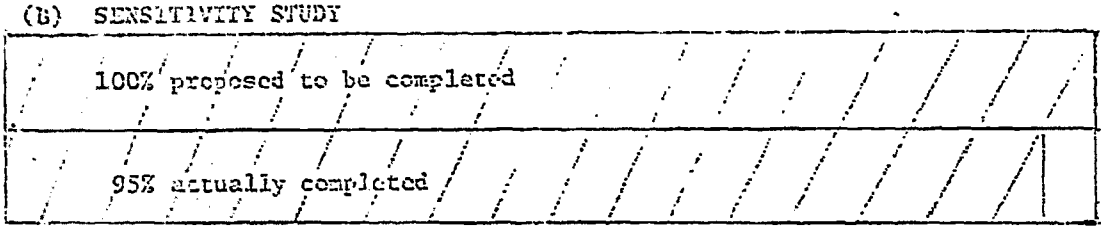

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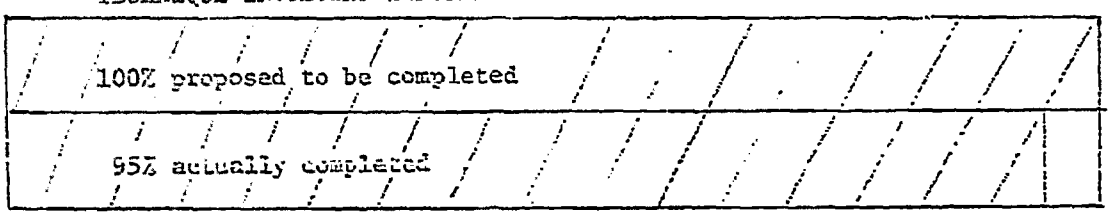

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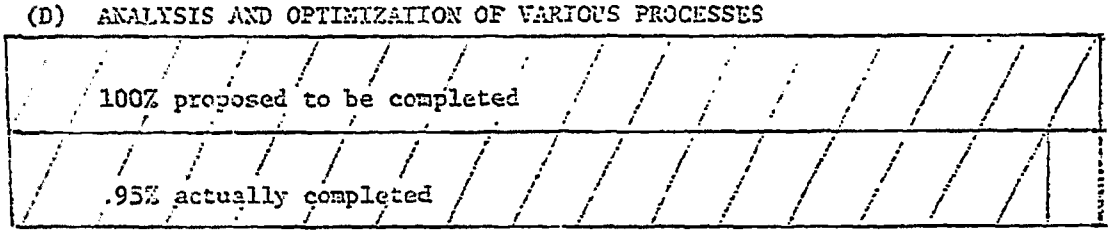

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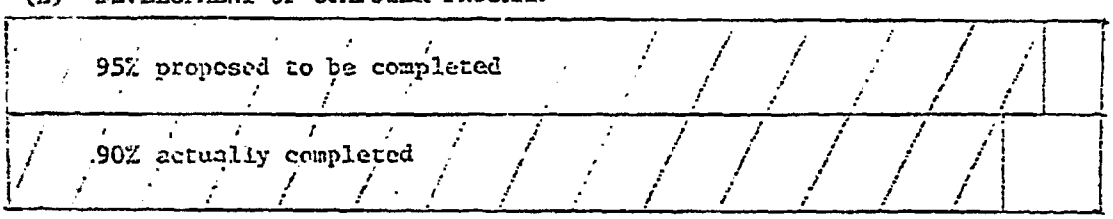

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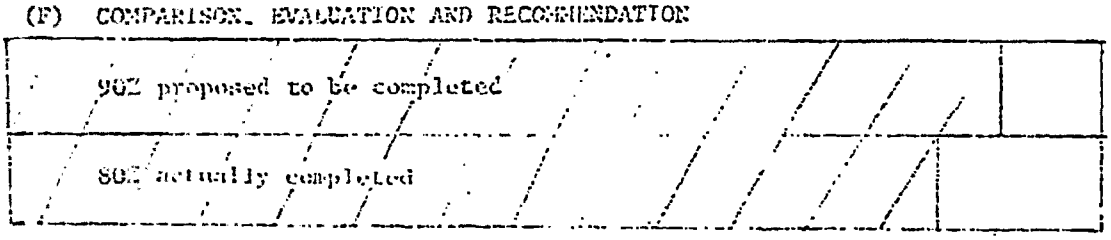

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 49
MARCH 31, 1971

to

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

Effects of temperature on a selected gasification system, consisting of primary gasification, secondary gasification, shift conversion, purification and methanation, have been studied. Based on several different temperatures and a set of constant inlet conditions, the hydrogasifier was simulated in a computer. Typical results are shown in the attached figures. Tons of coal used for each unit and for the entire system per MSCF of pipeline gas are plotted versus carbon conversion in the hydrogasifier. The balance operating line representing the condition of no excess or additional char needed for the entire gasification system is also shown in Figs. 1 and 2.

A similar system, but without hydrogasifier, has also been studied. This system is arranged in such a way that the gas leaving the gasifier is shifted to achieve a H_2-CO ratio approximately equal to 3. This gas is subsequently methanated after purification to remove CO_2 and H_2S. Fig. 3 presents the thermodynamic efficiency of the system in terms of number of tons of coal required to feed per thousand standard cubic feet of pipeline gas produced.

Apparently, more oxygen is required if the reaction is to be maintained at a higher temperature. It is also evident from the figure that for the same amount of the pipeline gas produced, the amount of coal required increases with an increase in temperature.

C. Y. Wen, Project Director

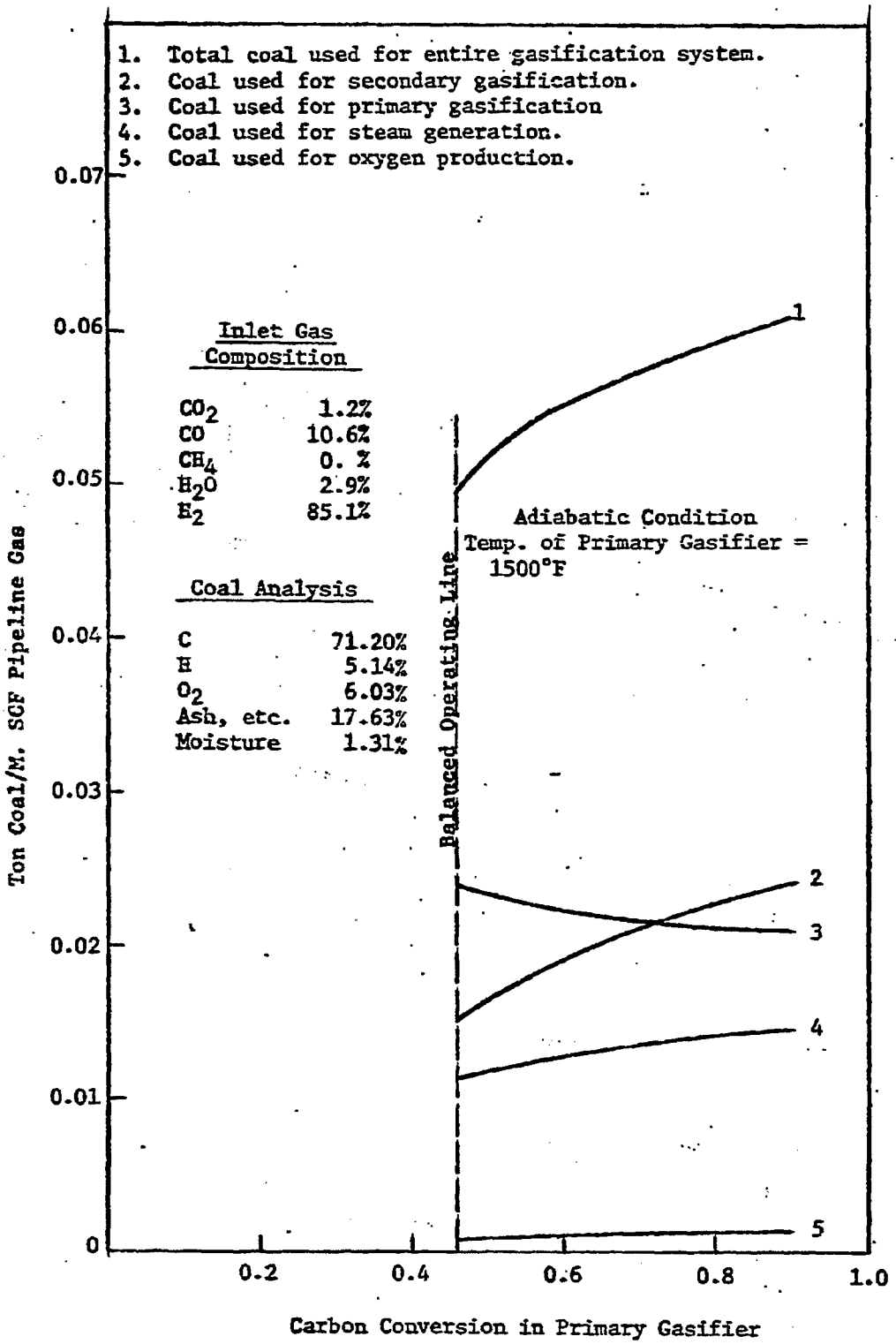

Fig. 1. Efficiency of Coal Gasification System, Case I

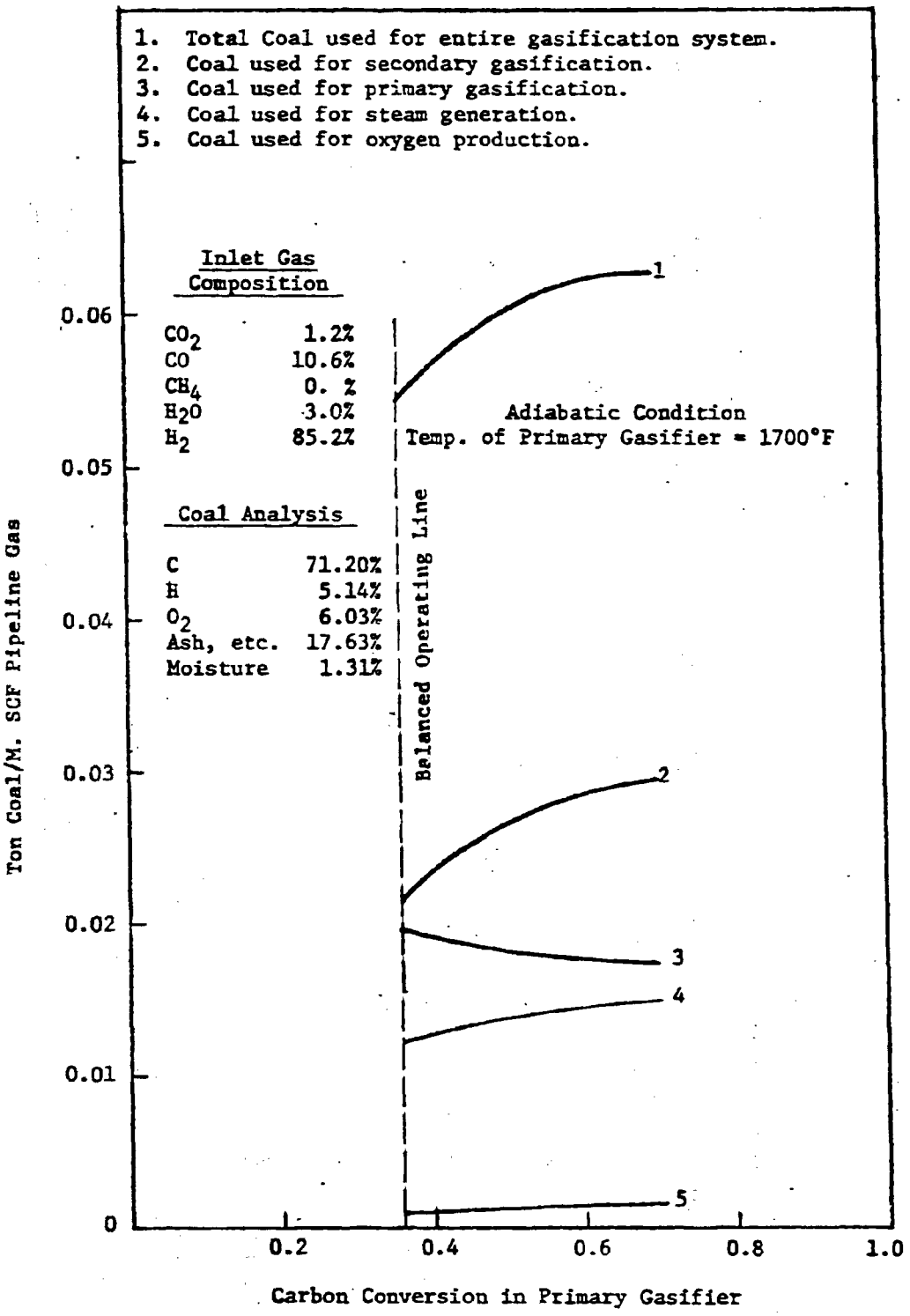

Fig. 2. Efficiency of Coal Gasification System, Case II

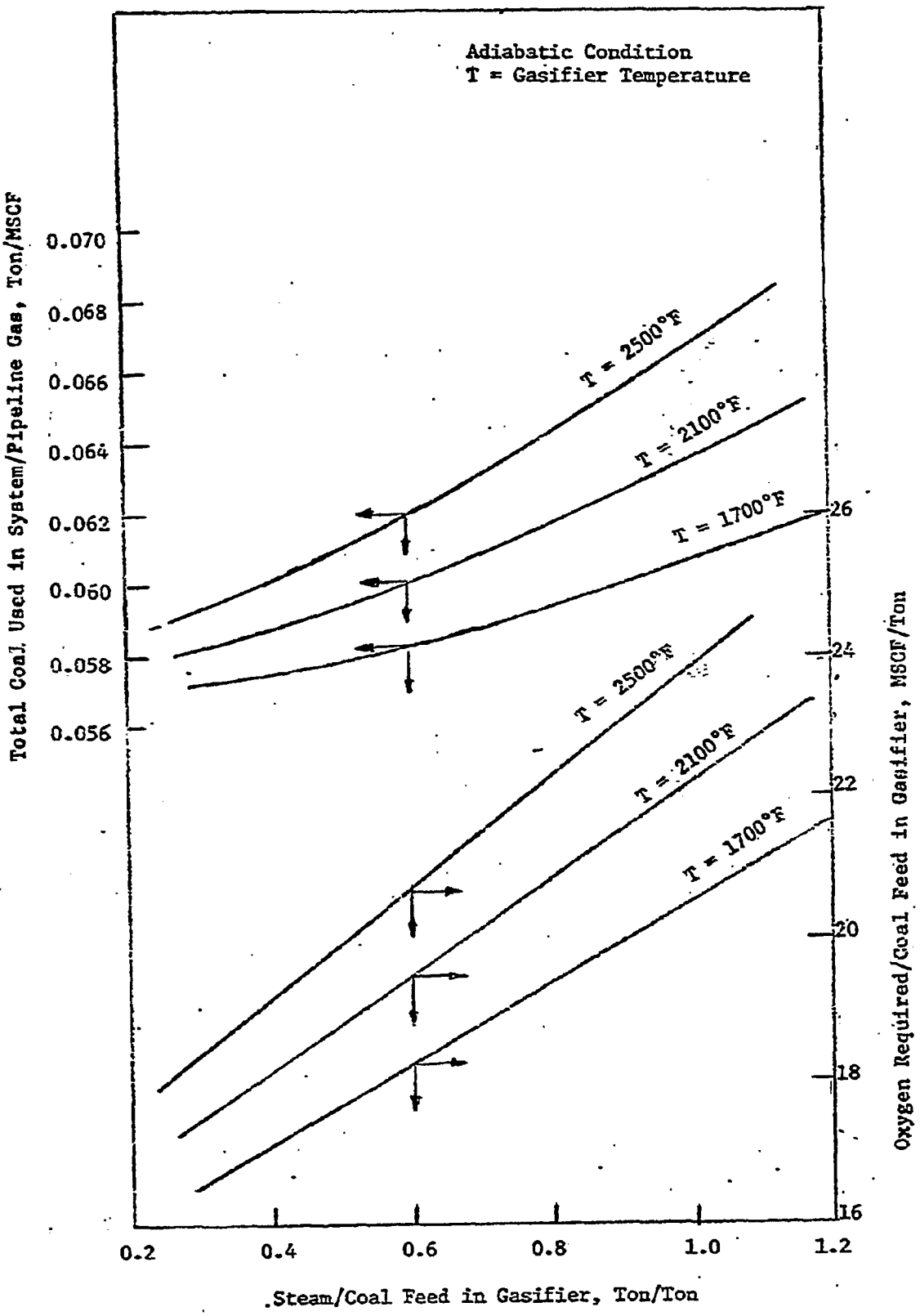

Fig. 3. Efficiency of Coal Gasification System and Oxygen Requirement, Case III

OPTIMIZATION OF COAL GASIFICATION PROCESSES
PROGRESS REPORT NO. 50
APRIL 30, 1971

to

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

A gasification process closely related to the B. C. R. Two-Stage Super-Pressure Gasification Process has been studied. The system was simulated in a computer. Assumptions made for the simulation are:

1. The temperature of the 1st stage is 2300°F and that of the 2nd stage is 1700°F.
2. Carbon is completely converted in the 1st stage.
3. No free oxygen is present in the 1st stage effluent gas.
4. The water-gas shift equilibrium is assumed in the 1st stage.
5. Both water-gas shift and carbon-hydrogen-methane equilibrium are assumed in the 2nd stage.

Parameters studied in the simulation are the amount of steam introduced in the 1st stage and the carbon conversion in the 2nd stage. Results are shown in the attached figure.

For a constant carbon conversion in the 2nd stage, an increase in the amount of steam introduced into the 1st stage increases the amount of coal required per unit amount of pipeline gas production. For a constant steam rate a higher carbon

conversion in the 2nd stage decreases the amount of coal required per unit amount of pipeline gas production.

From the results of the above simulation, it was found that most of the steam introduced into the 2nd stage was used for cooling, i.e., the degree of steam decomposition in the 2nd stage is not high. In order to study the effect of the amount of steam introduced into the 2nd stage on the pipeline gas production, a heat exchanger unit is inserted between the 1st stage and 2nd stage gasifier. By passing the hot 1st stage effluent gas through the heat exchanger, the temperature of the 2nd stage inlet gas can be controlled to any point as one desires. The temperatures used for the computer simulation are 2300°, 2100° and 1900°F. A typical result is shown in Table I. The result shows that the steam used in the 2nd stage decreases with a decrease in the temperature of the 2nd stage inlet gas. As a consequence of this reduction in steam consumption, a higher pipeline gas production per unit amount of coal is obtained.

C. Y. Wen

C. Y. Wen, Project Director

Carbon Conversion in 2nd Stage	0.3			0.35		
Coal fed into Gasifier 1b.	100			100		
Steam used in 1st Stage 1b-mole	6			6		
Temperature of 2nd Stage Inlet Gas °F	2300	2100	1900	2300	2100	1900
Steam used in 2nd Stage 1b-mole	7.103	5.333	3.432	5.496	3.654	1.536
M. SCF Pipeline Gas 1 Ton of Coal	16.572	17.156	17.829	17.404	18.064	18.888

Table I. Effect of Temperature of 2nd Stage Inlet Gas on Pipeline Gas Production.

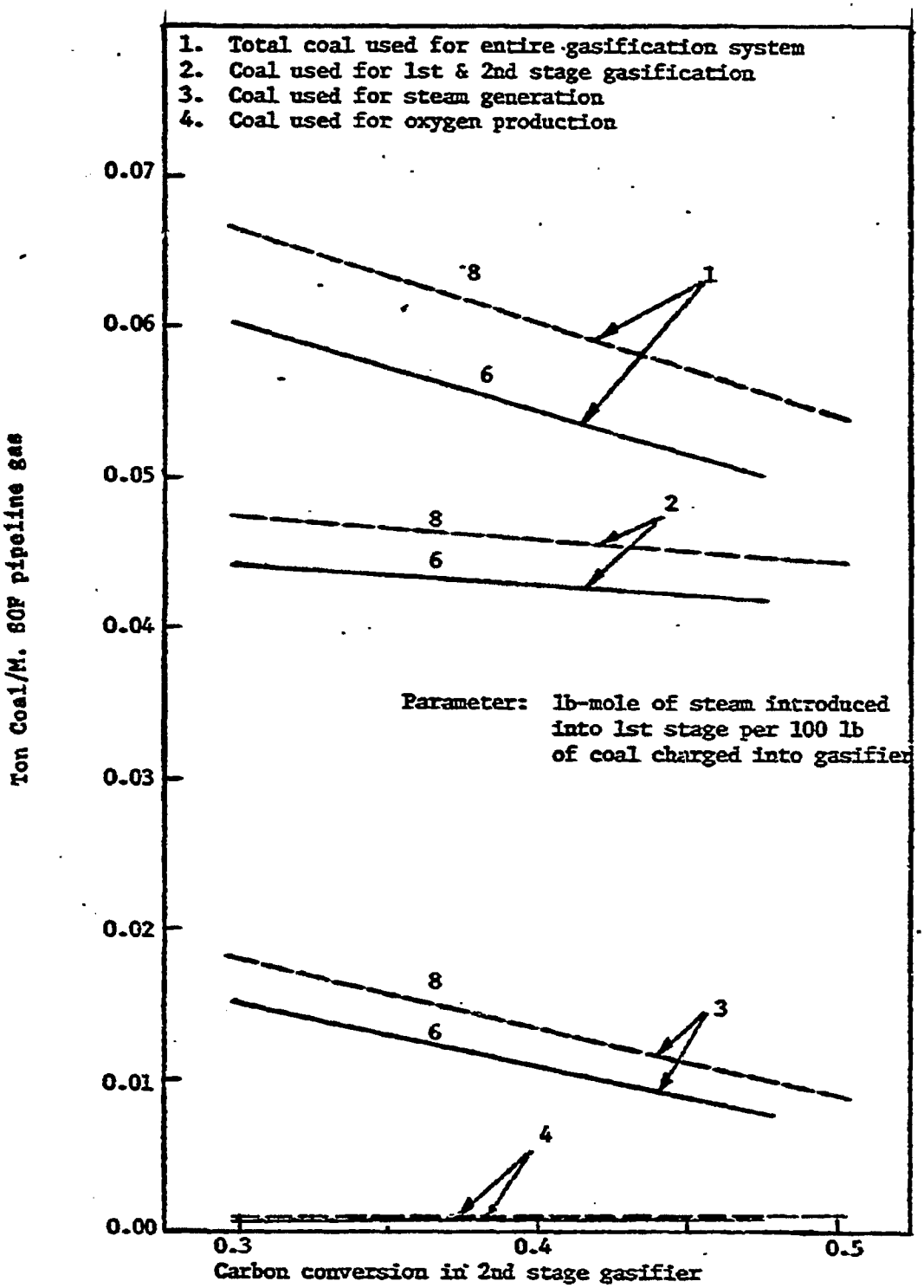

Figure 1. Efficiency of Coal Gasification

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PROGRESS OF WORK FOR OP[illegible]TION OF COAL GASIFICATION PROCESSES

JUNE 30, 1971

OCR CONTRACT 14-01-0001-497

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(B) SENSITIVITY STUDY

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(C) DEVELOPMENT OF GENERAL OPTIMIZATION TECHNIQUE INVOLVING INFORMATION UNCERTAINTY

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(D) ANALYSIS AND OPTIMIZATION OF VARIOUS PROCESSES

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(E) DEVELOPMENT OF COMPUTER PROGRAM

97% proposed to be completed

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(F) COMPARISON, EVALUATION AND RECOMMENDATION

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OPTIMIZATION OF COAL CONVERSION PROCESSES
PROGRESS REPORT NO. 51
NOVEMBER, 1971

to

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

The gasification process proposed by the Bureau of Mines, "Hydrane Process" was studied. Based on the available experimental data on Hydro-gasifiers and Devolatizers, the material and heat balances on shift conversion, purification gasification and methanation were calculated. The integrated gasification process has been developed and the price of pipeline gas was estimated.

New optimization techniques for the complex system have been studied. The optimization method used in the previous work is not as efficient as it was expected. The problem of tying up the sub-system optimizations together and obtaining an overall optimization is not an easy task. The multilevel optimization techniques discussed in an earlier report is one of the attractive methods to be used for this type of problem. However, when the number of variables in the systems are interacting, the multilevel method becomes too complicated and the efficiency decreases. The new approach is based on a simplified coal conversion plant such that all parts of the plant can be considered simultaneously. Using some sort of efficiency factor as an objective function the plant will be optimized. It is hoped that some relation can be established between this efficiency factor and the gas price. The new optimization techniques under study are: the Carroll-Fiacco penalty function, the created response surface, the Paviana, and the complex methods.

The production of fuel gas in the atmospheric pressure gas producer is compared with the production of high pressure pipeline gas from various coal gasification processes studied.

Instead of oxygen which is used for pipeline gas production, air from a blower is introduced into a gas producer where coal and steam are added to produce the raw gases. To obtain a cold clean gas from a hot raw gas, the raw gas may be passed through the gas cleaning system to remove impurities from the raw gas. The economic evaluation of fuel gas production processes will be made based on criteria developed for the coal gasification processes.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES
PROGRESS REPORT NO. 52
DECEMBER, 1971

to

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

A study is being made of the coal gasification system developed by the U. S. Bureau of Mines known as the "Synthane Process." This process scheme is similar to the "Alternate I" System described in our Final Report, Contract No. 14-01-001-497, September 15, 1971, except that the pretreatment and gasification sections, considered as separate units in "Alternate I", is combined into one step in the "Synthane Process". The material and heat balances have been completed for this process, using bituminous coal as the feed, and the optimization of this system and its comparative evaluation to other gasification processes are now being undertaken.

The previous computer programs for the high pressure coal gasification processes using oxygen to produce pipline gas have been reviewed with the intention of modifying the programs to use ambrient air at atmospheric pressure. The modified computer programs are now being written and debugged.

As discussed in Progress Report 51, the mathematical optimization technique used up to the present has been quite satisfactory in optimizing the individual units, but its efficiency in coordinating the sub-system optimizations to produce an overall optimized process is less than satisfactory. A new optimization technique called the "Complex Method", proven by other investigators to coordinate sub-systems more efficiently, is being tested for its usefulness in the study of the proposed coal gasification operations. The U. S. Bureau of Mines' "Hydrane Process" has been chosen as the first process to be tested by this new optimization method. The "Hydrane Process" has been mathematically

simulated and is now being optimized, using the process overall thermal efficiency as the objective function to be optimized. At this time the precise optimum independent parameters for the overall process have not been pinpointed; however, enough evidence have been gathered to prove that the "Complex Method of Optimization" can be used effectively in evaluating coal utilization processes of the type we are studying. Preparation of a supplemental report to our interim report on "Optimization of Coal Gasification Processes" is being contemplated.

The next phase of this project involves applying the previously developed optimization techniques to evaluate the coal liquidification processes. Some of the processes to be studied are; H-Coal Process (Hydrocarbon Research, Inc.), COED Process (F. M. C. Corporation), and the Solvent-Refined Coal Process (Pittsburgh & Midway Coal Mining Company). The next month will be devoted to the collection of process data from the respective companies and from published literature, and to the mathematical simulation of the various process sub-systems.

C. Y. Wen, Project Director

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