MASTER

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COLLEGE OF ENGINEERING
BUREAU OF ENGINEERING RESEARCH

QUARTERLY REPORT

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FEASIBILITY STUDIES OF IN-SITU COAL GASIFICATION
IN THE WARRIOR COAL FIELD

by

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Prepared for

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and
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The University of Alabama

October, 1978

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FEASIBILITY STUDIES OF IN-SITU COAL
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This project was initiated on May 15, 1975, under sponsorship of the National Science Foundation (NSF). On January 1, 1978, support of the research was taken over by joint funding from the Department of Energy (DOE) and the Appalachian Regional Commission (ARC). Because of some unexpended NSF funds, the ARC and DOE funds were not used until the late summer of 1978. Thus, this is the first quarterly report on work done under ARC and DOE funding and covers work done through October 1, 1978, on the tasks listed in the contracts. The tasks on the project have been divided into those sponsored by ARC and those sponsored by DOE. Since all of the research tasks fit together to form the overall project, a single report is being written, with subsections for ARC sponsored work and for DOE sponsored work so that each agency can see the overall results of the project, as well as the work it sponsored.

I. PROGRESS REPORT ON RESEARCH SPONSORED
BY THE APPALACHIAN REGIONAL COMMISSION

These studies are aimed at the effects of operating conditions in an in-situ gasification operation that affect the volume and quality of the gas produced.

A. Laboratory Combustor Studies: Mark Griffin, Graduate Assistant,
Mechanical Engineering

The laboratory combustor that was used for most of the work under the NSF contract is not suitable for some of the objectives of the continued research. In particular, it is not possible to adequately assess heat losses. Further, the system is so massive that the sensible heat requirements to bring it to operating temperature are excessive. In addition, previous work showed that it was not necessary to use a refractory lining in the vessel. Addition of water for the char-steam reactions will also pose problems in the horizontal combustor, because any condensed water will not flow into the combustion zone, but will be at the bottom of the combustor in any cool spots. For these reasons, a new combustor has been designed and continued development of a satisfactory combustor is in progress.

The combustor currently being used is constructed of stainless steel and has a cylindrical reaction zone 8 inches in diameter and 1.5 feet long. The combustor is insulated by diatomaceous earth poured into the annular space between the combustor and a thin steel jacket. Temperatures inside the bed are measured by thermocouples protruding into the fuel bed from a hollow central tube. The reactor is immersed in a water bath through which water is continuously

circulated. The heat losses can be determined from the temperature rise of the water in the bath.

The instrumentation and flow system is basically the same as for the previous combustor. At the present time, only runs with air as the oxidizing gas are being made. Gas flow into and out of the combustor is measured by d/p cells and orifice meters and composition of the off-gas is determined by a gas chromatograph. The oxygen content is continuously monitored on an oxygen analyzer. The flow rates, oxygen content of the off-gas, and temperatures are recorded on a data logger. Use of the data logger and the automatic gas chromatograph allow the system to operate with minimal attention.

Experiments in the apparatus, thus far, have been for testing of the apparatus. The runs have been made in forward combustion using air as the oxidant and commercial coke as the fuel. The runs to date have been without the addition of water, but the apparatus for water injection into the gas at the top of the combustor has been installed for later use.

In the next quarter, a series of runs using air at various flow rates without water addition are planned to establish a baseline. Then, runs will be made at the same flow rates of air, but with the addition of water. This apparatus will be used to attack directly the effects of the air velocity, influx of water, and heat losses on the gas quality.

B. The Effects of Heat Losses and Seam Thickness on Gas Quality:

Alan Bailey, Graduate Assistant, Mechanical Engineering

It was proposed, as part of in-situ coal gasification studies, to determine the effects of seam thickness and heat loss on off-gas quality.

An effort is being made to model in-situ coal gasification as a two-dimensional transient thermal system which utilizes conduction, convection, and heat generation. The desired analytical results should provide information on limiting seam thicknesses required to sustain combustion along with transient temperature distributions and heat losses in the system.

Currently a model which is made up of nine hundred and twelve nodal points with sixteen hundred and sixteen connectors between them is being used in conjunction with the NASA developed SINDA computer program to accomplish the proposed objectives.

An initial transient solution has been obtained and its corresponding analytical data produced using SINDA in order to analyze the effectiveness and usefulness of the model currently in use. It has been determined from this initial solution, however, that the use of SINDA to produce the desired data may be too costly to warrant its continued use. Therefore, a finite difference solution of the problem is being developed and coded in computer language as a check on the initial SINDA solution and as a check on a possible alternative to the use of SINDA to provide the desired data.

Once a limiting seam thickness is determined analytically, it will be possible to construct an experimental model that insures the proper lengths of the various combustion zones and that insures that the heat production versus heat loss ratio is of correct proportions. Once this experimental model is developed, experimental gas quality data may be produced and analyzed in order to fulfill the proposed objectives.

During the next quarter, efforts will continue with both SINDA and the local finite difference program to determine which will be more suitable for use on this project.

II. PROGRESS REPORT ON RESEARCH SPONSORED BY THE DEPARTMENT OF ENERGY

A. Application of the Shrinking-Core Model to the Combustion of Coke

Particles: Rajeev Mohan, Graduate Assistant, Chemical Engineering

Previous studies have shown that coke formed during in-situ gasification of bituminous coals is not sufficiently permeable for gas to flow through the coke itself, but must flow through cracks or channels around coke particles. The shrinking-core reaction model applies to the situation of combustion of a particle where the oxidant must diffuse through an ash layer to reach the reaction zone. As the reaction progresses, the core of unreacted material at the center of the particle becomes smaller, while the ash layer surrounding the core becomes thicker. The model includes extra particle diffusion, intra particle diffusion, as well as reaction rate limitations on the overall reaction rate. Since the reaction of coke with air is actually the reaction of carbon with air, the rate of reaction can be followed by the change in weight of the oxidizing particle. By making the proper plots of the weight of the particle and time data, information regarding the limiting step in the reaction process can be determined.

1. Experimental

The experimental apparatus is shown in Figure 1. The reactor consists of a 24 inch, 2.5 inch O.D. stainless steel tube which is heated by a Lindeberg heavy duty tube furnace. The coke sample basket is suspended in the reactor by a nichrome wire, which is connected to a load cell. This load cell is attached to an amplifier, and a millivolt signal proportional to weight is recorded on a chart recorder. Thus, throughout the experiment a continuous weight change is recorded versus time. The temperature of the

Fig. 1. Experimental Apparatus

region surrounding the coke piece and that of incoming gas is measured by thermocouples.

Air flow rate and nitrogen flow rate are measured by rotameters and % O_2 in the gas supplied to the reactor and in combustion gases is measured by an oxygen analyzer. A chart recorder records these oxygen percentages continuously throughout an experimental run.

2. Run Conditions

Typical run conditions for an experimental run are shown below:

Particle Size = a cube of 1.27 CM

Equivalent Spherical Radius, $R = 0.63505$ CM

Mass of Coke Particle = 2.44 gms

Gas Flow Rate = $7645.55 \text{ cm}^3/\text{min.}$ (0.27 SCF/min.)

Temp. Surrounding the Coke Piece = 1206°F

Temp. of the Incoming Gas = 286°F

% Oxygen in Incoming Gas = 21%

% Oxygen in Outgoing Gas = 18.5 %

3. Results Obtained

The run was carried out until there was no further change in weight. This happened after 104 minutes for the above run conditions and a conversion of 93.03% was achieved at this point.

The data obtained were tested to find which of the following three resistances in a typical shrinking core model are responsible for controlling the rate mechanism of a coke particle:

- a. resistance due to gas film
- b. resistance due to chemical reaction
- c. resistance due to ash diffusion

It was found that at the given run conditions, the resistance due to ash diffusion was the controlling resistance. A D_e value of $0.404175 \pm 0.029142 \text{ cm}^2/\text{sec}$ (95% confidence range) was obtained. The data between

40-104 minutes was used in finding this D_e value and this range of data had a correlation coefficient of 0.9915.

Another run at similar conditions but a different particle size ($R = 1.0319$ cm) was made to check if ash diffusion was indeed the rate controlling step. For the data obtained in this run a D_e value of 0.395518 ± 0.026326 cm²/sec (95% confidence range) was obtained. The correlation coefficient for these data is 0.995. A difference of only 2.7% was found between the D_e values of the two different sized particles.

The previous runs were made using commercial coke for the purpose of checking out the apparatus and data analysis. These tests show that the apparatus works well, and the analysis of data gives good results.

4. Future Plans

A coke making apparatus has been designed so that coke can be made from known coal under confinement in a furnace. This procedure will allow us to know under what conditions the coke was made and thereafter identical samples of coke can be obtained by following the same conditions.

This coke will then be used for further studying the application of the shrinking-core model. The effects of the following parameters will be studied:

- a. particle size
- b. temperature of the gas
- c. oxygen concentration in gas

B. Forward Combustion in Thin Seams of Swelling Bituminous Coal:

Alan Bailey, Graduate Assistant, Mechanical Engineering

It has been proposed as part of in-situ coal gasification studies to determine heat conduction rates and their effects in the forward combustion of coke.

A two-dimensional transient model has been developed utilizing conduction, convection, and heat generation phenomena in an effort to fulfill the proposed objectives. The desired analytical results should provide insight into the effect of conduction heat transfer in in-situ combustion of coke and corresponding transient temperature distributions within the system.

Currently the SINDA thermal analysis computer program developed by NASA is being used to simulate model systems similar to those found in in-situ gasification. The initial trial solutions however have shown the use of SINDA to be so costly that alternative solutions should be investigated.

A transient finite difference solution is now being developed and coded into computer language to determine its usefulness as a possible alternative to the use of SINDA and as a check on initial SINDA calculations.

Once the desired computations are completed and analyzed, the effects of conduction heat transfer on the in-situ combustion of coke can be assessed.

C. Properties of Char Produced from Eastern Bituminous Coal

1. Literature Survey: Tien-Shoe Wang, Graduate Assistant, Chemical Engineering; Yumwah R. Fong, Graduate Assistant, Mechanical Engineering

A systematic survey of the literature regarding coke and char properties is being conducted. Chemical Abstracts has been searched for general coke/char properties from 1950 to 1977, and for permeability, porosity, and thermal conductivity from 1907 to 1977. The Engineering Index has been searched from 1957 to 1978. Because the journal Fuel contains so many pertinent papers, it was searched from 1923 to 1978 in order to be certain not to miss any important articles.

Currently, we are preparing a bibliography of the literature searched thus far, and are making plans to complete the literature work early in 1979.

2. Thermal Conductivity and Thermal Diffusivity of Coke: Tien-Shoe Wang, Graduate Assistant, Chemical Engineering

Thermal conductivity and thermal diffusivity of coke are important properties because they determine the rate and extent of pyrolysis away from a burning zone, and they determine the rate of propagation of the flame front in reverse combustion. A review of the literature on methods of measuring coke thermal conductivities and diffusivities led to the conclusion that the transient methods of Badzioch, et al⁽¹⁾ were best suited for our measurements. There are two basic methods; the hot-wire method and the slab method.

With the hot wire-method, the thermal conductivity and thermal diffusivity can be determined from the same experiment, and then, by measuring the density of the coke, the specific heat of the coke can be calculated. The slab method can be used to evaluate only the thermal diffusivity, but with better reproducibility than the hot-wire method. These two methods are described as follows.

a. Hot-wire Method (see Figure 2)

A 2 mm diameter hole is drilled centrally through a lump piece of coke sample and then two other 2 mm holes are drilled parallel to the central hole; one as close as possible, and the second one further away. The heater wire is put through the central hole and thermocouple wire through the others. The thermal conductivity can be evaluated from the slope of a plot of $(\theta_r - \theta_o)$ versus nt as shown in equation 1. This plot is made from the thermocouple nearest the heater.

$$(\theta_r - \theta_o) = \frac{q}{4\pi k} \left(nt + n \frac{4}{r^2} - 0.578 \right) \quad 1$$

θ_r = Temperature at a point at radial distance r from the heater wire after time t

θ_o = Initial temperature

q = Heat supplied to the coke sample through the heater wire

k = Thermal conductivity

α = Thermal diffusivity

The thermal diffusivity can be evaluated from the following relationship:

$$(\theta_r - \theta_o) = \frac{q}{2\pi k} I(\beta) \quad 2$$

$$\beta = r/[2(\alpha t)^{1/2}] \quad 3$$

From equation 2, $I(\beta) = \frac{2\pi k}{q} (\theta_r - \theta_o)$, we get $\frac{2\pi k}{q}$ from the slope of equation 1. This calculation is made using the thermocouple furthest from the heater. Then, from a table of $I(\beta)$ vs β and equation 3, the value of α can be determined.

Fig. 2. Apparatus for Hot Wire Method
(from Reference 1)

b. Slab Method (see Figure 3)

A slab of coke sample approximately 3 mm thick is sandwiched between two steel plates. Two flat heating units are employed to heat the sample from both faces, usually asymmetrically as shown in Figure 4.

The thermal diffusivity is calculated from the following equation:

$$\alpha = \frac{ab (a + b)}{2 (a\Delta t_b + b\Delta t_a)} \quad 4$$

a,b = the distances from point A to point C and from point B to point C as shown in the figure

Δt_a = time interval between point A and point C to pass through the same temperature

Δt_b = time interval between point A and point C to pass through the same temperature

When carrying out the experiment, it is proposed to use a vacuum pump, desiccator and nitrogen tank to evacuate the air and water from the coke sample and fill the sample with nitrogen to prevent the sample from oxidizing at high temperatures. It is also proposed to use a furnace to bring the temperature of the coke sample to different initial uniform temperatures for both hot wire and the slab methods. A DC power supply will be used to energize the heater wire in the hot-wire method, and variable transformers will be used for the flat heating units of the slab method. The thermal conductivities and thermal diffusivities of various coke samples will be measured at temperatures ranging from near ambient to about 1200°F.

The necessary equipment has been ordered, and most of that which must be purchased has been received. Mr. Y. R. Fong has taken over the thermal conductivity research and will continue with construction and testing of the experimental apparatus during the next quarter.

Fig. 3. Apparatus for Slab Method
(from Reference 1)

Fig. 4. Temperature Profile within a Slab Heater Asymmetrically
through Its Faces at a Constant Rate
(from Reference 1)

3. Reactivity of Coke: Tien-Shoe Wang, Graduate Assistant, Chemical Engineering

The reactivity of coke toward air, CO_2 , and H_2O is important because it determines the reaction rate and the extent of reaction for underground coal gasification. Hence, it directly influences the feasibility of underground coal gasification.

The reactivities of coal char with air and CO_2 have been studied by P. L. Walker, Jr.,^(2,3) and the reactivities for several American coals have been reported. His method of measuring the reactivity of char is to heat (under a nitrogen blanket) the coke powder (-40 + 100 mesh) at a constant rate of heating, say $10^\circ\text{C}/\text{min}$, to a temperature, such as 500°C , which is held constant for about 15 minutes to achieve thermal equilibrium. Then air or CO_2 is passed across the heated sample. The weight of the sample will decrease by oxidation of carbon when reacting with these gases.

The reactivity is evaluated by:

$$R_T = \frac{-1}{W} \frac{dW}{d\theta} \quad 5$$

R_T = Maximum reactivity of coke at temperature $T^\circ\text{C}$

W = Initial mass of char

$\frac{dW}{d\theta}$ = Maximum rectilinear weight loss rate based on the
ash-containing basis

A typical reactivity graph is shown in Figure 5. The reactivity is determined from the linear portion of the graph.

Fig. 5. Reactivity Curve
(from Reference 3)

A Fisher thermogravimetric analyzer (TGA), the apparatus used by P. L. Walker, Jr., is currently available in the Chemical and Metallurgical Department. We plan to order some of the same coal samples used by Walker and run them on our TGA to be certain that our procedures and techniques give comparable results. We will then proceed with a series of runs on various coke samples. The method of coke formation and the type of parent coal influence the reactivity. We will investigate the relationship among reactivity, type of coal, and method of coke formation.

D. Review of In-Situ Gasification Tests at Gorgas, Alabama: Leon Y. Sadler, Associate Professor, Chemical Engineering

Copies of the Reports of Investigation on the Gorgas tests and published summaries of that work have been studied. Contacts have been made with some of those involved with the tests. A first draft of the report on the evaluation of the tests is in preparation for internal review and discussion. It is anticipated that this part of the project will be completed during the next quarter.

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**THE UNIVERSITY OF ALABAMA
COLLEGE OF ENGINEERING**

The College of Engineering of The University of Alabama (Tuscaloosa) has an undergraduate enrollment of more than 1,000 students and a graduate enrollment of 90-100. There are approximately 100 faculty members, a significant number of whom conduct research in addition to teaching.

Research is an integral part of the educational program, and interests parallel academic specialities. It is conducted in the classical engineering programs of aerospace, chemical, civil, electrical, engineering hydrology, engineering mechanics, environmental, industrial, mechanical, metallurgical, and mineral engineering. All of these programs offer the master's degree, and five programs offer the educational specialist and doctor of philosophy degrees.

Other organizations on the University campus that contribute to particular research needs of the College of Engineering are the Charles L. Seebeck Computer Center, Geological Survey of Alabama, Marine Environmental Sciences Consortium, Mineral Resources Institute—State Mine Experiment Station, Natural Resources Center, U.S. Bureau of Mines, Tuscaloosa Metallurgy Research Center, and the Research Grants Committee.

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