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GASIFICATION OF CHARS PRODUCED UNDER SIMULATED in situ PROCESSING CONDITIONS

Quarterly Report for the Period July–September 1975

by

J. Fischer, R. Lo, S. Nandi,
J. Young, and A. Jonke

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

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ABSTRACT

This effort, which is part of the Argonne National Laboratory energy program for ERDA, is being directed toward support studies for the national endeavor on *in situ* coal gasification. This task involves the investigation of reaction controlling variables and product distributions for the gasification of both coals and chars utilizing steam and oxygen. Included in this task is the investigation of the effects of using brackish water as the water supply.

SUMMARY

Gasification of Coal and Char for *In Situ* Gasification

The objective of this work is to investigate the reaction-controlling variables and reaction kinetics for the gasification of chars resulting from the pyrolysis of coal in underground gasification. This work will be relevant to all underground gasification projects being funded by ERDA. Primarily, the reaction of steam with a variety of coals and chars will be investigated using a laboratory-scale gasifier, and process variables will be correlated. The effects of introducing various components of brackish water will also be investigated since a number of these components are expected to have a catalytic effect on the steam/char reaction.

The laboratory-scale gasifier for this work is currently under construction by an outside contractor, with delivery expected in mid-October. The utilities and safety installation for this reactor system are currently being prepared at the Laboratory site.

In Situ Support Work

Two samples of chars were received from Oak Ridge National Laboratory. The chars were produced at ORNL by pyrolyzing a block of subbituminous coal under the conditions for the pyrolysis step of *in situ* gasification. Surface area, pore volume, and micropore volume for the two char samples have been determined. The results are presented.

The reactivities (the rate of reaction of the char in air at 500°C) have also been determined for the two char samples. The char produced at a lower temperature had a higher reactivity.

GASIFICATION OF COAL AND CHAR FOR *IN SITU* GASIFICATION

The objective of this project is to determine the reaction-controlling variables and reaction kinetics for the gasification of coals and chars resulting from the pyrolysis of coal in underground gasification. This work is relevant to all underground gasification projects being funded by ERDA. The data obtained from this work will be used in modeling *in situ* gasification systems, in order to understand and interpret field experimental data, and will be used in the design of future field experiments.

In the gasification of coal and char in a laboratory-scale gasifier using steam and oxygen, a number of variables will be investigated that are representative of actual *in situ* gasification conditions. These variables include total pressure (10 to 30 atm), temperature (500°C to 900°C), and partial pressures of steam and oxygen. Quantitative information about gaseous products such as hydrogen, methane, higher hydrocarbons, carbon monoxide, and carbon dioxide will be measured in order to establish the Btu value of gas obtained by gasification of the coal or char.

The water supply for *in situ* gasification projects will frequently be brackish, containing dissolved or suspended minerals such as carbonates, bicarbonates, halides, and hydroxides of alkali and alkaline earth metals, as

well as such transition metals as iron. The catalytic effects of these materials on char gasification will be investigated under conditions likely to be encountered in underground gasification.

The laboratory scale reactor system, previously described,[1] is under construction by an outside contractor, and will be delivered by mid-October. Work on the laboratory space with respect to utilities and safety provisions will be completed by the time the reactor system is received.

IN SITU SUPPORT WORK

At Oak Ridge National Laboratory, pyrolysis tests are being performed with large blocks of subbituminous coal obtained from the same seam (Wyodak-Anderson) as the coal with which Lawrence Livermore Laboratory is conducting *in situ* gasification tests. We have received two samples from ORNL--one (ORNL-650) pyrolyzed at a maximum temperature of 650°C and the other (ORNL-950) at 950°C.

The surface areas of these samples have been determined by nitrogen adsorption, using the B.E.T. equation. The micropore volume of the samples was estimated from carbon dioxide adsorption at 25°C, using the Dubinin-Polanyi equation. Total macropore volume of the samples was determined from helium and mercury densities. Estimates of the volume of the pores in the range 60Å to 40,000Å have been obtained by mercury porosimetry. These results are summarized in Table 1.

TABLE 1. Surface Area and Pore Volume of Coal Chars.

Sample	Surface Area, m^2g^{-1}		Total Open Pore Volume, cm^3g^{-1}	Micropore Volume, cm^3g^{-1}	Pore Volume with diameter between 40,000Å and 60Å, cm^3g^{-1}
	N_2	CO_2			
ORNL-650	4	320	0.15	0.13	0.09
ORNL-950	193	350	0.32	0.14	0.19

The surface area of the 950°C char using nitrogen adsorption at -195°C is larger than that of the 650°C char; however, the areas of the two samples measured, using carbon dioxide adsorption at 25°C, are nearly the same. From the consideration of the relative molecular size, the micropore area accessible to carbon dioxide at 25°C should be available to oxygen at temperatures higher than 25°C. Therefore the rate of char-oxygen reaction is expected to be dependent on the carbon dioxide measured area rather than the nitrogen measured area.

Rates of reaction of the chars with air have been determined at 500°C. These experiments were carried out using a thermogravimetric apparatus. The data are shown in Fig. 1. The 650°C-char is much more reactive. The maximum rate for the ORNL-650 samples was about three times greater than that for the ORNL-950 sample.

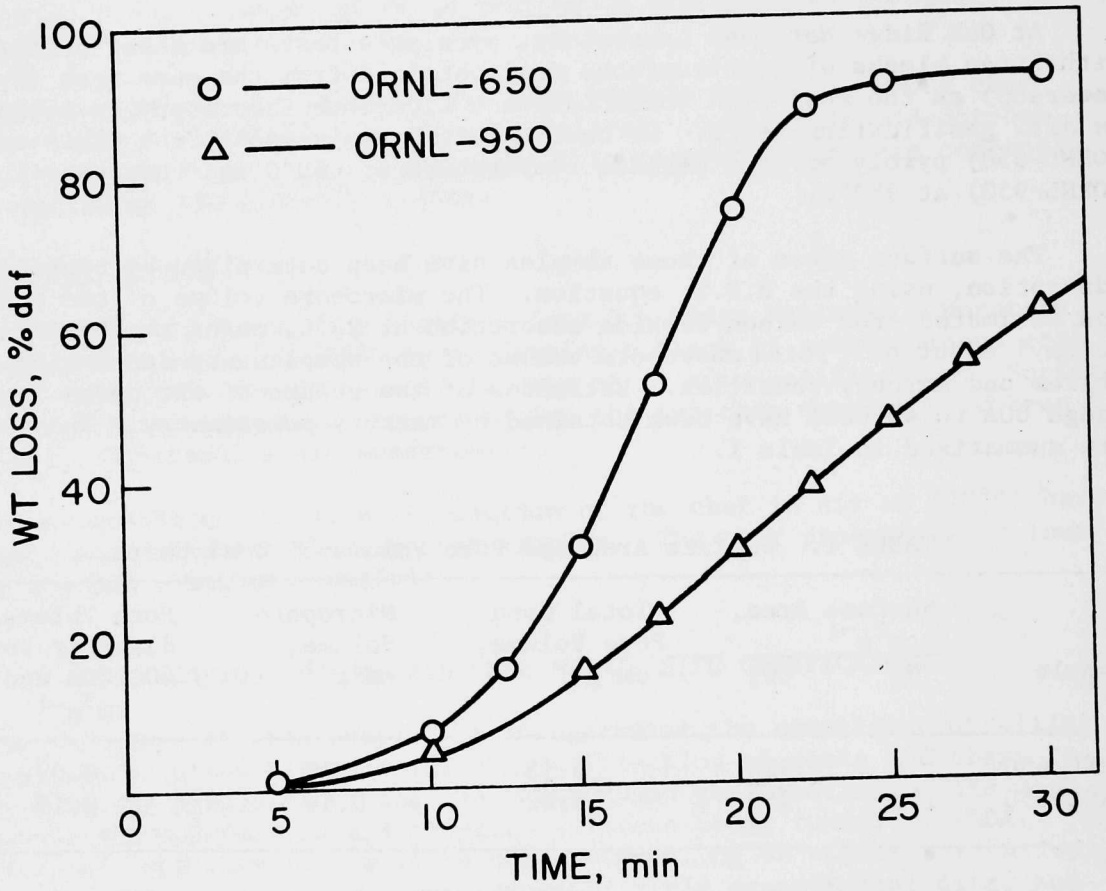

Fig. 1. Reaction in Air at 500°C
⊙ -- ORNL-650; △-- ORNL-950

Even though the 650 char has a surface area, measured by carbon dioxide, which is about the same as the 950 char, it has a higher reactivity with oxygen at 500°C. This may be indicative that, even though the surface area is the same for both chars, the char prepared at 950°C has fewer reactive sites per unit surface area, due to the chemical changes on the surface that occur at higher temperature.

MILESTONES FOR COAL AND CHAR GASIFICATION WORK

1. Complete and test gasifier apparatus to be received late in September 1975.

2. Installation of gasifier in October 1975; preliminary testing of the gasifier and analytical techniques to be completed by December 1975.

3. Preliminary data on kinetic and product distribution from gasification of subbituminous and other coal and char, made at low heating rates, delivered March 1976. Coal from the various sites of the national *in situ* program will be used.

4. Final data on kinetics and product distribution from gasification of coal delivered June 1976.

5. Data on effects of brackish water constituents on gasification of coal and on the effect of minerals in coal and in surrounding strata on gasification will be delivered October 1976.

6. Semiannual reports will be prepared. In addition, the ERDA contract officer will be provided with informal summary quarterly reports on the status of the work, including data. An annual report will be submitted.

REFERENCE

1. J. Fischer, S. Che, R. Lo, W. Podolski, S. Nandi, and A. Jonke, Chemical Engineering Division Coal Technology Semiannual Report, July - December 1974, ANL-8151.