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Energy
Program

**Fossil Energy Program
Progress Report For May 1979**

L. E. McNeese

OAK RIDGE NATIONAL LABORATORY
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FOSSIL ENERGY PROGRAM
PROGRESS REPORT FOR MAY 1979

L. E. McNeese
Program Director

Date Published: July 1979

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
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FOSSIL ENERGY PROGRAM REPORT FOR MAY 1979

ABSTRACT

This report - the fifty eighth of a series - is a compendium of monthly progress reports for the ORNL research and development programs that are in support of the increased utilization of coal and other fossil fuel alternatives to oil and gas as sources of clean energy. The projects reported this month include those for coal conversion development, materials engineering, a coal equipment test program, an atmospheric fluid bed combustor for cogeneration, engineering studies and technical support, process and program analysis, environmental assessment studies, magnetic beneficiation of dry pulverized coal, technical support to the TVA fluid bed combustion program, coal cogeneration/district heating plant assessment, and chemical research and development.

1. Summary

L. E. McNeese

Highlights of our progress in May are as follows:

Coal Conversion Development - Three experimental operations were conducted in the CLFS during the month. New flow curve data taken at 500 K are more consistent with expected trends than the previous data. Measurements of ΔP across the pipeline viscometer vs temperature of the slurry at the preheater exit indicate the same viscosity trends as in previous tests in which hydrogen was present. Also discussed is the preliminary analysis of the transition from laminar to turbulent flow. A series of reactions between bituminous coal and phenol have been completed and are being analyzed. Significant differences in conversion from the previous subbituminous runs are evident. Hydrogen transfer mechanisms are being explored using the Deno oxidation technique. During May several bugs were eliminated from the prototype electronics unit of the portable fluorescence spotter. A planning session for the field testing of the spotter, which will tentatively begin in September, was held at DOE headquarters. In support of in situ gasification (UCG), use of simulated UCG product gas had little effect on block pyrolysis of lignite, but the effect of H_2 purge on pyrophoricity has been linked to surface area changes. Data and correlations for coal enthalpy, specific heat, thermal diffusivity, and thermal conductivity are presented.

Chemical research and development - In continuing studies of pyrolysis of bibenzyl to further develop a free-radical model for coal conversion, the structure and dynamics of formation of a skeletally rearranged product, 1,1-diphenylethane, have been determined. Added phenol alters the pyrolysis products to a significant extent. The chemical assessment of the possible impact of Kölbel process concepts on advanced processes for indirect liquefaction is progressing on schedule.

Materials Engineering - The determination of the mechanical properties of 25-cm-thick 2 1/4 Cr-1 Mo steel plate was continued. The ductile-brittle transition of 1-in.-thick compact specimens (1T CS) appears to occur at slightly higher temperatures than for 0.394T CS. A postweld heat treatment of 40 h at 610°C had only a slight effect on tensile properties of this steel. In the task on weld overlay cladding with type 320 stainless steel, efforts are being made to place a subcontract to have a commercial manufacturer use the information gained from this task to develop and demonstrate a commercially viable technique for weld overlay cladding with this alloy. Examination of tube samples from the 4500-h experiment in the FluidDyne atmospheric fluidized-bed combustor continued. It is believed that air leaking from an air-cooled trimmer tube resulted in a nonuniform oxygen distribution in the bed, and this led to sulfidation/oxidation corrosion on tubes located in oxygen-deficient regions. In the Failure Prevention and Analysis task, analyses of corrosion coupons from Wilsonville and Fort Lewis solvent-refined coal pilot plants continued. Efforts to determine the cause of the recently experienced increased rate of corrosion in the Wilsonville T105 fractionation column showed that bottom liquids produced from the Kentucky coal used recently had about 10 times the chlorine content as those produced from the Indiana coal used previously. This higher chlorine content may have played a role in the accelerated corrosion of the fractionation column. In the task to evaluate materials for the ZnCl₂ recuperators of the ZnCl₂ Liquefaction Process, fabrication of the quartz glass test loop has begun, and test specimens are being machined. The study of stress corrosion cracking in coal liquefaction systems continued. The U-bend specimens exposed at the Fort Lewis SRC pilot plant are being examined metallographically. Although visual inspection of these specimens revealed no evidence of cracking, dye penetrant checks showed some indication of cracking, especially in the type 410 stainless steel coupons. Racks of coupons for insertion in the Wilsonville SRC pilot plant and the Exxon Donor Solvent pilot plant have been prepared. In the task to develop modified 9 Cr-1 Mo steel, considerable progress was made in demonstrating the weldability of modified 9 Cr-1 Mo to type 304 stainless steel and to 2 1/4 Cr-1 Mo steel tubing. In addition, a review of weight loss data after air oxidation at 593°C for 3700 h showed the weight loss of modified 9 Cr-1 Mo to be less than for 2 1/4 Cr-1 Mo by a factor of 1.7. The silicon content appeared to affect weight loss. An order was placed with Carpenter Technology for two 15-ton heats of modified 9 Cr-1 Mo. In the task to develop ceramic heat exchangers (recuperators), final negotiations are in progress to establish a subcontract with Hague International to evaluate silicon carbide heat exchangers exposed to coal-oil mixture combustion products. The modification to the refractories test facility at ORNL is on schedule with the firing of the castable tube support blocks in progress. Characterization of samples of candidate heat exchanger materials is in progress.

Coal Equipment Test Program - The final report proposing a coal feeder test facility (Dry Coal Handling/Feeding Test Facility - ORNL/ENG/TM-16) is currently in reproduction. Continuing work on this project will be directed towards surveying potential sites for the facility with emphasis to be placed on DOE gasification pilot plants currently scheduled for shutdown. Completion of the final report on the survey of coal handling equipment has been slowed by the delay in receiving Bechtel National's draft report. This information will be available in early June, and the report will be completed in June. The final report concerning the SRC R&D assessment was completed (ORNL/CF-79/213) and forwarded. Conclusions and recommendations were made for SRC I and SRC II valves, pumps, metering devices, and high-pressure oxygen compressors. The recommendations include proposed schedules and funding levels for projects currently under way and suggested for the near future.

Engineering Studies and Technical Support - Contacts with institutions active in coal liquefaction R&D have been essentially completed in our assessment of current R&D important to SRC development project. Preparation of the draft Interim Phase Report (ORNL/TM-6592) is well under way, but each will be delayed because of scheduling problems and visits with the Gulf Harmarville SRC-II PDU, Ft. Lewis SRC pilot plant, and the Texaco Gasifier pilot plant.

Process and Program Analysis - An assessment of methanol synthesis technologies has been completed and the draft final report "Production of Methanol and Methanol-Related Fuels from Coal" (ORNL-5564), is being reviewed internally. Major conclusions of the report are that current methanol synthesis technology is superior to all obsolete or discarded processes for the production of fuel-grade methanol and that recent catalyst advances in the conversion of such products to other fuels increases enormously the potential for new process development.

In the Fossil Energy Environmental Project, a new shipment of Grace/Ebasco/Texaco process solid waste was received and soils from the proposed site were obtained. Technical assistance was provided to DOE on all six demonstration projects: SRC-I, SRC-II, Grace, MLGW, CONOCO, and ICGG. The first public scoping meeting as defined by the new CEQ regulations was held for the Grace project in Henderson, Kentucky on May 16.

Magnetic Preparation of Dry Crushed Coal - The free-fall open-gradient separation has been modified in accordance with the findings of the mathematical model, and greatly improved separations were obtained.

A 20-minute narrated technical film on magnetic preparation has been completed and is available.

Two ORNL/TM reports are completed and are being prepared for publication.

The superconducting magnet has been received and will be installed when the laboratory space in 9201-3 is ready.

Mr. Thomas of TVA and Mr. Hise of ORNL witnessed tests of screening coal at 28 mesh in the plant of the Derrick Manufacturing Company.

Atmospheric Fluidized Bed Coal Combustor for Cogeneration (AFBCCC) - The CCC Program proposals were received from the vendors on May 31. A very good number of proposals were received, and they represent most of the leading gas turbine and fossil-fired furnace manufacturers.

TVA FBC Demonstration Plant Program - The 4' x 4' cold flow model system is now ready to begin bed slumping tests. Pressure drop measurements will first be taken across the distributor plate with the bed empty, and then the bed will be filled with limestone for the bed slumping tests. In the AFBC modeling task, work has begun on TVA/B&W's configuration simulation, using Wen's model which is already operational on the ORNL computer system. On the AFBC Bench Scale Model, the bed was filled with 12 x 30 mesh limestone and combustion testing was resumed on May 8. The limestone feeder was installed, and operation with continuous limestone addition was begun on May 16. Conditions were held fairly constant at 1530-1550°F, a fluidizing velocity of about 6 ft/sec, excess air level of 20%, and an expanded bed depth of 28-30 in. In assessment of PFBC systems, further progress has been made on the parametric study in which the effect of the furnace pressure and gas turbine inlet temperature on power plant performance is being investigated. In the Alternate Design Concepts Evaluation task, a general mass and energy balance computer program is being modified to conduct the parametric AFBC cost analysis. For the AFBC Technical Source Book, a consolidation of information on design parameters for fluidization velocity distributor trays, bed hydrodynamics, standpipe design, and elutriation was made. In the AFBC Dynamic Modeling task, a series of runs was made to investigate the natural open-loop (no control system) behavior of the fluid-bed boiler. Twelve parameters were individually reduced by 1%, and the system responses were determined.

Coal Cogeneration/District Heating Plant Assessment - A final draft on the Twin Cities District Heating Study has been delivered by Studsvik. A nonprofit company for the development of district heating in St. Paul has been formed by the mayor of St. Paul.

FBC Industrial Applications Project Survey - The committee reviews have been completed, and the reports are being finalized. The last three reviews were made during the past month.

2. COAL CONVERSION DEVELOPMENT

J. R. Hightower, Jr.

Coal conversion development activities are carried out in the Chemical Technology Division. This section discusses four projects conducted for the Division of Fossil Fuel Processing -- Physical Properties of Coal Liquids, Coal Slurry Preheaters, New Liquefaction Techniques, and In-Plant Environmental Monitors -- and one project conducted for the Division of Fossil Fuel Extraction -- Experimental Engineering Support for In-Situ Gasification Processes.

2.1 Physical Properties of Coal Liquids

G. E. Oswald and E. L. Youngblood

Physical properties (viscosity, density, thermal conductivity, and heat capacity) of both coal-solvent slurries and solids-free, coal-derived liquids will be measured at typical processing conditions, up to 31 MPa (4500 psig) hydrogen pressure and 810 K (1000°F) in a bench-scale, continuous flow system. The system includes a slurry preheater section and a hydrogenation reactor to simulate processing conditions prior to physical property measurement. Immediately after physical property measurement, the test fluids will be quenched and sampled for chemical characterization. Physical properties will be correlated with chemical characteristics of the test liquid.

The operation of the coal liquids flow system (CLFS) during this report period and plans for future work are discussed in this section.

2.1.1 Work accomplished

The CLFS was operated for two, one-week long periods. During the first operation period, replicate rheological characterization measurements were made on 35 wt % Illinois No. 6 coal (-170 mesh)/Wilsonville recycle solvent slurry at 500 K and 13.9 MPa overpressure. During the second operation period, the preheater and pipeline viscometer were operated within and beyond the slurry gelation temperature range to investigate the hydrodynamic behavior of the slurry in this region. Slurry was preheated, in liquid-phase-only flow, with incremental increases in preheater discharge temperature. The preheated slurry was passed directly through the pipeline viscometer and differential pressure recorded as a function of discharge temperature at a constant slurry mass throughput rate. This differs from a similar test reported earlier in that the earlier measurements were made on combined phase flow (slurry and hydrogen together).¹

During the first operations period four data points were established before the run was terminated by failures of the feed slurry circulation pump and the high pressure/high temperature vapor-liquid separator level controller electronics; both problems were corrected for the second period of operation. These data are discussed in Sec. 2.2.

Pipeline viscometer differential pressure measurements during the second operations period indicate the onset of the gelation stage, by a sharp rise in differential pressure, at 572 K (Fig. 2.1). As preheater discharge temperature was increased from 572 K to 644 K, differential pressure increased five fold. Increasing discharge temperature beyond 644 K resulted in decreasing differential pressure (not shown in the figure). At 700 K differential pressure had decreased to about the level observed prior to the onset of gelation. Increasing discharge temperature from 700 K to 750 K did not significantly reduce differential pressure below the 700 K observation. These observations were made at a constant slurry rate of 2 Kg/hr and 13.9 MPa overpressure. The slurry was combined with hydrogen (0.85 scmh) downstream from the pipeline viscometer and upstream of the reactor/dissolver. Reactor/dissolver temperature was 700 K. Pipeline viscometer temperature was increased to match the preheater discharge temperature. Operations were terminated when a small oil fire developed at a leak in a preheater tube fitting. The fire detection systems performed well and the CLFS was safety shut-down. The differential pressure vs preheater discharge temperature profile is almost identical to that observed for slurry in combined phase flow with hydrogen.¹ Thus, it appears that the presence of gaseous hydrogen during the preheating operation has minimal effect on the magnitude of the viscosity increase and the temperature range of the slurry gelation stage.

2.1.2 Work forecast

Slurry rheological characterization operations will continue. The Norcross falling ring viscometer, with modified ring, will be evaluated for viscosity measurements on slurry at elevated temperature.

2.2 Coal Slurry Preheaters

J. R. Thurgood and E. L. Youngblood

Experimentation and data analysis were continued in this report period to improve process understanding of coal slurry preheaters. This preheater project is principally concerned with thermal and rheological characterizations of slurry flow in preheaters at preheating conditions (pressures up to 31 MPa and temperatures up to 810 K). Experiments are made conjunctively with a companion project, Physical Properties of Coal Liquids. The data reduction and analysis are discussed in this section.

2.2.1 Data analysis

The flow curve for the rheological test made at 500 K is shown in Fig. 2.2. As was noted, only four data points were obtained. The data are sufficient, nevertheless, to show that they differ significantly from the data of the previously run test² at 500 K. The slope (n') of the new flow curve was determined to be 0.753; this is significantly

Fig. 2.1. Plot of pressure drop across the pipeline viscometer vs temperature for 35 wt % slurry at 13.9 MPa.

ORNL DWG 79-965

Fig. 2.2. Flow curve (plot of τ_w vs $8V/D$) of 35 wt % slurry at 500 K and 13.9 MPa, a repeated test.

different from the value of 0.503 determined in the previous test. These last test results indicate a slurry having less non-Newtonian character than the results of the previous test indicated. These new results are more consistent with data trends which are seen at lower temperatures; but because of the differences between these two sets of data, additional tests will be necessary to determine which data set, if either, is indicative of the slurry behavior at 500 K.

Inasmuch as the data above 400 K show the slurry to be non-Newtonian and pseudoplastic, an analysis of the transition from laminar to turbulent flow for such behavior was initiated. This analysis, of necessity, requires the use of a rheological model to describe the data. Because of the linearity of the data on the log-log flow curve plots, a power law model would describe the data fairly well and was selected as the basis for further analysis. In a power law fluid the shear stress is related to the shear rate as follows

$$\tau = K\dot{S}^n \quad (1)$$

where

- τ = shear stress,
- $\dot{S}$ = shear rate, and
- K, n = constants.

As more data are collected, use of other constitutive equations such as the Powell-Eyring model may be found more representative of the data.

Starting with the fundamental momentum equation and the constitutive power law equation, one can develop an expression describing the stabilized laminar pipe flow of a power law fluid.³ The friction factor (f), defined as

$$f = \frac{8c_{DAP}}{2\rho V^2 L} \quad (2)$$

where

- f = friction factor,
- ΔP = pressure drop across pipe of length L ,
- ρ = fluid density,
- D = pipe diameter,
- L = pipe length, and
- V = fluid velocity.

can be substituted in the developed equations to give

$$f = \left(\frac{16}{\text{Re}_{\text{PL1}}} \right) \left(\frac{1}{8} \right) \left(\frac{2 + 6n}{n} \right)^n \quad (3)$$

or

$$f = \frac{16}{\text{Re}_{\text{PL2}}} \quad (4)$$

where Re_{PL1} and Re_{PL2} are defined as alternate forms of a "power law Reynolds number," and are given as

$$\text{Re}_{\text{PL1}} = \frac{D^n v^{2-n} \rho}{K} \quad (5)$$

$$\text{Re}_{\text{PL2}} = \left(\frac{D^n v^{2-n} \rho}{K} \right) (8) \left(\frac{n}{2 + 6n} \right)^n \quad (6)$$

Both Re_{PL1} and Re_{PL2} reduce to the Newtonian Reynolds number when $n = 1$. These results can then be coupled with the Ryan-Johnson analysis³ to determine the critical velocity (at a given pipe diameter) at which the transition from laminar to turbulent flow begins. The Ryan-Johnson critical Reynolds number $(\text{Re}_{\text{PL2}})_c$ may be expressed as

$$\left(\text{Re}_{\text{PL2}} \right)_c = \frac{6464 n}{(1 + 3n)^2 \left(\frac{1}{2 + n} \right)^{(2 + n)/(1 + n)}} \quad (7)$$

Application of equation (7) to the rheological data collected on the 35 wt % slurries tested thus far indicate that all flows have been laminar. However, at the lower n values, such as the 0.3 value of the 700 K data run, the slurry begins to approach transitional flow. Additional work will be necessary to complete the analysis for all data collected thus far.

In addition to the flow transition work, Dr. R. W. Hanks of Brigham Young University (consulting for ORNL) is developing a correlation for the 35 wt % slurry data which takes into account the temperature dependency of K and n in the power law equation. His results will be reported upon completion. Dr. Hanks is also investigating possible correlations between the heat transfer data collected and the rheological data.

2.2.3 Future work

A continuation of both the rheological and heat transfer analysis of the data will be made. Also additional rheological characterization tests will be made as equipment operability and time permit.

2.3 New Liquefaction Techniques

J. W. Larsen,* B. R. Rodgers, and T. L. Sams

A series of reactions between Bruceton coal and phenol has been completed. Product samples have been sent out for analysis and complete results will be presented in the next monthly report.

An investigation into the nature of the reactions occurring when Wyodak coal is heated with phenol has begun. Our first goal is to determine, in so far as possible, the identity of the structures which are the sources and the receptors of the hydrogen which is transferred internally within the coal. To this end, we will oxidize the coal and the reaction products using Deno's procedure.⁴ This recently developed reaction oxidizes aromatic rings to CO₂ while leaving the aliphatic material intact as carboxylic acids. It is thus a unique and sensitive probe of the aliphatic structures in coals and coal-derived materials. By applying this reaction to the parent coal, the residue, and the extractable products, the change in the amount and type of aliphatic material present can be monitored. The proton nmr of the pyridine-soluble products in this reaction indicates a sharp increase in the number of methylene groups β or farther removed from an aromatic ring. We plan to analyze the products by gas chromatography of their trimethylsilyl esters. The gas chromatograph has been set up and authentic samples of the expected trimethyl silyl esters are being prepared for use in developing the GC procedures and in identifying the reaction products.

2.4 In-Plant Environmental Monitors

D. D. Schuresko

Technical progress during May on the portable fluorescence spotter primarily consisted of identifying and eliminating several bugs in the electronics unit. One problem, namely that the oscillator section of the mercury arc lamp supply and igniter was still operating at low level after lamp ignition, was due to a wiring error in this circuit. This problem generated lamp arc flicker which showed up as abnormally high signal noise. A second problem, the interference between the audio output circuitry and the synchronous detector card was eliminated by powering the audio circuit NE555 timer chip and the speaker from a separate, 9V transistor battery, rather than from the gel cells used to power the rest of the unit. In addition, an audio output transformer, which had been previously omitted from the circuit was installed. Debugging activities on this unit are progressing steadily and should be finished in June.

*Chemistry Division

A meeting was held at DOE headquarters in Germantown on May 8, 1979 to define a field test protocol and schedule for evaluating the fluorescence spotter. Present at the meeting were:

<u>Name</u>	<u>Affiliation</u>
Hershul T. Jones	DOE-FE/DFFP
M. A. Christensen	DOE-FE/FFP
J. Malcolm	DOE-FE/ETF, FFP, MEP
C. Harold Fisher	DOE-FE/FFP
T. K. Lau	DOE-FE/FFP
Paul Duhamel	DOE-Environmental Health & Safety
Daniel Lillian	DOE-Environmental Health & Safety
Barry Pally	NIOSH
Stephen P. Berardinelli	NIOSH/EIB
James M. Evans	Consultant from Enviro Control
H. D. Cochran	ORNL
D. D. Schuresko	ORNL
J. E. Mrochek	ORNL

The first part of the meeting was given over to a physical description of the instrument, the principles upon which its operation depends, and its sensitivity to pure polynuclear aromatic hydrocarbons (PAH) and various products of coal liquefaction. During and after this presentation, a discussion ensued on potential safety problems with the instrument in the operational areas of coal conversion plants. It was agreed that field testing in non-restricted areas of coal liquefaction plants should not be delayed while design modifications necessary to enable the spotter to operate in explosive atmospheres were looked into. It was also pointed out that since 110V AC power would be available at all anticipated testing locations, the spotter should be modified to run primarily on AC power.

Five operating pilot plant facilities were selected as potential sites for field testing the fluorescence spotter. They include the SRC Pilot Plant at Fort Lewis, Washington; the Grand Forks, Morgantown, and Pittsburgh Energy Technology Centers; and Hygas Pilot Plant in Illinois. First priority was assigned to the SRC plant with no order of priority attached to the remaining facilities. It was strongly suggested that each of these facilities be visited for 1 to 2 days by ORNL personnel to discuss and obtain preliminary concurrence of plant operating personnel for planning the actual field test protocol — dates, length of time, actual areas within the plant to be monitored, operating personnel participation, and any other necessary details concerning the actual field tests. It was suggested that planning visits should be completed and written field testing protocols for the five individual plants be submitted to DOE for their study and concurrence by the end of June with actual field testing to begin in September.

2.5 Experimental Engineering Support of In Situ Gasification Processes

P. R. Westmoreland, L. S. Dickerson, and B. R. Rodgers

Experiments and analyses were continued during this period to improve the understanding of physical processes and reactions in underground coal gasification (UCG). Items presented in this report are:

- Results from block pyrolysis of lignite in an atmosphere of simulated UCG product gas (Sec. 2.5.1),
- Surface areas of lignite chars as they affect char reactivity (Sec. 2.5.2), and
- Physical properties of coal (Sec. 2.5.3), including
 - enthalpy and specific heat correlations for low-rank coals,
 - review of literature data on thermal conductivity and thermal diffusivity of bituminous coal, and
 - correlation methods for thermal conductivity of low-rank coals.

This research program supports both the modeling and field development of in situ (or underground) coal gasification, and emphasizes study of the pyrolysis of large coal blocks. Pyrolysis of overburden and measurements of physical properties are also parts of the program.

In experiments which began at ORNL in 1975, 150-mm (6-in.-diam) right circular cylinders of lignite, subbituminous coal, and bituminous coal have been pyrolyzed by heating the blocks at 0.3-14 K/min (surface temperature) from ambient temperature to maximum temperatures of 773-1273 K (500-1000°C). Using an inert (argon) or reducing (hydrogen) purge gas at atmospheric pressure, gas- and vapor-phase reaction products are continuously swept from the reactor. Water, oils, and tars are collected in a water-cooled condenser and by filters, and the remaining noncondensable gases are metered and periodically sampled. In many of the experiments, block temperature profiles have been measured by internal thermocouples. These tests are designed to support modeling of field UCG experiments by Laramie Energy Technology Center (LETC), Lawrence Livermore Laboratory (LLL), Morgantown Energy Technology Center (METC), and Gulf Research & Development Company (GR&DC).

2.5.1 Block pyrolysis in a mixed sweep gas

A purge gas which simulates the product gas of UCG was used in block pyrolysis of lignite during experiment BP2-58, the second of a pair of similar experiments. In experiment BP2-57 on bituminous coal,⁵ steam and H₂ penetrated the coal from the purge gas, causing some steam gasification and hydrogasification. Steam flux out of the lignite is much

higher because of higher coal moisture content (37.5% vs 0.80% for bituminous coal). As a result, little reactant gas should penetrate a block of lignite.

In experiment BP2-58, Wilcox lignite was heated in the mixed gas at 3 K/min to 1073 K (800°C). The purge gas was changed to argon when the surface temperature reached 1073 K so as to isolate the effect of reactant gases on the drying, pyrolyzing block. Composition of the mixed gas is shown in Table 2.1, and Table 2.2 summarizes experimental conditions. Net yields were calculated by subtracting purge gas and coal moisture from the effluent gas and condensate.

These yields may be compared (Table 2.3) to previous experiments conducted in Ar and in H₂ to show the slight effects of the purge gas: (1) a slight penetration of the block by H₂ and (2) some shifts in the gas-phase equilibria from CO to CO₂ and H₂, probably by the water-gas shift reaction. As measured by oil cracking (decreased oil yield relative to the argon-purged experiment) and hydrogasification (increased CH₄ yield), some H₂ seemed to penetrate the block for reactions. The extent of penetration was about the same as during the hydrogen purged experiment. No other gas-solid reactions are apparent.

2.5.2 Char reactivity and surface area (G. L. Alexander,* B. V. Hu,* A. H. Kwai,* E. L. Fuller,** and P. R. Westmoreland)

Earlier, variations in pyrophoricity of lignite char were tentatively linked to the cracking of pyrolysis tars.⁶ After pyrolyzing blocks of lignite at different conditions, pyrophoricity (spontaneous heating) of room-temperature chars changed in definite patterns (Fig. 2.3). Specifically, chars produced using higher heating rates, wet blocks, and H₂ purge gas (instead of inert Ar) had lower pyrophoricity, as measured by temperature rise when the room-temperature char was exposed to air. By restricting diffusion of air to micropores, carbon deposits from tar cracking was speculated to have caused these changes.

Kamashita, Mahajan, and Walker studied the effect of carbon deposition on lignite char,⁷ finding a strong link between surface area changes and reactivity. Experimentally, a North Dakota lignite was pyrolyzed at 1128 or 1273 K. Carbon was deposited using the thermal cracking of CH₄, and reactivity to air was measured at 648 K. Relative to control samples (no carbon deposition), reactivities of these samples were lower. In addition, surface areas measured by N₂ adsorption (77 K) and CO₂ adsorption (298 K) were lowered by the deposits; the N₂ measurements, which have poorer accessibility to micropores, were lower than the CO₂ values and were affected more. Apparently, deposited carbon obstructed small pore openings, restricting the diffusion of air to reactive sites inside the micropores.

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Table 2.1. Composition of simulated UCG sweep gas
in experiment BP2-58

Gas	Composition (mol %)	
	Dry basis	Wet basis
H ₂	16.70	15.4
CH ₄	3.87	3.6
CO	13.84	12.8
CO ₂	13.77	12.7
Ar ^a	51.82	47.7
H ₂ O	---	7.9

^aSubstituted for N₂ which is present in UCG product gas.

Table 2.2. Conditions for experiment BP2-58

Coal used:	Lignite A Calvert Bluffs formation, Wilcox group Sandow, Milam Co., Texas
Coal cylinder:	4.353 kg as-received, 2.34 kg maf 149 mm diam (5-7/8 in.) 194 mm high (7-5/8 in.)
Reactor heating rate:	3 K/min (5°F/min)
Maximum temperature:	1073 K (1472°F)
Purge gas flow (dry):	0.1206 mol/min (0.0955 scf/min)

Table 2.3. Comparison of yields from block pyrolysis of Wilcox lignite. All experiments 3 K/min to 1073 K.

	Net yield (maf wt %)		
	In Ar	In mixed gas	In H ₂
Oil	5.7	4.3	3.4
Water (net)	-8.2	-0.8	-1.9
Subtotal	-2.5	3.5	1.5
Char	56.3	48.8 ^a	56.0
Gas - H ₂	2.20	2.29	1.983
CH ₄	3.10	6.21	5.78
C ₂	1.017	1.36	1.074
C ₃	0.298	0.37	0.369
CO	12.37	11.19	14.98
CO ₂	14.84	15.51	12.63
H ₂ S	0.52	0.40	0.40
Subtotal	34.35	37.33	37.21
Total	88.2	89.6	94.7

^aLow; char may have been lost by pyrophoric combustion.

Fig. 2.3. Relative pyrophoricity of lignite chars as affected by conditions of block pyrolysis.

Surface area and micropore volume have now been measured on three chars shown in Fig. 2.3.⁸ Samples came from the surface region of char blocks which had been prepared at 3 K/min to 1073 K. In order of decreasing pyrophoricity, one char came from a predried block pyrolyzed in inert gas (Ar), the second from a naturally wet block (37.5% H₂O) pyrolyzed in Ar, and the third from a wet block pyrolyzed in H₂. Brunauer-Emmett-Teller (BET) surface areas were calculated from adsorption isotherms of N₂ (77 K) and CO₂ (193 K), measured on a Cahn RG Electrobalance. Also from these isotherms, Dubinin-Radushkevich-Kaganer (DRK) micropore volumes were calculated.

These properties are compared in Table 2.4 for unreacted lignite⁹ and the three chars. Pyrolysis creates much new surface area, particularly by opening up micropores; this effect is shown by the large increase in N₂ surface area from dry lignite to the chars prepared in Ar. Predrying had no detectable effect on surface area or micropore volume, indicating that other factors cause that associated change in reactivity. However, both physical properties were nearly halved by pyrolyzing the lignite in H₂ rather than in Ar. Either H₂ has changed the thermal decomposition of the lignite (unlikely through either changed heating rate or altering of the solid), or deposited material such as carbon is blocking off micropores.

The source of deposited carbon must be pyrolysis or cracking of the pyrolysis products, particularly of the tars but possibly of CH₄ as well. Yield of organic liquids from blocks was previously shown² to be 50-70% less than yield from dry powder, indicating consumption. Apparently, tar vapors formed by pyrolysis inside the block have cracked as they escape through the hot surface region of the block. Such cracking to carbon, lighter oils, ethylene, and other gases was also observed in block pyrolysis of subbituminous and bituminous coals.¹⁰

Lower microporosity in the H₂-prepared block seems to result from more extensive cracking. Both in lignite² and in bituminous coal,¹⁰ yield of organic liquids was less in H₂ than in inert gas. Such promotion of cracking would seem contrary to hydrocracking experience, where in H₂ yield of coke and olefins is negligible and oil yield is higher, but hydrocracking is a high-pressure catalytic process, unlike block pyrolysis or UCG. Hydrogen probably affects cracking only in the surface region of the block because the countercurrent steam and product flux prevents deep penetration by H₂ diffusion.

An alternative explanation might be that H₂ inhibits steam gasification of the deposited carbon, but the facts do not support this hypothesis. Conceivably, cracking and deposition could occur unaffected by H₂ but H₂ could inhibit the gasification reaction. However, H₂ inhibition of gasification rate is not significant above 1023 K for small carbon conversions.¹¹ Furthermore, if this mechanism occurred, less oxygen as CO and CO₂ would be produced in the argon-purged experiment; on the contrary, oxygen yield from the wet block pyrolyzed in Ar or H₂ is the same within 0.6%. Promotion of cracking by H₂ is a more satisfactory explanation.

Table 2.4. Surface areas of lignite chars. All chars from surface region of blocks heated at 3 K/min to 1073 K.

Sample	Surface area (m ² /g)		Micropore volume (cm ³ /g char)	
	By N ₂	By CO ₂	By N ₂	By CO ₂
Dry, unreacted lignite ^a	2.3	238 ^b	--	--
Char from predried block pyrolyzed in Ar	279	288	0.092	0.118
Char from wet block pyrolyzed in Ar	240	272	0.096	0.113
Char from wet block pyrolyzed in H ₂	145	147	0.059	0.058

^a Darco mine, Texas, average of two samples (ref. 9).

^b Measured by CO₂ adsorption isotherm at 298 K using Dubinin-Polanyi equation.

2.5.3 Physical properties of coal

Correlations and summary of data on thermal properties of coal are presented in this section.

Enthalpy and specific heat correlations. — Based on data by Gomez et al.,¹² previously reported correlations of enthalpy and specific heat for low-rank coals¹⁰ are corrected and extended in Table 2.5. The method is based on a mass-weighted average of moisture, ash, and low-rank coal properties which has proved satisfactory.

Thermal diffusivity and thermal conductivity of bituminous coal. — Literature data 13-18 for dry, solid bituminous coal are presented in Table 2.6, listed in order of decreasing volatile matter. In the thermal conductivity data, significant scatter occurs. High mineral-matter content generally increases thermal conductivity, and petrographic make-up probably makes a difference (durain is more conductive than clarain). However, precision of these measurements on bituminous coal can be significantly affected (20%) by differences in handling.¹⁹ Thermal diffusivity is more consistent, averaging 0.151 ± 0.007 mm²/sec for the ten whole coal samples.

Correlations for thermal conductivity of low-rank coal. — Few thermal conductivity data are available for low-rank coals,⁵ but correlation of these data is desirable. No general moisture-conductivity relationship is available, but several models for conductivity in dry coal have been proposed. Each model seeks to correlate thermal conductivity k as a function of intrinsic conductivity k_s of the solid and of fractional porosity p . Fritz²⁰ tested the equations of Maxwell,

$$k = k_s \left(\frac{1 - p}{1 + 0.5 p} \right), \quad (1)$$

and of Burger,

$$k = k_s \left(\frac{1 - p}{1 + 0.67 p} \right), \quad (2)$$

using his own correlation of k_s with ultimate density of the solid (Table 2.7). While he rejected the correlations because they did not agree with his data on cokes, agreement with k of his dry lignite is good. For the respective methods, 0.168 W/m·K and 0.154 W/m·K are predicted, compared to the experimental value of 0.151 W/m·K. Another equation²¹ has been cited as a good approximation for thermal conductivity in a porous medium:

$$k = k_s p \left(\frac{k_f}{k_s} \right)^{1-p}, \quad (3)$$

Table 2.5. Correlations of enthalpy and specific heat for coals and chars as functions of temperature (K).

		Correlation
Enthalpy, kJ/kg		
Ash, 375-1031 K ^a	-181.9	+ 0.633 x T + 0.297 x 10 ⁻³ x T ²
Low-rank coal, maf, 305-450 K ^a	-203.1	+ 0.378 x T + 1.212 x 10 ⁻³ x T ²
Wilcox lignite, dry	-200.1	+ 0.414 x T + 1.084 x 10 ⁻³ x T ²
Wyodak subbituminous coal, dry	-202.0	+ 0.392 x T + 1.163 x 10 ⁻³ x T ²
Hanna No. 1 hvCb coal, dry	-196.4	+ 0.459 x T + 0.922 x 10 ⁻³ x T ²
Char from Wilcox lignite pyrolyzed at 500°C, dry, 368-724 K ^a	-169.8	+ 0.190 x T + 1.101 x 10 ⁻³ x T ²
Specific heat, kJ/kg·K		
Wilcox lignite, dry	0.414	+ 2.168 x 10 ⁻³ x T
Wyodak subbituminous coal, dry	0.392	+ 2.326 x 10 ⁻³ x T
Hanna No. 1 hvCb coal, dry	0.459	+ 1.845 x 10 ⁻³ x T
500°C Wilcox char, dry	0.190	+ 2.202 x 10 ⁻³ x T

^aData for correlation from Gomez et al.¹²

Table 2.6. Thermal diffusivity and thermal conductivity of dry bituminous coals.
Ranked in order of volatile matter (wt %, dry- and mineral-matter-free), excludes cannel coal.

Coal source (mine, seam, country)	Ref.	Mineral matter (wt %, dry)	Volatile matter (wt % dmmf)	Thermal diffusivity (mm ² /sec)	Thermal conductivity (W/m·K)	Temperature (K)
Cannel-like bituminous						
Sample 3, U.K.	13	9.1 ^a	48.4	--	0.163 ^b	288-373
Sample 2, U.K.	13	8.7 ^a	47.5	--	0.167 ^c	288-373
Sample 4, U.K.	13	7.7 ^a	43.4	--	0.159 ^b	288-373
High-volatile bituminous						
Binley, 9-ft., U.K.	14	6.4	42.2	--	0.184	423-673
Barnsley thick durain, U.K.	13	9.1 ^a	41.9	0.158 ^d	0.218 ^d	288-373
Polysaevskaya, U.S.S.R.	15	6.5 ^a	41.0	0.163	0.157	473-573
Pittsburgh seam, U.S.A.	16	9.3	40.6	0.155 ^e	0.213 ^e	423
				0.143 ^f	0.196 ^f	423
Woolaton, Tupton, U.K.	14	22.1	40.3	--	0.268	423-673
Woodside, U.K.	14	4.2	39.3	--	0.243	423-673
Hedwigswunsch, Germany	17,18	2.7 ^a	39.0	0.147 ^g	0.230 ^g	303
Radford, Tupton, U.K.	14	20.2	38.8	--	0.222	423-673
Hucknall, Main Bright, U.K.	14	6.1	38.4	--	0.227	423-673
Dearne Valley, Shafton, U.K.	14	5.6	37.6	--	0.205	423-673
Trencherbone clarain, U.K.	13	3.1 ^a	37.4	0.144 ^h	0.188 ^h	288-373
Hedwigswunsch, Germany	17	4.7 ^a	36.9	--	0.241 ^g	303
Clipstone, Low Main, U.K.	14	4.5	36.4	--	0.194	423-673
Vane Tempest Maudlin, U.K.	14	1.7	35.6	--	0.241 ⁱ	423-673
Barnsley Thick clarain, U.K.	13	1.7 ^a	35.1	0.120 ⁱ	0.155 ⁱ	288-373
Trencherbone durain, U.K.	13	7.6 ^a	34.1	0.152 ^j	0.230 ^j	288-373
Arley durain, U.K.	13	1.4 ^a	33.8	0.157 ^k	0.209 ^k	288-373
Arley clarain, U.K.	13	1.6 ^a	32.9	0.135 ^l	0.180 ^l	288-373
Dorstfeld, Germany	17,18	2.6 ^a	32.2	0.147 ^j	0.217 ^j	303
					0.280 ^j	303
Bilsthorpe, U. K.	14	15.8	31.9	--	0.266	423-673

Table 2.6. (continued)

Coal source (mine, seam, country)	Ref.	Mineral matter (wt %, dry)	Volatile matter (wt % dmmf)	Thermal diffusivity (mm ² /sec)	Thermal conductivity (W/m·K)	Temperature (K)
Medium-volatile bituminous						
Monopol, Otto, Germany	17	3.5 ^a	29.1	--	0.205 ^m	303
Monopol, Röttgersbank, Germany	17,18	6.0 ^a	28.6	0.156 ⁿ	0.229 ⁿ	303
Monopol, Ida, Germany	17	2.9 ^a	27.4	--	0.205 ^k	303
Monopol, Emil, Germany	17,18	2.4 ^a	26.8	0.150 ⁿ	0.215 ⁿ	303
Gleiwitzer, Germany	17	3.1 ^a	26.2	--	0.207 ^o	303
Gleiwitzer, Germany	17,18	3.7 ^a	25.9	0.158 ^o	0.212 ^o	303
Monopol, Rudolf, Germany	17	2.1 ^a	25.9	--	0.205 ^o	303
Cwmillery Garw, U.K.	14	4.3	25.5	--	0.29	423-623
Monopol, Wilhelm, Germany	17	1.3 ^a	24.9	--	0.194 ^o	303
Dorstfeld, Germany	17,18	1.7 ^a	24.2	0.153 ^p	0.210 ^p	303
Low-volatile bituminous						
Amalie, Dickebank I, Germany	18	3.7 ^a	20.3	0.142 ^q	0.195 ^p	303

^a Estimated using measured ash and 1% sulfur in Parr formula.^b Possibly contains 2.9% H₂O.^c Possibly contains 2.2% H₂O.^d Possibly contains 6.6% H₂O.^e Parallel to bedding planes.^f Perpendicular to bedding planes.^g Possibly contains 2.8% H₂O.^h Possibly contains 4.1% H₂O.ⁱ Possibly contains 9.9% H₂O.^j Possibly contains 1.3% H₂O.^k Possibly contains 1.4% H₂O.^l Possibly contains 1.5% H₂O.^m Possibly contains 1.0% H₂O.ⁿ Possibly contains 0.8% H₂O.^o Possibly contains 1.1% H₂O.^p Possibly contains 0.7% H₂O.^q Possibly contains 1.2% H₂O.

where k_f is the thermal conductivity of the interstitial fluid, but it predicts the value of $k = 0.26 \text{ W/m}\cdot\text{K}$, an unacceptably high value.

For unreacted, dry, low-rank coals, the best thermal conductivity correlation seems to be either Eqn. (1) or (2), using the Fritz correlation of k_s with ultimate density.

2.5.4 Future plans

Correlation of data and preparation of a summary report will continue. Thermal diffusivity measurements on subbituminous coal and char may have to be delayed into the next year because of resource limitations. However, thermal diffusivity and conductivity of anthracite and cannel coals will be reviewed next month in order to show a general correlation of thermal conductivity with rank from brown coal through anthracite. Also, based on data for thermal conductivity of wet and dry coals, correlations will be tested.

Table 2.7. Correlation of thermal conductivity for solid coal (zero porosity) with ultimate density.²⁰

Ultimate density of solid coal (kg/m^3)	Thermal conductivity of solid coal, k_s ($\text{W/m}\cdot\text{K}$)
1350	0.24
1400	0.284
1450	0.333
1500	0.401

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3. CHEMICAL RESEARCH AND DEVELOPMENT

M. L. Poutsma

3.1 Chemistry and Structure of Coal

M. L. Poutsma

Further data revealing the effect of conversion level on the product distribution from pyrolysis of bibenzyl (1) at various pressures are shown in Table 3.1. The rapid secondary pyrolysis of $\text{PhCH}_2\text{CHPhCH}_2\text{Ph}$ (4) and $\text{PhCH}_2\text{CHPhCHPhCH}_2\text{Ph}$ (5) to form largely PhCH_3 (2) and PhCH=CHPh (3) augment observations in earlier reports.

Last month we described Ph_2CHCH_3 (6) as a "secondary product." More detailed analysis of all data now in hand show that it is indeed a primary product whose proportion increases with increasing pressure of 1. At $366 \pm 1^\circ\text{C}$ and 1-2% conversion of 1, the proportion of 6 increases from <1% in the dilute gas to 15-20% in the neat liquid. Such behavior demonstrates that the 1,2-phenyl migration involved is rapidly reversible; radical 9 either reverts to radical 8 or is captured by hydrogen atom transfer with 1 to form 6. Being aware of such potential skeletal rearrangements may preclude errors in future attempts to deduce coal structure from thermally produced fragments.

To begin our investigation of the effects on the radicals present (7, 8, 9) of additives having structures representative of those in coal, we have carried out comparative gas-phase pyrolyses at $401 \pm 1^\circ\text{C}$ for 70 min. Under these conditions for 1 alone (0.25 atm), the total conversion was 6.0% to form 2, 3, 4, 5, and 6 in a carbon equivalent ratio of 27.3:17.9:36.0:17.0:0.4. Parallel pyrolysis of 1 (0.19 atm) in the presence of excess tetralin (2.45 atm) gave lower conversion (~2.5%) to form 2 but 3-6 were absent. This is of course the anticipated result if tetralin captures benzyl radicals (7) by hydrogen atom transfer before they can attack 1. Formation of dimers 4 and 5 was also largely eliminated by pyrolysis of 1 (0.20 atm) in the presence of a similar excess of phenol (2.92 atm); however 3 (along with 2) remained as a significant product, and small amounts of new products, presumably incorporating phenol, were detected. Hence, although phenol is less effective as a hydrogen atom donor than tetralin, it does produce a chemical effect worthy of further investigation. A diminution of the 4:2 and 5:2 ratios, as well as formation of new products, was also induced by the presence of excess anthracene, a representative of polycyclic aromatics.

TABLE 3.1

Thermolysis of Bibenzyl (1) at $401 \pm 1^\circ\text{C}$

Entry	p^a (kPa)	t (min)	Conv (%)	Product Distribution (Carbon Equiv. %)								
				PhCH_3	PhCH=CHPh^b	$(\text{PhCH}_2)_2\text{CHPh}$	$(\text{PhCH}_2\text{CHPh})_2$	Ph_2CHCH_3	PhH	Ph_2CH_2	Phenanthrene	Other
1	54	15 ^c	1.7 ^d	26.7	9.7	26.7	35.2	1.1	~ 0.6	e	e	-
2	52	1200	65.4 ^{f,g}	54.7	32.6	1.5	0.3	0.5	~ 1.6	1.7	5.4	h
3 ⁱ	99	15 ^c	1.1 ^d	21.5	7.1	23.6	47.7	j	k	e	e	-
4 ⁱ	96	1000	60.4 ^{f,l}	48.3	37.2	3.4	0.4	0.8	k	2.3	4.7	m
5	462	15 ^c	1.8 ^d	31.5	7.4	12.0	46.4	2.4	~ 0.4	e	e	-
6	493	1200	72.4 ^{f,n}	55.2	31.6	0.6	0.5	1.7	~ 0.7	5.0	2.1	o
7	Liquid ^p	15 ^c	1.4 ^d	30.0	10.6	3.3	44.6	11.2	~ 0.3	e	e	-
8	Liquid ^q	1200	85.0 ^{f,r}	58.8	7.3	1.0	2.2	3.4	~ 1.0	18.3	2.4	s

^aCalculated from tube volume by ideal gas law. The vapor pressure of 1 at 400°C (980 kPa) was extrapolated from data at lower temperatures. ^bTrans isomer only; see text. ^cIncludes heat-up time. ^dConversion = $(\sum \text{Products}) /$

$(\sum \text{Products} + (\underline{1})_f) \times 100\%$. ^eNot detected. ^fConversion = $\left(\frac{((\underline{1})_0 - (\underline{1})_f)}{(\underline{1})_0} \right) \times 100\%$. ^gMaterial balance = 103%.

^h $\sim 0.8\%$ PhEt, $\sim 0.5\%$ PhVi, and $\sim 0.3\%$ unknown (ret. time between 4 and 5). ⁱ $403 \pm 1^\circ\text{C}$. ^jTrace present but not quantified.

^kPhH not quantifiable in entries 3 and 4. ^lMaterial balance = 88%. ^m $\sim 1.0\%$ PhEt, $\sim 0.8\%$ PhVi, and $\sim 0.3\%$ unknown.

ⁿMaterial balance = 106%. ^o $\sim 1.2\%$ PhEt, $\sim 0.2\%$ PhVi, and $\sim 1.2\%$ unknown. ^p79% of 1 in liquid phase in equilibrium with

vapor at 980 kPa. ^q77% of 1 in liquid phase. ^rMaterial balance = 85%. ^s $\sim 3.7\%$ PhEt and $\sim 1.9\%$ unknown.

3.2 Kölbel Process Concepts

M. L. Poutsma

Various information sources on the Kölbel slurry reactor, the Kölbel-Engelhardt reaction, and the M-Gasoline process have been collected and compared. The first draft of the chemical assessment study is partly written and will be completed next month.

4. MATERIALS ENGINEERING

R. A. Bradley

The materials engineering and associated technology reported here are in support of activities directed or coordinated by the Materials Engineering Branch, Division of Planning and Systems Engineering, Fossil Energy. Other related work funded by the Division of Fossil Fuel Utilization and the Division of Fossil Fuel Processing is also included.

4.1 Pressure Vessel and Piping Materials

W. J. Stelzman, R. O. Williams, and D. A. Canonico

This task is concerned with the influence of an operating environment on the in-service reliability and safety of large pressure vessels for use in second generation coal conversion systems. The candidate steels from which these vessels will be constructed are subject to an environmentally induced embrittlement at the currently projected operating condition of these units. Of prime concern is the effect of hydrogen on both low- and high-temperature properties of these steels.

It has been known for many years that low alloy steels would develop internal bubbles of methane when exposed to high pressure hydrogen at elevated temperatures. Further, it was also known that the problem can be controlled by using alloy steels, specifically, steels which had alloying additions which formed stable carbides, the effect being simply to reduce the carbon activity and thus reduce the driving force for the formation of methane.

Even realizing this, the problem is rather complicated because the carbon activity is dependent upon prior history. Our program is currently addressing this question with the expectation that we can help select the most appropriate steel and the best heat treatment schedule, consistent with other requirements, which will give satisfactory service at a minimum cost. In addition, other aspects of the problem are also being considered, specifically, a more quantitative determination of the effect of stress on the susceptibility to hydrogen attack and the possible effects of such environments on crack propagation.

The primary reason why the carbon activity is history dependent is that the diffusion rates of the substitutional elements are always restricted under the conditions where the steel is undergoing transformations. One may obtain widely differing starting structures on the initial metallurgical transformations; specifically, pearlites having widely different spacings, bainite or martensite. The size of the carbides and their dispersion is highly dependent on the initial structure and the subsequent heat treatment. The carbon activity is controlled by the amount of the carbide-forming element which can diffuse to the carbide particle and on the particular carbides which form.

To make useful estimates on the time dependence of the carbon activity is relatively easy, but to try to obtain a quantitative treatment is very difficult and may not warrant the effort. Experimental verification is required in any case; and, because of this need, we are concentrating on these measurements.

Early in the program we further developed an existing computer program to calculate the equilibrium carbon activity in such steels. By taking the Nelson curve for plain carbon steels and assuming that attack for an alloy steel would occur at the same methane potential, it is possible to calculate the Nelson curves for the second steel. The agreement with the published Nelson curves was very satisfactory and verifies our premise that attack occurs at the same methane potential.

A direct measurement of the carbon activity would be of great help in this program and, in this connection, we have set up an experiment where we equilibrate our sample with a static hydrogen atmosphere and obtain the carbon activity from the concentration of methane which is found. This is a standard method for such measurements and is known to work at elevated temperatures. Such measurements will be of some value, but in the regime in which we are most interested, it appears that the kinetics may be too slow for the method to be useful.

A run has been made where samples of widely differing histories were exposed to hydrogen at elevated temperatures, but various experimental problems prevented sufficient exposure to develop hydrogen attack. These problems have been corrected such that we expect the next run to produce useful results. We are using high-temperature strain gages to monitor the attack, and our results so far indicate that this method will work satisfactorily.

We had a jig built for exposing samples under stress and have prepared the samples, but no runs have been made. We are also heat-treating material from which impact samples will be prepared and exposed.

A number of steels are candidates for the construction of large, second generation commercial pressure vessels. These steels include SA 516 Grade 70, SA 204 Grade B, SA 387 Grade 22, SA 533 Grade B, and SA 543. These grades are included in this program, and data concerning their fracture toughness properties are being obtained.

We have continued study on the mechanical properties of 24.8-cm-thick (9 3/4-in.) ASTM A 543 Class 1 steel plate (2 1/4 Cr-1 Mo). Four 1-in.-thick compact specimens (1T CS) were tested in the temperature range of -129 to 93°C (-200 to 200°F) and the results compared with previous results from 0.394T CS. All specimens were from the quarter thickness level. The ductile-brittle transition of the 1T CS appears to occur at slightly higher temperatures. The 110 MPa $\sqrt{m}$ (100 Ksi $\sqrt{in.}$) fracture toughness level occurs at -127°C (-190°F) for the 0.394T CS and approximately at -107°C (-160°F) for the 1T CS.

Tensile specimens [4.48-mm (0.176-in.) gage diam and 31.8-mm (1.250-in.) gage length] were also tested to extend the range of specimens tested at 23 and 343°C (74 and 650°F). The yield and ultimate stresses ranged from 743 and 852 MPa (107 and 123 Ksi), respectively, at -29°C (-20°F) to 531 and 565 MPa (77.1 and 82.1 Ksi), respectively, at 482°C (900°F).

We also subjected several tensile specimens to postweld heat treatment of 40 h at 610°C (1130°F) and tested them at two temperatures. The results were compared with the as-received plate results, and the change in yield and ultimate stresses is slight: about 28 MPa (4 Ksi) at 23°C (74°F) and essentially no change at 343°C (650°F).

4.2 Fossil Energy Welding and Cladding Development

D. P. Edmonds and J. F. King

Negotiations are continuing with commercial manufacturers to develop cladding techniques for type 320 stainless steel using the submerged-arc strip cladding process. A detailed proposal of planned work is expected in the near future. The information gained from the previous work on this program will be used to formulate strip electrode compositions that eliminate fissures in the clad deposits.

4.3 Fireside Corrosion of AFBC Tubes

T. G. Godfrey and J. H. DeVan

Examination of tube samples from the 4500-h experiment in the Fluidyne atmospheric fluidized-bed combustor (AFBC) is continuing. The analysis is not complete at this time, but a pattern seems to be emerging that might explain the severe corrosion of tube 9B (type 316 stainless steel) observed at the end of the test.

Tube 9B was inserted at the 1500-h point and remained in place during the following 3000-h period. In the nearby position 8C, three type 316 stainless steel tubes were used for the periods 1500-2000 h, 2000-3000 h, and 3000-4500 h. Metallographic examination indicates that the 8C sample exposed for the 2000-3000-h period experienced more corrosive attack than either the preceeding or the following sample. It was during this same 1000-h period that an air-cooled trimmer tube failed at mid-length from fatigue/stress. We believe that the failed trimmer tube actually leaked air for some time before it totally failed. This excess air was detected by the flue-gas oxygen analyzers which caused an increase in the coal feed by the control system. Since the total combustion air is held constant in the Fluidyne system, this increased coal feed rate would lower the excess oxygen within the fluidized bed while the flue gas would indicate the desired oxygen level. Thus, it is reasonable to conjecture that certain areas of the fluidized bed, such as 9B and 8C, were sufficiently oxygen-deficient that sulfidation/oxidation corrosion could occur.

4.4 Failure Prevention and Analysis

R. W. Swindeman

4.4.1 Examination of corrosion coupons from solvent-refined coal plants (V. B. Baylor, J. R. Keiser, E. J. Lawrence, and R. S. Crouse)

Analyses of coupons received from the Wilsonville and Fort Lewis solvent-refined coal (SRC) pilot plants are continuing. Racks of unstressed corrosion coupons have been assembled and shipped to Wilsonville for insertion into the repaired T105 fractionation column.

Chemical analysis of liquids provided by Wilsonville have been completed. As expected, the liquids produced from Kentucky coal feed had about 10 times the chlorine content as those produced from Indiana coal. The overhead product from the fractionation column was about the same for both coals, but at the bottom of the column, the Kentucky coal produced a product with higher chlorine content.

Microprobe analyses of samples of corroded trays from the Wilsonville fractionation column should begin soon.

4.5 Materials for ZnCl_2 Liquefaction Process

V. B. Baylor and J. R. Keiser

Fabrication on the quartz glass testing apparatus has begun at the glass shop. Several modifications in the design were made to enhance fabricability. Materials to simulate the regeneration system environment are being ordered, and specimens are being machined.

4.6 Materials to Resist Stress-Corrosion Cracking in Coal Liquefaction Pilot Plants

J. R. Keiser and V. B. Baylor

The U-bend specimens exposed at the Fort Lewis SRC plant are being examined metallographically. Although visual inspection revealed no evidence of cracking, dye penetrant checks showed some indication of cracking, especially in the type 410 stainless steel coupons exposed in all three separator vessels.

Two racks of U-bend samples were prepared for insertion into the T105 fractionation column at the Wilsonville SRC plant. An identical rack was delivered in March but has not yet been exposed due to failure of the column. The column is expected to be back in service soon. For each of the three locations of coupon racks, we are providing one rack of U-bends and one rack of flat coupons (see Section 4.4.1).

By agreement with Exxon, machined U-bend samples for insertion into the Exxon Donor Solvent (EDS) plant are being prepared for shipment. They have chosen which materials are to be tested. We will do the post-test analyses with information to be supplied to Exxon as soon as possible. The coupon-testing racks are to be inserted sometime soon even though the EDS plant will not be fully operational until 1980.

4.7 Development of Advanced 9 Cr-1 Mo Structural Steel

V. K. Sikka

Mechanical property characterization, fabrication, weldability, and steam corrosion studies continued on the experimental heats and two of the four DOE Reactor Research and Technology Division commercial argon-oxygen-deoxidization (AOD) process heats. Several accomplishments made during the last month are as follows:

1. Charpy impact testing of the first gas tungsten-arc (GTA) weld (PC-2) made during the previous month was completed. Data are currently being evaluated and compared with the base metal data.

2. A 16-mm-thick plate of the Quaker heat was welded using the filler wire made from the Quaker heat. Thus, this weld represents a combination of both the base and weld metal of the modified 9 Cr-1 Mo steel. The same filler wire was also used to make a weld in a 6.35-mm wall by 50-mm-OD tube made from the Quaker heat. The x-ray inspection of these welds have shown them to be defect free. The Charpy, tensile, and creep specimens are currently being machined from these weldments. The specimens will be tested during the next month, and the information obtained will be used in optimizing the postweld heat treatment and the filler wire composition.

3. The modified 9 Cr-1 Mo steel tube was also successfully welded to type 304 stainless steel and 2 1/4 Cr-1 Mo tubing. The joint between 9 Cr and type 304 stainless steel was made using Inconel 82 filler wire, and the 9 Cr to 2 1/4 Cr joint was made using 2 1/4 Cr filler wire. Tensile and creep specimens will be machined from these weldments for a limited mechanical property characterization during the next two months. A demonstration of successful weld between 9 Cr-1 Mo steel and type 304 stainless steel was required for inserting the 9 Cr-1 Mo tubing in TVA boilers which are currently tubed using type 304 stainless steel.

4. Weight loss data after air oxidation at 593°C for approximately 3700 h was compiled on 21 experimental heats of modified 9 Cr-1 Mo steel, the Quaker heat, and 2 1/4 Cr-1 Mo steel. The weight loss per 1000 h was lower by a factor of 1.7 for modified 9 Cr-1 Mo steel (based on average for 21 heats) as compared to 2 1/4 Cr-1 Mo steel. The Quaker heat with 0.36% Si showed less weight loss as compared to the experimental heats which contained less than 0.2 % Si.

5. Bids were obtained from various vendors, and an order for the two 15-ton heats was placed with Carpenter Technology. The ingots from these heats are expected to be delivered during the second week of September.

4.8 Ceramic Recuperators (Heat Exchangers)

V. J. Tennery, G. W. Weber, and G. C. Wei

As reported previously, discussions with Hague International of South Portland, Maine, have resulted in an effort to issue a subcontract to evaluate the suitability of silicon carbide heat exchangers for fossil-fired applications. A proposal from Hague relating to exposure of silicon carbide tubes to coal-oil mixture combustion products has been evaluated and suitable tasks identified. Exposure tests will be conducted at representative use temperatures and flows. Permeability and leakage will also be performed. Final negotiations are in progress to establish the contract during the next month.

The subcontract with Garrett-AiResearch (Torrance, California) to develop preliminary designs for ceramic heat exchangers is still incomplete. Completion is now scheduled during the next month with issuance of a final report encompassing the requirements of the steel, aluminum, and glass industries.

The modification to the refractories test facility to permit evaluation of ceramic heat exchanger materials is on schedule. The expected date of completion of fabrication of the test facility is June 14. Casting and curing of castable tube support blocks is complete, and firing is in progress.

Characterization of as-received samples is progressing. X-ray radiography revealed a crack in a Refrax-20 (Carborundum Co., Keasley, New Jersey) silicon carbide tube. Archive specimens are being prepared of all samples for chemical analyses, x-ray diffraction, metallography, scanning electron microscopy and fracture strength. Permeability measurements are also being conducted. An NC-430 (Norton Co., Worchester, Massachusetts) silicon carbide tube had a room temperature helium permeability of less than $2 \times 10^{-15} \text{ m}^3/\text{s}$ for a pressure differential of 276 kPa.

5. COAL EQUIPMENT TEST PROGRAM

J. M. Holmes and R. E. MacPherson

Work under the Coal Equipment Test Program (CETP) is currently divided into three sections:

- Coal Feeder Test Program
- Survey of Industrial Capability for Coal Handling Equipment
- Support for the Solvent Refined Coal Project

5.1 Coal Feeder Test Program

B. T. Thompson

The report covering the feasibility study and preliminary cost estimate of the Dry Coal Handling Feeding Test Facility (ORNL/ENG/TM-16) has been edited and turned over to reproduction for publication. The report should be published during the next reporting period. The level of activity on this project is low pending outcome of actions recommended in the report. However, a survey of potential sites for the facility will be implemented with emphasis placed on DOE gasification pilot plants currently scheduled for shutdown.

5.2 Survey of Industrial Capability for Coal Handling Equipment

F. C. Zapp, O. W. Thomas, M. D. Silverman, D. A. Dyslin

Approximately half of the equipment survey report has been typed in rough draft form on word processing equipment and is being corrected. After corrections have been made, an editor will review the partially completed report.

Bechtel National was to supply us with a rough draft of their report by May 8 but has supplied us with only a part of their report as of May 25. Information from the Bechtel report, needed to complete the ORNL report, is being forwarded, and the estimated completion date of a draft report is June 29.

5.3 Support for the Solvent Refined Coal Project

P. K. Carlson, L. F. Parsly, J. M. Holmes

During May, the information gathering phase of the SRC (Solvent Refined Coal) R&D Assessment was concluded, and findings of the individual investigators were combined into a final report. The contribution from Engineering Technology Division is entitled "Fluid Handling Components" (ORNL/CF-79/314) and includes evaluations of slurry handling valves,

pumps and metering instruments, and large oxygen compressors. Numerous planned and on-going projects concerned with furthering the technology of these components were examined to determine applicability and overall value to the SRC Demonstration Plants Project. Recommendations were made to extend or redirect current efforts, or if needed programs did not exist, they were proposed. Literature surveys, telephone conversations and trips to relevant work locations were the primary means used to gather data.

Two locations were visited in connection with the assessment of slurry handling valve development: Morgantown Energy Research Center and Fisher Controls, Inc. Neither facility had plans to utilize the hot, coal-derived, solids-containing slurries in test loops to simulate SRC process streams. It is considered essential that valve types proposed for demonstration-sized facilities undergo realistic testing prior to installation to provide assurance as to reliability, maintainability, etc. On that basis it was concluded that the present operating coal liquefaction pilot plants were the only realistic test beds.

A trip was made, in late April, to the SRC pilot plant at Wilsonville, Alabama. This facility, although certainly providing the necessary "fluid" properties, supplies only enough continuous throughput to accommodate very small valve sizes. Failure and wear information from testing of very small valves may not be strictly extendable to larger valves.

In reply to a questionnaire sent to Pittsburgh Energy Technology Center, operators of two Synthoil P.D.U.'s (400 lb/day and 1000 lb/day), the following information was received:

"...observed erosion appears to be directly proportional to the pressure drop (wear at 4000 psig is twice that at 2000 psig), and when the solids content is doubled, the erosion rate increases by a factor of three (3). Higher erosion rates than above are expected in SRC II operations because of the higher solids concentration at the letdown valve. In a run just completed on the 1000 lb/day plant at 2000 psig in the SRC II mode where solids content ran between 20 and 25%, higher wear rates of letdown valves were observed."

Final conclusions and recommendations, based on trips and other gathered information, were made for valves (P. K. Carlson), pumps and oxygen compressors (L. F. Parsly), and metering devices (J. M. Holmes). The recommendations include proposed schedules and funding levels for projects currently under way or suggested for the future.

6. ENGINEERING STUDIES AND TECHNICAL SUPPORT

R. W. Glass

Engineering studies and technical support are provided primarily for the DOE/FE Division of Fossil Fuel Processing. The effort includes: the development of analytical tools for use in the evaluation of processes and equipment; the technical and economic evaluation and comparison of coal conversion processes and subprocesses on a uniform basis; surveys of the need for coal conversion equipment and the capability of industry to provide such equipment; and studies of the magnitude and control of coal conversion plant emissions.

6.1 Process Modeling

R. Salmon, D. M. Lister, O. L. Culberson,
D. G. Ball, and K. W. Childs

6.1.1 Contract Objective

The objective is to assist DOE/FE in its plan for computer analysis and computer support for coal conversion studies. This includes assistance to Purdue and Lehigh Universities in the development of computer programs for this plan. Physical property data are being collected and computerized primarily by Purdue and will be used in support of programs prepared by both universities. Purdue's general design program will aim at material and energy balances, equipment size and costing, plant capacity, and general economics. Lehigh's dynamic simulation programs will address plant design primarily from the standpoint of process performance during transient operations, but can also be used for steady-state conditions. A single flowsheet will be selected to assess the operability and complementary utility of both design programs.

6.1.2 Status Summary

Quarterly Project Meeting: The regular quarterly project meeting was held May 23, 1979, at Morgantown Energy Technology Center and was attended by representatives of Purdue, Lehigh, METC, DARCOM, and ORNL. Status reports and future plans were discussed.

Purdue Physical Properties Package (PPROPS): James Mercer of METC reported that they have successfully run a number of problems using the version of PPROPS supplied by ORNL. However, the examples have not yet covered the areas in the program where ORNL has experienced difficulties.

At ORNL, efforts are continuing to run additional PPROPS examples based on a simple process flowsheet devised by ORNL. Comparisons are being made with results from the Phillips PDA program. Thus far, the PPROPS results have not been satisfactory. The subroutine LOADP has been rewritten and is being used. A summary of this work was prepared

in an effort to resolve these difficulties with Purdue and was delivered to Purdue at the project meeting.

Purdue reported that they will have a revised version of PPROPS and its documentation ready for delivery to ORNL by September.

Receipt of Additional Codes from Purdue and Lehigh: At the quarterly meeting, Lehigh distributed tapes containing their methanator model. No further codes or documentation were received during the month.

Both Purdue and Lehigh reported that their complete code packages and documentation would be delivered in September.

6.2 Coal Liquefaction Advanced Research Digest

F. M. O'Hara, Jr. and R. W. Glass

6.2.1 Contract Objective

The objective is to provide continuing technical assistance to DOE/FE by preparing digest reviews of current or potential subjects relating to coal conversion technology.

6.2.2 Status Summary

Working outlines of the papers "Mechanisms of Coal Liquefaction" and "Coal Depolymerization" were prepared, circulated for comment, reorganized, and approved. The writing of the rough drafts of these articles began and is now in progress.

6.3 Survey of Industrial Coal Conversion Equipment Capabilities

W. R. Williams, D. W. Hatcher, and J. R. Horton

6.3.1 Contract Objective

The objective of this project is to conduct surveys of industrial equipment capabilities that will identify the present capability of industry to supply the equipment needed. The project will also determine research and development needs, including lead time requirements, for producing equipment of advanced design for the various unit operations of critical importance to the Division of Fossil Fuel Processing.

6.3.2 Status Summary

(This section not received on time)

6.4 Environmental Controls for Low-Btu Gasification

S. P. N. Singh, M. S. Edwards, J. F. Fisher,
G. R. Peterson, and R. Salmon

6.4.1 Contract Objective

The objective of this project is to evaluate the various environmental control processes that might be used in connection with low-Btu gasification facilities and to determine the economic tradeoffs for various processes and levels of control.

The project is divided into two phases: Phase I consists of Tasks 1 through 5 of the work statement and covers the preparation of a detailed work plan and the selection of gasification and environmental control processes for use in the study. Phase II consists of Tasks 6 through 8 in the work statement and covers the collection and analysis of technical and economic data on the various environmental control processes and the preparation and analysis of flowsheets showing overall systems of environmental control processes used with various gasifiers.

6.4.2 Status Summary

DOE/Fossil Energy approval on the two draft reports titled Costs of Environmental Control Processes for Low-Btu Coal Gasification Plants (ORNL-5425) and Evaluation of Eight Environmental Control Systems for Low-Btu Coal Gasification Plants (ORNL-5481) has been received.

Copies of these reports have been distributed for proponent review. In-house editing will take place concurrently and issuance of the final reports is expected in July.

6.5 SRC R&D Assessment

M. S. Edwards, B. R. Rodgers, C. H. Brown, P. K. Carlson,
W. R. Gambill, T. M. Gilliam, J. M. Holmes,
R. P. Krishnan, and L. F. Parsly

6.5.1 Contract Objective

This project is an intensive, short-term assessment of current research and development activities of importance to the SRC Demonstration Project. The assessment includes acquisition and review of published information, discussions with R&D personnel involved in relevant activities, visits to sites of important R&D activities, monitoring of critical R&D operations, accessing, to the extent possible, the proprietary information of importance to the Project, and cross-matching R&D activities to the technical data needs of the industrial partners in the Demonstration Project. Based on the assessment of R&D activities against the data needs of the SRC Demonstration Project, recommendations will be

formulated, including: priority of activities; adequacy of the R&D program; the need for possible acceleration, extension, or redirection of current activities; and possible new activities required beyond the current program.

6.5.2 Status Summary

Contacts with institutions active in coal liquefaction R&D have been essentially completed. Preparation of the draft Interim Phase Report (ORNL/TM-6952) is currently under way. Because of scheduling delays in visiting the Gulf Harmarville SRC-II PDU, Ft. Lewis SRC pilot plant, and the Texaco Gasifier pilot plant, final recommendations for programs which should involve these institutions will not be contained in this initial draft of the Interim Report. Such recommendations will, however, be incorporated in the completed draft report which is expected to be issued in mid-June for comments.

Institutions contacted in May are listed below:

<u>Discussion Area</u>	<u>Institutions</u>
Separations, physical properties	Wilsonville SRC PDU
Vapor-liquid separations	Oklahoma State University
Solid-liquid separations	Kerr-McGee
Thermal properties	Bartlesville Energy Technology Center
Solid-liquid separations	Pittsburgh ETC
Vapor-liquid separations	Purdue University

A visit to the Harmarville SRC-II PDU is scheduled for June 1, 1979, and a Ft. Lewis SRC pilot plant visit is planned for June 6, 1979. Arrangements for obtaining information or a site visit to the Texaco Gasifier pilot plant are being pursued by DOE/ORO.

7. PROCESS AND PROGRAM ANALYSIS

R. W. Glass

Process and program analysis studies are being conducted for the DOE Fossil Energy Engineering Economics and Standards Section of the Planning and Systems Engineering Division. This effort includes research studies on most of the coal conversion and utilization processes. The program objective is to provide on a consistent basis, technical and economic evaluations of competing processes and systems for coal conversion and utilization.

7.1 In Situ Coal Gasification

M. S. Edwards and W. C. Ulrich

7.1.1 Contract Objective

The objective of this program is to provide technical and economic evaluations of candidate processes for the conversion of coal in situ to fluid products presently of interest. During FY 1977, technical and economic evaluations of the linked vertical well process applied to sub-bituminous coal were addressed. Three alternative end product configurations were considered - electricity, SNG, and syngas. In FY 1978, an evaluation was conducted of an in situ facility for producing gasoline from methanol via the Mobil-M process.

7.1.2 Status Summary

The final 1977 report, Process Designs and Economic Evaluations for the Linked Vertical Well In Situ Coal Gasification Process (ORNL-5341), and the final 1978 report, Evaluation of an In Situ Coal Gasification Facility for Producing M-Gasoline via Methanol (ORNL-5439), are in the final stages of editing and it is expected that both reports will be sent to Technical Publications in June for final issue.

7.2 HYGAS Modeling

J. P. Meyer, G. C. Frazier, J. W. Wells, and J. P. Belk

7.2.1 Contract Objective

The objective of this project is to develop a computer model of the HYGAS gasifier.

7.2.2 Status Summary

A copy of the HYGAS draft final report Mathematical Model of the HYGAS Pilot Plant Reactor (ORNL-5475) has already been forwarded to DOE for review and comment, but material to be included in the Appendix was not included. That material has been transmitted to DOE and final revision and publication is expected during the next quarter.

7.3 Liquefaction

R. W. Glass

7.3.1 Contract Objective

The objective of this project is to provide technical and economic evaluation of coal conversion liquefaction processes. Ralph M. Parsons Company is working under subcontract on the project with J. B. O'Hara as Project Manager. Major tasks included in the subcontract are: (1) a Survey of Liquefaction Processes and (2) a Detailed Review of High Potential Liquefaction Processes.

7.3.2 Status Summary

The revised final draft report for this project, Liquefaction Technology Assessment (ORNL/Sub-7186-20), has been reviewed by both DOE and ORNL and comments have been forwarded to Parsons for inclusion in the final report. Issue is expected in June.

7.4 High Btu Gas

R. W. Glass

7.4.1 Contract Objective

This subprogram is being analyzed under subcontract by the Scientific Design Company, Incorporated (SD) with A. S. West as Project Manager. The present work is divided into three phases as follows:

1. The objective of Phase I is to provide technical and economic evaluations of competing processes, concepts, and systems for the production of high Btu gas from coal.
2. The objective of Phase II is to monitor and analyze data from the HYGAS Pilot Plant.
3. The objective of Phase III is to perform a technical and economic evaluation of the Battelle Agglomerating Ash Burner Process for the production of medium Btu fuel gas, synthesis gas, and hydrogen from coal.

7.4.2 Status Summary

As mentioned in previous progress reports, Phase I activities in this project have resulted in the issue of a final report, Battelle Agglomerating Ash Burner Process for High-Btu Gas Applications, ORNL/Sub-7240/1. Further evaluation of the Battelle process for medium-Btu gas applications (Phase III) has been completed and minor changes in the draft final report by ORNL technical staff are being prepared for transmittal to SD. Issue of the report is expected in early July.

At IGT's HYGAS pilot plant, Test Run No. 79 has been completed. Prior to test initiation, an inventory of pretreated char (400 tons) was to be prepared and repairs to certain parts of the process facility were to be effected. Provision for magnetic separation of the coal feed was to be added, as well.

Accumulation of char (which began in early April) proceeded much more slowly than planned as a result of problems in the coal milling section and its feed equipment. These difficulties have led IGT to propose that further ROM tests be postponed.

SD engineers report that coal feed to the system for Test No. 79 began at 0600 on April 30 and the gasifier became "self-sustaining" at 2145. Phase I conditions included operation at 1.2 ft/s superficial velocity at a maximum SOG temperature of 1800°F. When the 400-ton char storage silos became depleted, the test was terminated (0500 hours, May 9). Phase II conditions were not attempted.

Reactor inspection after shutdown revealed a small amount of clinker on the steam-oxygen sparger coupling and some blown-out plugs in the pretreater gas distributor. A debriefing meeting for Test Run No. 79 was tentatively scheduled for May 30.

Present plans call for char accumulation for Test No. 80 to begin on June 1, with gasifier start-up around June 15. The test will utilize 1100 tons of ROM Illinois No. 6 coal.

7.5 Direct Combustion

E. C. Fox and T. D. Anderson

7.5.1 Contract objectives

The purpose of this study program is to assist DOE/FE in their effort to develop a national strategy to increase the near-term use of coal through direct combustion; the applications of interest in this study are the small-to-moderate industrial user and the large residential/commercial user. The following objectives will be accomplished.

1. Identify and quantify the important factors restricting the use of coal in the sectors of interest.
2. Evaluate potential technological and institutional solutions to the problems identified in (1) above.
3. Make recommendations to DOE/FE relative to the most promising approaches to increasing the near-term use of coal.

7.5.2 Status summary

The report entitled "Conversion to Coal in the Industrial Sector," ORNL/TM-6131, is being prepared for publication.

7.6 Advanced Power Conversion Systems

J. E. Jones Jr. and A. P. Fraas^a

7.6.1 Contract objective

The objectives of this project are to review selected major advanced power conversion systems and to assess these systems with respect to their basic R&D status.

7.6.2 Status summary

A total of eleven systems or components of systems were evaluated. Draft reports covering all of these topics, an overall summary report, and an executive summary report have been completed and are undergoing final review.

^aConsultant

7.7 Fuel-Grade Methanol Synthesis Technology Assessment

R. Salmon, M. S. Edwards, and R. M. Wham

7.7.1 Contract Objective

The objective of this work is to review and assess the present state-of-the-art of indirect liquid fuels synthesis, with particular emphasis placed upon those processes which produce methanol suitable for use as fuel as the primary or principal product.

7.7.2 Status Summary

A finished draft version of the final report of the project was completed. This draft is now undergoing internal review before being transmitted to DOE.

7.8 Liquefaction Technology Assessment Study (LTAS)

R. C. Forrester III, R. Salmon, M. S. Edwards,
A. R. Irvine, S. P. N. Singh, J. F. Fisher,
J. P. Meyer, and R. M. Wham

7.8.1 Contract Objective

The objective of this study is to provide a comparative assessment of the technical feasibility, economic competitiveness, and environmental acceptability of selected coal liquefaction processes representing different process classes on a uniform, consistent, and impartial basis.

This assessment encompasses four phases of work, identified as Phase 0, Phase I, Phase II, and Phase III. Each phase includes development of process designs, capital and operating cost estimates, process economic analysis, sensitivity studies, and assessment of technical feasibility and risk on as consistent a basis as possible. Existing process designs and cost estimates will be used whenever possible, with modification as necessary.

7.8.2 Status Summary

Phase 0 activities were described in some detail in the last report in this series, including a listing of process designs being considered, the general basis for design, and the scheduled completion date for the draft final report. Process designs for all processes (with the exception of methanol synthesis followed by conversion to gasoline via Mobil-M, which will not now be included in the process list) have been prepared, and both capital and operating costs are now being developed. Financial analyses will be performed in the early part of June.

Phase I activities will require substantial subcontractor involvement and an RFP has been issued which defines the scope of this work. Response is expected in late June and initiation of that part of the project is expected to take place early in July.

8. FOSSIL ENERGY ENVIRONMENTAL PROJECT

C. R. Boston

The Fossil Energy Environmental Project provides DOE with program assistance in the performance of environmental assessment functions related to the expansion of fossil energy conversion technologies, performs assigned technical assistance tasks, and conducts programmatic environmental investigations that are critical to the early realization of advanced fossil energy technologies.

8.1 Stored Solids Study

W. J. Boegly, Jr., and H. W. Wilson, Jr.

A shipment of Grace/Ebasco/Texaco (G/E/T) process solid waste was received at ORNL. The shipment consisted of four runs made in February, 1979, with two Kentucky #9 coals from the Zeigler #9 and Colonial #9 mines. Each coal was gasified at two carbon conversion levels and the slag was separated after quenching into coarse and fine fractions. The previous sample of G/E/T slag was produced from coal from the Providence #1 mine. Conversations with Grace on May 29 confirmed that this earlier shipment represents slag that will be most representative of waste produced by the demo plant.

On May 15, 16, and 17 a trip was made to the Grace/Ebasco/Texaco demonstration plant site for the purpose of collecting representative soil samples from the slag disposal area. The samples are being characterized and used in soil-waste interaction studies.

Plans are now being finalized for soil sampling trips to the SRC-II, MLGW and CONOCO demo plant sites.

All available batch and column leaching data for British Gas/Lurgi and Cogas solid wastes were transmitted to Hershel Jones, DOE Washington, for further transmittal to the respective developers.

8.2 Coal Conversion Demonstration Projects

8.2.1 Liquefaction projects - S. G. DeCicco

SRC-I and SRC-II - In terms of environmental assessment activity, both SRC projects are at the same point. For both the SRC projects the month was spent: (1) developing an overall environmental plan for DOE-ORO specifying all environmental steps required to fulfill the NEPA (EIS) requirements, and to fulfill environmental permitting and licensing requirements; (2) developing detailed site- and process-specific EIS outlines, including the site and process alternatives; (3) collecting information

for the EIS analyses such as site selection studies for each project; (4) preparing Notices of Intent to prepare an EIS for each project for publication by DOE-HQ in the Federal Register; (5) preparing for the Public Scoping Meetings to be held shortly for the purpose of soliciting the public's environmental concerns; (6) coordinating the roles that Battelle-PNL, Dames & Moore, Stearns-Roger, Gulf Mineral Resources, and Southern Company Services will play in preparing the EIS in cooperation with ORNL; and (5) preparing the environmental and health aspects of ORNL's SRC Market Penetration Study.

8.2.2 Gasification projects - A. J. Witten

MLGW - A planning session was held in Memphis on May 23 in preparation for the scoping meeting. Subsequently, a dry run was held in Memphis on May 30. The scoping meeting will be held at Christian Brothers College in Memphis on June 6.

Grace - The Grace scoping meeting was held on May 16 in Henderson, Kentucky.

ICGG - The NOI and IP were prepared for DOE.

CONOCO - The NOI and IP were prepared for DOE. The site soils sampling is unresolved due to the extensive disruption expected during site preparation. It appears that samples obtained now would not be representative of the graded site.

8.2.3 Processing of coal conversion wastes for disposal and resource recovery - R. M. Canon, G. Jones, Jr., and J. S. Watson

Initial investigations of aluminum recovery and trace metal removal from a number of advanced coal conversion residues are summarized below. (Results from the first two materials have been reported earlier.) Direct leach tests were performed with sulfuric acid of various concentrations. The residues were leached at 105°C for 16 hours. Three of the residues were also subjected to the Calsinter process which consists of a high temperature sinter of the residue with calcium sulfate and calcium carbonate followed by leaching with dilute sulfuric acid to recover the metal values. Residue 1 is the ash from combustion (at 900°C) of char material from ORNL's hydrocarbonizer facility. The studies to date indicate that Calsinter can be applied generally to most residues while the utility of simpler direct leach depends strongly on the residue to be treated.

<u>Residue</u>	<u>Aluminum recovery (%)</u>	
	<u>Direct acid leach</u>	<u>Calsinter</u>
1	95	88
2	2	94
3	96	--
4	77	85

Investigations of the fate of trace metals in residue processing have produced initial results. Behavior of trace metals from Residue 2 in the Calsinter process is summarized below. For several metals the material balance was poor, and these results should be viewed as only preliminary. One should refrain from drawing conclusions from these data until further studies are completed.

<u>Metal</u>	<u>% in solid</u>	<u>% in liquid</u>
Pb	88	12
Cr	50	50
Sr	90	10
Zn	33	67
Ag	79	21
As	1	99
Cu	46	54
Mo	2	98

Development of the XRF method of analysis is continuing. This method is expected to provide the capability to run an increased number of samples and gain statistical significance. Obtaining numerous accurate analyses of trace metals in coals and coal residue has been a difficult problem for all investigators in this field. We have made progress in this area, but unsatisfactory material balances and apparent errors are still too common to be satisfactory.

8.3 Gasification Test Facility (GTF)

S. G. DeCicco

Following several weeks of discussions with geographers in the Regional and Urban Studies Section a proposal for an ORNL site selection study for the GTF project was sent in draft form to DOE on May 25, 1979. The draft work statement proposes a list of site selection criteria and a preliminary methodology for locating ten prime sites for the facility. The funds for this work will be available due to the long slip in the GTF project's environmental program. If the work is undertaken, ORNL will present its findings by mid-August.

8.4 Atmospheric Fluidized Bed Combustion (AFBC)

S. G. DeCicco

8.4.1 Technology assessment

The objectives of this task are: (1) to assess the AFBC technology and determine the existing data base as applicable to the proposed 200 MWe AFBC demonstration plant; (2) to identify the most critical problem areas and R&D needs for the plant; (3) to recommend priorities and schedule for the required R&D activities based on the needs identified during the assessment. The final draft report of the AFBC demo plant technology assessment has been sent to more than 20 organizations for review and comments. Generally, the response was very positive.

Comments have been received either verbally or in writing from Oregon State University, Battelle Columbus Labs, Babcock & Wilcox, DOE (Steve Freedman), and TVA (Henry Withers). The most significant comment was that the report should go ahead and recommend which steps to be taken (and at which facilities) for solving the various problem areas mentioned. Although this is considered outside the scope of the report, an effort is being made this month to respond to this request in a limited way.

9. MAGNETIC PREPARATION OF DRY CRUSHED COAL

E. C. Hise and A. S. Holman

9.1 Objective

The objective of this program is to develop, demonstrate, and bring to commercial viability processes and equipment for the removal of pyrite and ash-forming minerals from dry crushed coal by either or both high-gradient magnetic separation and open-gradient magnetic separation.

9.2 Status Summary

The mathematical modeling of the free-fall open-gradient separator revealed the unanticipated information that if the magnet is operated in the vertical position, the more strongly paramagnetic particles actually cross the line of highest field strength and then oscillate across that line the rest of the way down the length of the magnetized cavity. Their line of departure from the cavity is, therefore, random and so the separations performed in this configuration contained some random distributions. The trajectory of these particles is about $2\frac{1}{2}$ degrees upgradient from vertical, so if the magnet is tilted at that angle these particles will track down roughly parallel to the maximum field line without crossing or oscillating. It then becomes necessary to remove the back plate from the pole pieces to permit the strongly diamagnetic particles to exit the pole piece gap down gradient before they reach the bottom.

The initial tests performed in this modified configuration gave the most selective separations that we have achieved by any of the physical separation methods. Figure 9.1 plots the percent of magnetics, the percent of product sulfur, and the percent of product ash vs the splitter location. A "+" location of the splitter signifies it is displaced upgradient from the line of vertical free-fall. Note that over the range of displacements tested the percent of magnetics and the percent of product ash varied as expected; however, the percent of product sulfur quite unexpectedly remained constant. This probably indicates that all of the liberated pyrite was deflected further upgradient than the most positive splitter location tested. Figure 9.2 plots these data as large squares along with the previously reported results from other separations. Note that the pyrite removal is essentially constant to 97% BTU recovery. These data emphasize again the strong incentive to seek an open-gradient configuration suited to processing in large quantities.

A technical film - 20 minutes, color, sound, 16-mm - on magnetic coal preparation has been completed. The film discusses the need for coal preparation, demonstrates laboratory-scale separations by specific gravity and three magnetic methods, shows possible production scale equipment for one magnetic method, and discusses the degree of cleaning achieved by the several methods. A loan print is available.

Figure 9.1. Percents of magnetics, product sulfur, and product ash vs the splitter location.

ORNL-DWG 79-5306R2 ETD

Figure 9.2. Recent free-fall open-gradient separations plotted as large solid squares on the previously reported graph of separations.

An ORNL/TM report entitled "Correlation of Physical Coal Separation Methods" has been completed, has received internal and external review, and is now being prepared for publication. An ORNL/FE report entitled "Separation of Dry Crushed Coals by High-Gradient Magnetic Separation" has been completed and is now receiving internal and external review.

The superconducting solenoid magnet for high-gradient and open-gradient laboratory experiments has been received. Installation is awaiting the preparation of expanded laboratory space in Building 9201-3. This space will include a small laboratory for chemical analyses and semi-precision work, a laboratory for the superconducting magnet, a laboratory for the other magnetic and gravimetric separations, and shared space for crushing and classifying equipment.

A visit, arranged by Mr. W. A. Thomas of TVA Chattanooga, was made to the Derrick Manufacturing Company, Buffalo, New York, to perform coal screening tests. The Derrick screens differ from conventional screens in several respects and are reported to have higher efficiencies and production rates. In order to continue with the engineering/economic analysis of the magnetic process portion of a coal preparation plant, it is necessary to specify the process flowsheet equipment for classifying the coal at 28 mesh. An earlier proposal by an A-E appeared to be unnecessarily complex and expensive. A 200-lb sample of 3/8" x 0 coal from the Paradise plant was tested at 28 mesh and at several levels of moisture content for screening efficiency and production rate. It appeared that good efficiency and production could be maintained up to about 6% surface moisture. More precise moisture contents, efficiencies, and production rates will be supplied in a final report. Mr. Derrick suggested that when the 3/8 x 0 feed is too wet to screen it can be adequately dried by blending in an appropriate amount of 1 1/2" coal crushed to minus 3/8". We propose to test this concept.

10. ATMOSPHERIC FLUIDIZED BED COAL COMBUSTOR FOR COGENERATION (AFBCCC)

R. S. Holcomb

10.1 Objective

The Coal Combustor for Cogeneration (CCC) Program is directed at the development of a fluidized bed coal combustion system heating air inside tubes to provide high temperature clean air to drive a gas turbine to generate electricity. The heat in the air leaving the turbine exhaust would be recovered to supply industrial process heat. The gas turbine is very well suited for cogeneration since the ratio of thermal to electrical energy is about 3 to 1 for the gas turbine cycle as compared to a ratio of about 5 to 1 for a back-pressure steam turbine, and the exhaust heat from the gas turbine is available at a higher temperature. The scope of the program includes the study of industrial cogeneration plants in the size range from 5 to 50 MW(e) and the construction and testing of a 0.3 MW(e) technology test unit.

10.2 Status Summary

The CCC Program proposals were received from the vendors on May 31. A very good number of proposals were received, and they represent most of the leading gas turbine and fossil-fired furnace manufacturers.

The evaluation will begin immediately and proceed as rapidly as possible. A period of 8-10 weeks may be required to complete the evaluation.

11. TENNESSEE VALLEY AUTHORITY (TVA) FLUIDIZED BED
COMBUSTION (FBC) DEMONSTRATION PLANT PROGRAM
TECHNICAL SUPPORT

J. E. Jones Jr.

Tennessee Valley Authority has assumed a lead role in the demonstration of FBC technology for application in large utility boilers. ORNL will provide technical support and services to TVA in FBC systems. This work is to support TVA Energy Research's objective to develop FBC systems for utility electric power generation which will burn high-sulfur coal and meet environmental emission standards.

TVA will be the lead agency in this work and will reimburse DOE for the work to be performed by ORNL. This work is to be conducted by ORNL under the terms and conditions of the Interagency Agreement between TVA, DOE, and ORNL regarding support for FBC research (reference: Agreement TV48296A, Subagreement 5).

11.1 AFBC Technology Support - Task 2

M. Siman-Tov and J. E. Jones Jr.

11.1.1 Contract objective

The objective of this program is to provide technical support of a general nature in FBC systems and respond to specific requests from TVA personnel. Such requests may include reviews, assessments, participation in TVA tasks, and similar activities.

11.1.2 Status summary

During this period, preliminary efforts to develop a coal feeding program were initiated. The first phase of this program will include fundamental coal feeding studies.

A materials test program for AFBC boiler materials is also being developed.

Preliminary efforts are under way to scope a cooperative DOE/TVA program for design and cost estimate of the Supercharged Fluidized Bed Combustor concept.

11.2 4 × 4 Cold Flow Model — Task 3

R. S. Holcomb and M. E. Lackey

11.2.1 Contract objective

The objective of this task is to experimentally investigate slumping of a portion of a fluidized bed using a sub-scale cold flow model. The scope of work includes design and minor modification of the 4 × 4 cold flow model for slumping and refluidization tests and conducting bed slumping tests.

11.2.2 Status summary

Design and modifications - The fluidizing-air plenum will be re-designed so that the air can be shut off to a portion of the 4 × 4 bed with the air flow continuing to the other portion. A new simulated tube bundle will be designed for the slumping tests. The design will be based on a 1/4 scale factor — i.e., the tube diameter, bed depth, and fluidizing velocity will be 1/4 that of the full-scale FBC boiler. The cold flow model has been modified to incorporate the design changes.

Testing - Tests will be conducted to investigate the effects of slumping a portion of the bed and continuing operation of the remainder. Observations will be made to study mixing between the active and slumped portions, fluidizing air bypass through the slumped section, elutriation from the fluidized section and deposit in the slumped section, and maximum buildup of the slumped bed. The fluidizing air will then be turned on to the slumped portion, and the action of the two sections will be studied during refluidization. These tests will be done over a range of fluidizing velocities from 1 to 2 ft/sec and bed depths from 1 to 1.5 ft to represent scale studies of values four times as large. Other operating data will be obtained incidental to these tests.

Progress to date - The original tube bundle was removed and the new one installed. Improvements were made in the existing pressure taps by adding metered purge air flow, and some new pressure taps were added.

The system is now ready to begin bed slumping tests. Pressure drop measurements will first be taken across the distributor plate with the bed empty, and then the bed will be filled with limestone for the bed slumping tests.

11.3 AFBC Modeling and Simulation - Task 4

M. Siman-Tov and J. W. Wells

11.3.1 Contract objective

The objectives of this program are to develop a simple steady-state model for conceptual design of the main cell and carbon burn-up cell and to incorporate in this model the ability to predict trends in bed performance under various feed and operating parameters.

11.3.2 Status summary

During this month, development of a new method for calculating bubble growth continued. A document summarizing this effort and comparing it to available data is being prepared. Also during the month, a reply was received from MIT on a convergence problem which was found in subroutine COMB of their code. MIT has eliminated this problem by "fudging" a constant. This was not the approach used in ORNL combustion routine. During an upcoming trip to MIT, this and other points will be discussed. MIT did not send the output from their code, but has sent to us a draft copy of Vol. 1 of the final report. This draft includes their complete system model for AFBC simulation

Work has begun on TVA/B&W's configuration simulation using Wen's model which is already operational on the ORNL computer system. Elements of the Wen model will be incorporated in the ORNL model combining the most advantageous features of each.

11.4 AFBC Bench Scale Model - Task 5

R. S. Holcomb, R. H. Guymon, and G. P. Zimmerman

11.4.1 Contract objective

The objective of this task is to experimentally investigate heat transfer, sulfur capture, carbon loss, and combustion of recycle carbon using the ORNL AFBC bench scale combustor.

11.4.2 Status summary

Test facility description - The combustor is 10-in. ID and about 15-ft tall. The combustor is designed for burning 10 to 30 lb/hr of coal and is equipped for limestone addition. The system is designed to operate with a bed fluidizing velocity in the range of 4 to 10 ft/sec and bed temperatures up to 1600°F. The bed is cooled by compressed air flowing through 0.5-in.-OD tubes immersed in the bed.

Test program - Heat transfer tests will be done for 1000 and 1900 μm mean size limestone over the fluidizing velocity range of 4 to 10 ft/sec at bed temperatures of 1400–1600°F. Sulfur capture and carbon loss tests will be run for selected coals and limestones of interest to TVA for several values of Ca/S over a fluidizing velocity and temperature range similar to that for heat transfer. Tests to investigate the combustion of recycle char removed by the cyclone separator will be run for various operating conditions.

Progress this period - The bed was filled with 12 x 30 mesh limestone and combustion testing was resumed on May 8. The bed was run with an expanded depth of about 22 in. and run with no addition of fresh limestone to establish a bed that would be sulfated to near the saturation point. A flue gas sample stream was taken off at near the top of the freeboard and passed through a continuous SO_2 analyzer. The SO_2 level increased for about 20 hr and then held fairly constant, indicating that the bed was sulfated to saturation.

The limestone feeder was installed, and operation with continuous limestone addition was begun on May 16. Conditions were held fairly constant at 1530–1550°F, a fluidizing velocity of about 6 ft/sec, excess air level of 20%, and an expanded bed depth of 28–30 in. A total running time of about 18 hr was accumulated at these conditions. The testing was interrupted at one point by the failure of four electric heater rods in the air preheater. The new air preheater that was on hand was installed in series with the original preheater, and this provided adequate power for heating the air.

Various problems were encountered with the SO_2 measurements such as interference from water vapor at the first wavelength selected for use and with reproducible calibration of the analyzer with standard gas samples. These problems prevented the acquisition of any reliable SO_2 readings as of the end of the month, but corrections have been made to all of them, and it appears that it will be possible to begin to obtain SO_2 emission data within the next few days.

11.5 Assessment of the State-of-the-Art of PFBC Systems - Task 6

R. L. Graves, M. E. Lackey, and A. P. Fraas^a

11.5.1 Contract objective

The purpose of this program is to provide TVA with an assessment and overview of the state-of-the-art for PFBC systems and their associated components.

11.5.2 Status summary

Further progress has been made on the parametric study in which the effect of the furnace pressure and gas turbine inlet temperature on power plant performance is being investigated. If the gas turbine inlet temperature is limited to 538°C (1000°F), the plant efficiency has been found to be practically independent of pressure with an efficiency advantage of 1.0 to 1.5 points better than an AFBC system. Definite optimum pressure ratios appear for higher allowable temperatures. For example, at 650°C (1200°F), the optimum pressure is between 7-10 atm, and the improvement in thermal efficiency is over half of the difference between the AFBC and a PFBC utilizing a 900°C (1650°F) gas turbine. Such trends are typical of cycle configurations as proposed by G.E. and AEP and not for the air-cooled PFBC being developed by Curtiss-Wright.

11.6 Analytical Support and Alternate Design Concepts Evaluation - Task 7

E. C. Fox and C. S. Daw

11.6.1 Contract objective

The objectives of this task are to assist TVA in determining the design parameters which are critical to an effective AFBC system from the standpoints of efficiency and cost and to provide direction as to better design options.

11.6.2 Status summary

A general mass and energy balance computer program is being modified to conduct the parametric AFBC cost analysis. Preliminary cost equations are being formulated to limit the cost parameters to be investigated. Initially, 13 parameters are being screened to determine which are the key variables. These will be reduced to a manageable amount for the final analysis.

^aConsultant

11.7 AFBC Technical Source Book and R&D Evaluation - Task 8

M. Siman-Tov and A. A. Khan

11.7.1 Contract objective

The objectives of this program are: 1) to develop a single comprehensive source book of technical data for design procedures and evaluation of AFBC facilities and programs, 2) to review and evaluate existing and proposed AFBC facilities to perform research and development for TVA, and 3) to interpret and translate results of test studies performed for TVA and further the knowledge in AFBC research and development activities.

11.7.2 Status summary

A consolidation of information on design parameters for fluidization velocity distributor trays, bed hydrodynamics, standpipe design, and elutriation was made. A summary of the topics was presented to the Fossil Energy Program management.

A review of Wen and MIT's model was made. Both models need much testing and development before they can be used as a design basis for AFBCs. Babcock and Wilcox empirical correlation for combustion and desulfurization is probably the best approach applicable for design purposes. Unfortunately, it does not allow for bubble sizes and bed hydrodynamics and thus is limited for designing systems with similar flow characteristics.

Next month, information on combustion, desulfurization, and NOx production kinetics in AFBCs will be summarized. Also, mass and energy balances for a simple AFBC module will be written up.

11.8 Materials Support for TVA Pilot and Demonstration AFBC Plants - Task 9

T. G. Godfrey, J. H. DeVan, and R. A. Bradley

11.8.1 Contract objective

ORNL proposes to assist TVA technically in the materials area. The unique part of an AFBC is the fluidized bed combustor and its associated hardware, since the balance of the plant closely resembles a conventional pulverized-coal supply system. The principal areas of concern are the in-bed heat-exchanger tubes and hangers, the air distributor, side walls, coal feed lines and nozzles, spent-bed removal hardware, and cyclones for separating elutriated material.

11.8.2 Status summary

Metallographic examination of the boiler tube materials from the first 100-h test at CURL (Leatherhead, England) has commenced. Thus far, we have observed no significant corrosion on these samples. In general, these British alloys appear to contain moderately high levels of manganese and sulfur as indicated by MnS inclusions throughout the structures. This makes the detection of surface-related sulfides somewhat more difficult.

11.9 Dynamic Modeling of the TVA Fluidized Bed Combustion Demo Plant - Task 10

O. L. Smith

11.9.1 Contract objective

The objective of this task is to provide dynamic modeling and transient systems analysis directly applicable to the TVA pilot plant. As an important benefit, the information obtainable from a dynamic model would help in the specification of such features as function, range, and type of instrumentation required to provide the desired plant operating characteristics.

11.9.2 Status summary

Previous monthly reports described the design of the preliminary dynamic model of the TVA fluid-bed pilot plant. Some applications of the model are reported here. A typical model run includes the sequential calculation of 1) the plant initial conditions; 2) the transient response during an interval of time following a specified disturbance; 3) the sensitivity of each of the system variables to the disturbance (% change in variable per % disturbance); and 4) the final equilibrium conditions. Output from a simulation consists of printed values of 100 system state variables at selected times during the transient plus optional plotting of any of the variables.

A series of runs was made to investigate the natural open-loop (no control system) behavior of the fluid-bed boiler. Twelve parameters were individually reduced by 1%, and the system responses were determined. The varied parameters are among those which may be collectively manipulated to control the boiler. Varying them individually provides insight into their separate functions as well as the ways in which they may tend to support or interfere with each other when coupled in a control system. While one must beware of placing too much weight on preliminary results, a number of interesting observations can be made about the natural dynamic behavior of the fluid-bed system as presently modeled.

Table 11.1 lists initial values of the parameters and some of the important state variables. Table 11.2 lists the changes in these variables that result from each of the parameter variations. Entries in Table 11.2 occur in pairs; the upper number of each pair is in the units indicated at the head of the column, and the lower number is percent change. For example, a 1% reduction in coal feed rate produces an increase in evaporator power generation of 0.019 MW (upper number of pair) or 0.22% (lower number). The percent change is referenced to evaporator power, not to total power. All computations in the model were performed in double precision (approximately 15 significant figures). For ease of presentation in Table 11.2, the numbers were rounded to two significant figures. Again for convenience, parameter variations of 1% were made. A variation of, say, 5% would produce changes in the variables

Table 11.1. Initial values of parameters and state variables.

<u>Parameter</u>	<u>Initial value</u>
Coal feed	1.28 lb/s
Air inlet damper	90% open
FD fan pressure	45.0 Inwg
Flue gas damper	90% open
ID fan pressure	-14.7 Inwg
Feedpump pressure	2982 psig
Attemperator valve	50% open
Throttle valve	90% open
Evaporator surface	720 ft ²
Primary superheater surface	4400 ft ²
Secondary superheater surface	1900 ft ²
Condenser air flow	145 lb/s

<u>State variable</u>	
Evaporator power	8.66 MW
Primary superheater power	3.04 MW
Secondary superheater power	2.88 MW
Condenser load (total power)	14.7 MW
Stack loss	1.06 MW
Bed temperature	1550°F
Primary superheater metal temperature	926°F
Secondary superheater metal temperature	1318°F
Drum temperature	688°F
Drum pressure	2829 psig
Throttle steam temperature	1000°F
Throttle steam pressure	2605 psig
Throttle steam flow	13.4 lb/s
Fluidizing air flow	13.2 lb/s
Furnace gas temperature	713°F
Stack gas temperature	285°F

approximately five times as large. Since a drum boiler is inherently unstable unless drum water level is regulated, a level controller is operating in these otherwise open-loop simulations. Effects of the controller will be apparent in some of the cases discussed.

This study was completed before the recent TVA pilot plant design specification (No. 4216) was available, and the model was parameterized for 15 MW rather than 20 MW. The model is being reparameterized to the new specification, but the qualitative conclusions drawn here probably will not change appreciably.

In the first case in Table 11.2, coal feed from the pulverizer was reduced by 1%. Figures 11.1 through 11.7 show the transient response to the disturbance. Figure 11.1 is total power; figs. 11.2, 11.3, and 11.4 are power generation in the evaporator, primary (above-bed) superheater, and secondary (in-bed) superheater, respectively. The total power level is seen to require a full half hour to approach a new equilibrium. Because of its high nucleate boiling heat transfer coefficient and comparatively small metal mass and heat capacity, the evaporator approaches equilibrium in about a third of this time. Sixty percent of the power is generated in the evaporator, and the bed temperature (Fig. 11.5) tracks the evaporator temperature fairly closely. The superheaters, with greater masses, smaller transfer coefficients, and larger time constants dominate the overall system response time.

Figure 11.1 shows the power level undershooting by about 25% before reaching the new equilibrium. The undershoot is the consequence of the system storing an increased amount of heat in metal and fluid masses and may indicate a behavior pattern that could assist a control system in load following. Under load changes, boilers have the natural tendency to either store heat in or release heat from the evaporators and superheaters. In conventional boilers, convective superheaters (such as the primary superheater in the pilot plant) typically store heat under load increase (and release it under load decrease). This deteriorates the ability of the plant to respond promptly to load change because increased firing initially goes partially into storage rather than load. Conventional boiler radiant superheaters on the other hand tend to release heat under load increase, which assists the control system by providing a relatively prompt supply of temporary additional heat.

The superheater in the bed of the pilot plant falls in neither the convective nor the radiant category, and its load following behavior remains to be determined. Evidence from the present simulation indicates the following behavior for the bed superheater. Since the air-cooled condenser inherently follows firing rate, the 1% reduction in coal feed caused a corresponding decrease of load (air cooling). The bed superheater, primary superheater, and evaporator heat storages increased by 0.8%, 0.39%, and 0.3%, respectively, the bed heat storage decreased by -0.14%, and the net change in system heat storage was positive, +0.3%. Thus, in the fluid-bed configuration currently modeled, the bed superheater appears to have beneficial heat storage dynamics, as does the

Table 11.2. Sensitivity of AFBC state variables to changes in selected system parameters.

Parameter reduced by 1%	Change (upper datum) and percent change (lower datum) in state variable															
	Evap. power (MW)	Prim. S.H. power (MW)	Sec. S.H. power (MW)	Condens. load (MW)	Stack loss (MW)	Bed temp. (F)	Prim. S.H. metal temp. (F)	Sec. S.H. metal temp. (F)	Drum temp. (F)	Drum press. (psig)	Throttle steam temp. (F)	Throttle steam press. (psig)	Throttle steam flow (lb/s)	Fluidiz. air flow (lb/s)	Furnace gas temp. (F)	Stack gas temp. (F)
Coal feed	0.019 0.22	-0.029 -0.97	-0.15 -5.3	-0.16 -1.1	0.0058 0.55	-2.2 -0.14	3.4 0.37	10 0.76	-4.4 -0.64	-78 -2.8	12 1.2	-74 -2.9	-0.51 -3.8	0.002 0.015	5.3 0.74	1.8 0.62
Air inlet damper	-0.0018 -0.021	-0.0091 -0.3	0.023 0.8	0.011 0.075	-0.011 -1.1	0.25 0.016	-1.7 -0.18	-1.6 -0.12	0.47 0.068	8.5 0.3	-2.2 -0.22	7.9 0.3	0.064 0.48	-0.1 -0.77	-3.1 -0.43	-1.5 -0.51
FD fan pressure	-0.014 -0.17	-0.051 -1.7	0.13 4.5	0.062 0.42	-0.062 -5.9	1.1 0.071	-9.3 -1.0	-9.4 -0.71	2.7 0.39	48 1.7	-12.8 -1.3	45 1.7	0.37 2.7	-0.55 -4.1	-17 -2.4	-8.0 -2.8
Flue gas damper	-0.0004 -0.0046	-0.0021 -0.069	0.0054 0.19	0.0027 0.018	-0.0027 -0.25	0.1 0.006	-0.38 -0.041	-0.3 -0.023	0.11 0.016	2.0 0.071	-0.51 -0.051	1.8 0.069	0.015 0.11	-0.024 -0.18	-0.72 -0.1	-0.34 -0.12
ID fan pressure	-0.0046 -0.053	-0.035 -1.2	0.088 3.1	0.046 0.31	-0.046 -4.4	1.2 0.077	-6.3 -0.68	-5.8 -0.44	1.8 0.27	33 1.2	-8.3 -0.83	30 1.2	0.24 1.8	-0.4 -3.0	-12 -1.7	-5.7 -2.0
Feedpump pressure	0.0058 0.067	0.0002 0.0066	-0.0064 -0.22	-0.0005 -0.0034	0.0005 0.047	0.4 0.026	0.35 0.038	0.9 0.068	-0.21 -0.031	-3.7 -0.13	1.8 0.18	-3.5 -0.13	-0.035 -0.26	0 0	0.33 0.046	0.12 0.042
Attenuator valve	0.0015 0.017	0.0001 0.0033	-0.0016 -0.056	-0.0001 -0.00068	0.0001 0.0054	0.1 0.0065	0.09 0.0097	0.2 0.0015	-0.05 -0.0073	-0.9 -0.032	0.4 0.04	-0.9 -0.035	-0.008 -0.06	0 0	0.08 0.011	0.03 0.01
Throttle valve	-0.034 -0.39	-0.0031 -0.1	0.038 1.3	0.0012 0.0081	-0.0012 -0.11	-1.6 -0.1	-0.98 -0.11	-4.7 -0.36	1.9 0.27	33 1.2	-5.0 -0.5	36 1.4	0.11 0.79	0 0	-0.77 -0.11	-0.27 -0.095
Evaporator surface	-0.001 -0.012	0.019 0.61	-0.023 -0.79	-0.004 -0.027	0.004 0.4	7.7 0.5	3.9 0.42	9.5 0.72	-0.98 -0.14	-18 -0.62	7.5 0.75	-16 -0.59	-0.15 -1.1	0 0	2.5 0.36	0.89 0.31
Primary S.H. surface	0.0017 0.02	-0.013 -0.42	0.0069 0.24	-0.005 -0.034	0.005 0.46	0.2 0.013	0.73 0.79	-0.4 -0.03	0.01 0.0015	0.2 0.0071	-0.81 -0.0081	0 0	0.007 0.052	0 0	3.7 0.52	1.3 0.45
Secondary S.H. surface	-0.0004 -0.0046	0.0045 0.16	-0.0035 -0.12	0.001 0.0068	-0.001 -0.1	0.4 0.026	-0.61 -0.066	-1.6 -0.12	0.46 0.067	8.2 0.29	-3.6 -0.36	7.3 0.28	0.072 0.54	0 0	-0.96 -0.13	-0.33 -0.12
Condenser air flow	-0.06 -0.69	-0.0016 -0.053	0.067 2.33	0.005 0.034	-0.005 -0.5	-4.1 -0.26	-3.7 -0.4	-9.4 -0.71	2.0 0.3	37 1.3	-9.0 -0.9	34 1.3	0.27 2.0	0 0	-3.6 -0.51	-1.3 -0.45

Figure 11.1. Total power generation.

Figure 11.2. Power generation in evaporator.

Figure 11.3. Power generation in primary (above-bed) superheater.

Figure 11.4. Power generation in secondary (in-bed) superheater.

Figure 11.5. Bed temperature.

Figure 11.6. Throttle steam temperature.

Figure 11.7. Drum pressure (upper curve) and throttle steam pressure (lower curve).

total system heat storage. Under load decrease, there is prompt internal storage of energy to assist the control system until firing rate can be adequately lowered.

Figures 11.2 through 11.4 and related data in Table 11.2 show that with reduced coal feed and load there is a shift in power distribution among the evaporator and superheaters; generation in the evaporator increases while that in the superheaters decreases. A similar pattern occurs in conventional boilers and can lead to large temperature shifts if not controlled. In the case of the fluid-bed system, the values in Table 11.2 indicate that most of the redistribution occurs between the evaporator and bed superheater — that is, the redistribution occurs primarily within the bed, the net change in bed power generation is relatively small, and the bed temperature change is correspondingly small. In Fig. 11.5 the bed temperature decreases approximately 7 degrees during the first five minutes of the transient and recovers to a final equilibrium 2 degrees below initial value. The 1% reduction in firing rate and load results in a bed temperature change of only -0.14%.

Decreased coal feed to the boiler causes a reduction of drum pressure and steam flow rate. Because of thermohydraulic nonlinearities, the decrease in flow is about 4% compared with the 1% reduction in heat generation. Consequently, throttle steam temperature (Fig. 11.6) increases by 12 degrees, close to the limit manufacturers allow for turbines. The inherent mismatch between change in firing rate and desired change in steam flow must be treated by the control system.

Table 11.2 further shows that the smaller size of the secondary superheater makes its metal temperature T_{sm2} more sensitive than the primary superheater metal temperature T_{sm1} to fluctuations in steam flow. With approximately equal heat generation in the two units, the ratio of changes in metal temperatures is roughly proportional to the inverse ratio of heat transfer surface areas,

$$\frac{\Delta T_{sm2}}{\Delta T_{sm1}} \propto \frac{A_{s1}}{A_{s2}}.$$

On a percentage basis, the quantities showing greatest sensitivity to the 1% change in coal feed and load are secondary superheater power generation (-5.3%), steam flow rate (-3.8%), throttle pressure (-2.9%), drum pressure (-2.8%), and throttle steam temperature (1.2%). (Throttle and drum pressures are shown in Fig. 11.7.) Virtually the least sensitive quantity is bed temperature (-0.14%). This insensitivity persists throughout the disturbances listed in Table 11.2. Because of its effect on SO_2 removal, bed temperature will presumably be one of the more important controlled variables. The noted tendency of evaporator and bed superheater power generation rates to respond in opposition acts to buffer the bed temperature and inherently stabilize SO_2 removal against system upsets.

At the end of 30 minutes of simulated plant operation, the transient calculation was terminated and the final equilibrium conditions computed. Equilibrium values were plotted, without lifting the Calcomp plotter pen, at the ends of the curves in Figs. 11.1 through 11.7. The resulting vertical tail on each curve gives the deviation from final equilibrium remaining when the transient was terminated. Examination of the curves in the various figures shows that the course of the transient is qualitatively clear after about the first ten minutes. Beyond that point is a slow, shallow, and predictable approach to equilibrium. For the remaining cases in Table 11.2, the transient calculations were therefore terminated at ten minutes and the new equilibrium determined, reducing computer time to one third. Because of space limitations, plots of these cases will not be included. Some cases will be discussed summarily.

Air inlet damper setting: In the second listed case in Table 11.2, closing the inlet damper by 1% reduces air intake, stack loss, and the flow dependent heat transfer coefficient of the primary superheater. There results a shift in heat transfer from the primary to the secondary superheater, and bed temperature increases slightly. Although drum temperature and pressure increase, heat transfer in the evaporator declines (in opposition to the bed superheater) because of reduced temperature differential across the evaporator metal. Although stack loss is reduced and steam generation is proportionately increased, thermohydraulic nonlinearities cause steam flow to increase six times as much as steaming rate, and the throttle steam temperature decreases.

Forced draft fan pressure: Reducing the fan pressure has qualitatively the same effect on the listed variables as closing the damper. The effect is proportionately greater, however, because air flow depends on the inlet-outlet pressure differential rather than on fan pressure alone.

Induced draft fan damper setting and pressure: For the variables listed, changes in these parameters have qualitatively the same effect as changes in the forced draft parameters.

The five preceding disturbances occurred on the gas side. The remaining seven occur on the steam side.

Feedpump pressure: Reduction of the feedpump pressure and flow causes a decrease of heat input to the drum via feedwater enthalpy. Drum pressure, temperature, and steam flow rate decrease; bed superheater output decreases, opposed by increased evaporator output. There is a net decrease of heat transfer in the bed, an increase in bed and flue gas temperatures, and increased stack loss.

Attemperator valve setting: For the variables listed in Table 11.2, closing the attemperator valve 1% has qualitatively the same effect as reducing the feedwater pressure.

Throttle valve setting: Closing the throttle valve by 1% has the perhaps surprising result of increasing throttle steam flow by 0.8%. This result, opposite to what was intended in decreasing the valve opening, is the consequence of drum water level controller interference. The detailed computer printout for this case shows that during the first two minutes of the transient, throttle steam flow does decrease. As throttle flow decreases, steam tends to back up in the drum, and drum pressure builds. Since the enthalpy of saturated steam varies conversely with pressure, steam flow from the drum then needs to increase to sustain heat removal. With increased steam flow, the controller opens the feed-water valve to maintain drum water level. Pressure and density at the throttle increase, and after the first two minutes of the transient, the increase in flow due to higher steam pressure and density more than compensates the reduced valve opening.

The next three parameters in Table 11.2 are the effective heat transfer areas of the evaporator, primary superheater, and secondary superheater. Each was varied by 1% to simulate the effects of manipulating heat transfer surfaces for purpose of boiler control.

Effective evaporator heat transfer surface: The reduction in evaporator surface represents the removal, as by bed slumping or whatever means available, of 1% of the evaporator heat transfer area from the high heat transfer rate regime. The resulting decrease of heat transfer to the evaporator is highly nonlinear, being only 0.012% compared with the 1% decrease in active surface. The nonlinearity is the result of a strong feedback reaction from the large evaporator heat transfer coefficient; reduction of heat to the evaporator causes drum pressure and temperature to drop which in turn increases the temperature differential across the drum metal and tends to restore heat transfer. The principal change in heat generation affected by reduction of active evaporator surface actually occurs in the bed superheater. Reduced drum pressure raises the evaporator steam enthalpy and necessitates lower steam flow to remove the nearly unchanged evaporator heat input; reduced steam flow through the secondary superheater then lowers its heat transfer by 0.8%.

Primary superheater transfer surface: Effective reduction of the primary superheater surface, as by dampering action, causes a much more linear response than the corresponding change in the evaporator. A 1% reduction produces a 0.42% decrease in heat transfer. Table 11.2 shows that heat transfer in the evaporator is nearly independent of this change in the superheater; there is only a 0.02% decrease. On the other hand, half of the heat no longer absorbed in the primary superheater is recovered in the bed superheater, which is downstream in the steam path. Most of the remainder is lost through the stack.

Secondary (bed) superheater transfer surface: A similar pattern occurs in the case of a 1% reduction in the secondary superheater surface. Heat transfer in the evaporator is nearly unchanged (-0.0046%). The primary superheater, downstream in the gas path, picks up most of the heat no longer absorbed in the bed superheater.

In short, changes in the evaporator are seen to have a strong effect on the superheaters, while changes in the superheaters have a comparatively minor effect on the evaporator. This is because both superheaters are downstream of the evaporator in the steam path, and disturbance signals generated in the evaporator propagate directly to the superheaters. On the otherhand, with the evaporator upstream of the superheaters, disturbance signals in these units reach the evaporator only roundabout through the condenser and feedwater loop and are largely damped out by high heat capacitances and impedences along that path.

The observed interaction between the superheaters in which the output of one tends to increase when the other decreases may be more characteristic of fluid-bed boilers than of some conventional boilers. Because of the location of the secondary superheater in the bed, the superheaters are each downstream of the other in one fluid path or the other. The primary superheater is downstream of the secondary superheater in the gas path, and the secondary superheater is downstream of the primary superheater in the steam path. There is thus direct coupling between them regardless of which one is disturbed.

The last parameter considered in Table 11.2 is air flow rate through the air-cooled condenser. Reduction of condenser air flow excites drum level controller interference analogous to that which occurred with throttle valve manipulation. When air flow was reduced 1%, heat removal decreased during the initial minutes of the transient as expected. Then, since firing rate was not changed, heat to the evaporator increased as did steaming rate, and it became necessary to increase feedwater flow to maintain drum water level. The increased steam flow and higher temperatures in the condenser eventually overshadowed the reduced air flow, and condenser cooling increased at equilibrium by a small amount (0.034%).

The data for fluidizing air flow (third from last column in Table 11.2) show it to be insensitive to all seven steam side disturbances investigated. This is because air flow is regulated primarily by the ID and FD fans. Steam flow does not show an analogous insensitivity to gas side disturbances.

Finally, it should be reported that one week of this month was spent in special training on the Cumberland Steam Plant Simulator at Chattanooga. Appreciation is extended to TVA for an excellent course of instruction on steam plant design and operation.

12. COAL COGENERATION/DISTRICT HEATING PLANT ASSESSMENT

M. A. Karnitz and R. L. Graves

12.1 Objective

The objective of this work is to provide the Fossil Fuel Utilization Division of DOE with an evaluation of the coal-fired closed-cycle gas turbine as a cogeneration power plant specifically for district heating in the Minneapolis-St. Paul area. This entails a preliminary design study, including a cost estimate. The design study is a cooperative effort between ORNL, United Engineers and Constructors (UE&C), and Northern States Power (NSP). Design of an extraction steam system for the same application is being carried out simultaneously by UE&C and will allow a comparative evaluation of both cogeneration plants. These design studies are part of a considerably larger program involving other divisions of DOE with the objective of evaluating district heating in Minneapolis-St. Paul.

12.2 Status Summary

The Mayor of St. Paul, George Latimer, has taken the initiative to form a nonprofit district heating development corporation. This company will attempt to design and implement the design plan for the first segment of a district heating system in the city of St. Paul. They hope to have the company formed and staffed by July 1, 1979. It now appears that the head of the organization will be Hans Nyman, presently a consultant with the Minnesota Energy Agency and formerly the chief engineer of the Uppsala, Sweden, District Heating System.

Studsvik delivered the final draft on the Twin Cities District Heating Study. There were minor changes between this report and the February report. The latest report does provide a significant amount of detail on a larger district heating scenario. The report will be published and distributed during the month of August.

On May 16, Mike Karnitz met with John Millhone, Buildings and Community Systems Branch, DOE, to discuss ORNL's ideas on a National District Heating Program. He was quite receptive to the ideas on the three-task program and encouraged us to continue developing the concepts. We plan to produce a small document on the program and distribute it to Buildings and Community Systems staff by early June.

The coal-cogeneration plant study with Northern States Power and United Engineers and Constructors was initiated in mid-May. UE&C is presently working on the 200 to 400 MW(e) reference plant design. There will be a meeting on June 11 in Philadelphia, Pennsylvania, to review the completed work up to that date.

The off-design model for the combined cycle district heating plant is complete and is being debugged after some minor modifications. The low-pressure steam turbine would operate at reduced mass flow rate when the demand for thermal energy is high requiring that its efficiency be appropriately corrected. Part load correction factors have been found in the literature and will be incorporated in the model.

The recuperated closed-cycle gas turbine cycle configuration has been completed and is ready for input on the computer. The maximum electric-to-heat ratio of this system appears to be slightly lower than the combined cycle when the recuperator effectiveness is limited to about 87%. Performance data on recuperators is being obtained from a vendor of these devices.

13. FBC INDUSTRIAL APPLICATIONS PROJECT SURVEY

K. K. Chipley, N. W. Durfee,
and M. E. Lackey

13.1 Objective

Part of the Fossil Energy decentralization includes the transfer of FBC industrial applications projects to Morgantown Energy Technology Center (METC). A review team has been organized by METC to provide a snapshot status with respect to cost, schedule, and technical problems of eight projects being transferred. After reviewing background information of each project, the team visits the contractor site for several days of intensive interaction with the contractor. A report of the findings of each project is then written and issued to METC.

13.2 Status Summary

The committee reviews have been completed, and the reports are being finalized. The last three reviews were of the Curtiss-Wright antracite culm AFB unit to be built at Shamokin, PA; the Foster-Wheeler/PER antracite culm AFB unit to be built at Wilkes-Barre, PA; and two FluidDyne units — an AFB antracite culm unit to be built in Towanda, PA, and an AFB process heater to be installed in Paynesville, MN.

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