27
8-25-81
JMS
4 to 11 TIS

②

B6673

ORNL/TM-7908

ornl

MASTER

OAK
RIDGE
NATIONAL
LABORATORY

UNION
CARBIDE

Fossil-Energy Program
Progress Report for June 1981

L. E. McNeese

Fossil
Energy
Program

OPERATED BY
UNION CARBIDE CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A07; Microfiche A01

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Contract No. W-7405-eng-26

FOSSIL-ENERGY PROGRAM
PROGRESS REPORT FOR JUNE 1981

L. E. McNeese
Program Director

Date Published - August 1981

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

**THIS PAGE
WAS INTENTIONALLY
LEFT BLANK**

CONTENTS

	<u>Page</u>
ABSTRACT.	1
1. SUMMARY	1
2. COAL CONVERSION DEVELOPMENT	8
2.1 Physical Properties of Coal Liquids.	8
2.2 Thermal Conductivity	12
2.3 Instrumentation for Measurement of CSD Feed Quality. . .	13
2.4 References for Section 2	14
3. CHEMICAL RESEARCH AND DEVELOPMENT	15
3.1 New Liquefaction Techniques.	15
3.2 Indirect Liquefaction Chemical Research.	16
3.3 Selective Beneficiation and Short Contact Time (SCT) Liquefaction	18
4. MATERIALS TECHNOLOGY.	22
4.1 Pressure Vessel and Piping Materials	22
4.2 Welding and Cladding Development	22
4.3 Corrosion of AFBC Heat Exchanger Materials	24
4.4 Failure Prevention and Analysis in Coal Liquefaction Systems.	25
4.5 Materials Research for Liquefaction Systems.	25
4.6 Development of Modified 9 Cr-1 Mo Structural Steel . . .	25
4.7 Evaluation of Materials for Use in Ceramic Heat Exchangers	26
4.8 Oxygen Measuring Systems for Fluidized Bed Combustors. .	27
4.9 Materials and Components for Coal Gasification Systems .	28
4.10 Assessment of Strategic Materials for Synfuels Plants .	30
4.11 References for Section 4.	30
5. COMPONENT DEVELOPMENT AND PROCESS EVALUATION.	31
5.1 Technical Support to Large Liquefaction Projects	31
5.2 New Initiatives in Coal Conversion	31
6. TECHNICAL SUPPORT TO MAJOR LIQUEFACTION PROJECTS.	33
6.1 Engineering and Design Review.	33
6.2 Liquefaction Technology Base	36
6.3 Components	50
6.4 Materials.	54
6.5 Environmental and Health	61
6.6 References for Section 6	63
7. PROCESS ANALYSIS AND ENGINEERING EVALUATIONS.	64
7.1 Liquefaction Technology Assessment (LTAS).	64
7.2 Direct Combustion.	65
7.3 Advanced Power Conversion Systems.	65

	<u>Page</u>
7.4 Process Modeling.	66
7.5 Coal Liquefaction Advanced Research Digest.	67
7.6 Indirect Liquefaction Environmental Control Technology Assessment (ILECTA)	67
7.7 Environmental Control Costs for an Indirect Coal Liquefaction Process.	68
7.8 Underground Coal Gasification	68
8. FOSSIL ENERGY ENVIRONMENTAL PROGRAM.	70
8.1 Fossil Energy Support	70
8.2 Synfuels Project.	71
8.3 Economic Regulatory Administration Support Project. . .	72
9. FLUE GAS DESULFURIZATION	76
9.1 Magnesia FGD Spray Absorption Technology.	76
10. COAL PREPARATION AND WASTE UTILIZATION	78
10.1 High-Gradient Magnetic Separation.	78
11. ATMOSPHERIC FLUIDIZED BED COAL COMBUSTOR FOR COGENERATION. .	83
11.1 Objective.	83
11.2 Status Summary	83
12. TENNESSEE VALLEY AUTHORITY (TVA) FLUIDIZED BED COMBUSTION (FBC) DEMONSTRATION PLANT PROGRAM TECHNICAL SUPPORT.	86
12.1 AFBC Modeling and Analysis - Task 4.	86
12.2 Analytical Support and Alternate Design Concepts Evaluation - Task 4b	87
12.3 AFBC Bench Scale Facility - Task 5	89
12.4 Coal Feed Tests - Task 11.	89
12.5 Tubular Flow Reactor Experiment - Task 13.	89
12.6 References for Section 12.	90
13. PFBC SYSTEMS ANALYSIS.	91
13.1 Objectives	91
13.2 Status Summary	91
14. FOSSIL FUEL APPLICATIONS ASSESSMENT.	93
14.1 District Heating Turbine Study	93
14.2 Comparative Assessment of Options for New Industrial Boilers Relative to Air Emission Regulations for Morgantown Energy Technology Center.	93
15. PERFORMANCE ASSURANCE SYSTEM SUPPORT FOR FOSSIL ENERGY PROJECTS	96
15.1 Objective.	96
15.2 Status Summary	96

	<u>Page</u>
16. INTERNATIONAL ENERGY TECHNOLOGY ASSESSMENT.	97
16.1 Liquefaction Technology (Including Gasifier Development Status)	97
16.2 International Survey of Coal Preparation Technology . .	97
16.3 International Survey of the Status of Technology of Critical Components for Coal Liquefaction Processes . .	98
16.4 Coal Liquefaction Materials	99
16.5 International Survey of Atmospheric Fluidized Bed Combustion Technology	99
17. GENERALIZED EQUILIBRIUM MODELS OF LIQUID AND GASEOUS FUEL SUPPLIES.	100
17.1 Background.	100
17.2 Status Summary.	100
17.3 References for Section 17	107
18. ANALYSES OF COAL PRODUCTION GOALS	108
18.1 Current Project Status.	108
18.2 Coal Transport System	109
18.3 Regional Demand Analysis.	109
19. FOSSIL ENERGY INFORMATION CENTER.	110

PREVIOUS REPORTS IN THIS SERIES

ORNL/TM-5044, Progress Report for August 1974
ORNL/TM-5045, Progress Report for September 1974
ORNL/TM-5046, Progress Report for October 1974
ORNL/TM-4787, Progress Report for November 1974
ORNL/TM-4796, Progress Report for December 1974
ORNL/TM-4850, Progress Report for January 1975
ORNL/TM-4873, Progress Report for February 1975
ORNL/TM-4892, Progress Report for March 1975
ORNL/TM-4946, Progress Report for April 1975
ORNL/TM-4966, Progress Report for May 1975
ORNL/TM-5010, Progress Report for June 1975
ORNL/TM-5037, Progress Report for July 1975
ORNL/TM-5092, Progress Report for August 1975
ORNL/TM-5124, Progress Report for September 1975
ORNL/TM-5186, Progress Report for October 1975
ORNL/TM-5214, Progress Report for November 1975
ORNL/TM-5246, Progress Report for December 1975
ORNL/TM-5301, Progress Report for January 1976
ORNL/TM-5321, Progress Report for February 1976
ORNL/TM-5430, Progress Report for March 1976
ORNL/TM-5479, Progress Report for April 1976
ORNL/TM-5532, Progress Report for May 1976
ORNL/TM-5595, Progress Report for June 1976
ORNL/TM-5611, Progress Report for July 1976
ORNL/TM-5654, Progress Report for August 1976
ORNL/TM-5674, Progress Report for September 1976
ORNL/TM-5717, Progress Report for October 1976
ORNL/TM-5752, Progress Report for November 1976
ORNL/TM-5770, Progress Report for December 1976
ORNL/TM-5819, Progress Report for January 1977
ORNL/TM-5858, Progress Report for February 1977
ORNL/TM-5883, Progress Report for March 1977
ORNL/TM-5932, Progress Report for April 1977
ORNL/TM-5980, Progress Report for May 1977
ORNL/TM-6003, Progress Report for June 1977
ORNL/TM-6038, Progress Report for July 1977
ORNL/TM-6066, Progress Report for August 1977
ORNL/TM-6104, Progress Report for September 1977
ORNL/TM-6137, Progress Report for October 1977
ORNL/TM-6217, Progress Report for November 1977
ORNL/TM-6262, Progress Report for December 1977
ORNL/TM-6274, Progress Report for January 1978
ORNL/TM-6329, Progress Report for February 1978
ORNL/TM-6385, Progress Report for March 1978
ORNL/TM-6386, Progress Report for April 1978
ORNL/TM-6454, Progress Report for May 1978
ORNL/TM-6489, Progress Report for June 1978
ORNL/TM-6518, Progress Report for July 1978

PREVIOUS REPORTS IN THIS SERIES (CONTINUED)

ORNL/TM-6592, Progress Report for August 1978
ORNL/TM-6630, Progress Report for September 1978
ORNL/TM-6666, Progress Report for October 1978
ORNL/TM-6682, Progress Report for November 1978
ORNL/TM-6767, Progress Report for December 1978
ORNL/TM-6815, Progress Report for January 1979
ORNL/TM-6829, Progress Report for February 1979
ORNL/TM-6886, Progress Report for March 1979
ORNL/TM-6923, Progress Report for April 1979
ORNL/TM-6928, Progress Report for May 1979
ORNL/TM-6997, Progress Report for June 1979
ORNL/TM-7031, Progress Report for July 1979
ORNL/TM-7057, Progress Report for August 1979
ORNL/TM-7095, Progress Report for September 1979
ORNL/TM-7144, Progress Report for October 1979
ORNL/TM-7171, Progress Report for November 1979
ORNL/TM-7210, Progress Report for December 1979
ORNL/TM-7251, Progress Report for January 1980
ORNL/TM-7285, Progress Report for February 1980
ORNL/TM-7322, Progress Report for March 1980
ORNL/TM-7375, Progress Report for April 1980
ORNL/TM-7414, Progress Report for May 1980
ORNL/TM-7444, Progress Report for June 1980
ORNL/TM-7483, Progress Report for July 1980
ORNL/TM-7535, Progress Report for August 1980
ORNL/TM-7573, Progress Report for September 1980
ORNL/TM-7610, Progress Report for October 1980
ORNL/TM-7635, Progress Report for November 1980
ORNL/TM-7682, Progress Report for December 1980
ORNL/TM-7723, Progress Report for January 1981
ORNL/TM-7763, Progress Report for February 1981
ORNL/TM-7795, Progress Report for March 1981
ORNL/TM-7826, Progress Report for April 1981
ORNL/TM-7865, Progress Report for May 1981

FOSSIL ENERGY PROGRAM REPORT FOR JUNE 1981

ABSTRACT

This report - the eighty-third of 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 as sources of clean energy. The projects reported this month include those for coal conversion development, chemical research and development, materials technology, component development and process evaluation, technical support to major liquefaction projects, process analysis and engineering evaluations, fossil energy environmental analysis, flue gas desulfurization, coal preparation waste utilization, atmospheric fluidized bed coal combustor for cogeneration, TVA FBC demonstration plant program technical support, PFBC systems analysis, fossil fuel applications assessments, performance assurance system support for fossil energy projects, international energy technology assessment, generalized equilibrium models for liquid and gaseous fuel supplies, analyses of coal production goals, and fossil energy information center.

1. Summary

Coal conversion development - The rheology of Kentucky No. 9 Wilsonville recycle solvent and Kentucky No. 9 coal at a 1.6 solvent-to-coal ratio was determined at a pressure of 17.24 MPa and temperatures of 423, 533, and 700 K. The apparent viscosities at the three temperatures and at a shear rate of 300 s^{-1} are 7.9 mPa·s, 41.4 mPa·s, and 2.0 mPa·s, respectively. The slopes of the flow curves were 0.953, 0.709, and 1.655, respectively. The gel region began at 500 K and the viscosity increased sharply as the temperature increased. By the time the temperature had reached 700 K, the viscosity had fallen to below the pre-gel region viscosity.

Experiments on thermal conductivity have been suspended pending repair of the line source gauge which was broken after measurements were completed on toluene.

Modification of our thirty-plate, spinning-band still by the manufacturer have resulted in doubling our solvent throughput. This greatly improves both sample concentration and solvent recovery. Concurrently, procedures were investigated which would more effectively recover dried fractions. Also, a repeat SESC run on CSD feed 217-C-MB ("good" SRC recovery) was made to determine the precision of the method.

Chemical research and development - Initial results for liquefaction of Bruceton bituminous coal in individual dihydroxybenzenes shows significant incorporation of these materials into coal-derived products, as had been observed previously for Wyodak coal.

Analytical results have been obtained for 9 fractions of a Kentucky #9 coal (Fies mine) separated by open gradient magnetic techniques. Initial results of liquefaction under SCT conditions show large enough differences to discriminate among these samples.

The ability to determine the position of incorporation of deuterium into polycyclic aromatics during isotope-exchange studies by direct ^2H nmr has been demonstrated. Further results have been obtained on relationships between liquid product composition (solvent fractionation) and reaction severity index under SCT conditions.

Materials technology - Testing of pressure vessel and piping materials for coal conversion applications was continued. Samples of modified 2 1/4 Cr-1 Mo from U.S. Steel Co. and from Japan Steel Works are being heat-treated in preparation for mechanical property testing. In the welding and cladding development task, the effect of postweld heat treatment on the fracture toughness of a 300-mm-thick 2 1/4 Cr-1 Mo weldment is being evaluated. Efforts in the study of fireside corrosion of AFBC heat exchanger materials continued. Studies of the deposition of CaSO_4 scale, which plays a role in the corrosion process, are under way. In the failure prevention and analysis task, tubing from the Kerr-McGee critical solvent deashing unit at the Wilsonville pilot plant are being examined. The investigation of materials performance in liquefaction systems continued. These studies include general corrosion and stress-corrosion cracking in direct liquefaction plants. In the task for development of modified 9 Cr-1 Mo steel, aluminum-coated samples are being prepared to study the effectiveness of such coatings in preventing sulfidation of this alloy. In the task to evaluate materials for use in ceramic heat exchangers, a 240-h exposure of several candidate ceramics to molten slag and the products of combustion of a coal-oil mixture was completed. Preliminary post-test observations indicated that the basic slag was very corrosive to the ceramic specimens. The evaluation of oxygen measuring systems (OMSs) for fluidized-bed combustors continued. Equipment is being assembled to evaluate ZrO_2 electrolyte and TiO_2 probes. In the task to provide technical support to METC on materials and components for gasification systems, a visit was made to Mountain Fuel Resources, Inc. to coordinate the placement of materials test coupons in the gasification process development unit by Metal Properties Council. A description of the process and some materials-related problems are discussed. Effort on the assessment of strategic materials for synfuels plants continued.

Component development and process evaluation - Proposals for five tasks in support of the Gasification Component Development Program were submitted to METC and DOE/HQ for final review. The formal package will be submitted in July.

Technical support to major liquefaction projects - Support is provided by Oak Ridge National Laboratory and Union Carbide Nuclear Division Engineering for the major liquefaction projects being managed by DOE Oak Ridge Operations--SRC-I and SRC-II Demonstration Plants, Tri-State and Breckinridge Commercial Plants, H-Coal Pilot Plant, and Exxon Donor Solvent Projects. Activities are reported in five broad categories--engineering and design review, liquefaction technology base, components, materials, and environmental and health.

At the request of Ashland Synthetic Fuels, we used a previously developed thermal model of the H-Coal reactor to assess the effects of refractory spalling on the pressure vessel; effects were not of serious concern--somewhat increased metal temperature but reduced thermal gradients. Additional experiments were performed to assess the rheology of slurries mixed at elevated temperature with the relatively light Wilsonville solvent. A report on remote-heat (surge-leg) pumping of slurries is nearing completion; the report includes an assessment of the state of the art and engineering analysis related to technical concerns. Commercial trim materials from slurry letdown valves are being examined. Final reviews were completed on the Final Environmental Impact Statement for the SRC-I project, substantially completing our responsibilities on this task.

Process analysis and engineering evaluations - To assist in the evaluation of gasifier efficiencies in the Phase II LTAS studies, a computer program was written that calculates the heat and material balance relationships and the overall thermal efficiency of an entrained-flow gasifier. The ORNL model was used to verify Fluor's calculations for both the Texaco and the Koppers-Totzek gasifiers. Good agreement with Fluor's results was obtained when the same input assumptions were used. A preliminary draft of the Phase II report is undergoing internal review.

Fossil energy environmental program - In the Fossil Energy Support project, regulatory and legislative review highlights were submitted to DOE and the first newsletter is scheduled for distribution on July 15. In the Synfuels project, the SRC-I Final EIS underwent DOE review and final revisions for an expected July issuance. Reviews of environmental documents for the Breckinridge project continued. In the Economic Regulatory Administration support project, comments on the Ravenswood DEIR were received on June 8. Submission of the Final DEIRs for Arthur Kill and Ravenswood are scheduled for July 3 and 17 respectively. All other planned deliverables have been submitted for the site specific analyses. A peer-reviewed draft of the health effects technical support document for the Northeast Regional EIS was submitted to DOE on June 12. Responses to comments on the latest revision of the Regional EIS were provided to ANL for incorporation into the next revision. Work is continuing on Dispatch Analysis and Rate Impact Modeling.

Flue gas desulfurization - The bench-scale spray dryer has been modified to improve temperature monitoring and water removal. Several successful runs were completed in which the SO₂ removal efficiency ranged from 28% to 85%.

Coal preparation and waste utilization - The HGMS test series on the core samples from the TVA Paradise stockpile have been completed and some results have been obtained from analytical chemistry. The early results indicate that there is a problem separating coal which has a coating on the particles. We are exploring methods of preparing the HGMS feed to reduce or eliminate this problem. The raw coal fines removal facility is approximately 90% complete, but completion of the facility will have to await settlement of the current labor strike.

Atmospheric Fluidized Bed Coal Combustor for Cogeneration - The scoping document for redirection of the Test Unit was prepared by ORNL and reviewed by METC.

Progress on the Reference Plant Design includes preparation of three views of the combustor island arrangement drawing, design of the spent bed material letdown system, and determination of the specifications for the FD and ID fans, boiler circulation pumps, baghouse and the steam coil air heater.

The Baseline Project Plan and Cost Estimate for the TTU has been reviewed and approved by ORNL and submitted to ORO.

Progress on the Test Unit design includes work on combustor layout drawings, structural engineering and water flow analysis on the water jacket, tube bundle design, and specifications for the FD and ID fans, all by B&W; and work on the combustion air preheater, combustion air and flue gas systems, air compressor, instruments and controls, and coal and limestone preparation by UCC-ND Engineering and ORNL.

Tennessee Valley Authority (TVA) Fluidized Bed Combustion (FBC) demonstration plant program technical support - In the AFBC Modeling and Analysis task, work continued on the simulation of the 20 MWe AFBC Pilot Plant. The heat transfer heat balance/subroutine was successfully run and the SO₂ capture code was run for the first time for the 20MWe AFBC configuration. Also during this month, modifications were made to the freeboard subcode to simulate the 20 MWe AFBC freeboard configuration. This included the addition of the coal ash balance and modification of the code to account for varying freeboard cross-sectional area. These modifications are presently complete.

PFBC systems analysis - The Office of Coal Utilization (OCU) replied to the recommendations for future work that ORNL submitted last month. The areas to be studied by ORNL are:

1. Advanced PFBC power plant concepts.
2. Modelling and analysis of PFBC control systems.
3. Packaged coal-fired industrial boilers, including a PFB.

Fossil fuel applications assessments - H. I. Bowers met with Burns and Roe staff to review the progress of the study. The project continues to fall behind schedule primarily because of the extended delays in obtaining district heating turbine data from General Electric. It is unlikely that Burns and Roe can meet the presently scheduled completion date of September 30.

The CONCEPT computer code developed by ORNL for DOE to estimate the capital investment costs for utility power plants is being modified to allow estimating the capital cost of a variety of industrial steam supply systems. Preliminary cost models have been prepared for representing 56 boiler configurations.

Performance assurance system support for fossil energy projects - The bi-monthly status report was presented to the DOE Task Manager at the DOE facility in Germantown, Maryland. Plans are being made to hold a workshop on the "Failure and Plant Operational Reporting System" during the last week in July at METC.

International energy technology assessment - Oak Ridge National Laboratory is supporting the Lawrence Livermore Laboratory in a broad program funded by the DOE Office of International Affairs. The program is designed to alert DOE management to foreign energy-related technologies of potential interest to the United States.

ORNL has responsibility for several areas of work including liquefaction technology, coal preparation technology, international survey of the status of technology of critical components for coal liquefaction processes, coal liquefaction materials, and the international survey of atmospheric fluidized bed combustion technology.

The pictorial report on SASOL is currently undergoing review by representatives of SASOL. Questionnaires requesting information on coal preparation technology were sent to six countries. Letters were sent to 69 foreign manufacturers requesting information on pumps, valves, and heat exchangers. Comments on the international assessment of atmospheric fluidized bed combustion technology draft report have been received from Lawrence Livermore National Laboratory and are being incorporated into the final report.

International energy technology assessment - Oak Ridge National Laboratory is supporting the Lawrence Livermore Laboratory in a broad program funded by the DOE Office of International Affairs. The program is designed to alert DOE management to foreign energy-related technologies of potential interest to the United States.

ORNL has responsibility for several areas of work including liquefaction technology, coal preparation technology, international survey of the status of technology of critical components for coal liquefaction processes, coal liquefaction materials, and the international survey of atmospheric fluidized bed combustion technology.

The pictorial report on SASOL is currently undergoing review by representatives of SASOL.

Questionnaires requesting information on coal preparation technology were sent to six countries.

Letters were sent to 69 foreign manufactures requesting information on pumps, valves, and heat exchangers.

Comments on the draft report on the international assessment of atmospheric fluidized bed combustion technology task from Lawrence Livermore National Laboratory have been received and are being incorporated into the final report.

Generalized equilibrium models of liquid and gaseous fuel supplies - The Oak Ridge National Laboratory is conducting a research program in the modeling of liquid and gaseous fuel supplies to provide support in decision and benefit-cost analyses for the Division of Policy and Strategic Planning, DOE/Fossil Energy. Near term objectives focus on assessing and reviewing existing models of enhanced oil recovery, developing a sensitivity theory based approach to decision analysis, and initiating advanced data tasks. ORNL's Engineering Physics Division has the lead responsibility for the program.

June 1981 activities concerned: (1) determination of a sample problem to address policy issues of interest to DOE/FE; (2) calibration of the prototype LFS model to ARC-80 projections; (3) implementation of an expanded LFS model and of a prototype GFS model; (4) treatment of the undiscovered resource base; (5) continued development of the Decision Analysis methodology.

Analyses of coal production goals - Uncertainties regarding project funding levels for FY 82 led to a revision in the FY 81 work plan to concentrate effort on those tasks and subtasks which could be completed with current funding. This approach will cause no major inefficiencies in returning to the original project work when FY 82 funding levels are determined. Research topics which could possibly be completed within the four months remaining in FY 81 were identified and prioritized during a June 19th meeting with LANL staff. These improvements will be incorporated into a new coal model based on the LACUMS (LANL) and the National Coal Model (EIA) should additional funding become available in FY 82. In the area of coal supply data, revision of reserve estimates received first priority. Transport research will concentrate on development of engineering cost estimates for coal movements by rail. The demand analysis continued on schedule as previously planned and will be completed in July or early August.

Fossil energy information center - The center has begun work on a critical review of the worker exposure and potential health effects of indirect coal liquefaction. The process description has been completed. Two new databases were established: Synfuels Assessment Database and Synfuels Substances Database.

2. COAL CONVERSION DEVELOPMENT

B. R. Rodgers

Coal conversion development activities are carried out in the Chemical Technology Division. This section discusses three projects conducted for the major liquefaction projects being managed by the DOE Oak Ridge Operations. The projects are (1) Measurement of Physical Properties of SRC-I Slurries, (2) Measurement of Slurry Thermal Conductivity in Support of the SRC-I and SRC-II Demonstration Plants, and (3) Instrumentation for Measurement of Critical Solvent Deashing Feed Quality. The first two projects are closely related to a project being done for the Office of Coal Processing - Physical Properties of Coal Liquids.

2.1 Physical Properties of Coal Liquids

D. D. Lee, M. R. Gibson, and T. L. Sams

The objective of this project is to measure and correlate physical properties (viscosity, density, thermal conductivity, and heat capacity) at typical processing conditions, up to 31 MPa (4500 psig) hydrogen pressure and 810 K (1000°F) in a bench-scale, continuous flow system. This system includes a slurry preheater and a hydrogenation reactor to simulate processing conditions prior to physical property measurement. Immediately after the physical property measurement, the test fluid is quenched and sampled for chemical characterization. Physical properties are ultimately correlated with the chemical characteristics of the test liquid to provide information useful to designers.

Results of the rheological characterization of Kentucky No. 9 coal/Wilsonville recycle solvent at various temperatures and 17.24 MPa pressure are presented. The rheological measurements were fitted to the power law and Bingham plastic models.

2.1.1 Work accomplished

The rheological characterization of Kentucky No. 9 coal/Wilsonville recycle solvent slurry at a 1.6 solvent to coal ratio was made at 17.24 MPa and 423, 533, and 700 K. One flow rate was measured at 560 K. The experimental results are presented in Figs. 2.1 and 2.2. The rheological characterization was carried out by passing the slurry through the preheater to reach the desired temperature, and then through the pipeline viscometer (PLV) at various flow rates. The plots of the wall shear stress, τ_w , vs $8V/D$, the Rabinowitsch-Mooney flow parameter, in log-log format are shown in Fig. 2.1 for the three temperatures studied. The results were analyzed using the power law model to correlate the data. The power law model for rheology is

$$\tau = k(t)\dot{\gamma}^{n(t)},$$

Fig. 2.1. Log-log plot of shear stress vs $8V/D$ for Kentucky No. 9 coal solvent-slurry.

ORNL DWG 81-823

Fig. 2.2. 38.5 wt % Kentucky No. 9 coal in Wilsonville recycle solvent, 17.24 MPa, 1.1 g/s mass rate.

where n is the slope of the flow curve and k is the consistency factor, which is determined from the flow curve by

$$k(t) = \tau_w \left(\frac{3n+1}{4n} \right)^{-n}$$

at $8V/D = 1$. The units are defined as:

$$k(t) = \text{mNs}^n/\text{m}^2$$

$$\dot{S} = \text{s}^{-1}$$

$$\tau = \text{mN/m}^2$$

The power law models for the three temperatures are:

$$\tau_w = 10.3 \dot{S}^{0.953} \text{ mN/m}^2 \text{ at } 423 \text{ K}$$

$$\tau_w = 217.6 \dot{S}^{0.709} \text{ mN/m}^2 \text{ at } 533 \text{ K}$$

$$\tau_w = 0.047 \dot{S}^{1.655} \text{ mN/m}^2 \text{ at } 700 \text{ K}$$

The apparent viscosities at $\dot{S} = 300 \text{ s}^{-1}$ for the three temperatures are: 7.9 mPa·s (7.9 cP) at 423 K, 41.4 mPa·s (41.4 cP) at 533 K, and 2.0 mPa·s (2.0 cP) at 700 K.

Figure 2.2 is a plot of viscometer ΔP (an indication of viscosity) versus the slurry temperature at 1.15 g/s slurry mass flow rate. As shown, the slurry begins to thicken at 500 K and increased to at least 10 times the minimum ΔP at 533 K. At 700 K, the slurry has passed the gel region and the ΔP is below that at the reaction minimum. The point at 560 K is the only rate obtained at this temperature because the PLV pressure taps plugged after the measurement and could not be opened sufficiently for continued operation.

The data were also analyzed assuming Bingham plastic behavior for the Rabinowitsch-Mooney analysis. This results in:

$$8V/D = \frac{\tau_w}{\eta} - \frac{4}{3} \frac{\tau_y}{\eta} + \frac{\tau_y^4}{3\eta\tau_w^3},$$

where τ_y is the yield stress (N/m^2) and η is the plastic viscosity (Ns/m^2) in the plastic constitutive equation:

$$\tau_w = \tau_y + \eta \dot{S}.$$

The Bingham plastic models for the three temperatures are:

$$\tau = 0.112 + 0.00746 \dot{S} \text{ mN/m}^2 \text{ at } 423 \text{ K}$$

$$\tau = 3.60 + 0.0284 \dot{S} \text{ mN/m}^2 \text{ at } 533 \text{ K}$$

$$\tau = -0.407 + 0.0035 \dot{S} \text{ mN/m}^2 \text{ at } 700 \text{ K}$$

The apparent viscosities using the Bingham model at 300 s^{-1} shear rate are 7.8, 40.4, and $2.1 \text{ mPa}\cdot\text{s}$ (cP), respectively. The negative yield stress for the third model has not been explained, but the data were fit only over a very narrow shear rate range and this could very easily cause some problems at the zero shear rate point. More data on low shear rates would be needed to resolve this question.

2.1.2 Discussion

The curve shown in Fig. 2.2 is very similar to the one produced at 35 wt % Kentucky No. 9 coal/solvent slurry.¹ The point where the gel region begins is the same ($\sim 500 \text{ K}$) and the steepness of the increase in PLV pressure drop with temperature is similar. However, the ΔP is about 4-5 times that at the lower coal concentration. The flow curve (τ_w vs $8V/D$) at 700 K is also somewhat unexpected. Previous experience with Illinois No. 6 coal showed a continued drop in the flow index, n , as the slurry temperature increased above the gel temperature. The data obtained at 700 K showed a flow index of 1.655, significantly greater than 1. It also showed a very low viscosity, but this was expected. As yet, there is no explanation for this behavior, as we have ruled out major problems with the PLV instrument during the sampling procedure.

2.1.3 Future work

The rheological analyses of the Kentucky No. 9 coal-solvent slurries at a 1.6 solvent to coal ratio will continue through June 30, 1981, at which time work on this project will cease. The work that will begin on July 1 is the study of residence time effects on the rheology of Kentucky No. 9 slurry at 38.5 wt % solids and the measurement of coal/recycle solvent slurries downstream of the vapor/liquid separator. A final report on the coal-solvent mixture density and rheology will be written.

2.2 Thermal Conductivity

J. E. Mrochek and J. B. Overton

The objective of this project is to develop an instrument for measurement of the thermal conductivity of coal-solvent slurries under typical process conditions present in SRC and H-Coal liquefaction processes. The thermal conductivity instrument being developed is based on the transient hot-wire measurement technique. Instruments of this type have been successfully used for measurement of thermal conductivity of solids-free organic liquids; however, additional development and testing is required for use with coal slurries at elevated temperature and pressure. The ultimate objective of the project is to develop an instrument suitable for making thermal conductivity measurements in the Coal Liquids Flow System.

2.2.1 Progress

Experiments have been suspended pending repair of the line source gauge which was broken after measurements were completed on toluene.

2.3 Instrumentation for Measurement of CSD Feed Quality

M. S. Denton, S. R. Dinsmore, and W. D. Bostick

The objective of this project is to design, construct, and test a CSD feed quality monitor for initial installation at the Wilsonville pilot plant and for eventual use at the SRC-I demonstration plant. Economics of the SRC-I process are sensitive to SRC recovery from the Kerr-McGee CSD unit which is dependent on the asphaltene/preasphaltene (ASP/PASP) ratio of the feed. The ASP/PASP ratio may be controlled to some degree through control of the severity of treatment in the dissolver. Present methods of determining the ASP/PASP ratio rely on time-consuming laboratory extraction and analysis. On-line sampling and rapid analysis of the CSD unit feed quality would permit process control closer to optimum.

2.3.1 Work accomplished

Representatives from B/R Instrument Corp., Pasadena, Maryland, visited our laboratory to discuss means of increasing our solvent throughput with the spinning-band distillation unit. Our solvent recovery rate has been doubled (to ~2.6 L/h) by several modifications in the electronic controllers. It may be possible to double this rate again with a modification in the still glassware.

Concurrently, we investigated procedures to more effectively recover the dried solids from the collected fractions. The most effective procedure that we have found is to redissolve or resuspend the solids in a minimal volume of THF and hexane, evaporate the suspension to dryness in a water bath (~90°C), and place the solids in a vacuum oven (50-60°C, -70 KPa) for a minimum of one day. This azeotropic procedure appears to more efficiently remove adsorbed or occluded moisture and original solvent.

We performed a repeat SESC run for sample 217-C-MC ("good" SRC recovery). In general, the distribution of recovered solids was very similar to that of the first run. There was some variation of the distribution within the three fractions (Nos. 3-5) representing asphaltenes (ASP), although the sum of these fractions was very similar (53 vs 57 weight percent).

2.3.2 Future work

The next scheduled run will be that of a CSD feed with a high ASP/PASP ratio of 3.2 (Wilsonville Soxhlet extraction values). This will complete the third sample in a series of varying CSD feed qualities.

2.4 Reference for Section 2

1. L. E. McNeese (ed.) *Fossil Energy Program Quarterly Progress Report for the Period Ending June 30, 1980*, ORNL-5671, Oak Ridge National Laboratory, Oak Ridge, TN (October 1980).

3. CHEMICAL RESEARCH AND DEVELOPMENT

M. L. Poutsma

This Section describes three projects carried out for the Office of Coal Processing. All three involve joint efforts of the Chemistry and Chemical Technology Divisions while one (Sec. 3.3) also includes work in the Metals and Ceramics and Engineering Technology Divisions. Additional work in the Chemistry Division sponsored by the Office of Basic Energy Sciences is not reported monthly but is described in the Fossil Energy Program Quarterly Reports.

3.1 New Liquefaction Techniques

B. R. Rodgers,* J. W. Larsen, B. M. Benjamin,
M. S. Hendricks, and T. L. Sams*

The overall objective of this project is to explore new reactions of coal with a view toward formulation and initial experimental laboratory evaluation of new process concepts to convert coal to liquid fuels. The present focus derives from our observations that coals can be extensively liquefied by heating in the presence of phenol in the absence of externally supplied hydrogen. We have conceptualized a closed-loop process in which oxidation of a portion of the feed coal or char would generate a mixture of polycarboxylic acids which would be oxidatively decarboxylated to produce a mixture of polyhydroxybenzenes for liquefaction. Recent efforts have focused on the liquefaction performance of the dihydroxybenzenes as compared with phenol and on the oxidative decarboxylation reaction applied to benzenepolycarboxylic acids.

The previous few reports described scoping studies of the reactions of Wyodak sub-bituminous coal with the three individual isomeric dihydroxybenzenes. Although high conversion of coal to pyridine-soluble material could be achieved, extensive incorporation of the dihydroxybenzenes into coal-derived products accompanied the solubilization. A parallel set of scoping experiments is now in progress for a Bruceton bituminous coal. Conversion in hydroquinone was 82% at 460°C (860°F), 67% at 441°C (825°F), and 45% at 400°C (752°F). Incorporation was high at all three temperatures, amounting to more than half the recovered material at 460°C. Incorporation of resorcinol into the coal-derived product was also severe at all temperatures, being 4 times the original weight of coal at 460°C, and 3 times at 400°C. Conversion with resorcinol was 87% at 460°C and 72% at 441°C. Results with resorcinol at 400°C and results with catechol are not yet complete. We are currently studying the literature accounts of the thermal reactions and free-radical reactions of the dihydroxybenzenes in an effort to find ways to reduce incorporation of these materials into the coal-derived products.

*Chemical Technology Division.

The Cu^{2+} -catalyzed oxidative decarboxylation of a simulated mixture of benzenepolycarboxylic acids containing isophthalic, trimellitic pyromellitic, trimesic, and terephthalic acids in a weight ratio of 5:32:40:9:14 continued to give operating problems with our present reactor system. Another run was attempted using only the di, tri-, and tetra-benzenecarboxylic acids which were most prevalent in the mixture (terephthalic - 16%, trimellitic - 37%, pyromellitic - 47%). However, the same type of problems occurred with this mixture. Various mixture melting points are currently being run to better define reactor operating conditions. The 230°C run on the full mixture that was reported last month has been separated and is being analyzed. Thus far, phenol and isophthalic, terephthalic and benzoic acids have been identified. The latter is particularly interesting since benzoic was not present in the original mixture.

3.2 Indirect Liquefaction Chemical Research

This project is focused on improved understanding of the behavior of Fischer-Tropsch catalysts under typical operating conditions. We are currently investigating the significance of olefins as gas-phase intermediates in determining molecular weight distributions of products as well as exploring the effects of steam in controlling catalyst aging.

3.2.1 Fischer-Tropsch mechanism studies - (R. A. Strehlow, E. C. Douglas, and B. M. Benjamin)

Decarbonization of Fischer-Tropsch catalysts by hydrogen is well known to produce methane. We attempted to use deuterium in one series of experiments to determine if it were possible to assay the hydrogen content of waxes normally assumed to exist in the pores of used catalyst. Adding deuterium after having quenched the CO/H_2 reaction with helium (until the pressure of hydrogen was negligible) led to the results shown in Table 3.1. Negligible CH_3D was observed. Although d_4 -methane dominated the mixture for 40 minutes, there appeared to be a continuing source of CH_4 which did not equilibrate with the deuterated methanes. After 41 minutes of deuterium exposure, the system was flushed and the deuterium was replaced by hydrogen. Within a few minutes the deuterated products had significantly decreased and CH_3D was observed. The amount of protium observed was ~50 cc (STP) from ~1 g of catalyst.

We believe that experiments of this type may be developed to permit identification of some surface CH_x groups. The presence of CD is indicated but not proved in the present experiment at 45 minutes, while large amounts of CH_2 groups were not observed in the initial deuteration.

In a separate determination relating to waxes and other products produced in Fischer-Tropsch syntheses, an analysis was made of a residue in the reactor system after shutdown. Although the work reported last month showed unusual concentrations of aromatic compounds, the accumulated high molecular weight products were quite normal with straight-chain

Table 3.1. Deutero-methanes produced by deuterium treatment of a used FT catalyst

Species	Minutes, %			
	2	12	15	45*
CD ₄	36	37	43	14
CHD ₃	28	27	27	15
CH ₂ D ₂	18	24	19	16
CH ₃ D	--	--	--	17
CH ₄	17	11	10	39

*Four minutes after flushing and switching gas to H₂.

alkanes and alkenes dominating the product mixture and with about 1% alkylbenzenes (formed by dehydrocyclization of olefins).

3.2.3 Fischer-Tropsch catalyst aging studies - (J. H. Wilson,* S. L. LeStrange,* T. V. Dinsmore,* and B. R. Rodgers*)

Last month it was reported that essentially no catalytic activity was evident when the synthesis gas conversion unit was started up with water injection. Upon terminating water injection, conversion was observed. After the unit operation appeared to be at a steady-state condition with a H₂/CO ratio of 2/1 in the feed gas, water was again injected into the reactor. As a result, the conversion of hydrogen and carbon monoxide decreased, but not drastically. However, upon lowering the H₂/CO ratio to 1/1, the reaction rate dropped appreciably. These results appear to be consistent with the kinetic rate equation, reported by Dry [Ind. Eng. Chem., Prod. Res. Dev., 1976, 15, 282] which states that

$$r = k \left(\frac{\rho_{CO} \cdot \rho_{H_2}}{\rho_{CO} + a \rho_{H_2O}} \right),$$

*Chemical Technology Division

where r is the reaction rate, k is the kinetic rate constant, ρ_{CO} , ρ_{H_2} , and ρ_{H_2O} are partial pressures of the indicated components, and $\frac{r_a}{r_d}$ is the ratio of the rates of adsorption and desorption of water and carbon monoxide. To offset the decrease in reaction rate caused by increased levels of CO and H₂O, higher reaction temperatures will be investigated. Upon establishing conditions which produce an acceptable reaction rate, the effect of water injection on catalyst life at a low H₂/CO ratio in the feed gas will be studied.

3.3 Selective Beneficiation and Short Contact Time (SCT) Liquefaction

3.3.1 Selective beneficiation for liquefaction by magnetic separation - (E. C. Hise,* L. A. Harris,** B. R. Rodgers***, and B. M. Benjamin)

The objective of this task is to explore the potential of open-gradient magnetic separation (OGMS) to prepare beneficiated fractions and/or blends for SCT liquefaction. A sample drum of coal marked "Kentucky #9, underground Fies" was received from Catalytic, Inc., Wilsonville, Alabama. The size consist as received was 3/4" x 0. The coal was air dried, crushed, screened into size fractions at 30 and 100 mesh, and stored in an inert atmosphere. Two representative samples of the 30 x 100 size fraction yielded the chemical analyses: total S, 3.05, 2.93%; pyritic S, 0.45, 0.46%; ash, 7.82, 7.83%. A 630-gram sample was selectively beneficiated in the magnetic separator into nine fractions. The weight % and chemical analyses of the fractions are shown in Table 3.2. For this particular separation of this coal, 42.6 wt % (or about 47% of the heating value) was obtained as a "pure" fraction containing 2.48% sulfur and 4.55% ash. Fractions 2 through 6 could be considered a "middling" product and aggregate 37.4 wt % averaging 2.95% sulfur and 8.9% ash. Fractions 7 through 9 could be considered the "refuse" and aggregate 20 wt % averaging 3.43% sulfur and 14.2% ash. However, because of the remarkable analysis of the feed material the "refuse" fraction is appreciably better than ROM Kentucky #9.

As noted above, the feed contained only 0.45% pyritic sulfur so that little sulfur reduction in the clean fraction or concentration in the refuse could be expected. A similar argument applies to ash. The Bureau of Mines Report of Investigation, R.I. 8118, lists analyses of channel samples (containing no out-of-seam material) for 14 different locations of the Kentucky #9 seam. These analyses are summarized in Table 3.3.

*Engineering Technology Division.

**Metals and Ceramics Division.

***Chemical Technology Division .

Table 3.2. Analytical results for OGMS fractions
from Kentucky #9 coal (Fies)

Sample # ^a	Wt %	Analyses ^b				
		% C	% H	% N	% S	% Ash
Feed	-	72.15	5.15	1.44	2.74	7.71
1	42.6	75.19	5.58	1.54	2.48	4.55
2	8.9	72.26	5.25	1.49	2.82	7.65
3	7.6	72.27	5.29	1.49	2.93	7.76
4	7.8	72.60	5.31	1.49	2.96	9.25
5	7.4	71.47	5.20	1.47	2.95	9.56
6	5.7	67.94	5.11	1.40	3.16	11.05
7	5.4	66.88	5.31	1.26	3.22	12.50
8	6.9	64.66	4.87	1.10	3.40	14.12
9	7.7	60.85	4.98	1.32	3.63	15.38

^aNumbers increase from the diamagnetic to the paramagnetic fractions.
^bAverage of duplicate analyses.

Table 3.3. Reported analyses of coal
from Kentucky #9 seam

	Total Sulfur	Pyrite Sulfur	Ash
High	4.79	3.02	20
Low	3.60	1.49	8.1
Average	4.22	2.3	12.2

The ROM samples that we receive from TVA Paradise site are comparable to the average to high figures. Clearly, the Fies sample is from an extraordinarily clean deposit and/or has been washed. This is desirable as regards the properties of the fraction #1. However, if a concentration of pyrite in fraction #9 is desirable to test as a catalyst, that concentrated pyrite will have to be obtained elsewhere.

These samples are being liquefied in a blended SCT solvent from Conoco Coal Development Corp. Runs are being made in tubing bombs at 425°C for 5 min with a 3 min heatup time. Initial results are shown in Table 3.4.

Table 3.4. Elemental analysis and conversion results for selected beneficiated samples (see Table 3.2)

Sample	C (%)	H (%)	N (%)	S (%)	Ash (%)	MAF Conversion (%)
Feed	72.15	5.15	1.44	2.74	7.71	79
Fraction No. 1	75.19	5.58	1.54	2.48	4.55	89
Fraction No. 9	60.85	4.98	1.32	3.63	15.38	71

These preliminary results indicate that there are indeed differences among the beneficiated fractions when they are processed under SCT conditions. The fraction with the highest ash content and lowest carbon content (Fraction No. 9) exhibits the lowest ash-free conversion. This relatively low conversion was somewhat surprising in view of the catalytic effect of mineral matter reported in much of the literature. It might be a result of a lower percentage of reactive macerals present in the beneficiated sample or it could be due to an unexplained inhibitory effect of the mineral matter. Further tests will be performed to determine whether or not the recorded differences are statistically significant.

3.3.2. Solvent performance correlations - (B. M. Benjamin and E. C. Douglas)

The objective of this task is a search for correlations between the chemical properties of recycle solvents and their SCT performance. To this end, one of the chemical properties we will investigate is the ability of the solvent to serve as a hydrogen transport or hydrogen shuttling agent. Our first experimental approach will be to determine specific types of hydrogens which participate in hydrogen shuttling as indicated by hydrogen-deuterium exchange.

In the previous report we described the advantages, limitations, and applications of ^2H nmr at 47,000 Gauss. We have now applied ^2H nmr to several of our samples which have undergone thermal exchange with diphenylmethane- d_2 . Thus the ^2H nmr spectrum of 1,2-benzanthracene, exchanged for two hours at 400°C , integrated against natural abundance deuterium in the solvent, 1,2-dichloroethane, showed 4.03% exchange. This is compared with 3.92% exchange determined by gc-ms. The spectrum showed two strong peaks at $\delta = 9.13$ ppm and 8.32 ppm indicating exchange principally at H-9 and H-10. Smaller amounts of exchange were apparent in other positions as indicated by peaks at $\delta = 8.04$ ppm, 7.73 ppm, and 7.58 ppm. The almost complete absence of a peak at $\delta = 8.75$ ppm indicates that exchange is slowest at position 1. All the features mentioned above were more prominent in the spectrum of the sample exchanged for five hours. Chrysene exchanges fastest at the 1, 4, 5, 6 positions and to a lesser extent at the 2,3 positions. The 1-position of perylene exhibited more exchange than the 2-position while almost no exchange occurred at the 3 position. Exchange was not positionally selective for triphenylene while the chemical shift range was not large enough to distinguish the various positions in pyrene.

We have investigated hydrogen-deuterium exchange for three heterocyclic aromatics. The results are as follows: dibenzofuran and dibenzothiophene do not exchange significantly with diphenylmethane- d_2 at 400° in five hours. However, the nitrogen-containing analogue, carbazole, was 6.1% deuterated in 2 hours and 19.8% deuterated in 5 hours.

3.3.3 SCT product stability - (J. E. Wortman,* R. K. Hessley,* T. V. Dinsmore,* and B. R. Rodgers*)

Fractionation of SCT product obtained from Kentucky No. 9 coal and Wilsonville recycle solvent continued. Several runs in the reaction severity region of 20-30 have been made. Preliminary results are shown in Table 3.5. The results for the $R_s = 30$ run represent an average of the analyses of two samples which were run simultaneously in the tubing bombs. The data for the $R_s = 24$ run were obtained from the analysis of the products from one bomb; replicate analysis is currently underway. Although no firm conclusions can yet be drawn from these data, the fact that there is a higher conversion for the lower severity run might indicate that there is an optimum value of severity in the $R_s = 20$ to 30 region. Further experiments will explore this possibility.

Table 3.5. Fractionation analysis (wt % composition) of SCT products

Reaction Severity	Preasphaltenes (%)	Asphaltenes (%)	Oils (%)	Residue (%)
30	20	17	47	16
24	18	28	46	8

*Chemical Technology Division

4. MATERIALS TECHNOLOGY

R. A. Bradley

This section describes the research and development performed on the Advanced Research and Technology Development (AR&TD) Fossil Energy Materials Program supported by the Department of Energy's Fossil Energy Office of Advanced Research and Technology. It includes tasks on pressure vessels and piping materials, welding and cladding development, corrosion of AFBC materials, failure prevention and analysis in coal liquefaction plants and fluidized-bed combustion systems, materials research for liquefaction systems, development of modified 9 Cr-1 Mo alloy, materials for ceramic recuperators, and identification and quantification of the critical materials requirements for designated synthetic fuels facilities. In addition to the above tasks on the AR&TD Fossil Energy Materials Program, this section includes work sponsored by the Pittsburgh Energy Technology Center on ceramic heat exchangers and by the Morgantown Energy Technology Center on an oxygen monitoring system for fluidized-bed combustors and an assessment of materials and components experience in gasification pilot plants.

4.1 Pressure Vessel and Piping Materials

W. J. Stelzman and D. A. Canonico

The purpose of this task is to investigate the fracture toughness and hydrogen attack of pressure vessel steels. During this period we have completed the DATA TRAK portion of the heat treatments of the $12.7 \times 12.7 \times 127$ -mm bars ($1/2 \times 1/2 \times 5$ in.) from the six 19-mm-thick ($3/4$ -in.) modified 2 1/4 Cr-1 Mo-1/2 Ni steel plates from U.S. Steel. We have simulated the quench cycle of 254- to 305-mm-thick (10-12 in.) plate at the surface and at the quarter-thickness depth and are tempering bars for 6 h at 663°C (1225°F). The temper will be followed by a postweld heat treatment (PWHT) of bars for 28 h at 691°C (1275°F), air cooling after each heat treatment.

The bars from the Japan Steel Works V-Ti-B modified 2 1/4 Cr-1 Mo have been machined into Charpy-V and tensile specimens and are awaiting testing.

4.2 Welding and Cladding Development

D. P. Edmonds and G. M. Goodwin

The purpose of this task is to investigate and develop techniques for welding and cladding components for coal conversion. During this reporting period we have evaluated data from room-temperature Charpy impact testing for specimens taken from the 300-mm-thick (12-in.) plate of 2 1/4 Cr-1 Mo steel obtained from Chicago Bridge and Iron Company. These specimens have been exposed to simulated weld heat-affected zone (HAZ) thermal cycles shown in Table 4.1. Simulation was performed using Gleeble testing

Table 4.1. Thermal cycles for heat-affected zone simulation study

Cycle number	Aim thermal cycles [Peak temperature (°C)/cooling rate (°C/s)]		
	First	Second	Third
A	1370/44		
B	1370/22		
C	1370/17		
D	955/22		
E	955/17		
F	955/11		
G	730/17		
H	730/11		
J	730/6		
K	1370/44	955/17	
L	1370/22	955/17	
M	1370/44	730/11	
N	1370/22	730/11	
P	955/22	730/11	
R	955/17	730/11	
S	1370/44	955/17	730/11
T	1370/22	955/17	730/11

equipment. Thermal cycles were monitored using Chromel-alumel thermocouples, spot welded to each specimen, and were recorded on strip charts.

For each of the thermal cycles, four weak-direction specimens (test plane parallel to rolling direction) were prepared, two for testing as welded and two in the PWHT condition. Four additional weak-direction specimens were prepared using thermal cycle B, to investigate the effects of PWHT time. Several strong direction specimens were also prepared using thermal cycles B, E, and H, to investigate directionality of properties. Specimens were then machined to final size, notched, and impact tested at room temperature. Effects of cooling rate and PWHT on impact energy of the single cycle specimens are summarized below.

There is not a significant variation in the as-welded impact energy with cooling rates from temperatures above the A_{c3} (955–1370°C). Impact energy shows only a slight increase with increasing cooling rate from 1370°C and a slight decrease with increasing cooling rate from 955°C. One would expect a slight decrease in impact energy with increasing cooling rates from these temperatures. For specimens cooled from 730°C, which is below the A_{c1} , high impact energies were observed with no significant variations with cooling rates. These high values would be expected, since heating in this range only tempers the microstructure.

As expected, significant improvements in impact energy result from PWHT of specimens heated to the two higher peak temperatures. Only slight improvements result from PWHT of specimens heated to the lower peak temperature. Impact energies for the strong direction are significantly lower than for the weak direction, except for specimens heated to 1370°C peak, most of which fall on or near the lower shelf energy. Finally, as peak temperature increases impact energy of as-welded specimens decreases significantly and impact energy after PWHT increases. In conclusion, it appears that peak temperature has a greater affect on impact energy of the single cycle specimens (simulating the HAZ of a single pass weld) than does expected variations in cooling rate.

Additional evaluation of data is under way for the multicycle simulated specimens simulating the HAZ of multipass weldments. Also, micro-hardness testing is being performed for tested specimens in an attempt to correlate the above Charpy impact data to observations made for an actual weldment HAZ in this base metal.

4.3 Corrosion of AFBC Heat Exchanger Materials

J. H. DeVan and P. J. Ficalora

The purpose of this task is to perform tests to evaluate the oxidation-sulfidation response of candidate heat exchanger alloys as a function of oxygen and sulfur partial pressures at 850°C and to determine the role of CaSO_4 in the corrosion process.

A glass fluidized bed has been constructed in an effort to determine the conditions under which a CaSO_4 film can be formed on a heated metal substrate. Two 16-h experiments have been completed to date. The bed material in both experiments was CaSO_4 and the metal substrate was type 308 stainless steel wire. In the first experiment the substrate was heated to 500°C and in the second to 800°C. After each experiment the wire was examined optically and that part of the wire immersed in the bed was compared with a section of the wire which was at the same temperature but protected by an alumina sheath. The specimen held at 500°C had been attacked by the CaSO_4 but was not covered by a sulfate film. The specimen held at 800°C also showed signs of attack and was coated by a noncontinuous film of sulfate. These experiments will be continued for longer times at 800°C and under conditions where the bed is the eutectic CaO-CaSO_4 composition.

The equipment to measure the rate of reaction on a rapidly changing P_{O_2} is being assembled. The pumping system is now completed and the main chamber has been constructed and mounted on the pumping system. The quadrupole mass analyzer and titanium sublimation pump have been added to the main chambers and are functional. The flange which contains the gas inlet valves, equilibrating furnace, and specimen has been machined and is being assembled.

4.4 Failure Prevention and Analysis in Coal Liquefaction Systems

R. W. Swindeman

4.4.1 Support for the Wilsonville SRC Pilot Plant — J. R. Keiser and G. C. Marsh

Four sections of tubing from the Kerr-McGee critical solvent deashing (CSD) unit at the Wilsonville SRC pilot plant were sent to ORNL for examination. Each section included a 12-in.-length of 3/4-in. tubing which served as a jacket around the 3/4-in. tubing. A section which failed, apparently from corrosion on the inner diameter of the smaller tubing, was sent to Kerr-McGee for examination. Adjacent pieces sent to ORNL are currently being examined metallographically.

4.5 Materials Research for Liquefaction Systems

R. R. Judkins

4.5.1 Studies of general corrosion in coal liquefaction plants — J. R. Keiser, M. Howell, and J. F. Newsome

The purpose of this work is to determine the potential for general corrosion in coal liquefaction plants. The corrosivity of the fluids is measured by exposing corrosion coupons in a number of vessels in the Fort Lewis and Wilsonville SRC Pilot Plants, and the Catlettsburg H-Coal Pilot Plant. No coupon racks were shipped or received during this month. Examination was completed on four racks of coupons removed from the Catlettsburg H-Coal N-202 fractionator. Results are presented in Sect. 6.4.2 of this report.

4.6 Development of Modified 9 Cr-1 Mo Structural Steel

V. K. Sikka

Large heat fabrication, mechanical property characterization, and weldability studies continued this last month.

The modified 9 Cr-1 Mo has high-temperature strength properties, but it offers limited resistance to corrosion in sulfur-containing environments. To improve corrosion resistance in these environments, two types of coatings will be examined. These will be of aluminum and chromium type. The aluminum coatings will be put on many test coupons, tubing, tensile and fatigue test bars and some plate for weldability studies. An order to do this work was placed with Alon Company in Pennsylvania. The chromium coating will also be tried on similar kinds of test material. This will be done at Combustion-Engineering in Chattanooga, Tennessee. Coupons will be installed in a gasifier for corrosion response, whereas tensile and fatigue bars will be used to check any influence of coatings on mechanical properties.

4.7 Evaluation of Materials for Use in Ceramic Heat Exchangers

V. J. Tennery

4.7.1 Tubular materials — M. K. Ferber

In this reporting period, the Ceramic Recuperator Analysis Facility (CRAF) Test 3 was completed. In this experiment, several candidate ceramic materials for high-temperature heat exchanger applications were exposed to the combustion products of a basic coal carried in a Venezuelan crude-derived No. 6 fuel oil. The materials included two tubes each of KT SiC, α -SiC, Coors SC-2 SiC, and AD 998 Al₂O₃ plus one tube each of CVD SiC, CVR SiC, three types of sialon ceramics, and one NC 430 SiC containing a proprietary butt-joint at tube midspan. The three sialons are designated as GE-128, GE-129, and GE-130. Descriptions of all materials with the exception of the SC-2 and CVR SiC have been given elsewhere.¹⁻³ The SC-2 SiC is a siliconized silicon carbide which is very similar to KT and NC 430 SiC. The CVR SiC is an experimental material that is prepared by initially reacting Si with a graphite mandrel at 1800°C and then applying a chemically vapor deposited (CVD) overlay of SiC. During the exposure which lasted for approximately 240 h, the tubes achieved a nominal temperature of 1230°C.

Observations made of the tubular specimens during combustion gas exposure in CRAF Test 3 indicate that the slag from the Hanna Seam (Wyoming) coal used in the coal-oil-mixture (COM) fuel was very fluid at the exposure temperatures of about 1230°C, as anticipated. This fluid condition coupled with the relatively basic chemistry of the slag is anticipated to be the most corrosive long-term exposure of structural ceramics conducted anywhere to date.

During this experiment, approximately 18.9 Mg of fuel was burned including 3778 kg of coal which included about 189 kg of ash. In the next quarter, the structural ceramic specimens from this experiment will be analyzed to determine their general stability in this environment and to determine the mechanisms of corrosion as well as its effect upon the mechanical properties. Air delivered by a secondary fan and flowing through the tubes was heated to about 340°C during this experiment.

The report of CRAF Test 2 was completed in draft form and typed in preparation for internal review and publication.

Discussions are under way concerning potential contract work oriented to an analysis of the energy and performance benefits possible due to use of ceramic heat exchangers in selected fossil energy systems.

4.7.2 Property studies — P. F. Becher

Flexure bar-type samples of three silicon nitride (NC-132,* NC-34,* and SSN-522[†]) and three silicon carbide (NC-203,* KT,[‡] and sintered- α) ceramics were placed in KT SiC fixtures in the flue of the CRAF. These samples were then exposed for about 240 h at about 1220°C to the combustion products of a mixture of 20% coal (basic ash) and No. 6 fuel oil [Combustion Exposure (CE) Test 2]. The test was completed late in the month and some preliminary observations are worth noting. The basic nature of the slag, which was quite fluid at temperature, was much more aggressive in attacking the above ceramics than the acid slag produced in CE-1. After CE-2, very few of the ceramic specimens remained intact, and those that did remain reasonably intact appear to have fallen into the combustion chamber early in the test. In fact, visual observations during the run indicated that the samples ($\sim 0.25 \times 0.5$ cm) corroded completely through their cross sections some time between about 70 h and 100 h of exposure. The few bars that experienced environmental conditions less severe than those existing in the flue, as well as a few very thin sections of bars that were caught on the exit flue surface, are being analyzed.

4.8 Oxygen Measuring Systems for Fluidized Bed Combustors

J. I. Federer

Stainless steel and nickel-based alloy steam generator tubes tend to corrode in low oxygen-high sulfur environments of fluidized bed combustors (FBCs) burning coal. An oxygen measuring system (OMS) is needed to aid in interpreting corrosion behavior and to establish and maintain optimum combustion conditions. Ceramic electrolytes have greater potential for making the required measurements in an FBC than any other commercially available device. Preparations are being made to test ceramic electrolyte oxygen probes in a laboratory apparatus under controlled conditions. The test apparatus including the test chamber, gas metering/mixing system, and signal display system are mostly available and are being assembled; however, some components of the test chamber are still not available.

Two oxygen probes furnished by Corning are on hand and will be tested when the apparatus is ready. These probes consist of stabilized zirconia electrolytes in alumina protection tubes. The two probes are similar except that one has a porous ceramic protective layer over the electrolyte. The response time of the probes, one of the key characteristics to be evaluated, may be adversely increased by the protective layer. Delivery of two other probes from another source is still anticipated. Since these are not provided with protection tubes, our own design will be used. The protection tube/electrolyte assembly will be designed to promote rapid response time to changes in oxygen concentration.

*Product of Norton Company, Worchester, Massachusetts.

[†]Product of Carborundum Company, Niagara Falls, New York.

[‡]Product of AirCasting Company, Torrance, California.

An assembly has also been designed and is being prepared for further testing of titanium dioxide thermistors. As reported last month, these thermistors exhibit large variations in electrical resistance as a function of oxygen concentration of the surrounding atmosphere at 750°C. The new assembly will allow the response time of the thermistors to be evaluated in the test apparatus that is being assembled.

4.9 Materials and Components for Coal Gasification Systems

J. P. Hammond

In company with representatives of IIT Research Institute (IITRI) and the Metal Properties Council, Inc. (MPC), a visit was made to the Mountain Fuel Resources, Inc. (MFRI), Salt Lake City, Utah, on June 26, 1981, for the purpose of planning for surveillance testing (Phase II of the MPC erosion-corrosion program) in the Mountain Fuel coal gasification process development unit (PDU), which is presently being designed. The current MPC contract specifies fabrication of six racks for testing. Since it now appears that construction on the PDU will not begin until 1982, there will be ample time to provide access for test racks in the PDU, and IITRI will shortly submit a proposal to MFRI for the placement of racks in the PDU. During the visit, we had an opportunity to discuss some of the design and materials problems associated with the PDU, which are briefly discussed below.

This process uses a single-stage, entrained-flow, intermediate-pressure [2.07 MPa (300 psig)], oxygen-blown, ash slagging gasifier. It is intended to use both caking and noncaking varieties of coal (Utah bituminous of <1.0% S at the start) of a size of 70%, 200 mesh and will be aimed at an intermediate heating value gas [11.2 MJ/m³ (300 Btu/scf)] suitable for industrial use. The current PDU design has a capacity of 30 tons of coal per day, which was developed from a laboratory gasifier of 0.5 tons/day size. Studies for a 600 tons/day commercial plant are under way.

Unique features of the Mountain Fuel process include the incorporation of a radiant heat exchanger in the gasifier that cools the downflowing product gases from the combustor from a temperature of 1566 to 871°C (2850–1600°F). An abrupt increase in flow area at the entrance of this heat recovery unit is provided to cause the slag flowing down the walls of the combustor to fall as droplets through the heat exchangers into a slag quench system located below. The outflowing product gas possibly will receive moderate water quenching before or after exiting the gasifier, at which point it passes through two convective heat exchangers. The first of these cools the product gases to about 682°C (1260°F) which preheating boiler feed water that is supplied to the radiant heat exchanger. The second superheats steam [>413°C (755°F), 4.34 MPa (530 psig)] raised from the radiant heat exchanger, for various uses in the gasifier system. The product gases, on emerging from the heat exchangers, pass through a particulate removal system that features a Venturi scrubber and a glycol dryer. The water and solids (5% of the original coal, composed equally of ash and char) from the scrubber are disposed of whereas a fraction of the product gas is used as

the vehicle for fuel transport. Standard off-the-shelf acid removal and sulfur production units would be used in a commercial plant and therefore do not constitute areas of development.

The fuel from the coal preparation system is brought into the pressure envelope of the gasifier system and quenched slag removed from it, through separate lockhopper systems. The pulverized coal, after pressurization, is dropped into a feed hopper, from which it is metered into the feed line by twin helical augers. From here the coal is transported to a single fuel injection nozzle at the top of the gasifier by "high-density fluid transport," a newly emerging technology for pneumatic transport. As the term implies, the fluid is carried at a significantly higher density than conventional and whereas erosion is less of a problem, propensity for plugging is greater.

The fuel injection unit passes coal plus product gas [at 38°C (100°F)] and oxygen plus superheated steam [399°F (750°F)] into the combustion chamber of the gasifier where it is burned. This chamber contains a 10.2-cm-thick (4-in.) refractory liner, the inner component of which presumably will be high in chromia content to resist the high-temperature molten slag. The radiant heat exchanger extends up to the top of the combustion chamber and thus provides some cooling for the refractory liner. The gasifier pressure vessel is to be built of the conventional tube-to-web, water wall construction that controls the temperature of the vessel.

Of the three waste heat recovery systems, the steam superheater is expected to present the most severe materials problems. Incoloy 800 presently is being considered for this unit. Since carbon and/or low alloy steel (1 1/4 Cr-1/2 Mo) will be used from the coal preparation system up to this point, welded transition joints at relatively high temperatures will be required to span the changeovers to metal of significantly different physical properties.

Interestingly, the earliest test of a construction material for the radiant heat exchanger was said to involve either types 316 or 321 stainless steel and this gave a service life of only 2 to 3 h. This testing was performed with the laboratory-scale gasifier and the heat exchanger at this time was a coil of tubing approximately 25.4 cm (10 in.) in diameter. Whereas it was cautioned that the feed water for the unit should be demineralized to guard against chloride stress-corrosion cracking, it was nevertheless stated that the tubing was thought to fail from the gas side (outside). Subsequently, a copper coil was substituted for the stainless steel one and this gave good performance. Finally, the present construction, that of a two-wall, annular exchanger fabricated of carbon steel, was developed. As has been repeatedly the case with other gasifier heat exchanger systems that are water-cooled, the carbon steel seems to have performed excellently.

Since the radiant heat exchanger will be directly exposed to the raw product gases of the gasifier, the Mountain Fuel process will be dependent upon a "stuffing" mechanism for shredding char-ash deposits that tend to

build up on the surfaces. Soot blowers for aiding in the removal of solids will probably be required within the gasifier as well as in the convective heat exchangers downstream.

4.10. Assessment of Strategic Materials for Synfuels Plants

D. L. Lennon and A. R. Olsen

The purpose of this task is to identify and quantify the critical materials requirements for designated synthetic fuel facilities, with the initial effort directed to a generic direct coal liquefaction facility.

The take-off of material requirements from the engineering data for the direct coal liquefaction facility continues. A search of literature and data banks has been initiated to determine material compositions of various equipments to minimize the labor involved in the engineering estimate.

The critical materials have been sorted into categories with priority being placed on quantification of those materials that are most critical by virtue of the combination of the U.S. dependence on unfriendly or potentially unreliable sources and their importance to the United States in general and the direct coal liquefaction facility specifically.

4.11 References for Section 4

1. G. C. Wei and V. J. Tennery, *Evaluation of Tubular Ceramic Heat Exchanger Materials in Residual Oil Combustion Environments*, ORNL/TM-7578 (April 1981).
2. V. J. Tennery and M. K. Ferber, *Evaluation of Tubular Ceramic Heat Exchanger Materials in Acidic Coal Ash from Coal-Oil-Mixture Combustion*, ORNL/TM (in press).
3. A. Gatti and M. J. Noone, *Methods of Fabricating Ceramic Materials*, DML-TR-77-135 (November 1977).

5. COMPONENT DEVELOPMENT AND PROCESS EVALUATION

D. M. Eissenberg

The objective of component development and process evaluation activities is to ensure that coal conversion (liquefaction, gasification, pyrolysis) processes, subsystems, and components have satisfactory functional performance, lifetime, reliability, and safety for their intended applications, and that sufficient component and subsystem performance data are available to permit process design optimizations. Activities to be carried out include performance and cost analyses; assessments of operating plants; field tests; operation of test loops; and the development of advanced processes, subsystems, and components.

Present activities are primarily those carried out as part of the technical support to large liquefaction projects. In addition, studies are being initiated aimed at the development of processes, subsystems, and components for more generic coal conversion applications.

5.1 Technical Support to Large Liquefaction Projects

P. K. Carlson, T. B. Conley, T. L. Dahl,
W. A. McAuley, L. F. Parsly and A. N. Smith

Activities in this area are in support of the H-Coal and SRC Demonstration Projects, and are described in more detail in Chapter 6 and Chapter 15.

5.2 New Initiatives in Coal Conversion

D. M. Eissenberg

As part of the Engineering Technology Division strategic planning activities, assessments are being carried out to identify and propose new initiatives in coal conversion. Current activities include an assessment of coal pyrolysis technology and a review of critical component technology for coal gasification processes.

5.2.1 Coal pyrolysis - D. M. Eissenberg, E. C. Fox, and A. P. Fraas

Objective - A review and assessment of coal pyrolysis technology and economics is being carried out to determine the feasibility of utilizing pyrolysis plants in conjunction with utility coal-fired power plants to produce useful liquids from the feed coal, with the utility burning the solid residue (char) as a substitute boiler fuel and either selling the coal liquids as syncrude or utilizing them as gas-turbine or oil-fired-boiler plant fuel.

Status summary - A preliminary comparison between a coupled coal pyrolysis system using a fluidized bed pyrolyzer and a fluidized bed combustor was made with a Lurgi-Ruhrgas pyrolyzer providing char into a conventional pulverized-char furnace. While there are some technical advantages to using the fluidized bed system, the thermal efficiency advantages, at least at atmospheric conditions, are small.

A planning meeting for a joint study between ORNL and several interested utilities is being organized. This meeting, which is tentatively scheduled for August, would initiate and make plans for a two-phase study of utility oriented coal pyrolysis. The emphasis of the study will be to assess the techno-economic issues related to utility coal pyrolysis in general and, in the second phase, to each individual utility.

5.2.2 Gasification component development - D. M. Eissenberg

Objective - The objective is to develop and test improved and advanced components for use in advanced coal gasification processes which provide cost-effective increased performance, reliability, efficiency, and safety. This work supports the gasifier component development program managed by METC for the DOE/FE, Division of Gasification.

Status summary - Draft FTP/A's for five tasks in support of the Gasification Component Development Program were submitted to METC and DOE/HQ for final review. Modifications have been made as requested, and the formal package will be submitted in July.

6. TECHNICAL SUPPORT TO MAJOR LIQUEFACTION PROJECTS

H. C. Cochran

Support is provided by Oak Ridge National Laboratory and Union Carbide Nuclear Division Engineering for the major liquefaction projects being managed by DOE Oak Ridge Operations--SRC I and SRC II Demonstration Plants, Tri-State and Breckinridge Commercial Plants, H-Coal Pilot Plant and Exxon Donor Solvent Projects. Activities are reported in five broad categories -- engineering and design review, liquefaction technology base, components, materials, and environmental and health.

6.1 Engineering and Design Review

C. B. Smith

Objective

This section reports on six work elements involving reviews, evaluations, and analyses of process, engineering, and designs presented in project documents for major coal liquefaction projects managed by the DOE Oak Ridge Operations Office. The objectives are to assess conformance of project technical elements with the data bases, to identify data gaps and technical problems, and to investigate identified anomalies and problems as directed and/or authorized by DOE-ORO. The projects on which these objectives are focused are defined below.

The SRC-I project involves the design, construction, and operation of a coal liquefaction plant for the production of a clean solid boiler fuel. The SRC-II project is for the production of a clean liquid boiler fuel. The detail design phase of the SRC-I project is cost-shared by the U. S. Government and the International Coal Refining Company (ICRC). The SRC-II detail design phase is cost-shared by the U. S. Government with Solvent Refined Coal International, Inc. (SRCII) and the governments of Germany and Japan.

The Tri-State project, a cooperative agreement project between the U. S. Government and the industrial entities, Texas Eastern Synfuels, Inc. and Texas Gas Synfuels Corp., involves the process design, cost estimate, and construction and operations planning for a commercial plant to produce transportation fuels and SNG with a SASOL-type process.

The Breckinridge Project is cost shared by the U. S. Government, Ashland Synthetic Fuels, Inc. (ASFI) and AIRCO Energy Corp. It involves the preparation of a preliminary design and cost estimate, and plans for construction and operation of a commercial scale H-Coal plant.

6.1.1 Document reviews - J. J. Kurtz, A. R. Irvine, A. R. Olsen,
W. R. Reed, J. Horton

Scope - To review project technical documents for objectivity, adequacy and accuracy in areas of interest requested by ORO and subject to available information.

Status summary - The SRC-I Utilities and Offsites DBM - Rev. 1 was reviewed and commented on. Comments were also offered on ICRC resolutions of specific issues raised in the review of the previous issue of the DBM. The majority of comments addressed omissions which were considered gaps in the basic description of Utilities and Offsites systems.

For the Breckinridge Project, three Phase 0 preliminary design reports, addressing seven major functional process areas, were reviewed and commented on. The comments identified a wide variety of inconsistencies, suggested several design modifications, and noted some uncertainties in the design base.

6.1.2 Design Reviews - J. J. Kurtz

Scope - To review the technical adequacy of engineering designs, and conformance with data base, subject to available detail, ORO review interests and review site considerations.

Status summary - Action was initiated for arranging a nondisclosure agreement for GKT proprietary data to allow UCC-ND/ORNL participation in the SRC-I Gasification Unit review at the ICRC office in mid-July.

6.1.3 Technical meetings - J. J. Kurtz

Scope - To monitor or participate in project meetings, as requested by ORO, as an aid in assessing project progress, status of issues, and problem areas.

Status summary - The SRC-I Project Technical Status Review meeting was attended. The project is currently proceeding at a prescribed pace to accommodate a certain funding level directed by DOE.

6.1.4 Process design reviews - A. R. Irvine, J. F. Fisher, K. H. Lin,
and B. R. Rodgers

Scope - To provide analysis of key areas of technical concern where the data base is insufficiently delineated or the process area is of considerable significance to direct liquefaction processes.

Status summary - Corrosion related work was undertaken to identify process modifications that might be useful in reducing corrosion in atmospheric pressure fractionators.

The experience of the M&C Division and of IMMR in distilling coal liquids has been examined in an effort to gain insight into the behavior of chlorine in a direct coal liquefaction plant. Three tests have been carried out, two at ONRL and one (possibly more) at IMMR in which a batch of chlorine containing oil was batch distilled. In all cases, there existed above the boiling liquid, a section of tubing which provided a degree of rectification. Differences existed in the size and nature of the tubing above the boiling liquids and no doubt there were differences in the rates of boilup. In all cases, the preponderance of the contained chlorine was evolved over a temperature range of $\sim 40^{\circ}\text{C}$. However, the temperature of the vapor at the top of the rectifying section when the chlorine came over varied from 185 to 250°C . The temperature of the liquid within the pot was not measured. A possible explanation for this phenomenon is that the products of dissociation of a coal liquid hydrochloride did not recombine with sufficient rapidity to trap dissociated hydrogen chloride in dissociated organic base as it refluxed back into the liquid. Thus, the temperature observed at the top of the rectifying section during the time of peak chlorine concentration could vary according to the effectiveness of the rectifying section and to the rate of boilup. Another possibility that seems less likely is that the decomposition temperature varied between tests. Inasmuch as two of the experiments were carried out with identical feed materials, this possibility seems unlikely.

Two additional simple tests to determine the nature of chlorine volatilization from coal liquids were devised. These tests will show the effectiveness of removal of chlorine from a relatively volatile coal liquid when it was under greater than 1 atmosphere pressure. In the first proposed test, 10% of the liquid will be vaporized and collected while the liquid is held at 270 to 300°C ; in the second case, no significant quantity of liquid will be vaporized, but corrosive gases volatilizing from the liquid phase will be trapped in the vapor space by a reactive metal surface.

6.1.5 Engineering support - R. A. Just, C. B. Smith

Scope - To perform technical studies, analyses and evaluations of specific engineering design subjects, as requested and/or authorized by DOE-ORO, focusing on project problems affecting plant design and operability.

Status summary - Pursuant to an informal request from the H-coal Pilot Plant management, and with informal approval from DOE-ORO, assistance was provided in evaluating the effect of refractory liner spalling on the H-Coal reactor wall temperature. Agreement between temperature measurements and results of a UCC-ND/ORNL developed computer model was obtained for an actual case. Reactor wall temperatures were projected for two hypothetical cases of refractory spalling.

6.1.6 General technical support - K. H. Lin, G. C. Frazier, R. Edwards, V. C. A. Vaughen, B. R. Rodgers, and C. B. Smith

Scope - To perform evaluations of documented R&D activities for the projects, and to perform intensive studies of limited scope on selected subjects requested and/or authorized by DOE/ORO.

Status summary - Further analysis of the coking data for the fired preheater from the Wilsonville Plant resulted in an improved correlation that can relate incipient coking to the heteroatom content of feed coal in addition to the inlet H₂ partial pressure, coal feed slurry concentration and residence time (estimated), preheater coil skin temperature (at the location of coke deposit) and solvent quality. The validity and usefulness of this preliminary correlation are expected to be strengthened as the coking data base is broadened. A limited amount of the dissolver coking data from the Harmarville P-99 unit was acquired, but has not yet been analyzed in detail. The data from the Ft. Lewis Plant and the EDS facility have not been received. Preparation of a final report on the coking study is underway.

6.2 Liquefaction Technology Base

B. R. Rodgers

This section reports on nine work elements with the overall objective of accumulating, evaluating, and maintaining a broad base of technical information on coal liquefaction

6.2.1 Liquefaction technology overview - K. H. Lin, V. C. A. Vaughen, and B. R. Rodgers

Objectives - The primary objectives of this task are: (1) To keep abreast of significant developments in coal liquefaction technology, (2) to evaluate and systematically document technical data of importance to plant design and operation derived from such developments, (3) to provide liaison between the major liquefaction pilot plants and DOE/ORO through technical representatives at these sites, and (4) to serve as a center for expediting flow of technical information pertaining to coal liquefaction technology.

Schedule, scope, and progress against milestones - The major effort will be directed toward evaluation of (1) R&D activities relevant to the liquefaction process data base, and (2) technical and experience data from pilot plants and PDUs that are crucial to the design and operations.

The task objectives will be accomplished through the following activities: 2.1.1 Liquefaction Technology File, 2.1.2 Direct Liquefaction Data Source Book, 2.1.3 Liquefaction Overview Report, 2.1.4 Technical Site Representatives, 2.1.5 Monitor R&D Meetings, 2.1.6 Property Data Base, and 2.1.7 Process Data Base Evaluations.

The key milestones for activities 2.1.1, 2.1.3, and 2.1.7, and progress toward them are listed below.

<u>Activity</u>	<u>Milestones</u>	<u>Completion Date</u>	<u>Status</u>
2.1.1	a. Complete indexing of up-to-date proprietary documents	Indefinitely postponed	On hold
	b. Complete indexing of most of earlier (prior to 1979) documents while maintaining file on recent (1979 and later) documents current	Indefinitely postponed	On hold
2.1.3	a. Complete first topical report	March 1981	Completed
	b. Complete second overview report	May 1981	Postponed in order to complete R&D evaluations
<u>Activity</u>	<u>Milestones</u>	<u>Completion Date</u>	<u>Status</u>
2.1.7	a. Complete Kerr-McGee data base compilation and initial evaluation for consistency.	February 1981	Completed
	b. Complete research for correlations between data base and process parameters.	March 1981	Interim report completed. Final report delayed.

Status summary

Liquefaction technology file (J. K. Huffstetler) - As of the end of June, approximately 500 citations are on the interactive computer data base. Four routings of documents received were sent to each of 16 program managers in the direct liquefaction file.

Data source book (J. P. Belk and W. R. Williams) - No activity this month.

Overview report (K. H. Lin, J. F. Fisher, A. R. Irvine, and F. M. O'Hara) - The revised drafts of individual contributions have been updated to cover significant developments through March 1981. Consolidation of the updated drafts is continuing.

Site representatives (S. P. N. Singh) - The H-Coal Pilot Plant Technical Advisory Committee (TAC) meeting held on June 3, 1981, was attended by the H-Coal Pilot Plant technical site representative designee (S. P. N. Singh). The plant was shut down for repair and maintenance during June 1981, and is expected to resume operation by July 1, 1981. A trip report summarizing the minutes of the TAC meeting was completed, and has been distributed. Among the significant developments was the loss of ebullation in the H-Coal reactor with a subsequent temperature excursion [up to $\sim 820^{\circ}\text{C}$ ($\sim 1500^{\circ}\text{F}$)] which led to termination of Run 7. During the run (7 days prior to shutdown), the plant had a net positive oil make, and no clarified slurry oil (petroleum-derived make-up solvent) was used.

R&D meetings (J. H. Wilson) - The Wilsonville Technical Review Meeting and the Planning and Scheduling Meeting were attended on June 23 and 24, respectively. The hydrotreater has been operating on SRC feed with 689 K (780°F) as the primary target temperature. The catalyst addition and withdrawal system is scheduled for installation this fall. The Critical Solvent Deashing unit was recently run at a feed rate of over 318 kg/h (700 lb/h) with very smooth operation. New controllers, which are not as sensitive to voltage drops, have been ordered for the heaters. Since the last meeting, 30 power drops have occurred that were sufficient to cut off the heaters. There was an apparent elevation in corrosion rate in T102 tower (vacuum column) when the entry point for T102 (Light Organics Recovery column) bottoms was moved up the column. More will be known about this in a few weeks. Beginning July 1, the pilot plant will be operated to obtain low severity data at 672 K (750°F) and a high space rate. The hydrotreater will be operated from 617 to 717 K (650 to 830°F) for one week. The operation will then continue for approximately two additional weeks at a temperature estimated to give 50% SRC conversion.

Properties data base coordination (B. R. Rodgers) - No activity this month.

Process data base evaluation (B. R. Rodgers) - Completion of the Kerr-McGee correlations have been delayed by another month.

6.2.2 Coal slurry mixing tests - J. K. Johnson, L. S. Dickerson, and B. R. Rodgers

Objective - The objective of this project is to study the changes that occur in physical properties (particularly viscosity) in coal slurries during mixing at temperatures up to 533 K (500°F). The system includes a small scale mix tank with an agitator and slurry circulation system of the type used for feed makeup in the SRC processes. Continuous viscosity measurements are made with on-line pipeline viscometers. The ultimate objective of the study is to establish conditions that will permit the slurry preparation system in the SRC demonstration plants to be operated at increased temperature, thereby improving the overall process thermal efficiency and cost.

Schedule, scope, and progress against milestones - New milestones have been requested and are being negotiated with DOE.

Status summary - The study of slurry rheology for Kentucky No. 9 coal in Wilsonville solvent has continued. The analysis of data obtained previously has been performed and two experimental runs were attempted.

An analysis was completed of data from runs SRC-I-3 and SRC-I-5 to determine why each pipeline viscometer produced a rheogram with a different slope¹. The findings show that the data previously reported are confounded by a least two phenomena: wall slippage and turbulence. The data of the Ft. Lewis solvent-Kentucky No. 9/14 system exhibit the effect of wall slippage in the viscometers. Compensation can be made for this effect using existing data. Furthermore, the behavior of the Wilsonville solvent-Kentucky No. 9 system appears to be explained by the onset of turbulence in the viscometers. However, in addition to these complications, the possible effect of solids settling in the experimental system is being investigated. Efforts are being made to quantify the effect and to correct it if necessary. Because of these problems, it must be stressed that all data previously reported are preliminary. The reported apparent viscosities will be corrected for non-Newtonian behavior and the aforementioned effects in the final report.

During the month of May, three tests were run. The first, SRC-I-6J, studied a 38.5 wt % slurry of Kentucky No. 9 coal (70% -200 mesh) at 450 K (350°F). After the addition of the coal to the preheated solvent, several plugs developed in the viscometer line and in the check valves of the metering pump. While the check valves were being cleaned, an obstruction formed in the discharge line of the metering pump, which forced the termination of this experiment.

Two tests were made to study the operability of the system at different temperatures, runs SRC-I-7 and SRC-I-8. The first studied a 38.5 wt % slurry of Kentucky No. 9 coal (70% -200 mesh) and Wilsonville solvent at 422 K (300°F). The coal was added to the preheated solvent over a period of 7 min. Difficulties with the check valves caused a delay of data acquisition of 52 min, after which the system ran for 330 min before the test was ended. During the run, the pressure taps on the intermediate size viscometer also plugged. The data for the vertical viscometer as well as the two remaining horizontal viscometers are shown in Fig. 6.1. The slope of this Rabinowitsch-Mooney plot is 0.910, indicating pseudo-plastic behavior. After correcting for non-Newtonian behavior,² the data were analyzed for both the Bingham plastic and the Casson models. Figure 6.2 shows the curve for the Bingham plastic model, while Fig. 6.3 shows that for the Casson model. Since the models should be linear on the respective coordinates used, it is evident that the Bingham plastic model is slightly better at this temperature.

ORNL DWG 81-861

Fig. 6.1. Rabinowitsch-Mooney plot for SRC-I-7.

ORNL DWG 81-856

Fig. 6.2. Bingham plastic model for SRC-I-7.

ORNL DWG 81-857

Fig. 6.3. Casson model for SRC-I-7.

Run SRC-I-8 examined the behavior of the slurry with a hot mixup at 478 K (400°F). Problems were encountered with the system which were apparently due to vaporization of the solvent. Thirteen percent of the solvent vaporized prior to the addition of the coal, and was collected in the condenser. Also, the dP readings were erratic as a result of vaporization of solvent in the lines. The first data were taken after a residence time of 61 min, but the taking of data was terminated when plugs developed in the pressure taps of three of the four viscometers. Due to the limited number of data points, all taken at the same flow rate, the results were inconclusive.

Run SRC-I-6K studied the 38.5 wt % Kentucky No. 9 slurry in Wilsonville solvent at 450 K (350°F). The procedure for coal addition was modified which permitted data acquisition to begin after an average residence time of 30 min. The Rabinowitsch-Mooney plot of these data is shown in Fig. 6.4. This figure shows behavior which could be attributed to the onset of turbulent flow, as previously discussed. A rheological characterization was made based on the lower curve, the results of which indicates pseudoplastic behavior. Only data from the horizontal viscometers were included; however, much of the initial data were in the apparent turbulent region. In addition, both the Bingham plastic and the Casson models were utilized to analyze the data. The results of these analyses are presented in Fig. 6.5 for the Bingham plastic model, and in Fig. 6.6 for the Casson model. It is evident that the Casson model produces a somewhat better fit to the experimental data.

During preparation for the next test, the connecting rod of the circulation pump was broken. While a new connecting rod was being installed, the braided teflon packing was replaced by a teflon impregnated asbestos material, which should provide greater dimensional stability at high temperatures.

Run SRC-I-6L was then attempted at the same conditions as the previous run. After the coal was added to the preheated solvent, plugs developed in the circulation line. After several obstructions in the intake of the circulation pump were removed, a plug developed which could not pass through the pump, and the run was terminated. Upon disassembly, it was found that the connecting rod had sheared during the run. The rotor, stator, and connecting rod were replaced, and an in-line strainer was added between the mix tank and the pump intake to prevent large particles from entering the pump. The system is currently being flushed in preparation for the next run.

6.2.3 Wet grinding studies - W. A. McAuley and D. M. Eissenberg

No activity this month.

Fig. 6.4. Rabinowitsch-Mooney plot for SRC-I-6K.

ORNL DWG 81-859

Fig. 6.5. Bingham plastic model for SRC-I-6K.

ORNL DWG 81-860

Fig. 6.6. Casson model for SRC-I-6K.

6.2.4 VSB viscosity - J. H. Wilson and B. R. Rodgers

Objective - The objective of this project is to provide a tested and calibrated instrument for installation at the Ft. Lewis SRC pilot plant or other suitable site which is capable of providing on-line viscosity measurement of residuals obtained from the vacuum still on the SRC-I and SRC-II processes. This type instrument is necessary to provide indication of the onset of irreversible polymerization or coking problems which would interfere with controlled feeding of vacuum still bottoms to a gasifier.

No activity this month.

6.2.5 Thermal conductivity - J. E. Mrochek, J. R. Hightower, and B. R. Rodgers

Objective - The objective of this project is to develop an instrument for measurement of the thermal conductivity of coal-solvent slurries under typical process conditions present in SRC and H-Coal liquefaction processes. The thermal conductivity instrument being developed is based on the transient hot-wire measurement technique. Instruments of this type have been successfully used for measurement of thermal conductivity of solids-free organic liquids; however, additional development and testing is required for use with coal slurries at elevated temperature and pressure.

Experimental measurements of the thermal conductivity of coal-solvent slurries are needed (by Gulf Research and Catalytic, Inc.) to verify models to be used for design and analysis of the fired slurry preheaters for SRC demonstration plants.

Schedule, scope, and progress against milestones - This work element includes completing fabrication of the high-pressure cell, calibration of the instrument with standard materials, installing it in the Coal Liquids Flow System at ORNL and making measurements using fresh coal liquids generated therein.

The following progress toward significant milestones has been achieved.

1. Operation of the high-temperature, high-pressure cell has been verified in the flow-through mode with isolating valves to 350 K (185°F).

Technical highlights - Breakage of the line source gauge has temporarily suspended further experimentation.

6.2.6 Rheology and density of H-Coal samples - D. D. Lee, M. R. Gibson, and B. R. Rodgers

Reporting on this project ended with the May monthly. A preliminary final report has been issued and a final report is in preparation.

6.2.7 Coal solvent mixtures - D. D. Lee, M. R. Gibson, J. H. Wilson,
and B. R. Rodgers

Objective - The objective of this work element is to provide measurements of rheology and density of coal-solvent mixtures simulating SRC-I conditions at high temperature and pressures using ORNL's existing capabilities for such measurements.

The International Coal Refining Company (ICRC) requires reliable measurements of the rheology and density of coal/recycle solvent slurries made from Kentucky No. 9 coal for design of feed pumps and the preheater for the SRC-I demonstration plant. The ICRC requires measurements of density and rheology of slurries of Kentucky No. 9 coal in Wilsonville recycle solvent at the following conditions: solvent-to-coal ratio (S/C) of 1.6, temperature in the range 300 to 730 K (250 to 850°F), and pressure in the range 0.1 to 17.2 MPa (14.7 to 2500 psia). They also require the variation in density over these temperature and pressure ranges at other solvent-to-coal ratios (in the range of 1.2 to 2.5).

Schedule, scope, and progress against milestones - The required information can be obtained using the Coal Liquids Flow System (CLFS) with coal on hand and solvent from a pilot plant run at Wilsonville at demonstration plant conditions (mid-January 1981).

The following progress toward significant milestones has been achieved.

1. Complete subtask 2 - February 28, 1981. Completed.
2. Complete subtasks 1, 3 and 4 - March 13, 1981. Subtasks 1 and 4 have been completed. Subtask 3, delayed due to priority work on EIS, will not be completed due to truncation of funds.
3. Complete subtask 5 - May 15, 1981. This subtask was delayed due to priority work on EIS.
 - A. Subtask 5 sub (a) - The rheology has been measured at 423, 450, 478, 505, 533, and 700 K and 17.24 MPa. Measurements will not be made at 588, 644, and 728 K due to truncation of funds.
 - B. Subtask 5 sub (b) will not be completed due to truncation of funds.
 - C. Subtask 5 sub (c) will not be completed due to truncation of funds.

Technical highlights - The rheology of Kentucky No. 9 Wilsonville recycle solvent and Kentucky No. 9 coal at a 1.6 solvent-to-coal ratio was determined at 17.24 MPa and temperatures of 423, 533, and 700 K. The apparent viscosities at the three temperatures and a shear rate of 300 s^{-1} are 7.9 mPa·s, 41.4 mPa·s, and 2.0 mPa·s, respectively. The gel region appears to begin at about 500 K and end between 650 and 700 K. The apparent viscosity increased sharply as the temperature increased above 500 K. The flow curves at the three temperatures gave slopes of 0.953, 0.709, and 1.655 at 425, 533, and 700 K, respectively.

6.2.8 Instrumentation for measurement of CSD feed quality - M. S. Denton, J. R. Hightower, and B. R. Rodgers

Objective - The objective of this work is to design, construct, and test a feed quality monitor for initial installation at the Wilsonville pilot plant and for eventual use at the SRC-I demonstration plant.

Economics of the SRC-I process are sensitive to SRC recovery from the Kerr-McGee CSD unit which is dependent on the asphaltene/preasphaltene ratio of the feed. The asphaltene/preasphaltene ratio may be controlled to some degree through the control of the severity of treatment in the dissolver. Present methods of determining the asphaltene/preasphaltene ratio rely on time-consuming laboratory extraction and analysis. On-line sampling and rapid analysis of the CSD unit feed quality would permit process control closer to optimum.

Schedule, scope, and progress against milestones - A system for CSD sampling and rapid analysis will be designed; the principle of operation of the system will be automated solvent elution chromatography. Commercially available chromatography system components will be procured and assembled. The prototype system will be calibrated and tested at ORNL on samples from the Wilsonville pilot plant. After calibration and testing, the system will be delivered to the pilot plant for field evaluation with the goal of ultimately installing a similar system on the SRC-I demonstration plant.

Significant milestones are discussed below.

1. Purchase and assemble equipment - May 1981. The project was frozen by DOE/ORO before any of the capital purchases could be made.
2. Develop sample loading protocol and solvent elution sequence - August 1981. On schedule. This is being carried out on in-house chromatographic equipment.

Technical highlights - Electronic control modifications of our spinning-band distillation unit have resulted in a doubling of our solvent throughput (to ~2.6 l/h). A further glassware modification promises to double this efficiency again. This cuts both our sample and solvent recovery times in half. An azeotropic procedure (described in Chapter 2) has been developed which solves the problem of retaining moisture in the recovered fractions. Finally, a repeat run of CSD feed sample 217-C-MB was run to determine the precision of the SESC fractionation (see Chapter 2).

6.2.9 CSD feed rate measurement - J. K. Johnson and B. R. Rodgers

This work element is on hold pending DOE/ORO decision to continue.

6.3 Components

D. M. Eissenberg

This section reports on activities related to analyzing and improving the performance (reliability, availability, and maintainability) of critical components in coal liquefaction service. Activities include identification and characterization of critical components for coal liquefaction demonstration plants, development of improved methods for critical component design and selection, development and testing of improved or advanced critical components, and assisting DOE/FE in organizing, implementing, and coordinating related critical component development and test activities.

6.3.1 Component design reviews - D. M. Eissenberg

Objective - Provide reviews and critical assessments of deliverables prepared by SRC-I and SRC-II Demonstration Plant contractors. The assessments will be directed toward the major components and subsystems and will be aimed at identification and resolution of potential problems pertaining to functional performance, reliability, cost, maintainability, and safety.

Schedule, scope and progress against milestones - No milestones are currently required for this task.

6.3.2 Valve reliability - T. L. Dahl, A. A. Khan, and L. J. Ott

Objectives - The objectives of this subtask are 1) to collect information and data on past slurry valve performance and flashing slurry flow, 2) to develop the methodology for characterizing and predicting multi-component, multiphase, non-Newtonian flow behavior within letdown valves and devices, and 3) to analyze the fluid flow in the entire letdown region of the process. Recommendations, correlations, and guidelines will be provided for use in the design and modifications of demonstration plant slurry valves and systems.

Schedule, scope, and progress against milestones

1. Develop preliminary 1D model by June 1, 1981; status: complete. Debugging and testing remain to yield analytical results. Efforts continue to debug and strengthen the model.
2. Modify letdown valve loop by October 1, 1981; status: all work remains on hold.
3. Inspect pilot plant valves by October 1, 1981; samples from Wilsonville are being reviewed.
4. Prepare reports on commercial letdown valve operating history by October 1, 1981; status: on schedule.

Technical discussions - The Grayson-Steed correlation is being used for predicting the equilibrium ratios in flash calculations. Use of this correlation in our model is being verified. Also, compressibility was calculated by a more efficient method which reduced the number of iterations required in the calculations. Both the Redlick-Kwong and the Redlick-Kwong-Soave equations of state were used for predicting gas fugacity and compressibility.

Algorithms for the Lockhart-Martinelli and Dukler frictional pressure drop correlations have been debugged and checked out in developing the final analytical model. In addition, the Hughmark, Lockhart-Martinelli, and Dukler correlations for liquid holdup in horizontal flow have also been debugged and tested. Efforts are now in progress to test the two-phase vertical flow pressure drop and holdup correlations.

This basic logic of the 1D model as discussed in last month's report was presented at the Pilot Plant Operators' Critical Component Meeting in Chicago on June 11. The needs for valid data was discussed as an agenda item.

The commercial letdown valve operating history for Wilsonville and Fort Lewis has been extracted and collected in rough form. Evaluation and review of the information is in progress.

6.3.3 Packed bed letdown valve - P. K. Carlson

Objective - The objective of this study is to develop an improved slurry pressure letdown system for possible application to the SRC-I and SRC-II Demonstration Plants. The improved system utilizes a packed bed for pressure drop, with flow control provided by addition of vapor or clean liquid which volatilizes at the temperature/pressure conditions within the packed bed.

Schedule, scope, and progress against milestones - There have been no significant changes in scope or milestones since the May monthly report. In an attempt to include the maximum amount of data in the analysis of the final report, some slippage in the deadline for completion of experiments is likely to occur.

1. Complete development experiments June 30, 1981; status: experiments are under way, probably about two weeks behind schedule.
2. Issue draft report of development experiments July 30, 1981; status: preparation is under way, awaiting completion of experiments.

Technical discussion - During June, a presentation and paper entitled Packed Bed Letdown Studies was given in San Francisco at the Symposium on Instrumentation and Control of Fossil Energy Processes.

A draft report is currently being prepared to record the results of this project. It was hoped that some additional experiments could be undertaken in late June and July with findings included in the report; however, it appears that this may not be possible. The experiments, if undertaken, will consist of a series of high gas/low liquid throughput runs at low and moderate pressures to study the behavior of two-phase pressure drop per unit length " $(\Delta P/\Delta L)_{T.P.}$ " at low values of Lockhart and Martinelli's two-phase parameter " χ ".

6.3.4 Heat exchanger technology - W. R. Williams, A. A. Khan, J. P. Belk, and L. M. Brown

Objective - Provide a focus for information, data analysis, and technology development leading to improved reliability and performance of fired heaters and heat recovery exchangers used in direct coal liquefaction demonstration plants.

Schedule, scope, and program against milestones - The key milestone remaining for this activity and progress toward it is as follows.

Summarize and analyze methods for design of fired heaters, stressing tube side (slurry) heat transfer by October 1, 1981. This activity should be completed on schedule.

Technical discussion - Two-phase flow correlations for pressure drops and flow pattern regimes were surveyed. Pressure drop correlations reviewed were those of Dukler, et al; Lockhart and Martinelli; Baker, and Clisholm. Flow maps of Baker; Mandhane, et al; Taitel and Dukler; and Weissman, et al, were examined. Articles by Shaver and Merrill; Dodge and Metzner; Quader and Wilkinson; Metzner and Reed; and Heywood and Charles were surveyed for non-Newtonian turbulence parameters for slurries.

Institute of Gas Technology reports were surveyed for viscosity, heat transfer coefficient, and other flow data. Reports of work done by the Chemical Technology Division of ORNL to produce rheological data for coal liquids were procured.

6.3.5 Indirect slurry pump technology evaluation and demonstration - T. B. Conley

Objectives - Evaluate the technology and economics of indirect slurry pumping systems (pumping of slurry utilizing a clean intermediate liquid) for application to large direct liquefaction coal conversion plants. Demonstrate indirect slurry pumping systems in large direct liquefaction plants. This work is part of the coordinated effort with the Office of Engineering and Component Management.

Schedule, scope, and progress against milestones

1. Complete rough draft of a state-of-the-art, techno-economic analysis on surge leg pumping and deliver to DOE/ORO April 1, 1981; status: writing continuing, 100% typed, in review/editing, August 3.
2. Decision point on surge leg pump testing May 1, 1981; status: decision to be made after draft of SOA, see #1.
3. Complete rough draft of a state-of-the-art, techno-economic analysis on hydraulic displacement pumping July 1, 1981; status: writing initiated; rough draft 10% completed; due September 1981.
4. Decision point on hydraulic displacement pump testing August 1, 1981; status: decision to be made after draft of SOA, see #3.
5. Surge leg pump testing progress report September 30, 1981; status: not started, see #2.
6. Complete final state-of-the-art report(s) on remote-head technologies September 30, 1981; status: rough drafts initiated - no delay expected.

Technical discussion - The draft of the surge leg report will be delayed into July or August due to delays in word processing and to planned revisions to the report. The revisions are intended to provide additional analysis of technical problems, primarily factors that determine the volumetric efficiency of the pump.

During the delay of the surge leg report, the rough draft of the hydraulic displacement pumping assessment was started, with 10% having been written to date.

Also this month, conversations with Ingersoll-Rand have produced some interesting results. I-R has expressed interest in a cooperative project with ORNL in order to study surge leg pump characteristics. I-R would provide a pump for a small fee if the Lab will operate and test it. A letter to this effect is on its way from Stanley Morgan, Manager of Synfuel/Pipeline Marketing for Reciprocating Pumps. Details remain to be worked out internally at I-R, as well as between them and ORNL; but, we are in general agreement on what the critical areas of study are, namely; 1) solids mixing and migration through the barrier fluid, 2) barrier fluid and pumpage temperatures control, 3) pump speed effects, and 4) flush requirements. A task description is being written to take advantage of this situation.

6.3.6 Component development support to DOE/HQ - D. M. Eissenberg

Objective - Provide assistance to the DOE/FE Office of Engineering and Component Management in developing and implementing their projects aimed at improving the performance and reliability of critical components needed in major liquefaction projects. The assistance will be provided until such time that OECM can obtain sufficient direct funding.

Schedule, scope, and progress against milestones - No milestones are currently required for this task.

6.4 Materials

This section reports on five subtasks in the area of materials technology: materials design review and coordination of materials research and development for SRC projects, H-Coal materials testing and failure analysis, investigation of corrosion in fractionation areas of liquefaction plants, valve materials, and mechanical properties data for pressure vessels.

6.4.1 Materials design review and coordination of materials research and development for SRC projects - A. R. Olsen, R. R. Judkins, and J. R. Keiser

Objectives - The objectives of this task are to assist in the review of contractor documents for materials selection, to review and provide input to materials testing and failure analysis plans, and to coordinate materials research and development for SRC projects.

SRC-I design materials review

Schedule, scope, and progress against milestones - The key milestones for this activity are as follows:

1. Complete review of preliminary design materials selections for SRC process areas - December 23, 1980. Completed.
2. Complete review of preliminary design materials selections for Coker Calciner - April 15, 1981. This milestone was deleted by DOE/ORO on May 5, 1981.
3. Complete review of preliminary design materials selections for gasification and gas treatment areas - July 15, 1981. Current information indicates material for review will be available about July 15.
4. Complete review of preliminary design materials selections for coal preparation area - July 15, 1981.

5. Complete review of preliminary design materials selections for L-C Finer area — September 15, 1981.

To achieve these milestones we perform a number of reviews of material as it becomes available from the prime contractor. These reviews generally constitute intermediate events with a completion date scheduled at the time the material is made available for review. To date all such reviews have been completed on time.

Status — Materials selections for the SRC-I Phase I Design Area 15 (gas systems) shift section were reviewed this month. In general the materials selections appeared to be generally appropriate. This conclusion is contingent on the removal of chlorine and fluorine from the feed gas in the proprietary section of the gas system which precedes this shift section. Comments were transmitted to DOE/ORO on June 26.

Selected nonproprietary portions of the proprietary sections of the gas system which included the gasifier, heat recovery, and gas washing processes were scanned to define the scope of the materials review which is planned for next month at Allentown, Pennsylvania.

SRC-II design materials review

Schedule, scope, and progress against milestones — The key milestones for this activity are as follows:

1. Complete review of preliminary design materials selections for Area 10, primary process plants (Units 11, 12, and 13) — July 15, 1981.
2. Complete review of preliminary design materials selections for Area 20, hydrogen production systems (Units 21, 22, 23, 24, and 25) — July 15, 1981.
3. Complete review of preliminary design materials selections for Area 30, refining and gas systems (Units 31, 32, 33, and 34) — July 15, 1981.

To achieve these milestones we perform a number of reviews of material as it becomes available from the prime contractor. These reviews generally constitute intermediate events with a completion date scheduled at the time the material is made available for review. To date all such reviews have been completed on time.

Status — No new materials for review were submitted during this month. We have continued to monitor all available SRC-II quarterly reports and the activities at the Fort Lewis SRC pilot plant.

Breckinridge project reviews

We are participating in the engineering reviews of Phase 0 submissions from the Breckinridge Project. Our emphasis is on the materials selection for the plant with concentration on the H-Coal process and gasification areas.

As indicated last month, because of scheduling and funding restrictions, the extent of these reviews has been reduced in scope. During the past month we reviewed Volumes 4, 6, and 7 of the Breckinridge Project Initial Effort Report IV. These volumes covered Plant 7 (gas plant), Plant 15 (oxygen plant), Plant 18 (naphtha hydrotreating and refining), and Plant 12 (gasification and purification). No materials data were presented for Plant 18 and significant portions of Plant 12 are proprietary, so materials comments could not be made in these areas. In general, most materials selections in these volumes appear appropriate and adequate for cost estimation purposes. A number of inconsistencies in materials selection were noted.

All comments on materials selections were forwarded to the UCC-ND Engineering Division for incorporation with other comments in transmittals to DOE/ORO.

6.4.2 H-Coal materials testing and failure analysis — R. W. Swindeman

Objective — The objective of this task is to assist Ashland Synthetic Fuels, Inc. (ASFI) and associated contractors in developing and implementing a materials testing, surveillance, and failure analysis plan for the H-Coal Pilot Plant at Catlettsburg, Kentucky. The scope of work involves the review of the materials of construction, participation in materials testing effort, and assistance in the preparation and implementation of a failure analysis plan. The review of the materials of construction is complete, and no additional work is reported.

Schedule, scope, and progress against milestones — The key milestones for this activity and progress toward them are as follows:

1. Draft report on first group of stress-corrosion cracking coupons from the H-Coal Pilot Plant — August 1981: About half of the samples have been metallographically examined for evidence of cracking.
2. Draft report on second group of stress-corrosion cracking coupons from the H-Coal Pilot Plant — Open: We expect that samples currently being exposed will not be returned to ORNL before September.
3. Recommend revisions to improve the implementation of the failure analysis plan — June 30, 1981: Plan working well; revisions not required.
4. Provide metallurgical assistance when requested: Examination of valve plungers is completed.

Materials testing — J. R. Keiser

Corrosion rates were reported previously³ for a set of coupons exposed on tray 11 of the N-202 fractionator at the Catlettsburg, Kentucky, H-Coal pilot plant. At that time, four other coupon racks, located on trays 9, 10, 12, and 13, were left in the tower. These four racks have since been removed and examined at ORNL. Results of the examination of all five racks are given in Table 6.1. These results show that carbon steel suffered extensive corrosion on all five racks, but corrosion was most severe on trays 10 and 11. Except for monel, all nickel-base alloys performed very well. Only two samples of type 321 stainless steel were exposed, but these did not perform nearly as well as type 321 stainless steel has in the fractionation towers of the SRC pilot plants. The iron-base high-molybdenum alloys, 904L, Haynes 20 mod, and Crucible 6M, demonstrated very good corrosion resistance. These five corrosion racks have been rebuilt and returned to Catlettsburg for exposure during the next operating period.

Table 6.1. Corrosion rates of samples exposed in Catlettsburg fractionator

Alloy	Corrosion rates, mils/year ^{a, b}				
	Tray 9	Tray 10	Tray 11	Tray 12	Tray 13
Hastelloy G	<0.1	<0.1	<0.1	<0.1	<0.1
Inconel 625	<0.1	<0.1	<0.1	<0.1	<0.1
Hastelloy C-4	<0.1	<0.1	<0.1	<0.1	<0.1
Alloy 904L	<0.1		<0.1		<0.1
Titanium	0.1	<0.1	<0.1	<0.1	0.1
Haynes alloy 263	0.1	<0.1	0.2	0.1	<0.1
Haynes 20 modified	<0.1	<0.1	<0.1	0.3	<0.1
Crucible 6M	0.2	0.1	0.1	0.1	0.1
RA 333	0.2	0.1	<0.1	<0.1	0.2
Hastelloy B-2	0.3	0.3	<0.1	0.3	0.3
Incoloy 825	<0.1	0.4	0.7	0.1	0.1
Inconel 600	0.5	0.5	<0.1	0.3	<0.1
2RE69	<0.1	0.5	1.3	0.6	<0.1
San 2205	0.2	1.3	1.5	1.8	<0.1
Carpenter 20 Cb 3	1.3	1.4	4.5	1.4	<0.1
Type 317 stainless steel	2.4	7.0	7.4	1.2	<0.1
Monel 400	12.9	11.5	4.5	5.9	4.4
Type 321 stainless steel		15.8		20.7	
Type 347 stainless steel	32.1	29.9	21.7	19.3	<0.1
Type 409 stainless steel	45.1	261.6	300.1	210.5	0.2
Carbon steel	582.0	803.6	759.9	700.4	295.0

^aExposure times: tray 11, 45 d (1080 h); trays 9, 10, 12, and 13, 49 d (1176 h).

^bCalculated by assuming uniform removal of material.

Failure analysis — A. R. Olsen, R. J. Gray, and R. W. Swindeman

The M-209 reactor effluent vapor trim cooler at the H-Coal pilot plant developed leaks after a major repair operation. The alloy 800 tubing (Fe-32% Ni-21% Cr) was removed and replaced with a nickel-base alloy. Several of the alloy 800 tubes are being shipped to ORNL for inspection.

The failure analysis plan has been reviewed as intended (Milestone 3 above) and we have concluded that no major revisions to the plan are required.

6.4.3 Investigation of corrosion in fractionation areas of liquefaction plants — J. R. Keiser, M. Howell, and R. R. Judkins

Objective — Severe corrosion has been observed in the fractionation areas of the SRC pilot plants. A concentrated effort is being made at ORNL to identify materials with sufficient corrosion resistance for use in the fractionation towers and to develop methods to control the corrosion.

Schedule, scope, and progress against milestones — The key milestones for this activity and progress toward them are as follows:

1. Identification of alloys for fractionation tower — June 1981: A draft was prepared and is being reviewed.
2. Identification of corrodents — August 1981: Studies are proceeding at a slower rate because of reduced funding. Supplemental funding for this effort has been requested.
3. Identification of corrosion inhibitors and/or corrodent removal techniques — August 1981: Complete.
4. Report of Phase II activities — September 1981: This milestone is to be deleted because of reduced funding. In lieu of the topical report, a summary report was prepared for submission to the *Journal for Materials for Energy Systems*.

Status — The major efforts on this program during the month of June were directed toward identification of the chlorine-bearing compounds which we feel are essential in the severe corrosion process observed in the SRC pilot plant fractionation columns. Chemists from our Analytical Chemistry Division (ACD) have used Fourier transform infrared spectroscopy to study the organic components from Fort Lewis recycle process water tank (RPWT) water. These studies have shown that amine hydrochlorides are present in this sample. Further studies using negative chemical ionization mass spectrometry are being carried out by ACD chemists to identify the amine hydrochlorides. These techniques offer a very promising way to identify the corrodents, but reduced funding will prevent us from making a complete study.

In last month's report, we described the distillation studies we are performing which we feel indicate that a thermal decomposition reaction occurs to release hydrogen chloride from coal liquefaction oils. We are currently conducting vacuum distillations with selected oils and oil/water mixtures in an effort to provide enough information that we can better explain the behavior of the chloride-bearing compounds.

6.4.4 Valve materials — E. L. Long, Jr.

Objective — This materials task originally consisted of distinct elements that were directed toward both near- and long-term objectives of the slurry letdown and block valve support program developed jointly by METC and ORNL. However, because of budget limitations recently imposed, this materials task will be limited to the near-term objective of characterizing the more popular commercial trim materials, performing erosion tests at Battelle-Columbus Laboratories, and following the performance of trim materials in various pilot plants.

Schedule, scope, and progress against milestones — The key milestones for this activity were revised to accommodate the short-term effort of this activity. The key milestone for this activity and progress toward it is as follows:

1. Issue draft report on detailed characterization studies of commercial material (September 1981): On schedule.

Status — Funding for this task was authorized in February 1981 and work was initiated on characterizing the more commonly used commercial trim materials in letdown valves. This work is continuing. Work on material systems for candidate advanced trim has been stopped because of a reduction and redirection of the remaining funds for this activity. The valve testing program at H-Coal is continuing to be followed and trim material from some of the valve tests are being evaluated. A trip was made to Fort Lewis to review their plans for a letdown and block valve testing program. At that time their plans were to initiate their testing program this fall; however, at the present time with the uncertain future for the Fort Lewis facility, this does not appear likely.

Three stems from Wilsonville letdown valves LV 415 A/B were received from Air Products and Chemicals, Inc. this month for characterization studies. These three stems are reportedly of the same design and material but were removed from service at significantly different intervals: 1200, 2000, and 4000 h. We expect to receive an additional letdown valve stem and seat that was removed from service after less than 300 h. The findings of this characterization study will be reported as work progresses. The details of the progress on commercial trim characterization are given below.

Commercial materials — C. S. Yust and V. J. Tennery

Study of the dendritic component of the K-602 microstructure has been continued. Electron diffraction data had previously shown that most of this material is the ternary carbide $\text{Co}_3\text{W}_3\text{C}$, but this microstructural constituent is itself polycrystalline and the composition of each grain in the dendrite may not be identical. Diffraction data have been acquired from other dendrite regions, and the results show that some dendritic areas have the structure of the ternary carbide $\text{Co}_3\text{W}_9\text{C}_4$. The presence of $\text{Co}_3\text{W}_3\text{C}$ had been confirmed by x-ray analysis of the K-602 material, and several of the x-ray lines had remained unidentified. The determination of $\text{Co}_3\text{W}_9\text{C}_4$ by electron diffraction is confirmed by the previously unidentified x-ray lines, which correspond to those for this compound.

6.4.5 Pressure vessel materials data — R. W. Swindeman

Objective — The objective of this activity is to procure mechanical properties data needed for reliability and safety analyses of SRC dissolver vessels. Time-dependent data for the materials of construction are being collected and assessed according to the criteria established in Section VIII Division 1 of the *ASME Boiler and Pressure Vessel Code*. In addition, creep fatigue and associated stress-strain data are being gathered. The results of the study will be used to recommend a plan of action to verify or alter the design stress allowances to be used in conjunction with the rules in Section VIII, Division 2 of the *ASME Boiler and Pressure Vessel Code*.

Schedule, scope, and progress against milestones — The key milestones for this activity and progress toward them are as follows:

1. Complete compilation of available mechanical properties data for the materials of construction of dissolver vessels — March 31, 1981: completed.
2. Determine the time-dependent stress allowances from literature data for SA-387 Grade 22 Class 2 based criteria from Section VIII, Division 1 of the *ASME Code* — June 30, 1981: completed.
3. Recommend a plan of action to verify the design stress allowables in Section VIII, Division 2 of the *ASME Code* for the materials used in liquefaction vessels — August 31, 1981: Efforts are on schedule.

Time-dependent stress allowables for the materials of construction — M. K. Booker and R. W. Swindeman

Status — A report on the analysis of stress-rupture data for 2 1/4 Cr-1 Mo steel (SA-387 grade 22 class 2) is being prepared. Examination of creep behavior obtained from unpublished sources was completed, and we found that rupture strength, not creep strength, controlled the time-dependent allowable stresses. These data will be included in the final report that constitutes Milestone 3 above.

Creep-fatigue studies of the materials of construction — J. P. Strizak and R. W. Swindeman

Status — Exploratory creep-fatigue testing of 150-mm plate of 2 1/4 Cr-1 Mo steel (SA-387 grade 22 class 2) has been completed. We found that hold-time effects existed at 482°C and that tensile strain holds were more damaging than compression strain holds at 2% strain range. Tests on materials without a final 690°C simulated postweld heat treatment were performed to examine the effect of ultimate strength on fatigue response. We found that the stronger material had worse fatigue resistance at high strain levels. Cyclic tests to explore the softening behavior were initiated, and a series of 100-h relaxation tests were completed. Sufficient exploratory test data should be available by the end of August to aid in the development of the recommended plan identified as Milestone 3 above.

6.5 Environmental and Health

This section reports on the work elements in the area of environmental and health effects of direct liquefaction technology — preparation of environmental impact statements for SRC-I and SRC-II, critical review of environmental and health effects, and assistance to DOE in environmental and health monitoring.

6.5.1 SRC-I and SRC-II environmental impact statements — C. R. Boston and S. G. DeCicco

SRC-I

The Final Environmental Impact Statement (FEIS) for the SRC-I demonstration project went through its final review sequence during the month of June. Review documents were produced on June 6, June 19, and June 29 for DOE review — each edition responding to reviewers' comments up through that point.

The FEIS was prepared in response to comments received on the Draft EIS. Written comments on the Draft EIS were received from 67 individuals, groups, and agencies. In addition, 106 speakers commented on the Draft at three public hearings. After combining all redundant comments, 468 specific and distinct comments remained. Each of these comments along with a response is presented in Appendix A of the FEIS, and represent the basis for revising the document from draft to final form. While comments were directed at health effects, DOE policy, site selection, plant design, and floodplain/wetlands, the socioeconomic impacts projected for the project received the most attention (108 specific comments) from reviewers.

By the conclusion of the EIS process, the environmental issues which had surfaced as the most important were: health effects for synfuel workers, traffic congestion from commuting construction workers, possible cumulative adverse socioeconomic impacts with nine other nearby projects, encroachment on floodplain/wetlands areas, withdrawal of prime farmland, and the presence of a Federally-listed endangered species.

Some of the environmental issues could not be quantitatively assessed in the EIS due to the absence of a detailed plant design, site monitoring data, and/or basic scientific understanding of the effects of synfuel chemicals on the environment. In these cases, monitoring and mitigation measures were defined to observe and correct adverse impacts. However, with the uncertain role of DOE, the Synthetic Fuels Corporation, and other possible sponsors, it became unclear who would carry out the monitoring and mitigation program described in the EIS. The EIS assesses only the proposed action which assumes DOE's involvement and commitment to the terms of the EIS. Should DOE's involvement come to an end and another sponsor undertake the project, the new sponsor would not be bound to the proposed action described in DOE's EIS (including the proposed pollution control, monitoring and mitigation program). This situation is clearly identified in the EIS which concludes that even under other sponsorship, the project would require environmental permits with their own monitoring and mitigation requirements. In addition some of the permits are likely to incorporate a NEPA review (i.e., EIS).

6.5.2 Environmental and health status of SRC and H-Coal processes - C. J. Oen

The objectives of this work are to complete and publish critical reviews of selected issues relating to environmental and health effects of direct liquefaction processes.

A description of test procedures and interpretation has been drafted for the carcinogenesis report. Results of experimental work at ORNL, Dupont, and PNL have been summarized in table form. Any pertinent data from Air Force documents will be incorporated when they are received. Efforts are underway to find recent human epidemiological data.

A small revision was made in Chapter 5 of the mutagenesis document at the suggestion of L. E. McNeese; the distribution lists were revised and updated. The document was ready for reproduction on June 5.

6.5.3 Environmental and health monitoring - C. R. Boston

No activity this month.

6.6 References for Section 6

1. Richard W. Hanks, Analysis of Rheological Data for SRC Solvent Coal Slurries: Ft. Lewis and Wilsonville Solvents, Richard W. Hanks Associates, Orem, Utah, May 25, 1981, pp. 3-5, 11-15.
2. A. H. P. Skelland, Non-Newtonian Flow and Heat Transfer, John Wiley and Sons, New York, 1967, p. 31.
3. J. R. Keiser, M. Howell, and J. F. Newsome, "Studies of General Corrosion in Coal Liquefaction Plants," pp. 22-26 in *Fossil Energy Program Prog. Rep. for April 1981*, ORNL/TM-7826 (June 1981).

7. PROCESS ANALYSIS AND ENGINEERING EVALUATIONS

V. C. A. Vaughen

Process analysis and engineering evaluation studies are being conducted for DOE/FE to provide technical and economic assessments and evaluations of processes and systems for coal conversion and utilization on a consistent basis.

7.1 Liquefaction Technology Assessment (LTAS)

R. M. Wham, R. Salmon, S. P. N. Singh, J. F. Fisher,
W. C. Ulrich, and P. J. Johnson

7.1.1 Objective

The objective of the Liquefaction Technology Assessment is to provide technical information, cost information, and economic evaluations needed by the Department of Energy (DOE) to compare, coal liquefaction processes on a consistent basis. The assessment is being carried out in several phases, starting with processes employing available technology and progressing to those which are in earlier stages of development. ORNL and the Pittsburgh Energy Technology Center (PETC) select the processes to be evaluated. ORNL, in conjunction with a subcontractor, develops technical and cost information which serves as the basis for the detailed technical and economic evaluations reported by ORNL.

7.1.2 Status summary

To assist in the evaluation of gasifier efficiencies in the Phase II LTAS studies, a computer program was written that calculates the heat and material balance relationships and the overall thermal efficiency of an entrained-flow gasifier. The ORNL model was used to verify Fluor's calculations for both the Texaco and the Koppers-totzek gasifiers. Good agreement with Fluor's results was obtained when the same input assumptions were used. Further results will be reported in the *Fossil Energy Program Quarterly Report for the Period Ending June 30, 1981*.

A preliminary draft of the Phase II work was completed in late June. The draft will be circulated for an internal review prior to release to DOE and process developers for review.

Discussions with DOE and Fluor concerning future phases of LTAS are continuing.

7.2 Direct Combustion

E. C. Fox

7.2.1 Objective

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.

7.2.2 Status summary

The main report, "Conversion to Direct Coal Combustion in the Industrial and Commercial/Residential Sectors - A Study of the Barriers to Implementation in the Near Term," ORNL/TM-6139, is being prepared for final publication.

7.3 Advanced Power Conversion Systems

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

7.3.1 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.

7.3.2 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. The reports entitled "Summary of the Research and Development Effort on Open-Cycle Coal-Fired Gas Turbines," ORNL/TM-6253, "Summary of Research and Development Effort on Air and Water Cooling of Gas Turbine Blades," ORNL/TM-6254, "Summary of the Development of Open-Cycle Gas Turbine-Steam Cycles," ORNL/TM-6252, "Summary of the Research

^aConsultant

and Development Effort on Steam Plants for Electric Utility Service," ORNL/TM-6250, "Summary of the Research and Development Effort on the Supercritical CO₂ Cycle," ORNL/TM-6236, and "Summary of Research and Development Effort on Closed-Cycle Gas Turbines," ORNL/TM-6237, have now been published.

7.4 Process Modeling

R. Salmon, P. J. Johnson, and W. C. Ulrich

7.4.1 Objective

The objective of this project is to provide DOE with computerized models for the analysis and support of coal conversion studies. Generally this effort includes documentation and testing of various computer codes; verification and validation of process simulators; modeling, computing, and systems engineering support; and developing, installing, and evaluating process models and systems engineering codes. Current work includes the implementation of ASPEN at ORNL and the modification and testing of the Purdue and Lehigh process modeling codes installed at Morgantown Energy Technology Center (METC).

7.4.2 ASPEN

The May 1981 version of the ASPEN process simulation code was obtained from MIT and installed on the ORNL computer system. The code was successfully verified through test cases supplied by MIT. Familiarization runs are being continued with the new version.

7.4.3 Support to METC

The two draft reports summarizing ORNL work on the Purdue PPROP code have been reviewed internally and are now undergoing technical editing prior to publication. These reports concern the review and evaluation of the PPROP (physical properties) code and the ORNL modification of the code to permit the handling of streams containing solids. Both reports have been transmitted to METC for review.

Work continued on the modification of the Purdue PCOST (cost estimation) and BED (generalized fluidized bed) codes to make these codes compatible with IBM systems. A number of subprograms that were specific to the Purdue CDC system have been replaced. PCOST is now operational on the ORNL IBM system but the code is malfunctioning on one of the seven test examples. The source of this error is still being traced.

The BED program uses a number of numerical analysis routines from the proprietary IMSL library which are available at both ORNL and METC. Other installations that do not have the IMSL package will not be able to use the program. Several other routines called by the program were not available on the tape supplied by Purdue. An effort is being made to obtain these routines or replacements for them.

7.5 Coal Liquefaction Advanced Research Digest

F. M. O'Hara, Jr.

7.5.1 Objective

The objective of this activity is to provide continuing technical assistance to DOE/FE-DFFP by preparing digest reviews of subjects related to coal-conversion technology that are of current or potential interest.

7.5.2 Status summary

Corrections were made for the illustrations of the article "Chemical Reactions of Coal Liquefaction."

Writing was completed on the article "Free-Radical Chemistry of Coal Liquefaction," and the manuscript was circulated for internal review.

7.6 Indirect Liquefaction Environmental Control Technology Assessment (ILECTA)

S. P. N. Singh, J. F. Fisher, R. Salmon,
R. M. Wham, and E. L. Youngblood

7.6.1 Objective

The objective of ILECTA is to prepare a technical information manual on the pollution abatement aspects of indirect coal liquefaction plants. The manual will present the current state of knowledge on the effluents and on the processing routes that can be used to control the effluents from commercial indirect coal liquefaction plants in an environmentally acceptable manner.

The indirect liquefaction process examined in the assessment consists of syngas production via coal gasification, conversion of the syngas to methanol (using the ICI process), and production of principally gasoline from the methanol (using the Mobil MTG process). This assessment will focus on the examination of three alternate gasification systems namely, Lurgi, Texaco, and Koppers-Totzek in the above sequence.

7.6.2 Status summary

A computer program called DMEG has been developed to evaluate the discharge stream severity of emission streams from the conceptual indirect coal liquefaction plants proposed to be evaluated in this study. DMEG was developed using EPA's DMEG (discharge multimedia environmental goals) methodology. The DMEG computer program is operational and example stream analyses are being run to check out the program capabilities.

A preliminary design for the Texaco gasification case (up to the methanol synthesis step) has been completed including the estimation of the waste stream flowrates. In addition, approximate effluent flows have been developed for most of the ancilliary processes such as the acid gas recovery process, raw water treatment, and the boiler circuit.

A block flow diagram has been prepared for the K-T gasification case.

Work on ILECTA was side-tracked for about 10 days in early June to review EPA's "Pollution Control Guidance Document (PCGD) for Lurgi-based Indirect Liquefaction Facilities." The ILECTA task force members (along with others) completed the review and the results were delivered to DOE/Fossil Energy.

7.7 Environmental Control Costs for an Indirect Coal Liquefaction Process

P. J. Johnson, S. P. N. Singh, R. M. Wham,
and J. F. Fisher

7.7.1 Objective

The objective of this study is to examine the effect of several degrees of stringency of pollutant emission control requirements on the economics of an indirect liquefaction process for several sizes of liquefaction facilities. The work was initiated by the DOE Assistant Secretary for the Environment's Office of Environmental Assessments (OEA) [formerly Office of Technology Impacts (OTI)]. Technical and cost information was provided by Fluor Engineers and Constructors through a contractual agreement with the Oak Ridge National Laboratory (ORNL). ORNL provided guidance in the development of environmental emission control requirements and provided economic evaluations based on cost information developed by Fluor.

7.7.2 Status summary

This work will be reported in the *Fossil Energy Program Quarterly Progress Report for the Period Ending June 30, 1981* in the section titled "Life Sciences Synthetic Fuels Program."

7.8 Underground Coal Gasification

W. C. Ulrich

7.8.1 Objective

The objective of this project is to assist the Department of Energy (DOE) in evaluating the state of development of various technologies for underground coal gasification (UCG) and the potential offered by these processes by means of technology and economic assessments.

7.8.2 Status summary

This project was completed during May.

8. FOSSIL ENERGY ENVIRONMENTAL PROGRAM

C. R. Boston

Environmental support is provided to DOE/Fossil Energy and DOE/Economic Regulatory Administration. The effort includes: (1) preparation of NEPA-required assessments and statements related to synfuels demonstration programs and fuel conversion implementation; (2) programmatic environmental studies that are critical to the early realization of advanced fossil technologies and minimization of the use of petroleum and natural gas; and (3) general environmental technical assistance.

8.1 Fossil Energy Support

C. R. Boston

Specific work areas include:

Environmental, Safety and Health Support - Provides technical and management support to the Environmental Safety and Health Branch in the areas of occupational safety and health and industrial hygiene.

Regulatory and legislative reviews - Provides a continuing review of all regulatory and legislative items, present and planned, and their effects on fossil energy programs.

8.1.1 Environmental, Safety and Health Support - R. C. Martin

A draft FTP/A has been prepared and discussed with both ASFE/OPTA and ORO. Questions relating to the responsibilities of ASFE/OPTA with respect to federal employee health and safety programs and the utilization of contractors for audits and functional appraisals have been referred to the Assistant Secretary for Administration. Finalization of the FTP/A will be delayed pending resolution of these issues; however, interim authorization to proceed with three initial tasks is anticipated:

1). Review of the Model Industrial Hygiene Program Project.

This program for development of a model program for ASFE facilities is being administered through an interagency agreement with the Air Force. ORNL has been requested to review the program manual and a proposed sampling and characterization program for technical adequacy and to make recommendations for modifications to increase the usefulness to the Energy Technology Centers.

2). Review of Revised DOE Orders.

Most of the DOE orders relating to health and safety are undergoing revision. ORNL will review the proposed orders to identify impacts on ASFE programs and facilities and make recommendations to ASFE regarding implementation.

3). Development of Tasks and Schedules for FY 82.

This task provides for prioritization of support needs and development of statements of work and tentative milestone schedules for work to be performed during FY 82.

8.1.2 Industrial Hygiene/Occupational Medicine Workshop -
C. R. Boston

Draft materials are being edited by an ORNL editor in preparation for publication of the proceedings document.

8.1.3 Regulatory and Legislative Review - A. W. Reed

Four transmittals of environmental regulatory/legislative news items were received from the Information Division in June. A summary of highlights was telefaxed to DOE-FE (M. Rogowsky) on June 23, 1981. A return telefax indicating which highlights should be emphasized in the July newsletter was received at ORNL on June 26, 1981. Work on the newsletter progressed toward a July 15, 1981 deliverable date.

8.2 Synfuels Project

C. R. Boston

This 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.

8.2.1 Coal conversion demonstration projects

Liquefaction projects - S. G. DeCicco

This activity is reported in Chapter 6.

Gasification projects - C. R. Boston

No Activity.

8.2.2 Breckinridge ER/EIS Reviews - R. D. Roop

ORNL is providing assistance to DOE/ORO in the review of supporting documents for the Breckinridge H-Coal Commercial Project. Portions of Report VII, (Environmental, Socioeconomic, Safety, and Health Report) were received and initial review efforts have begun. The available deliverables covering design and specifications for various parts of the facility have been examined for information relevant to the environmental assessment. Review of Report VII, Part 3, (Cultural Resources Assessment and Socioeconomic Baseline Report) was completed in June. Ashland Oil Co. has been delayed in its delivery of the remaining portions of Report VII, which were expected in June. Further review of Part 2 (Environmental Baseline Report) will proceed when Part 1 (Environmental Management Plans) is available (expected early July).

8.2.3 Grace Site Evaluation Report - R. D. Roop

No activity.

8.3 Economic Regulatory Administration Support Project

R. C. Martin

The mission of this project is to provide technical assistance to the Economic Regulatory Administration (ERA) of the Department of Energy in its implementation of the Powerplant and Industrial Fuel Use Act of 1978 (FUA). This act has as a general purpose the encouragement of increased utilization of alternate fuels, in a manner consistent with applicable environmental requirements, through the minimization of the use of petroleum and natural gas as primary energy sources. The scope of FUA includes both new and existing electric powerplants and new and existing major fuel burning installations. Within ERA the Office of Fuels Conversion (OFC) is responsible for implementing FUA and meeting the requirements of the National Environmental Policy Act. The Fuels conversion Analysis Division (FCAD) supplies the technical support for OFC.

ORNL is providing technical support to OFC in the implementation of the FUA. This support includes both programmatic and site-specific research and analysis related to program management, alternative fuel/control options, environmental impacts, environmental regulations, engineering feasibility, and fuel supply and transportation.

On March 6, 1981, Mike Carosella provided guidance regarding the phase out of the ERA programs including schedules for remaining deliverables and authorized expenditures. The Arthur Kill and Ravenswood analyses will be continued through the Final Draft EIR. Work on the Salem Harbor and Northport engineering and environmental analyses will be discontinued as soon as possible. The Environmental Regulations Technical Report, EIS Implementation Plan and Fuel Supply and Transportation Analysis will be terminated after completion of the next deliverable, Uncosted balances remaining on subcontracts will be recovered where possible.

8.3.1 Program management

Programmatic activities continued to focus on recovery of uncosted balances of subcontract obligations. Final contract modifications are expected to be issued in early July.

8.3.2 Arthur Kill - N. E. Hinkle

Preparation of the Final Draft Environmental Impact Report is in progress; submission is scheduled for July 3, 1981 and no problems are anticipated.

All other deliverables have been submitted and no further activity is planned.

8.3.3 Ravenswood - N. E. Hinkle

Interagency review comments on the Draft EIR were received during the week of June 8th and preparation of the Final Draft is in progress. Submission is scheduled for July 17, 1981; no problems are anticipated.

All other deliverables have been submitted and no further activity is planned.

8.3.4 Northport - D. J. Wilkes

This analysis has been terminated.

8.3.5 Salem Harbor - A. W. Reed

This analysis has been terminated.

8.3.6 Northeast Regional Analysis

Air quality - F. C. Kornegay

Responses to comments on the revised Draft EIS were provided to ANL for incorporation into the next revision.

A draft report on the stochastic model development effort was submitted to ERA the week of June 22. Development work is continuing.

Health effects - P. J. Walsh

A peer-reviewed draft of the health effects technical support document "Health Effects of Air Pollution: A Technical Backup Document for Oil to Coal Conversion Under the Fuel Use Act" was submitted to ERA on June 12, 1981.

Responses to comments on the revised Draft EIS were submitted to ANL for incorporation into the next revision.

8.3.7 Electric utility dispatch analysis - The analysis of the effectiveness of alternative strategies to coal conversion was concluded during June. This work was in support of the regional Environmental Impact Statement as required by EPA. The revised PRODCOST simulations and generation mix plots were sent to DOE.

Work continued on the documentation package for the power pool simulations.

8.3.8 Rate impact model development - Reviewers comments were incorporated into the code report and the report was sent to the Division Reports Office in June. The report currently is in editing.

8.3.9 Milestones

The following schedules are based on guidance provided by OFC on March 6, 1981.

<u>Deliverable</u>	<u>Scheduled Delivery</u>	<u>Status</u>
<u>Arthur Kill Powerplant</u>		
Final Draft EIR	July 3, 1981	In preparation
<u>Ravenswood Powerplant</u>		
Final Draft EIR	July 17, 1981	In preparation

Northport

No further activity planned

Salem Harbor

No further activity planned

9. FLUE GAS DESULFURIZATION

A. D. Kelmers

Magnesia slurry scrubbing is a regenerable system for removing SO_2 from flue gas by reaction with magnesium oxide (hydroxide) to form hydrated magnesium sulfite. The magnesium sulfite is then decomposed at high temperature to yield MgO for recycle to the scrubber and more concentrated SO_2 gas which can be used to produce sulfuric acid or sulfur. The use of spray absorption in conjunction with the regenerable magnesia FGD system could lead to significant simplification of the conventional magnesia FGD system through elimination of several processing steps, while simultaneously reducing the amount of slurry handling involved. The objective of this program is to explore the technical feasibility of combining the spray absorption technique with the magnesia FGD system.

9.1 Magnesia FGD Spray Absorption Technology

B. Z. Egan

The bench-scale apparatus simulating a spray dryer has been modified to provide better temperature monitoring and to obtain better water removal from the exit gas. A schematic diagram of the apparatus is shown in Fig. 9.1. Flue gas is simulated by a mixture of SO_2 and N_2 . The heated gas is mixed with a magnesium hydroxide slurry and the mixture is sprayed into a drying tower. Water is condensed from the exit gas and the gas is analyzed for SO_2 . Higher concentrations of SO_2 (>2000 ppm) are measured by gas chromatography; lower concentrations are presently estimated using Bendix Gastec analyzer tubes. An SO_2 analyzer will be installed to obtain more accurate measurements of low concentrations of SO_2 .

Several successful runs were completed using the spray dryer. Gases containing 0.1, 0.25, and 1.0% SO_2 in nitrogen were used to simulate flue gas. Slurry concentrations of $\text{Mg}(\text{OH})_2$ in water were 4, 7.6, and 10%. Inlet gas temperature varied from 110 to 130°C, while the temperature inside the spray dryer was 80-120°C. The average molar ratio of $\text{Mg}(\text{OH})_2:\text{SO}_2$, calculated from the gas and slurry flow rates, ranged from 0.7 to 5. The SO_2 removal efficiency ranged from 28% (with a 1% SO_2 stream, 10% slurry, and a $\text{Mg}(\text{OH})_2:\text{SO}_2$ ratio of 0.7) to 85% (with a 0.25% SO_2 stream, 10% slurry, and a $\text{Mg}(\text{OH})_2:\text{SO}_2$ ratio of 5).

Fig. 9.1. Schematic diagram of apparatus for magnesia spray absorption of SO_2 .

10. COAL PREPARATION AND WASTE UTILIZATION

E. C. Hise

The objectives of this program are: to develop, demonstrate, and bring to commercial viability, processes and equipment for the removal of pyrite and ash forming materials from dry crushed coal by either or both processes of high-gradient magnetic separation (HGMS) and open-gradient magnetic separation (OGMS); to integrate the magnetic process into the coal preparation system to achieve the most effective and economic preparation of the raw coal; and to develop processes to minimize the refuse disposal by efficiently utilizing the heating value and concentrated mineral resources in that refuse.

10.1 High-Gradient Magnetic Separation

E. C. Hise, A. S. Holman, and M. T. McFee

During May of 1980, a complete test series was performed on the stockpile coal from the TVA Paradise coal cleaning facility. The results from these tests are being received from analytical chemistry, and we are in the process of reviewing them. For these tests, each of the stockpile samples (samples were for depths of 10-20, 20-30, 30-40, 40-50, 50-60, 60-70, 70-80, 80-90, and 90-100 feet) was screened to +30M, 30M x 100M, 100M x 200M, 200M x 325M, and -325M. Each of the size fractions from 30M to 325M were processed in two different cannisters both with the magnet off and with the magnet energized to a field of 20 kG.

The magnet-off tests were performed to determine the amount of material which would be mechanically trapped by the mesh. The results of these tests are shown in Table 10.1.

Table 10.1. Percent material retained in mesh with magnet off

Size	Mesh A	Mesh B
30M x 100M	< 1%	< 1%
100M x 200M	< 1%	1%
200M x 325M	1.5%	< 1%

This data clearly shows that with the magnet off, there is no problem with mechanical entrapment for the two mesh tested.

The next step was to perform separations with the magnet on. These tests were performed in the laboratory superconducting magnet operating with a background field of 20 kG. With the magnet energized, it was found that some flush air was required to reduce mechanical entrapment as

the mesh loaded. Both the product and the magnetic fractions from each test were sent to Analytical Chemistry for determination of ash and sulfur content. At this time, results are available for the 100M x 200M, 200M x 325M, and the 100M x 325M size fractions.

In addition, float-sink tests were performed on the 30M x 100M samples to use as a reference. These samples have also been sent to Analytical Chemistry, but the results are not available at this time. Float-sink tests are now being performed on the 100 x 200 mesh fractions.

Overall, these tests show no significant reduction in the total sulfur content. We are now in the process of submitting several samples to Analytical Chemistry for a determination of the forms of sulfur present in both the feed and the product coal. It is quite possible that as a result of weathering, the stockpile coal contains little or no pyritic sulfur which is the only form which HGMS removes.

With respect to ash reduction, the magnet generally removed 10-15% of the ash with a 75-85% heat value recovery. Figures 10.1-10.3 show the performance with respect to ash reduction for those tests for which we have chemical results.

The basic problem encountered during these tests was that all the particles were coated with a grey film which appears to be magnetic. This of course causes all the particles to behave somewhat magnetically, even the more or less clean coal particles. This tendency reduces the selectivity of HGMS and is one we are currently trying to eliminate or reduce.

This particular set of tests were performed in a dry mode of operation and the samples were prepared by dry screening the raw coal. We will be exploring the effects of air classifying and wet screening to see if either of these techniques can help reduce or eliminate this coating problem. We will also be carefully analyzing this first set of tests in an effort to locate areas where we can improve our experimental technique for the test series we will be performing in the future.

Construction of the fines removal screen test facility at the Y-12 steam plant is 90% complete, but completion and operation of the facility must now await the settlement of the strike by the Atomic Trades and Labor Council which began on June 19, 1981. During the interim, our efforts will be concentrated on the second phase of the fines removal work. This involves determining the means by which the underflow from the initial cut of run-of-mine coal can be effectively dried and further classified so as to yield suitable HGMS feed material. Inquiries are being made to equipment manufacturers about the use of their research facilities for this experimental work, and a program plan will be developed as the results of these contacts are evaluated.

ORNL-DWG 81-8420 ETD

Fig. 10.1 Magnetic separation of stockpile coal 100 x 200 mesh.

Fig. 10.2 Magnetic separation of stockpile coal 100 x 325 mesh.

ORNL-DWG 81-8422 ETD

Fig. 10.3 Magnetic separation of stockpile coal 200 x 325 mesh.

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

R. S. Holcomb

11.1 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 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 testing of a 0.3 MW(e) technology test unit.

11.2 Status Summary

R. S. Holcomb, R. H. Guymon, N. W. Durfee, and W. A. Hartman

The scoping document for redirection of the Test Unit was prepared by ORNL and submitted to METC for review. It was reviewed by METC and has been revised by ORNL and sent to METC for concurrence.

Reference Plant Design

The Reference Plant Flow Schematic and Heat Balance Diagram was reviewed by ORNL and has been approved.

One side view and two plan views of the combustor island arrangement drawings have been completed. The water circulation requirements for the combustor waterwalls and the convection boiler bank have been developed.

Work has continued on the design of the auxiliary systems. The spent bed material letdown system has been designed. The hot flue and ductwork to and from the tubular air preheater has been laid out.

The design requirements and specifications have been determined for several auxiliary equipment items. These include the FD and ID fans, boiler circulation water pumps, baghouse and the steam coil air heater.

The baghouse design specifications are based on the EPA New Source Performance Standard for particulate emission of 0.03 lb solids per million Btu input and a design value of 75% for the cyclone separator efficiency and a 75% recycle rate, both of which are conservative values compared to the expected performance.

Test System Design

The Baseline Project Plan and cost estimate has been reviewed and approved by ORNL management and has been submitted to ORO.

B&W continued work this month on the test unit layout drawings, structural engineering and design engineering. Structural engineering work on the water jacket enclosure, involving the determination of necessary plate thicknesses, stiffener sizes and locations, and support and tie locations, has been completed. A water jacket circulation analysis has also been completed. The analysis determined the quantity and size of downcomers and door jumper tubes required to ensure adequate water circulation in all parts of the enclosure.

Engineering work has begun on the convection pass and in-bed tube bundles, headers, and inter-connecting piping. Layout sketches have been developed and finalized design conditions determined. Header, piping, and tube thickness calculations are nearly complete. A preliminary layout and support arrangement for the inter-connecting hot air pipe has been developed and is currently undergoing flexibility analysis. A preliminary in-bed tube support arrangement has been developed and support locations determined. A vibration analysis of the in-bed tube bundle and support arrangement has begun.

Specifications for the FD and ID fans have been developed by B&W and are currently being reviewed by them.

UCC-ND Engineering continued work on the test system design during the month. They revised the Engineering Flow Diagram to agree with an updated heat and mass balance received from B&W. A proposal and quotation were received from Harrison Radiator for the combustion air preheater, but because their design did not meet the thermal performance requirements, Harrison has been asked to review and improve their proposal. The design criteria for the Combustion Air and Flue Gas System have been approved and are in the process of being issued.

Instruments and Controls - The preliminary instrument application diagram is being updated to include a real-time data acquisition system and its interfacing to the combustor, and the deletion of the turbine-generator.

Work to define control strategies is awaiting information from B&W.

A list of direct digital control (DDC) vendors is being prepared. This list will be composed of vendors who have systems which could satisfy the needs of the TTU. Each vendor will be contacted and asked to supply detailed technical and pricing information. If, in the future, the decision is made to use a DDC system for control of the combustor, the most likely candidate vendors will be reviewed in detail and asked to demonstrate their systems. A performance specification would be written and put out for competitive bid.

Coal and Limestone Preparation - The estimated cost for the coal and limestone preparation facility was much higher than had been anticipated and as a result of this it was decided to investigate the feasibility and cost of buying the coal and limestone already dried and sized for feeding. Two limestone suppliers advise that they can provide the stone to meet the TTU requirements. They can deliver the stone in hopper trucks and unload them into the feed bunker.

A number of coal suppliers have been contacted and none of them contacted thus far have facilities for drying the coal to meet the TTU specifications. Blue Diamond Coal Co. volunteered to make a survey in an attempt to locate a supplier. A letter has been written to the "Facts About Coal in Tennessee" organization asking for their assistance. Efforts to try to find a supplier of prepared coal are continuing.

Air Compressor - Direction by DOE to omit the gas turbine from the TTU has imposed the requirement to provide a large motor-driven air compressor for supplying the combustor tube bundle cooling air. Use of a compressor will require that the electrical capacity in building 9401-1 be increased by running in a larger service line and installation of a stepdown transformer. Also, an air-to-air heat exchanger will be required to preheat the compressed air going to the combustor tube bundle by absorbing heat from the hot discharge air. These requirements are expected to result in a significant cost increase for the TTU. Several alternative schemes are being studied that make use of a circulating blower or air jet compressor in conjunction with the air compressor to reduce the compressor capacity and reduce the size of or eliminate the heat exchanger in an effort to find a way to reduce the cost.

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

E. C. Fox

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

TVA is the lead agency in this work and will reimburse DOE for the work to be performed by ORNL. This work is being conducted by ORNL under the terms and conditions of the Interagency Agreement between TVA, DOE, and ORNL regarding support for FBC research (reference: Agreement TV-48296A, Subagreement 5).

12.1 AFBC Modeling and Analysis - Task 4

J. W. Wells

12.1.1 Objective

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

12.1.2 Status Summary

On June 16, 1981, a meeting was attended with members of the Engineering Technology Division, and Meyer Steinburg and Patrick McGauley of Brookhaven National Laboratory. Steinburg and McGauley gave a presentation on artificial sorbent and the regeneration of these sorbents after sulfation. Their laboratory scale work has shown that calcium oxide silicate ($(\text{CaO})_x \cdot \text{SiO}_2$), common cement, may be a reasonable alternative to the "throw away" limestone sorbent. The main advantages of cement sorbent are claimed to be its attrition resistance and the ability to be regenerated after sulfation. This work is currently being funded by Morgantown Energy Technology Center (METC).

Work continued on the simulation of the 20 MWe TVA AFBC Pilot Plant. A summary of the heat transfer results to the submerged surfaces is given in Table 12.1. These results are for a superficial velocity of 244.0 cm/sec (8 ft/sec), expanded bed height of 122 cm (4f) and no recycle. The resulting fireside bed temperature found by closing the

energy balance was 1124.6°K (1564°F). These results are based on input from the B&W design basis.¹ Also, the SO₂ capture code was run for the first time for the 20 MWe AFBC configuration. During this process, a bug in the programming of SO₂ capture code was discovered and corrected. This correction caused the per cent SO₂ capture in the bed of 20 MWe AFBC to change from 86.7% to 80.6%. This result is for a 122 cm (4 ft) expand bed, a superficial velocity of 244 cm/sec (8 ft/sec) and no recycle. Further testing of both the heat transfer and SO₂ capture subcode will be performed during the next month.

Also during this month modifications were made to the freeboard subcode to simulate the 20 MWe AFBC freeboard configuration. This included the addition of the coal ash balance and modification of the code to account for varying freeboard cross-sectional area. These modifications are presently complete. Preliminary results for elutriated material from the freeboard are significantly lower than those predicted by the ORNL elutriation and attrition subcode.² This difference is currently being investigated and will hopefully be corrected by varying the solid flux from the bed, the injection velocity of solids from the bed or other possibilities not yet considered. The material balance portion of the freeboard code has been completed. During the next month the heat transfer surfaces in the freeboard will be included and the energy balance about the freeboard completed. The freeboard code will then be incorporated into main bed simulation to form the overall AFBC simulation of the TVA/EPRI 20 MWe AFBC Pilot Plant.

12.2 Analytical Support and Alternate Design Concepts Evaluation - Task 4b

C. S. Daw, W. K. Kahl, and E. C. Fox

12.2.1 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.

12.2.2 Status summary

The draft report detailing the trade-offs in design parameters and evaluating the economics of various design options is being prepared.

Table 12.1 Preliminary Summary of Calculated Heat Duties of
Submerged Surfaces

Type	Tube Side Temperature				Tube Side Pressure		Average Fireside	
	Inlet		Outlet		Inlet	Outlet	Wall Temperature	
	$^{\circ}\text{K}$	$(^{\circ}\text{F})$	$^{\circ}\text{K}$	$(^{\circ}\text{F})$	psia	psia	$^{\circ}\text{K}$	$(^{\circ}\text{F})$
Boiling Bundle	628.3	(670.9)*	628.3	(670.9)	2549.0*	2549.0	637.0	(686.6)
1st SSH**	667.8	(742.0)*	746.2	(883.2)	2538.0*	2485.1	738.2	(868.8)
2nd SSH**	723.6	(842.5)	811.1	(1000.0)*	2468.9	2415.0*	795.8	(972.4)
Waterwalls	628.3	(670.9)*	628.3	(670.9)	2549.0*	2549.0	673.8	(752.8)

Type	Steam*		Heat Duty		Heat Transfer Coefficient	
	Mass Flow					
	gm/sec	(lbm/hr)	Kcal/sec	(Btu/hr)	cal/cm ² ·s· $^{\circ}\text{K}$	(Btu/ft ² ·hr· $^{\circ}\text{F}$)
Boiling Bundle	72790.2	(577700.0)	2480.0	(3.54 x 10 ⁷)	.00716	(52.8)
1st SSH**	14017.2	(111247.6)	823.9	(1.18 x 10 ⁷)	.00661	(48.7)
2nd SSH**	14017.2	(111247.6)	805.5	(1.15 x 10 ⁷)	.00681	(50.2)
Waterwalls	99006.1	(785762.7)	1107.5	(1.582 x 10 ⁷)	.00620	(45.7)

* - A given condition

** - A secondary superheater

12.3 AFBC Bench Scale Facility - Task 5

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

12.3.1 Contract objective

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

12.3.2 Status summary

The testing program for sulfur capture performance of TVA limestones has been completed. Chemical analyses concerning carbon burn-up have also been completed. The raw data are being tabulated and analyzed. A complete report to TVA covering the entire bench scale test series is in the process of being prepared.

12.4 Coal Feed Tests - Task 11

C. S. Daw and V. R. Brantley

12.4.1 Objective

The objective of this task is to experimentally investigate feeding techniques and equipment for AFBC applications. Fundamental tests will be conducted in order to establish the key operating variables over which reliable coal and limestone pneumatic feeding can be achieved.

12.4.2 Status summary

The draft report for all phases of the coal feed test program has been approved by TVA and is now in the publications office.

12.5 Tubular Flow Reactor Experiment - Task 13

C. S. Daw

12.5.1 Objective

The goal of this program is to develop reliable kinetic expressions for the combustion of devolatilized Western Kentucky No. 9 coal (a swelling bituminous coal) in an atmospheric fluidized bed combustor. A series of small-scale experiments will be run to identify the key variables that affect char combustion and to provide the data needed for a quantitative model.

12.5.2 Status summary

We have suspended further activity on this project per request of TVA. It is anticipated that the project will be resumed in October.

12.6 References for Section 12

1. J. R. Byrd, Tennessee Valley Authority, Chattanooga, TN, 1981, personal communications to J. W. Wells.
2. J. W. Wells, M. H. Culver, and R. P. Krishnan, TVA Atmospheric Fluidized Combustor Annual Report, January 1 - December 31, 1980, ORNL/TM-7847.

13. PFBC SYSTEMS ANALYSIS

R. L. Graves

13.1 Objectives

The engineering systems analysis of PFBC power plants systems is intended to provide data, analysis, and supporting logic for the expanding PFBC program in DOE in order to achieve rapid commercialization of this technology. The analyses will be useful in evaluating the "evolutionary" approach to PFBC development as well as the "advanced" versions under consideration by DOE. Studies quantifying the trade-offs between costs, emission control, and plant efficiency are to be performed for various levels of PFBC development.

13.2 Status Summary

The Office of Coal Utilization (OCU) has replied to the recommendations for future work that ORNL submitted last month. The activities authorized by OCU reflect advice from METC also. The areas to be studied by ORNL are:

1. Advanced PFBC power plant concepts.
2. Modelling and analysis of PFBC control systems.
3. Packaged coal-fired industrial boilers, including a PFB.

The report from Task I is also to be completed and the review of new data from experimental facilities is to continue at a low level of effort.

The study of advanced systems is intended to be a screening analysis of high performance and novel PFBC power cycles. Some of the systems to be evaluated are:

1. Advanced air-cooled PFBC systems with and without gas turbine reheat.
2. Hybrid steam- and air-cooled PFBC combined cycles.
3. PFBC combined cycles utilizing coal pyrolysis to generate liquid and gaseous fuels for high temperature gas turbines.

The study is not limited to the above concepts.

The control analysis effort will emphasize the integration of turbine, compressor, and fluidized bed characteristics. The control schemes that have been proposed for the Curtiss-Wright pilot plant will be evaluated as part of this task. In addition, based on findings of the analytical effort, new control methods can be proposed and evaluated.

The task on packaged boilers will focus on assessing the potential of compact PFBC boilers in the industrial sector. Due to its high volumetric energy release, the PFBC appears to be the ideal choice for shop-fabricated industrial boilers. These boilers would not produce net power as would a utility PFBC power plant, but would be turbocharged to moderate pressures for the purposes of size reduction, improved SO₂ reduction, and high combustion efficiency. The PFBC packaged boiler will be evaluated relative to the AFBC and conventional boilers.

ORNL is currently developing a detailed task description and schedule for these three activities. The schedule will be provided in this progress report when completed.

14. FOSSIL FUEL APPLICATIONS ASSESSMENT

14.1 District Heating Turbine Study

H. I. Bowers

14.1.1 Objective

The purpose of this task is to assess the technical and economic factors related to modifying the design of new power plants to provide thermal energy for district heating by using the cogeneration process. Most of the work will be accomplished under a subcontract with Burns and Roe (B&R).

14.1.2 Status summary

H. I. Bowers met with B&R staff on June 23 to review the progress of the study. GE-Schenectady has provided revised performance data and heat balance diagrams for the 400- and 800-MW(e) district heating turbines. Final cost data and dimensions were promised by June 20, but have not yet been received at B&R. Preliminary cost estimates from GE for the 400-MW(e) turbines are $\$25.9 \times 10^6$ for a conventional condensing turbine and $\$37.2 \times 10^6$ for the district heating design, almost 50% higher. This is primarily because the district heating turbine design requires an additional element on the same shaft. GE-Lynn has also provided performance data and heat balance diagrams for the 200-MW(e) turbine, but no cost estimates or dimensions. Burns and Roe has developed piping schematics and general arrangement sketches for the 200-MW(e) turbine room allowing space for future district heating heat exchanges and circulating pumps. They are also developing equipment sizes and collecting cost data for equipment.

The project continues to fall behind schedule primarily because of the extended delays in obtaining district heating turbine data from GE. It is unlikely that B&R can meet the presently scheduled completion date of September 30.

14.2 Comparative Assessment of Options for New Industrial Boilers Relative to Air Emission Regulations for Morgantown Energy Technology Center

O. H. Klepper

14.2.1 Contract objective

1. Objectives: The purpose of this work is to define the technologies required to meet the range of allowable emissions for new industrial boilers, the relative merits of these technologies, and to identify needed research and development.

Industrial boiler capital costs developed in this program will be incorporated in the CONCEPT computer program for use in this and future studies.

14.2.2. Status summary

Subtask A — Selection of Emission Standards and Associated Boiler Criteria

No significant effort was devoted to this topic.

Subtask B — Steam Supply System Characteristics

Sections 11 and 12 were received from Foster-Wheeler (F-W) for their Phase I draft report on design concepts and costs for conventional coal-fired boilers, oil-fired boilers, and atmospheric fluidized bed boilers. These sections, dealing with operating costs and system reliability, have been reviewed and comments have been forwarded to F-W. The issues that remain to be resolved include the following:

1. The cost of disposing of ash and flue gas desulfurization (FGD) waste needs to reflect the total disposal cost incurred by a contractor who picks up waste at the boiler site and disposes of it permanently at his own site. The cost estimated by F-W at \$2.50/ton appears insufficient to cover more than just waste transportation cost.
2. The operating cost for steam/electricity in Section 11 for the boiler fans and FGD systems needs to be consistent with the plant operating requirements given in other sections of the report.
3. The basis for F-W's estimate of FGD reagent needs to be explained more clearly.
4. F-W needs to describe the basis for the boiler plant availability cited.

The target date for F-W revision of the Phase I report (including the comments received from METC) is the end of July 1981 — that date is about four weeks later than anticipated. We are reviewing our work schedule to determine the impact of the above delay.

Subtask C — Engineering Economic Evaluation

The cost submodels for the economic assessment, based on the first draft F-W costs, are complete and ready for use in the

code. Changes in these cost models are anticipated after revisions are received from F-W. Code modifications were completed to account for variations in internal steam uses between systems.

A description of the methodology to be used in the economic assessment and a sample code output was sent to Bill French, METC, Morgantown.

Subtask D - Characterization of Low- and Medium-Btu Gasification Systems

A draft of F-W's Phase II report dealing with steam supply systems fueled with gasified coal was received at the beginning of the month; system capital and operating costs were received by the middle of the month. This material is being reviewed at ORNL; copies have been sent to METC. Lacking from the F-W information is a cost breakdown of the boiler installation; F-W has been asked to provide this.

Subtask E - Inclusion of Industrial Boiler Cost Data in the CONCEPT Code

The CONCEPT program has been modified for handling industrial boiler cost models. This version of the computer code has been named INDCEPT. Fifty-six preliminary cost models for representing a variety of coal- and oil-fueled boilers and associated emission control systems have been assembled.

Work was begun on the preparation of a draft user's manual. The development of cost models for the steam supply systems fired with gasified coal remains to be done.

15. PERFORMANCE ASSURANCE SYSTEM SUPPORT FOR FOSSIL ENERGY PROJECTS

B. R. Everman, H. A. Nelms, L. F. Parsly, and A. N. Smith

Performance assurance support is being provided for major DOE-Fossil Energy projects. This support covers the areas of reliability, system safety, and quality assurance. Current activities include support for the liquefaction projects being managed by DOE and a failure modes and effects analysis.

15.1 Objective

The ORNL Performance Assurance System Support Office is responsible for acquiring, generating, and disseminating information relating to performance assurance (PA). The Support Office will provide performance assurance related technical support services to those Fossil Energy programs under the decentralized management control of the Oak Ridge Operations (ORO) Office and to programs under the direct management control of the Washington Headquarters Office. The Support Office will, as required, design and develop appropriate procedures, tools, and methodology necessary to provide the PA support services indicated.

15.2 Status Summary

Task 1: Assistance to the Fossil Energy Office of Control Management, Program Director for Major Programs - The bi-monthly status report was presented to the DOE Task Manager at the DOE facility in Germantown, MD.

Task 2: Critical Coal Liquefaction Components - The results of this study are being summarized in a topical report. The first draft of this report has been completed and is being circulated for comment.

Task 3: Selected Reliability Studies - A draft report is being prepared on the effort to produce a parametric study of the time and cost to demonstrate on-stream factors of 50-90% at confidence levels greater than 50%.

The topical report, "A Failure Modes and Effects Analysis of a Coal Slurry Preheater," has been finalized. Publication of the report is awaiting go-ahead from DOE-Headquarters.

Task 4: Failure and Plant Operational Reporting System - Meetings were held at four of the gasifier projects which will participate in the reporting system. Plans are being made to hold a workshop for the participants during the last week in July.

16. INTERNATIONAL ENERGY TECHNOLOGY ASSESSMENT

Oak Ridge National Laboratory is supporting the Lawrence Livermore National Laboratory (LLNL) in a broad program funded by the DOE Office of International Affairs. The program is designed to alert DOE management to foreign energy-related technologies of potential interest to the United States.

ORNL has responsibility for the following three areas of work: coal liquefaction including gasifier development status, coal liquefaction materials, and atmospheric fluidized bed combustion. These efforts are closely coordinated with similar activities underway at Argonne National Laboratory in the areas of pressurized fluidized bed combustion and coal gasification materials.

16.1 Liquefaction Technology (Including Gasifier Development Status)

W. C. Ulrich

16.1.1 Objective

Broad objectives of the IETA program are to report foreign technology developments of current interest and to identify and assess those developments of significance to U.S. programs. Detailed assessments in selected areas will also be provided. A specific objective of the ORNL effort is to provide a substantive technical review of the status of foreign technology for the liquefaction of coal, including gasifier development status.

16.1.2 Status summary

Work continued on the survey of indirect coal liquefaction and gasifier technology. Of seven authors contacted, three provided us with preprints of papers which they were to present at the Coal Technology Europe '81 Conference in Cologne.

The pictorial report of SASOL is currently undergoing review by representatives of SASOL.

16.2 International Survey of Coal Preparation Technology

J. C. Moyers, K. O. Johnsson

16.2.1 Objective

The objectives of this survey are to assess the general state of the technology of coal preparation in foreign countries, to identify

and describe development work in progress, and to identify and assess particular categories of technical problem areas which need additional emphasis.

16.2.2 Status summary

Questionnaires requesting statistical information on current practices and technical information on new developments were sent to appropriate governmental agencies in Australia, India, Poland, South Africa, United Kingdom, and West Germany. A. W. Deurbrouck, of the Pittsburgh Mining Technology Center, was visited on June 9 to discuss the survey and to learn of significant developments of which he is aware. The search for and review of pertinent literature continued.

16.3 International Survey of the Status of Technology of Critical Components for Coal Liquefaction Processes

W. R. Williams, K. O. Johnsson, T. B. Conley, and T. L. Dahl

16.3.1 Objective

The objective of this survey is to carry out an assessment of the state-of-the-art of foreign technology related to three critical coal liquefaction plant components: slurry valves, slurry pumps, and slurry heat exchangers. The assessment will consider the current generation components as well as those of improved designs and/or utilizing advanced technology, and will focus on components for use in demonstration plants and commercial plants. Foreign components will be assessed in terms of their applicability to liquefaction processes under development in the U.S. and will be compared where possible to comparable U.S.-made components. Recommendations for follow-up efforts to benefit from the foreign technology will be made.

16.3.2 Status summary

During June, letters which included general specifications for equipment and questions on current design capabilities and proposed research and development activities were prepared for mailing to foreign manufacturers. Manufacturers have been requested to respond by July 31 with information on their capabilities to supply the specified equipment and with the name of a person to discuss their research and development activities. Manufacturers may choose to respond in writing to the research and development questions. Letters have been sent to 22 pump manufacturers and 26 valve manufacturers. Letters are going out to 21 heat exchanger manufacturers on July 1.

16.4 Coal Liquefaction Materials

A. R. Olsen and G. M. Caton

16.4.1 Objective

The objectives of this phase of the assessment program are to identify materials research and development programs in foreign countries in support of liquefaction processes and to assess the programs and findings in terms of their status, applicability to U.S. coal liquefaction demonstration and commercialization programs, and the potential value of possible cooperative agreements.

16.4.2 Status summary

Lawrence Livermore National Laboratory comments on the materials section of the draft report were reviewed and appropriate editorial modifications were made. We are continuing to monitor foreign publications for materials information.

16.5 International Survey of Atmospheric Fluidized Bed Combustion Technology

R. P. Krishnan, E. C. Fox, and K. O. Johnsson

16.5.1 Objective

The objective of this program is to provide an international assessment of the status of atmospheric fluidized bed combustion (AFBC). The assessment will describe the applications, critical problem areas, and the current developmental projects that address these problem areas in AFBC technology in foreign countries.

16.5.2 Scope

This assessment is part of a broader program designed by the DOE Office of International Affairs (IA) and managed by Lawrence Livermore National Laboratory (LLNL) to alert DOE Management to foreign energy-related technologies of potential value to the United States. ORNL and Argonne National Laboratory (ANL) have been assigned the area of fluidized bed combustion. ORNL will survey AFBC, and ANL will survey pressurized fluidized bed combustion (PFBC).

16.5.3 Status summary

The draft report on this task has been reviewed by Lawrence Livermore National Laboratory. The comments have been received and the report is being revised.

17. GENERALIZED EQUILIBRIUM MODELS OF LIQUID AND GASEOUS FUEL SUPPLIES

J. Barhen

17.1 Background

In support of DOE/Fossil Energy (FE), Oak Ridge National Laboratory is conducting a research program in the modeling of liquid and gaseous fuel supplies. The principal objectives of this program are as follows:

- a. Complete the development of a Liquid Fuels Supply (LFS) model based on a prototype model developed by Decision Focus Incorporated in collaboration with Lewin and Associates, and provide operational support in decision analyses, benefit-cost analyses, etc., for the Division of Policy and Strategic Planning, DOE/FE.
- b. Develop a Gaseous Fuels Supply (GFS) model and provide operational support for FE's use of the model.
- c. Develop and demonstrate a decision making strategy based on sensitivity theory.
- d. Provide operational support to DOE/FE in the use of all versions of GEMS and LEAP and in the interpretation of model results including data and model limitations.

Decision Focus Incorporated (DFI) has developed the Generalized Equilibrium Modeling System (GEMS) and associated Model Data Base Management System (MDMS). GEMS is a system of computer programs designed to aid analysts in constructing models of regional, national and international economic markets, in particular those associated with energy, and their linkage to the rest of the economic system. The resulting models could be applied to evaluate the impact of specific public policy or private sector investment alternatives. The GEMS system was also used to construct the LEAP model, which is the Energy Information Administration's (EIA) principal long range energy model.

17.2 Status Summary

Progress on subtasks currently active is reported in the following sections.

17.2.1. Subtasks 0.1 and 3.1: Program definition and objectives. R. G. Alsmiller, J. Barhen, V. A. Kuuskraa, F. Morra, D. M. Nesbitt, R. L. Phillips, C. R. Weisbin

It is proposed¹ that the main focus of the expanded LFS model be directed toward addressing the relative funding allocation priorities among various transitional technologies (e.g. EOR) and the long-term backstop (i.e. synthetic fuels), in order to study the strategic issue of achieving U.S. liquid fuels supply self-sufficiency.

A recent study² by the MITRE Corporation, which examined some options for eliminating oil imports by the year 2000, has determined that liquid fuels are the only critical domestic energy resource in the year 2000. An independent analysis³ by R. H. Clark, president of the American Association of Petroleum Geologists (AAPG) estimates that, depending on commitment (e.g. financial), the U.S. has the resource base and technology to make itself self-sufficient in oil within five years. Furthermore, a comprehensive study⁴ on national energy issues has just been completed at ORNL. The proposed broad strategy for shaping the U.S. energy future emphasizes the urgent need to reduce oil imports below the 20% level, and provides suggestions to solve current problems with currently available solutions, without precluding the use of better solutions when they become available.

Several additional studies⁵⁻⁷ argue that the U.S. can attain energy independence within the next decade through leasing of new acreage and acceleration of drilling. The implications of these claims have major impact on the types and levels of R&D and technology deployment that would be sponsored by Fossil Energy.

Using the expanded LFS model currently being implemented at ORNL, we propose to develop options which reflect careful study, documentation, and public availability, for increased supplies of domestic liquid fuels. If necessary, additional options to reduce the total demand for liquids⁴ (e.g. by improving engine efficiencies and downsizing or weight reduction in the transportation sector, and by fuel substitution in the industrial, residential/commercial and utility sectors) could be assessed using the LEAP-80 macro-energy model.

The funding allocation decisions among the various transitional technologies and the long-term backstop shall provide a measure of total economic impact in terms of required capital investment increase over the "business-as-usual" framework, versus the potential cost of oil imports. This impact will be quantitatively determined using the Decision Analysis/Sensitivity Theory capabilities under development at DFI and ORNL.

17.2.2. Subtask 1.3: Comparison of prototype LFS results to ARC-80/LEAP projections. J. Barhen, J. E. Horwedel, L. Stewart, R. W. Sturm

The task of "calibrating" the exogenous processes specified in the prototype LFS model to the results of the macro-energy model ARC-80/LEAP

is well under way. Preliminary results appear most interesting. The plot in Fig. 1 shows the LFS high and low demand trajectories for liquid fuels, as compared to the ARC-80 low, medium, and high projections. It should be recalled that, anticipating the benefits for EOR to be accelerated in a high-demand scenario, the previous DFI study⁸ attempted to be conservative in the selection of an oil-demand track. It turns out, however, that, as shown on the graph, even the low LFS demand track is quite higher than the highest ARC-80 projections. The impact of these differences on the final results is being investigated. It is also planned to calibrate the synthetics and imports exogenous processes.

17.2.3. Subtask 1.4: Review and critique of the data base and its use in the prototype LFS model. V. A. Kuuskraa, F. Morra

During the month of June three products were submitted to ORNL for consideration. The first two continued the treatment of the undiscovered resource component, while the third sought to create options for future use of the model.

A. Report on Finding Rates

Lewin and Associates prepared a report on the rate of finding reserves of oil and gas as a function of drilling effort. The implication of various methods of calculating finding rates on forecasts of conventional reserves was studied. This analysis will make a strong contribution to the conventional reserve portion of the Oak Ridge system. It will be possible to make much more accurate forecasts by extrapolation from this statistical series of finding rates, given a small number of assumptions, because conventional reserves are supported by a large, historical data base; and because the discovery of this resource is reasonably mature.

At the heart of most models of conventional reserves is the finding rate, defined as the ratio of reserves added to the amount of effort expending. While simple in concept, practical applications of finding rates are relatively complex:

- There are from four to six independent classification of reserve additions, yielding from twelve to sixty-three possible definitions of the numerator
- There are seven classifications of drilling effort activity, yielding 119 definitions of the denominator.

Analysis of published literature on modeling the undiscovered conventional reserves component indicates some confusion about which of the 7447 possible definitions of finding rate are being used. Some studies take the ratio of all reserves added to all drilling effort, other studies focus only on pure wildcatting (i.e., new field discoveries divided by new field wildcats). Each different assumption about the finding rate has

clear implications on the type of model necessary to account for reserves addition and the amount of reserve forecast to be added.

Lewin and Associates prepared a summary review of the literature on this subject and organized existing data on drilling and reserves into an interactive system which permitted the user to:

- Explicitly specify a definition of the finding rate (with possibility of selecting any of the 7447 possible definitions)
- Calculate finding rates using this definition for existing data
- Forecast finding rate into the future; the user can select size of the undiscovered resource base based on the PGC, USGS or RAND Corporation estimates
- Make reasonable projections of the implications of definitions of finding rate for production in future years.

Economics were not a part of this assessment. The amount of future drilling activity is really a function of both productivity and product price; for this particular study, drilling was exogenously specified.

B. Documentation of the Finding Rate System

The analysis of finding rate required a computer system to manipulate the large data base. The individual data bases for drilling and reserves are organized in different fashion and must be placed in common terms. A large number of errors in both data bases were noted and corrected. Most prevalent were minor typographical errors, although some conceptual errors were also found. (These have to do with the impact of tax treatment on dryhole rate for offshore drilling.)

The finding rate system is composed of the data base and analysis routines. Because the system is likely to be used and reused in the future, it was made interactive. That is, the program requests many of the parameters from the user who may supply a wide range of values. This permits others to study questions which were not addressed in the report discussed above.

Some of the options that are available to the user are listed below:

- Level of analysis: The user may select a simple onshore/-offshore breakout or a Lower 48 vs. Alaska breakout or a more elaborate breakout according to the NPC regions.
- Product: The user may select oil or gas, which can also be subdivided into associated and nonassociated gas.
- Effort: The user may choose to specify effort in terms of wells drilled or total drilling footage.

- Reserves: The user may select from any of the API/AGA reserves classifications.
- Drilling: The user may select from the AAPG categories of drilling effort.
- Dry Holes: The user has complete freedom to specify the allocation of dry hole footage among products.
- Ultimate Recovery: The user may fit a curve to the historical set of finding rates so that the curve yields ultimate recovery of hydrocarbons according to either the Potential Gas Committee (PGC); the United States Geological Survey (USGS); or the recently released report by the RAND Corporation.
- Future Drilling: The user may select on a regional basis future scenarios about drilling, including options permitting constant rate, linearly increasing rate, geometrically increasing rate, or any particular empirical drilling scenario.
- Ratio of Reserves-to-Production: The user may select a constant or changing ratio of reserves-to-production with the same options as the drilling statistics.
- Time: The user may specify any time frame between 1982 and 2010 for forecast reports.

In the documentation, all of the routines and data bases are described and the sample runs are presented to enable the interested user to operate the system.

C. Strategy Paper

The paper describes the options for the "specific work project" to be conducted to test the liquid and gaseous fuels model. In addition, the paper discusses the impact of choice of a work problem on the nature of model development activities.

The paper summarizes the basic policy options available to the Federal government, in the context of ultimate long-term goals of the modeling project, and sets the stage for the discussion of strategic options.

A second section discusses the work which would be required to develop the liquid and gaseous fuels models as a policy analysis tool. This includes: improvement of the prototype liquids model (both data improvement and validation); and expansion of the liquids model to treat more disaggregate view of the technologies; and a more disaggregate view of geography. Additional suggestions for improvement included: disaggregation of the "non-EOR" sources; incorporation of uncertainty into the model; or the development and further refinement of the gaseous fuels model.

The third section indicates the extent to which the work could be used to address four kinds of policy issues. Included are the impacts of providing information sponsoring R&D; changing the tax structure; and changed regulatory activities. This document has been submitted to all parties concerned, for review, comment and critique.

17.2.4. Subtask 1.5: Design of an expanded LFS model. B. Toney, J. E. Horwedel, D. M. Nesbitt, R. L. Phillips

During June, DFI constructed a first order expanded Liquid Fuels Supply model (LFS). This model explicitly considers the competition among 13 different sources of domestic oil (including synthetical with imported oil to serve domestic oil demand. It also explicitly models shale-oil upgrading, Alaskan oil pipeline economics, and the economics of transportation of Western oil. DFI built this model on their DEC VAX 11/780 computer using internally generated data. The model was run using this base-case data and a price-quantity forecast was produced for all the technologies in the model. Since this data has not been verified these results are not defensible. Final base case data will be developed by the DFI/Lewin/ORNL project team. Listings of the data and the results for this model were sent to ORNL. Attempts by ORNL staff to implement the above model on the DOE/FCF system have, as of now, not been successful because of potential inconsistencies in defining the network model.

17.2.5. Subtask 2.1: Design of a prototype GFS model. B. Toney, J. E. Horwedel, D. M. Nesbitt, R. L. Phillips

DFI constructed a prototype Gaseous Fuels Supply Model (GFS) based on the design previously presented in the project memorandum "Designs of Domestic Oil and Gas Models for Research and Development Funding Allocation Decisions" (March, 1981). This model explicitly considers the competition among 12 sources of domestic natural gas, including both synthetics and unconventionals, with imported gas. Both Alaskan and domestic gas pipelines are explicitly, modeled. As with the expanded Liquid Fuels Model, DFI built this model on their DEC VAX 11/780 computer using internally generated data. A base case run was made using this data to produce forecasts for all the technologies represented in the model. Listings of the data and the results for this model were sent to ORNL. ORNL staff is currently implementing the GFS model on the DOE/FCF system.

17.2.6. Subtask 3.5: Automated Decision Analysis/Sensitivity Theory Capability. D. M. Nesbitt, R. L. Phillips

DFI continued its research in this area. In particular the problem of optimal research and development funding allocation in the case where both funding decisions and outcomes occur over time was considered. In addition, an application of the analysis for a deterministic static economy was developed for a linear economy. These results will be documented in the final version of "A Methodology for Determining an Optimal Allocation of R&D Funds".

Fig. 17.1. Comparison of total liquid fuel demand projections between the LFS Model and ARC-80/LEAP.

17.3 References for Section 17

1. "ORNL/DFI/L&A Strategy for Developing a Capability to Analyze Liquid and Gaseous Fuels Policies for DOE/FE/OGST," draft strategy paper, June 1981.
2. "U.S. Energy Strategies: Some Options for Eliminating Oil Imports by the Year 2000," The MITRE Corporation, April 1981.
3. "U.S. Oil Self-Sufficiency Timetable Set," R. H. Clark, Oil and Gas Journal, p. 47, June 1981.
4. "Toward a Desirable Energy Future: A National Perspective," R. S. Livingston, et al., ORNL/PPA-81/6, Final Draft, March 1981.
5. Erickson, E. W., "Natural Gas and the Natural Gas Policy Act: A Pragmatic Analysis," Natural Gas Supply Association, January 1981.
6. Hann, J. D., "Future of Petroleum Exploration in the United States", Lewin and Associates, private communication to J. Barhen, June 1981.
7. Merklein, H. A., "Drilling: The Key to Ending U.S. Oil/Gas Imports by 1994", World Oil, June 1981.
8. D. M. Nesbitt, et al., "A Decision Analysis of National R&D Funding for Unconventional Oil Technologies," DFI/1029, pp. 1-16, December 1980.

18. ANALYSES OF COAL PRODUCTION GOALS

W. F. Barron

The analysis of coal production goals by ORNL and LANL involves improvement in both the structure and data for a model of regional coal markets. The model tentatively titled the Regional Coal Allocation Model (R-CAM) is a modification of the LACUMS (LANL) and the National Coal Model (EIA). Originally, the project was designed as a two year effort with the ultimate objective of assisting DOE in developing regional coal production goals. Those goals would then be incorporated into the DOI decision making process with regard to the leasing of Federal lands. Uncertainties regarding project funding levels for FY 82 have led to a redirection of project effort to emphasize tasks and subtasks which could be completed by the end of FY 81. This redirection will result in no major loss of efficiency in the overall work effort should funding for FY 82 become available. It should be noted that funding levels for FY 82 have not yet been set. The decision to redirect project is, however, considered a prudent one until the FY 82 budget is determined. We hope and expect that additional funding will be available to complete the tasks as originally set out in the two year work plan.

18.1 Current Project Status

Early in June project staff at ORNL and LANL in conjunction with DOE decided that funding uncertainties for FY 82 were sufficient to warrant an emphasis on work tasks which could be completed during FY 81. This approach will permit development of finished products which can be employed in later coal modeling efforts by ORNL, LANL or others. Staff in each of the three major topical areas (supply data, transport costs, and demand estimates) identified and prioritized segments of the work effort which could be completed with funds available in the FY 81 budget.

18.1.1 Coal supply data

Tasks in coal supply analysis were prioritized and activities are proceeding in the following areas:

- (1) Revising coal reserve estimates by region and by BTU and sulfur content.
- (2) Estimating the variability of regional coal reserve estimates utilizing several data bases.
- (3) Revising the project model to allow a "maximum leasing" solution under uncertainty, in terms of:
 - altering some of the LP constraint inequality conditions,
 - improving the reserve margins and ambient SO₂ constraints,
 - altering capacity construction costs,

- eliminating water demand and supply which have negligible impact on the solution and which are not well-specified in LACUMS,
 - eliminating oil shale from the model (same reason as above),
 - identifying production goal bounds and their probabilities based on the ranges in coal reserve estimates (stochastic LP),
 - introducing an explicitly dynamic representation that reflects depletion of reserves and long-term contracts between coal suppliers and utilities,
 - determining a "maximum leasing" solution using the high case scenario and the results from the stochastic LP and hop-skip-and-jump solutions, and
 - improving computational efficiency via Wolfe and Dantzig's Decomposition Principle.
- (4) Initiating a study (but no final documentation) to re-estimate county-specific coal reserves:
- considering recent state geologic survey reports and maps,
 - minability factors from those reports, and
 - information on ownership patterns.

18.2 Coal Transport System

Engineering cost estimates will be used to forecast coal transport rates. These estimates will include amortized construction costs for new spur lines needed to serve developing supply regions as well as the operating and maintenance costs to move coal between origin and destinations.

The revised FY 81 work plan calls for estimating an origin-destination movement cost matrix based on preliminary traffic volume estimates. Existing traffic volumes on the rail network have been determined. Research is in progress on other aspects of the cost functions.

18.3 Regional Demand Analysis

A decision was made jointly by ORNL and LANL staff that coal demands would be regionalized by state with a few exceptions. This level of aggregation will facilitate the regionalization of industrial coal demand forecasts and provide for a more interpretable model outputs. The development of coal demand projections for the export and synfuels sectors will be completed by the end of July. Reports documenting these projections and allocations to states will be completed by mid-August.

For the industrial demand component work is currently underway at synthesizing the various coal demand forecasts to be used in the model. During this reporting period it was also decided to include for completeness a residential and commercial coal sector.

19. FOSSIL ENERGY INFORMATION CENTER

Carol Oen

A review of worker exposure and potential health effects of indirect coal liquefaction is being carried out under the leadership of Dr. Nancy Munro. A draft of the process description has been completed and descriptions of carcinogenesis and teratogenesis testing have been drafted. Background work has begun for the chapter on worker exposure. Numerous inquiries have been made to obtain information pertinent either to an adequate exposure assessment or to toxicity testing results.

Development of the Synfuels Assessment and Synfuels Substances databases is continuing with the investigators of several other related topics contributing technical analysis of documents.

Copies of pertinent documents have been shared with various investigators—Bert Hakkinen, Jeanne Calle and others in Walsh's group, Wanda Haschek and Carol Heckman.

Dr. Wanda Haschek, toxicologist, will review the validity of the basis for the current methanol standards as requested by Dr. Pat Buhl.

INTERNAL DISTRIBUTION

1. S. P. Baker	42-44. L. E. McNeese
2. J. Barhen	45. C. A. Mills
3. B. M. Benjamin	46. J. E. Mrochek
4. W. J. Boegly	47. B. Niemann
5. C. R. Boston	48. C. J. Oen
6. R. A. Bradley	49. A. R. Olsen
7. V. R. Brantley	50. G. E. Oswald
8. C. H. Brown	51. L. F. Parsly
9. G. H. Burger	52. T. W. Pickel
10. D. W. Burton	53. M. L. Poutsma
11. H. D. Cochran, Jr.	54. L. W. Rickert
12. K. E. Cowser	55. B. R. Rodgers
13. C. S. Daw	56. M. W. Rosenthal
14. N. W. Durfee	57. R. Salmon
15. D. P. Edmonds	58. C. D. Scott
16. D. M. Eissenberg	59. M. Siman-Tov
17. J. L. Epler	60. C. B. Smith
18. J. I. Federer	61. G. P. Smith
19. D. E. Ferguson	62. I. Spiewak
20. C. W. Gehrs	63. R. W. Swindeman
21. R. W. Glass	64. V. J. Tennery
22. T. G. Godfrey	65. J. F. Thomas
23. G. M. Goodwin	66. D. B. Trauger
24. R. L. Graves	67. W. C. Ulrich
25. W. A. Hartman	68. V. C. Vaughen
26. J. R. Hightower	69. J. S. Watson
27. M. R. Hill	70. G. C. Wei
28. J. K. Huffstetler	71. J. R. Weir
29. G. R. Jasny	72. C. R. Weisbin
30. J. K. Johnson	73. J. W. Wells
31. K. O. Johnson	74. B. Wham
32. P. J. Johnson	75. W. R. Williams
33. J. E. Jones, Jr.	76. J. H. Wilson
34. J. R. Keiser	77. J. Wortman
35. A. D. Kelmers	78. E. L. Youngblood
36. A. A. Khan	79. G. P. Zimmerman
37. R. P. Krishnan	80. Patent Office
38. D. D. Lee	81-84. Laboratory Records
39. E. L. Long, Jr.	85. Laboratory Records - RC
40. R. W. McClung	86-87. Central Research Library
41. C. J. McHargue	88. Document Reference Section

EXTERNAL DISTRIBUTION

DOE-ORO, Oak Ridge, TN 37830

- 89. R. N. Collier, Jr.
- 90. C. W. DiBella
- 91. L. L. Radcliffe

DOE-Office of Fossil Energy, Washington, DC 20545

92. T. Atwood	99. C. A. Kinney
93. D. L. Bauer	100. T. K. Lau
94. P. Buhl	101. C. V. McGurl
95. W. M. Crim	102. G. A. Mills
96. S. J. Dapkunas	103. E. S. Pierce
97. S. I. Freedman	104. D. K. Stevens
98. J. F. Geffken	105. R. E. Verner

DOE Denver Projects Office, P.O. Box 26300, Lakewood, CO 80226

- 106. R. A. Flinn
- 107. D. P. Lessig

DOE-Morgantown Energy Research Center, P.O. Box 800, Morgantown,
WV 26506

108. J. Byam	110. L. Headley
109. J. S. Halow	111. R. E. Schafer
	112. J. S. Wilson

DOE-Pittsburgh Energy Technology Center, P.O. Box 10940, Pittsburgh,
PA 15236

113. S. Akhtar	118. R. E. Hucko
114. J. P. Barreca	119. J. J. Lacey
115. D. Bienstock	120. L. Lorenzi
116. A. W. Deurbrouck	121. R. R. Schehl
117. J. D. Hickerson	122. A. G. Sharkey
	123. T. M. Torkos

Electric Power Research Institute, 3412 Hillview Ave., Palo Alto, CA 94304

- 124. S. B. Alpert
- 125. E. Aulisio

International Coal Refining Co., P.O. Box 2752, Allentown, PA 18001

- 126. S. M. Morris
- 127. G. C. Rappe

Tennessee Valley Authority, 1020 Chestnut St., Tower 2, Chattanooga, TN 37401

128. J. R. Byrd	132. G. A. Hollinden
129. D. Daugherty	133. K. LuePhang
130. R. L. Frank, Jr.	134. R. L. Lumpkin
131. W. D. Goins	135. A. M. Manaker
	136. S. R. Smith

U.S. Environmental Protection Agency, Research Triangle Park, NC 27711

- 137. J. McSorley
- 138. C. D. Sedman

- 139. H. Beuther, Gulf Research and Development Co., P.O. Box 2038, Pittsburgh, PA 15230
- 140. B. Crynes, School of Chemical Eng., Oklahoma State Univ., Stillwater, OK 74074
- 141. C. W. Edington, Office of Health and Env. Rev. (EV), USDOE, E-201, Washington, DC 20545
- 142. W. R. Epperly, Exxon Research and Engineering Co., P.O. Box 101, Florham Park, NJ 07932
- 143. H. L. Falkenberry, DOE/Resource Applications, Coal Resource Mgt., 1200 Pennsylvania Ave., N. W., Mail Stop 3344, Washington, DC 20461
- 144. O. F. Ghaly, Bechtel Corp., P.O. Box 3695, San Francisco, CA 94119
- 145. C. R. Greene, SRI International, 333 Ravenswood Ave., Menlo Park, CA 94025
- 146. N. A. Greenlee, P & M Coal Mining Co., P.O. Box 199, Du Pont, WA 98237
- 147. E. O. Gurmen, Stearns Magnetics, 6001 S. General Ave., Cudahy, WI 53110
- 148. O. J. Hahn, Univ. of Kentucky, Institute for Mining and Minerals Research, 213 Bradley Hall, Lexington, KY 40506
- 149. G. Heunisch, Research Division of Conoco Coal Development Co., Library, PA 16129
- 150. E. Huffman, Southern Company Services, Fuel Processing Programs, P.O. Box 2625, Birmingham, AL 35202
- 151. J. E. Jones, Kentucky Center for Energy Resources, P.O. Box 11888, Ironworks Pike, Lexington, KY 40502
- 152. D. L. Keairns, Westinghouse Electric Corp., 1310 Beulah Rd., Pittsburgh, PA 15235

153. H. F. Lewis, Catalytic, Inc., P.O. Drawer 239, Wilsonville,
AL 35186
154. W. J. Lochmann, Ralph M. Parsons Co., 100 W. Walnut St., Pasadena,
CA 91124
155. D. H. Maylotte, GE R&D Center, P.O. Box 8, Bldg. K 1, Rm. 4B-26,
Schenectady, NY 12301
156. M. V. Mehta, ICRC, P.O. Box 2752, Allentown, PA 18001
157. T. Modrak, Babcock & Wilcox Res., 1562 Beeson St., Alliance,
OH 44501
158. T. E. O'Hare, Dept. of Energy and Environment, Brookhaven National
Laboratory, Associated Universities, Inc., Upton, LI NY 11973
159. G. J. Pappaionau, Union Carbide Corp., Linde Div., 1500 Polco St.,
Indianapolis, IN 46224
160. E. G. Pierick, General Electric Co., M/C V02, Vallecitos Nuclear
Center, P.O. Box 460, Pleasanton, CA 94556
161. D. Rimmer, City Svc. Co., 1305, 4-ND, Box 300, Tulsa, OK 74102
162. T. E. Scott, Ames Laboratory, 126 Metals Development Bldg., Iowa
State University, Ames, Iowa 50011
163. W. R. Siegart, Texaco, Inc., 2000 Westchester Ave., White Plains,
NY 10650
164. C. Streed, Process Res. and Dev. Div., Mobil Res. and Dev. Corp.,
Billingsport Rd., Paulsboro, NY 08066
165. J. J. Turner, Office of Plans & Tech. Assessment, DOE, Mail
Stop C0125, Germantown, Washington, DC 20545
166. B. M. Weiss, Catalytic, Inc., Centre Sq., West, 1500 Market St.,
Philadelphia, PA 19102
167. F. E. Witmer, DOE/EV/OECO/ECT, MSE-201, Washington, DC 20545
- 168-194. Technical Information Center