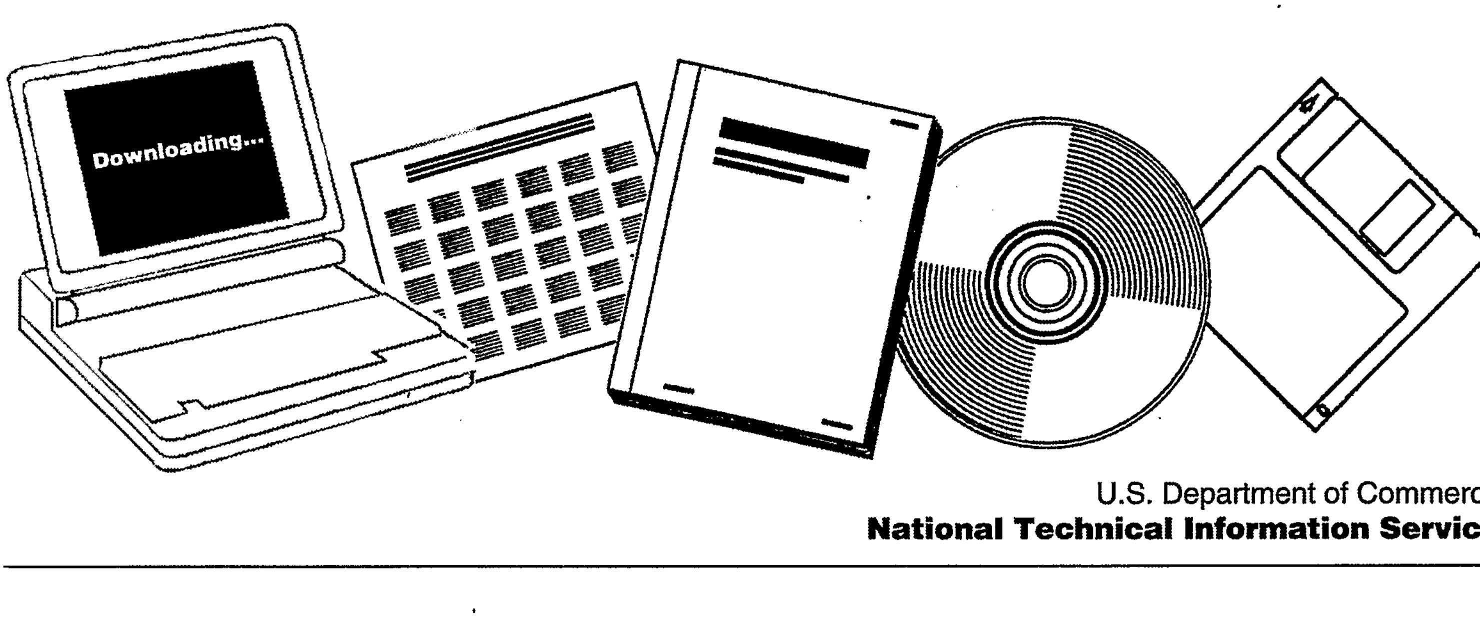
MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES: SIXTH QUARTERLY REPORT, JANUARY 1-MARCH 31, 1988

ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

MAR 1988



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D.G. Hamblen
M.A. Serio
L.D. Smoot
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Work Performed Under Contract No.: DE-AC21-86MC23075

For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
Morgantown, West Virginia

By
Advanced Fuel Research, Inc.
East Hartford, Connecticut
and
Brigham Young University
Provo, Utah

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87 Church Street
East Hartford, Connecticut 06108
and
Brigham Young University
Provo, Utah 84602

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ABSTRACT

The overall objective of this program is the development of predictive capability for the design, scale up, simulation, control and feedstock evaluation in advanced coal conversion devices. This technology is important to reduce the technical and economic risks inherent in utilizing coal, a feedstock whose variable and often unexpected behavior presents a significant challenge. This program will merge significant advances made at Advanced Fuel Research, Inc. (AFR) in measuring and quantitatively describing the mechanisms in coal conversion behavior, with technology being developed at Brigham Young University (BYU) in comprehensive computer codes for mechanistic modeling of entrained-bed gasification. Additional capabilities in predicting pollutant formation will be implemented and the technology will be expanded to fixed-bed reactors.

The foundation to describe coal-specific conversion behavior will be AFR's Functional Group (FG) and Devolatilization, Vaporization, and Crosslinking (DVC) models, developed under previous and on-going METC sponsored programs. These models have demonstrated the capability to describe the time dependent evolution of individual gas species, and the amount and characteristics of tar and char. The FG/DVC models will be integrated with BYU's comprehensive two-dimensional reactor model, PCGC-2, which is currently the most widely used reactor simulation for combustion or gasification. The program includes: i) validation of the submodels by comparison with laboratory data obtained in this program, ii) extensive validation of the modified comprehensive code by comparison of predicted results with data from bench-scale and process scale investigations of gasification, mild gasification and combustion of coal or coal-derived products in heat engines, and iii) development of well documented user-friendly software applicable to a "workstation" environment.

Success in this program will be a major step in improving the predictive capabilities for coal conversion processes including: demonstrated accuracy and reliability and a generalized "first principles" treatment of coals based on readily obtained composition data.

During the sixth quarter of the program, progress was made in several areas, as summarized below.

For Subtask 2.a, samples of demineralized Zap coal were subjected to ion-exchange with Mg and Ca, in order to further understand the role played by ion-exchangeable cations on char reactivity. Chars were prepared by heating in a TGA at 30°C/min to 900°C or 1000°C and reactivity measurements were done in both air and CO_2. In both gases, the loading of sufficient amounts of Mg or Ca produced a char which was equal or more reactive than chars produced from the raw coal.

Char samples obtained from drop tube experiments done with Pittsburgh Seam coal were prepared for SEM analysis by potting and polishing. The SEM photographs were taken and were analyzed to obtain quantitative information such as bubble size and wall thickness, which can be used for validation of the viscosity and swelling models. Our preliminary analysis indicates that maceral effects may be important.

Work resumed on the viscosity model and continued on using the FG-DVC model to model the baseline pyrolysis data obtained for the 10 coals from the EFR and TG-FTIR reactors, as well as from FIMS analysis at SRI International. Some refinements were made to the treatment of internal and external transport in the model. Work was also done on comparing the FG-DVC model to the statistical model of Pugmire and Grant at the University of Utah, which is based on percolation theory.

Entrained flow reactor experiments continued with three coals and additional FIMS analysis experiments were done at SRI.

For Subtask 2.b, char samples were prepared in the simple hot-tube reactor and in the BYU gasifier. Seven char samples were analyzed along with a sample of Utah bituminous coal. Construction of the high-pressure, controlled-profile reactor continued. Improvements were made in the reactor design to reduce cost and increase reliability. A program was developed to test and characterize the reactor.

For Subtask 2.c, data collection was temporarily suspended as the FT-IR spectrometer was needed for a different project.

For Subtask 2.d, SEM/dispersive x-ray analysis was performed on individual ash spheres that were recovered from the eight stages of a cascade impactor for experiments in the Transparent Wall Reactor (TWR) with Zap lignite coal. It was determined that the small particle sizes collected in the impactor may not give quantitative analysis results in our x-ray system. It was decided to modify the instrument conditions and use some pure mineral oxide standards in the appropriate size ranges for calibration.

For Subtask 2.e, the design of the fixed bed reactor system was completed during the past quarter, parts were ordered and construction was begun. This reactor will have on-line analysis of evolved volatile products, functional group composition, and particle temperatures.

For Subtask 2.g, predictions of thermal NO in the integrated submodel were physically unrealistic. The literature on chemistry/turbulence interactions was reviewed. A new approach at calculating pollutant concentrations with chemistry/turbulence interactions was developed. A sorbent chemistry submodel was evaluated and compared with recent data at short residence time under independent funding at The University of Utah. The chemistry of sulfur in flames was reviewed from the literature.

For Subtask 2.h, modifications of the cold-flow facility were completed and tests were initiated. Three injection jets for sorbent were found to be more effective than one. Work on modifying the gasifier for sorbent injection tests was continued. Modifications are being made to insert thermocouples and to make FTIR measurements.

For Subtask 3.a, work continued on incorporating the FG-DVC submodel under the SSPV and MSPV methods. Converged solutions were obtained for a combustion case and a gasification case with two progress variables tracking coal offgas. The approaches of tracking volatiles and char oxidation offgas separately and of tracking hydrogen separately from all other elements were both investigated. Results showed that variability in offgas composition, offgas enthalpy, or both, is important. For a swirling combustion case, the use of two progress variables decreased the size and severity of the fuel-rich region. Burnout and gas composition were both significantly affected. The FG-DVC submodel was delivered by AFR to BYU. The comparison of the FG-DVC with other coal reaction submodels continued.

For Subtask 3.b, equations for an improved fixed-bed model were developed and coding is now approximately 80 percent completed. Physical property and transport correlations applicable to fixed beds were reviewed and documented. Sources of fixed-bed gasifier data were also reviewed and summarized.

For Subtask 4.a, work was completed on preparing a version of the FG-DVC model for transfer from AFR to BYU. The time for the combined programs to run varied from 4.5 to 5.5 hours depending on the coal and conditions.

For Subtask 4.b, no work was scheduled.

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