MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION: QUARTERLY REPORT, JANUARY-MARCH 1987

ADVANCED FUEL RESEARCH, INC.
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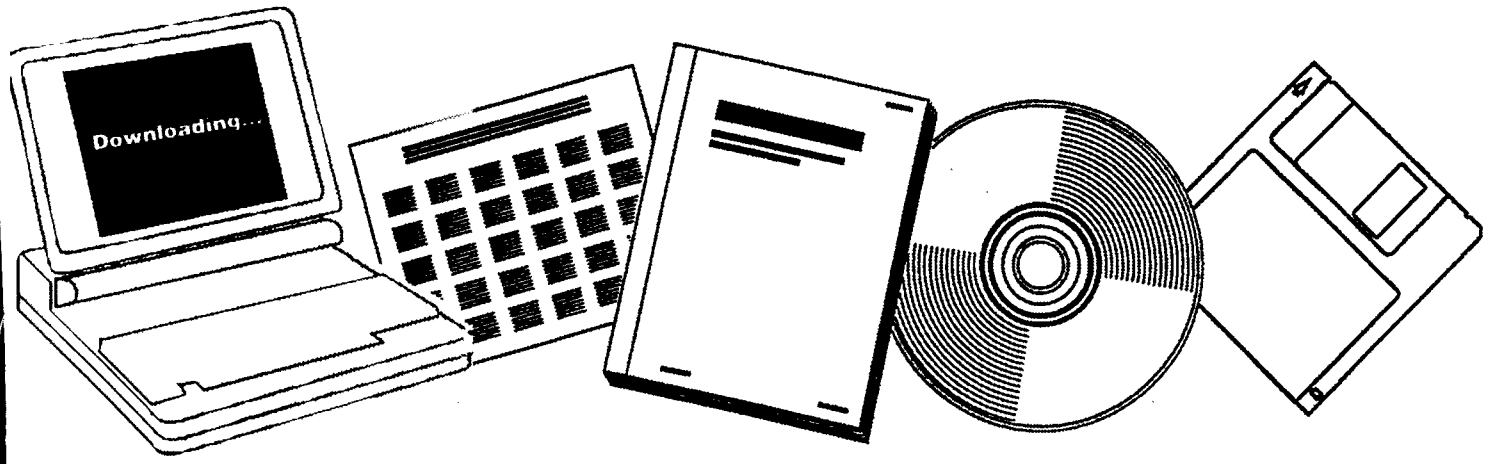
MAR 1987



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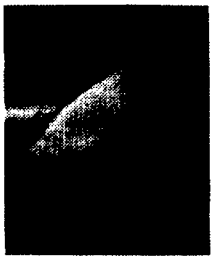

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Measurement and Modeling of Advanced Coal Conversion

Quarterly Report, January-March 1987

P.R. Solomon
D.G. Hamblen
M.A. Serio
L.D. Smoot
S. Brewster

March 1987

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, Conneticut
and
Brigham Young University
Provo, Utah

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ABSTRACT

The overall objective of this program is the development of computer-aided reactor engineering technology for the design, scale up, simulation, control and feedstock evaluation in advanced coal conversion devices. This technology, based on a systematic database and reactor simulation software, 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. Current computer-aided reactor engineering technology has shown significant potential, but there is a need to bring the technology to a higher level of generality, accuracy and acceptability. This program will merge significant advances made at Advanced Fuel Research, Inc. (AFR) in predicting coal conver-sion 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 second quarter of the program, staffing requirements for the work were filled. Experiments were performed to obtain information on soot formation, ignition, and particle optical properties. The PCGC-2 code was installed on AFR's Apollo DN580 workstation and integration of the FG/DVC submodel was started. Alternative approaches for incorporating submodels into the PCGC-2 comprehensive code were also identified.

MEASUREMENT AND MODELING OF COAL CONVERSION PROCESSES

Contract No. DE-AC21-86MC23075

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B - Response to "Extension of Emission-Transmission Technique to Particulate Samples Using FT-IR", submitted to Combustion and Flame, (1987).

C - "Application of FT-IR E/T Spectroscopy to Study Coal Combustion Phenomena", being presented at the International Coal Combustion Symposium, Beijing, China, (Fall 1987).