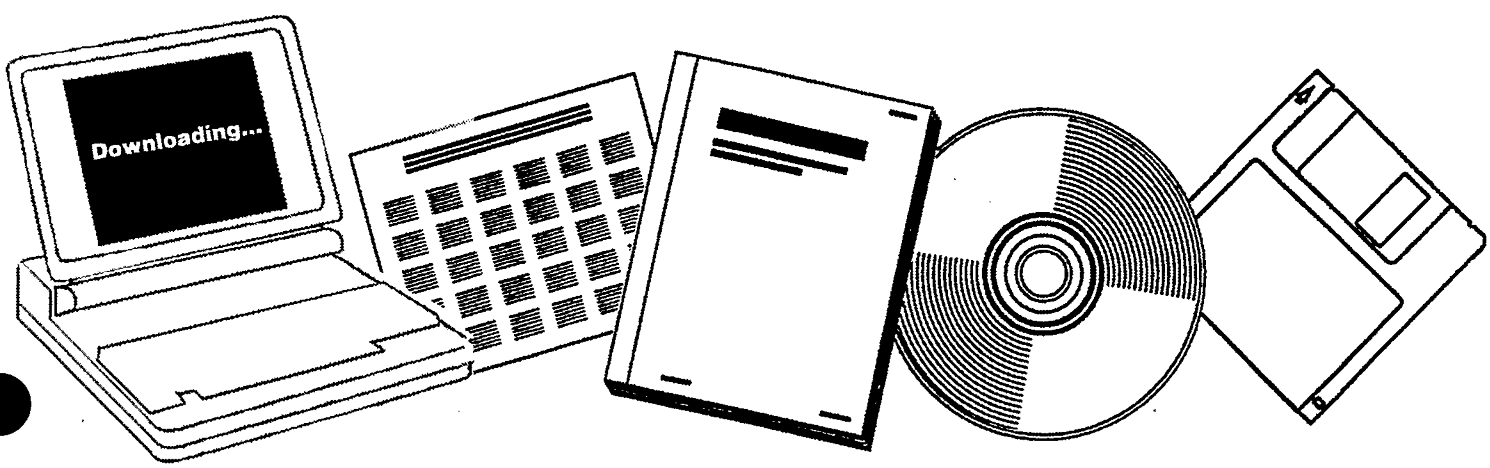
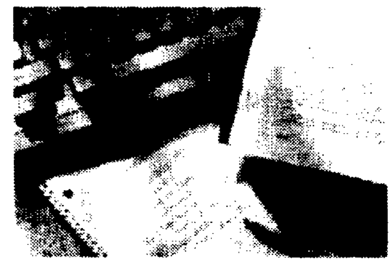
MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION: ANNUAL REPORT, OCTOBER 1, 1986-SEPTEMBER 30, 1987

ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

OCT 1987





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Measurement and Modeling of Advanced Coal Conversion

Annual Report, October 1, 1986-September 30, 1987

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

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For
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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

RELEASE OF CONTRACTED RESEARCH DOCUMENTS

12/18/87

Contract No.	DE-AC21-86MC23075
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Name & Phone No. of DOE COTR	Justin L. Beeson (304) 291-4571

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U.S. Department of Energy
Morgantown Energy Technology Center
P.O. Box 880, 3610 Collins Ferry Road
Mail Stop I05, ~~T-44~~, Attn: Ms. M. L. Mehalic
Morgantown, West Virginia 26507-0880

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A. CONTRACTOR INFORMATION (CONTRACTOR COMPLETES PART A. 1-5)

1. Document Title: "MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION" 1st Annual
2. Type of Document: [X] Technical Progress Report [ ] Topical Report [ ] Final Technical Report [ ] Abstract [ ] Technical Paper [ ] Journal Article [ ] Conference Presentation [ ] Other (please specify): ______
3. In order to meet a publication schedule or submission deadline, patent clearance by ASAP (date) is desired.
4. This document has been reviewed for possible inventive subject matter (Subject Inventions) and:
   - [X] a. no Subject invention is believed to be disclosed therein.
   - [ ] b. describes a possible Subject Invention relating to ______
     - i. Contractor Docket No. ______
     - ii. A disclosure of the invention was submitted on ______
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5. Remarks:

Signed *Michael A. Serio* (contractor) Date November 12, 1987

Position Manager, Chemical Engineering Science - Michael A. Serio

B. PATENT COUNSEL ACTION (PATENT COUNSEL COMPLETES PART B. 6-7)

[X] 6. Patent clearance for release of the above-identified document is granted.
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cc: — METC Technology Communications Manager Contractor

MEASUREMENT AND MODELING OF COAL CONVERSION PROCESSES

Contract No. DE-AC21-86MC23075

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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 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 first year of the program, progress was made on all of the tasks. Under Subtask 2.a, "Coal to Char Chemistry Submodel Development and Evaluation", characterization by FT-IR, TGA and pyrolysis were carried out on most of the coal samples to be used. Demineralized samples were also produced and characterized. The literature search on transport properties during pyrolysis was completed and a simple model of tar transport was developed and successfully tested. The combined FG/DVC model has been improved and installed on a Sun workstation. Work was initiated on computing the optical properties of particles during the coal to char transformations.

Under Subtask 2.b, "Fundamental High-Pressure Reaction Rate Data", the interdisciplinary research team has been organized. Appropriate literature has been reviewed and the high pressure reactor and support systems have been designed.

Studies of ignition and soot formation were performed in the transparent wall reactor (TWR) under Subtask 2.c, "Secondary Reaction of Pyrolysis Products and Char Burnout". Attention is being focused on what controls ignition (heterogeneous or homogeneous oxidation) and what controls soot formation. Measurements for four samples have been completed and analysis of the results is continuing.

The literature search for Subtask 2.d, "Ash Physics and Chemistry Submodel" was completed to identify the important effects of coal minerals in determining coal behavior. Mineral characterization experiments were begun on coal samples. Work was also initiated to study the mineral transformation during coal conversion.

For Subtask 2.e, "Large Particle Submodels", a literature review of heat and mass transport effects in coal pyrolysis was completed. In addition, calculations were done to define regimes of internal and external heat and mass transport control for conditions of interest. This was done to define the boundary regions where such considerations become important.

Under Subtask 2.g, "SO_x-NO_x Submodel Development", the existing NO_x submodel in PCGC-2 was evaluated by comparing model predictions with experimental data obtained at high pressure and under fuel-rich conditions. The model gave accurate predictions for bituminous coals but not for lignite. A kinetic model for predicting formation of thermal NO was developed from the literature and coding changes were initiated to incorporate this model into PCGC-2. A literature search of sulfur chemistry in combustion flames was initiated.

For Subtask 2.h, "NO_x/SO_x Submodel Evaluation", graduate research assistants have been hired, the experimental program defined, and fabrication of the modified test facility initiated. A cold-flow facility has been designed to simulate the gasifier, providing optical access for laser measurements and flow visualization. A device has been designed to produce smoke so that the flow can be visually observed. A method of extracting gas samples from the flow, with on-line sampling and minimal flow disturbance, has been designed so that mixing rate data can be collected.

For Subtask 3.a, "Integration of Advanced Submodels into Entrained-Flow Code, with Evaluation and Documentation", a doctoral student was recruited and began work on this project. Three alternatives are being considered concurrently to integrate the Functional Group (FG) devolatilization model into the comprehensive entrained-bed code. Code modifications have been made to test all three.

A literature review of existing fixed-bed coal gasification codes and experimental data was conducted for Subtask 3.b, "Comprehensive Fixed-Bed Modeling Review, Development, Evaluation, and Implementation". Three available 2-D codes were installed and tested. Potential improvements over existing models were identified, and an outline of an improved fixed bed model was developed. A review meeting with external consultants was held to evaluate the proposed model. Several sets of experimental data were obtained for model evaluation.

Under Subtask 4.a, "Application of Generalized Pulverized Coal Comprehensive Code", installation of PCGC-2 on the AFR Apollo DN 580/T computer was completed to allow testing of performance. The test code took approximately 4 times longer than expected based on the Apollo specifications. The Apollo was returned and Sun Workstations were purchased. PCGC-2 was installed on the Sun Workstation. The reference case for PCGC-2 takes 3.25 hours to run on a SUN 3/260, this compares to 7 hours on the Apollo DN 580 T.