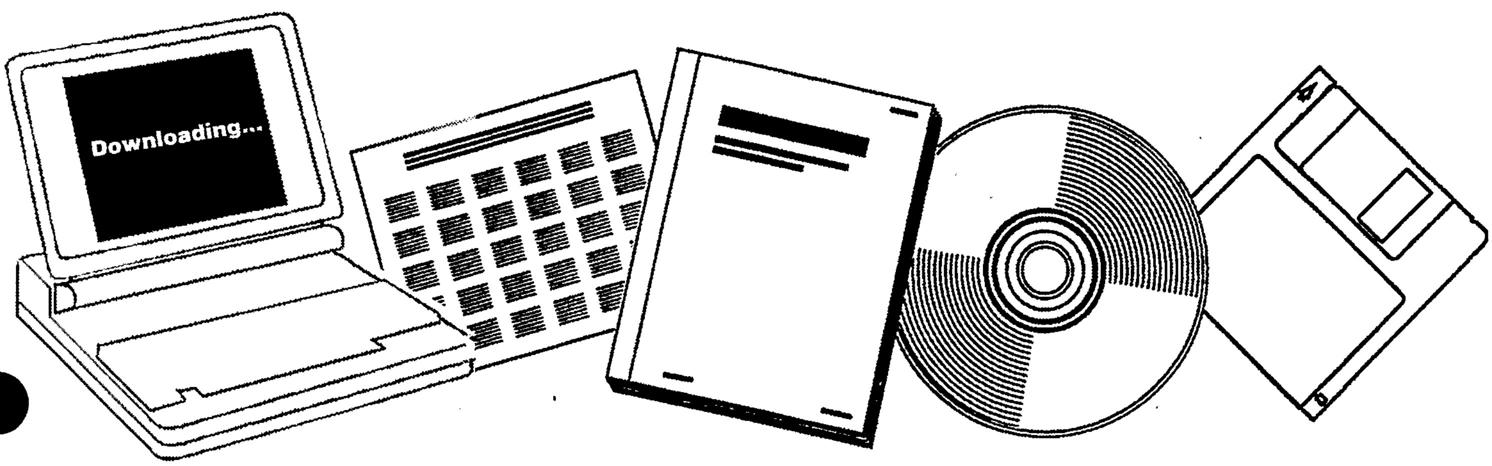
DE88001057

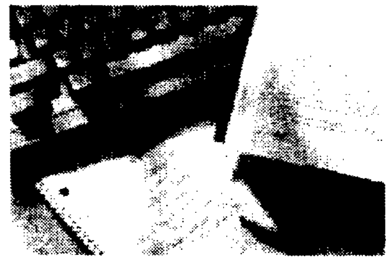
MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION: 5TH QUARTERLY REPORT, OCTOBER 1, 1987 TO DECEMBER 31, 1987

ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

MAR 1988



U.S. Department of Commerce
National Technical Information Service



DE88001057

LEGIBILITY NOTICE

A major purpose of the Technical Information Center is to provide the broadest dissemination possible of information contained in DOE's Research and Development Reports to business, industry, the academic community, and federal, state and local governments.

Although a small portion of this report is not reproducible, it is being made available to expedite the availability of information on the research discussed herein.

1

DE88001057

DOE/MC--23075-2555

DE88 001057

Measurement and Modeling of Advanced Coal Conversion

5th Quarterly Report
October 1, 1987 to December 31, 1987

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

March 1988

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

DOE MC 23075 2555
DE88001057

Measurement and Modeling of Advanced Coal Conversion

5th Quarterly Report
October 1, 1987 to December 31, 1987

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

March 1988

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

Available from the NTIS Energy Distribution Center, P O Box 1300, Oak Ridge, TN 37831.

Price: Printed copy A09
Microfiche A01

Codes are used for pricing all publications. The code is determined by the number of pages in the publication. Information pertaining to the pricing codes can be found in the current issues of the following publications, which are generally available in most libraries: *Energy Research Abstracts (ERA)*, *Government Reports Announcements* and Index (*GRA* and *I*); *Scientific and Technical Abstract Reports (STAR)*, and publication NTIS-PR-360 available from NTIS at the above address.

DOE/MC/23075-2555
(DE88001057)

Measurement and Modeling of Advanced Coal Conversion

5th Quarterly Report, October 1, 1987 to December 31, 1987

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

Work Performed Under Contract No.: DE-AC21-86MC23075

For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
P.O. Box 880
Morgantown, West Virginia 26507-0880

By
Advanced Fuel Research, Inc.
87 Church Street
East Hartford, Connecticut 06108
and
Brigham Young University
Provo, Utah 84602

March 1988

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 fifth quarter of the program, progress was made on all of the tasks.

For Subtask 2.a, a review of internal pore transport models was prepared by Professor Eric Suuberg of Brown University. It was determined that differences in the pressure drops calculated by the Simons and Gavalas approaches to internal transport were primarily due to different assumptions regarding the pyrolysis rate. The geometry of the Simons approach makes it the easiest model to use in predicting swelling and so it will be used in the future swelling model. However, the model will be modified to reflect the fact that transport in the finest pores needs to be described by an activation diffusion process. The review is presented in Appendix A.

Additional characterization of the coal samples for Subtask 2.a was performed by TG-FTIR, Field Ionization Mass Spectrometry (FIMS) and swelling in a drop tube furnace.

For Subtask 2.b, Utah bituminous coal was selected for the initial char oxidation studies. Preparations were continued to obtain char from the BYU gasifier. Samples were also prepared in a simple hot-tube reactor. The high pressure reactor design was completed, and construction was initiated. Orders have been placed for the reactor components. The literature review of sulfur capture by sorbents was continued.

For Subtask 2.c, studies of ignition and soot formation in flames were continued in the transparent wall reactor (TWR).. Seven additional samples have been completed in addition to the four reported in the Annual Report. A comparison of the ignition of several samples suggests that the rate of ignition correlates with the initial rate of weight loss in air in a TGA experiment. Ignition of chars is heterogeneous; ignition of high rank coals is homogeneous; but low rank coals exhibit both homogeneous and heterogeneous contributions to ignition. Soot formation in combustion correlates well with tar yield in pyrolysis suggesting that tar is the chief precursor of soot.

For Subtask 2.d, two sample collection probes were constructed that can be inserted into the transparent wall reactor (TWR) to allow for the collection of char with its transforming mineral matter from the flame at various stages of burnoff, and of fly ash from above the flame. Initial sample collections were performed.

For Subtask 2.e, the literature review of heat and mass transport effects in coal pyrolysis was completed. A critical evaluation was made of two models from the literature that have been used to describe coupled reaction and transport in large particles. A major effort was made on design of the fixed-bed reactor. This reactor will have on-line analysis of evolved volatile products and on-line measurement of weight loss, functional group composition and particle temperature.

For Subtask 2.g, a revised NO_x submodel has been completed. A literature survey of SO_x chemistry was initiated to determine the key reaction mechanism and identify the important aspects of predicting SO_x behavior. This effort will receive increased emphasis in the upcoming quarter. With the thermal NO_x rate of formation turned off, prediction of fuel NO_x by the revised model matched that of the former code for a swirling-flow, coal combustion case. Efforts are currently being made to validate predictions with thermal NO_x included.

For Subtask 2.h, work continued on the cold-flow study for turbulence and mixing measurements with cross-flow injection. Fabrication of the clear plastic flow chamber was completed. A new research team for the gasifier was organized, and training in gasifier operation was initiated. A sorbent particle feeder was designed and is being constructed.

For Subtask 3.a, work continued on the Single Solids Progress Variable (SSPV) and Multiple Solids Progress Variables (MSPV) methods for incorporating the FG/DVC model into PCGC-2. Work is also continuing to review an advanced research version of PCGC-2. Under the MSPV method, calculations were continued to investigate the effect of using two progress variables to track coal offgas. Other accomplishments include selection of the UNIRAS graphics software for examining code output, and installation of the advanced research version of PCGC-2 on the Sun workstation at AFR. The FG/DVC model and a model developed at The University of Utan (Grant et al., 1988), based on percolation theory, are being reviewed and evaluated.

For Subtask 3.b, a research plan for developing an advanced fixed-bed model was prepared based on the written comments and recommendations of expert consultants. This plan was presented to AFR and METC at the annual contract review meeting. Data comparisons and a sensitivity analysis of the Washington University 2-D model were performed. A plan for developing a simplified fixed-bed code with several of the advanced model features was formulated.

For Subtask 4.a, the FG/DVC model was successfully integrated with PCGC-2. After mkaing several modifications to FG-DVC and to the criteria under wnich it is called, we were able to obtain a converged solution for the integrated code in a little over four hours. For this calculation, the FG/DVC model takes less than 20% of the total time.

MEASUREMENT AND MODELING OF COAL CONVERSION PROCESSES

Contract No. DE-AC21-86MC23075

TABLE OF CONTENTS