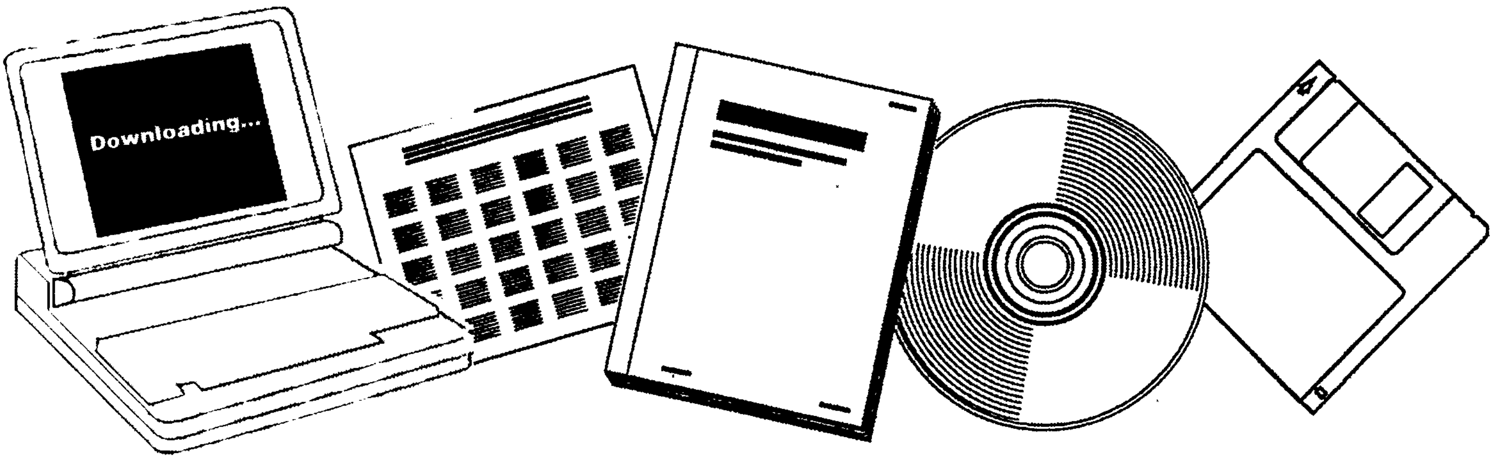
MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES. 13TH QUARTERLY REPORT, OCTOBER 1-DECEMBER 31, 1989

ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

FEB 1990



One Source. One Search. One Solution.

NTIS

Providing Permanent, Easy Access to U.S. Government Information

National Technical Information Service is the nation's largest repository and disseminator of government-initiated scientific, technical, engineering, and related business information. The NTIS collection includes almost 3,000,000 information products in a variety of formats: electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.

Search the NTIS Database from 1990 forward

NTIS has upgraded its bibliographic database system and has made all entries since 1990 searchable on **www.ntis.gov.** You now have access to information on more than 600,000 government research information products from this web site.

Link to Full Text Documents at Government Web Sites

Because many Government agencies have their most recent reports available on their own web site, we have added links directly to these reports. When available, you will see a link on the right side of the bibliographic screen.

Download Publications (1997 - Present)

NTIS can now provides the full text of reports as downloadable PDF files. This means that when an agency stops maintaining a report on the web, NTIS will offer a downloadable version. There is a nominal fee for each download for most publications.

For more information visit our website:

www.ntis.gov

U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161

FOSSIL ENERGY

MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES

13th Quarterly Report #523043-42
October 1, 1989 to December 31, 1989

By
Peter R. Solomon
Michael A. Serio
David G. Hamblen
L. Douglas Smoot
B. Scott Brewster

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
Dr. Richard Johnson
COTR

By

Contractor

Advanced Fuel Research, Inc.
87 Church Street
East Hartford, CT 06108
(203) 528-9806

Program Director

Peter R. Solomon
President

Subcontractor

Brigham Young University
Provo, Utah 84602
(801) 378-4326

Program Director

L. Douglas Smoot
Dean and Professor

DOE/MC/23075--2814

DE90 010628

DISCLAIMER

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 is 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 combined FG-DVC model 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.

The progress during the thirteenth quarterly of the program is summarized below.

For Subtask 2.a., a significant amount of work was done in the area of tar transport, work was resumed on the addition of polymethylenes to the FG-DVC model, and work also continued on the swelling model.

In addition, work continued on examining a percolation theory approach to doing the network decomposition calculations. A version of the model was developed which incorporates two different types of bonds, the so-called two-σ model. The Monte Carlo and two-σ predictions of the tar yield and of the coal fluidity data agree reasonably well with each other and with the data.

Work also continued on examining the rank dependence of the pyrolysis kinetic rates. So far, comparisons have been made with Pittsburgh Seam bituminous coal TG-FTIR data from experiments at four different heating rates. In this case, rank dependent kinetics have been determined which provide an excellent fit to the evolution profiles and yields for each heating rate.

Finally, a comparison was made of intrinsic reactivity measurements for Montana Rosebud coal determined from the non-isothermal test to the plot

developed by Smith (1982) for a range of carbons over a wide range of temperatures. The agreement at low temperatures was within a factor of two when compared to Smith's data for brown coal chars. When the results were extrapolated to high temperatures using E = 35 kcal/mole, again good agreement was obtained with Smith's data for coal chars (within a factor of two).

For Subtask 2.b., work continued on developing the optical particle-imaging system for the HPCP reactor. A new particle injection probe with smaller diameter and thicker insulation is being fabricated to reduce the thermal impact of the probe on the preheated inlet stream. A suction pyrometer for reactor centerline temperature characterization is also being fabricated. Work continued on the analytical procedure to measure titanium content for determining char burnout.

For Subtask 2.c., work continued on doing coal flame experiments in the transparent wall reactor (TWR). For a Montana Rosebud flame, tomographic reconstruction techniques were applied to line-of-sight FT-IR Emission/Transmission (E/T) measurements to derive spectra that correspond to small volumes within a coal flame. From these spectra, spatially resolved point values for species temperatures and relative concentrations can be determined as functions of distance from the flame axis and height above the coal injector nozzle. Initial measurements (reported last quarter) were made at 6 cm and 12 cm above the coal injector nozzle, with the ignition point occurring at 10 cm. During this quarter, two more slices of data, at 16 cm and 20 cm above the nozzle were collected and tomographically reconstructed.

For Subtask 2.d., the work on the study of mineral transformations in the entrained flow reactor (EFR) was temporarily suspended due to manpower and funding constraints. Temperature Programmed Desorption (TPD) experiments were done in air for chars produced from all of the Argonne coals. The CO_2 desorption and the O_2 adsorption show a consistent trend with the char reactivity as measured by the Critical Temperature (T_{cr}).

For Subtask 2.e., the work on the AFR fixed-bed reactor (FBR) system was continued. Experiments were done at two bed depths and two flow rates with samples of Illinois No. 6, Pittsburgh No. 8, and Upper Freeport bituminous coals. Over the range of bed depths examined, there did not appear to be a large effect on tar yield and composition. We were restricted from using larger bed depths because problems with tar deposition in the gas cell. However, the ability to bypass some of the tar from the cell has recently been added which will allow larger samples to be used.

For Subtask 2.f., work was initiated on this subtask. A literature search of large particle oxidation and high-pressure reactor systems was conducted. An experimental approach was selected which includes using reactor tubes containing fixed beds of large char particles inserted in the HPCP reactor from Subtask 2.b.

For Subtask 2.g., work continued on evaluating the thermal NO submodel using data from the BYU/ACERC laboratory-scale reactor. Problems with the high gas temperature previously predicted by PCGC-2 have been resolved, and thermal NO predictions have been compared with experimental data. The NO concentration is underpredicted by approximately 30 percent, but it is not certain that this disparity is a result of neglecting prompt NO. Several coal gasification cases have been simulated, and the gas temperature and major species concentrations agree reasonably well with the experimental data. Evaluation of the combined fuel and thermal NO mechanism is ready to begin.

For Subtask 3.a., several improvements in PCGC-2 were made during the last quarter. A major error was discovered and corrected in the radiation submodel. This correction apparently resolved the previously reported problem with unreasonably high temperature predictions in some cases. A new option was also added to the code for solving the radiation submodel for gaseous combustion (no particles). Converged solutions were then obtained for several cases being used in Subtask 2.g to evaluate the extended NO_x submodel, and for the gasification case chosen previously as a standard test case. Additional model validation data were also obtained from AFR, and work continued on modeling the TWR reactor facility. Development of a user-friendly, graphical interface on the Sun workstation was also continued.

For Subtask 3.b., work continued during the last quarter on coding chemical and physical submodels and model validation. Improved temperature profiles and pressure profiles have been obtained from the one-dimensional, fixed-bed code. Predictions and comparisons to experimental data include effluent gas compositions and temperatures, temperature profiles, and axial pressure variation. Additional predictions with comparison to limited data include carbon conversion, variable particle size, and species concentration profiles. The relative importance of char oxidation resistances to bulk film diffusion, ash diffusion, and chemical reaction are identified. For the cases examined, chemical resistance dominates in the cool regions at the bottom and top of the reactor while ash diffusion resistance competes with chemical resistance throughout most of the reactor.

For Subtask 4.a., this subtask has not been initiated.

For Subtask 4.b., work continued on collecting fixed-bed design and test data from organizations and individuals involved in fixed-bed research. Eighteen sets of data have been obtained, but some of the most important ones have not been obtained yet. Work also continued on collecting fixed-bed experimental data from the open literature. Further testing and validating of the advanced fixed-bed code developed in Subtask 3.b was performed.

MEASUREMENT AND MODELING OF COAL CONVERSION PROCESSES

Contract No. DE-AC21-86MC23075

Table of Contents