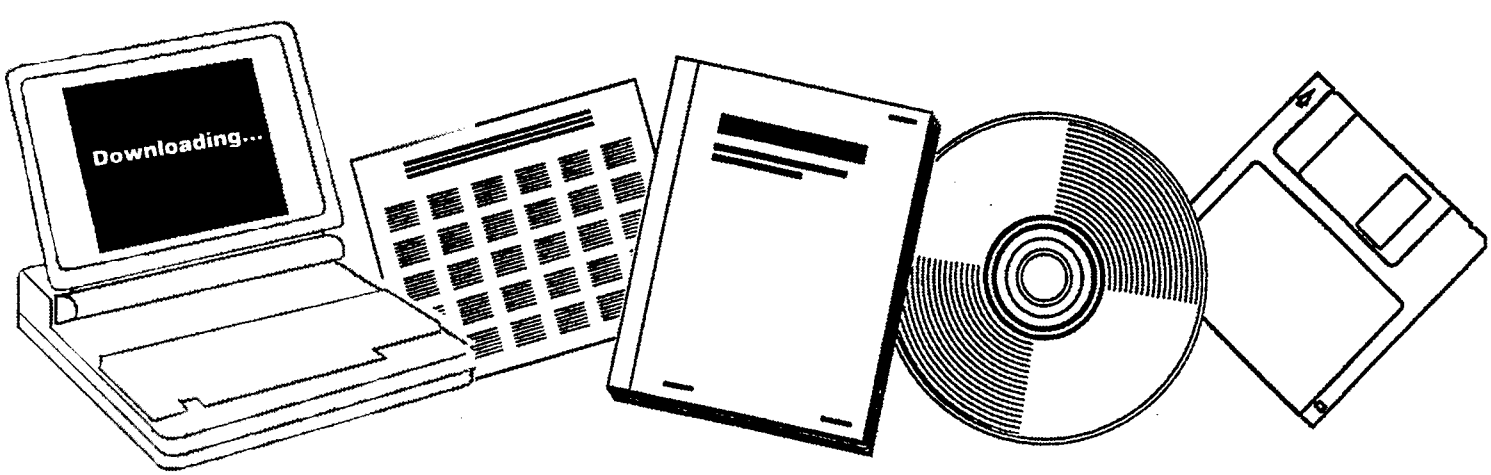
MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES. TWENTY-SIXTH QUARTERLY REPORT, JANUARY 1, 1993--MARCH 31, 1993

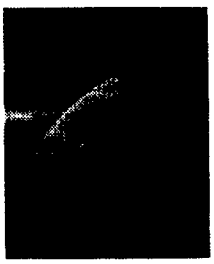
ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

1993



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

MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES

26th Quarterly Report #523043
January 1, 1993 to March 31, 1993

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. Norman Holcomb
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

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 twenty-sixth quarter of the program is summarized below.

For Subtask 2.a., Work continued on the reactivity model. Suggestions for the interpretation of the parameter for the mean pore radius/tortuousity ratio were offered during a group meeting. In particular, comments were made that the model should account for not only the overall particle size, but also the wall thickness, since the char contains numerous bubbles. Future studies in that direction are being planned.

Work continued on the swelling submodel to determine the effect of air on coal swelling. A set of drop tube experiments was performed in air and in N_2 at 540 ^{o}C using 200 x 325 Pittsburgh #8 seam coal. SEM photographs of the char particles did not show any obvious differences in swelling between the two atmospheres.

Work continued on the sulfur and nitrogen experiments. Previously collected data was organized and current literature was reviewed for the preparation of a manuscript and presentation titled "Sulfur and Nitrogen in the Argonne Coals: Experiment and Modeling." The presentation was made at the 1993 ACERC meeting in Utah and the manuscript will be submitted for publication in "Energy and Fuel."

For Subtask 2.b., The contribution to the final report for this subtask was completed.

For Subtask 2.c., no work was scheduled.

For Subtask 2.d., no work was scheduled.

For Subtask 2.e., no work was scheduled.

For Subtask 2.f., The contribution to the final report for this subtask was completed.

For Subtask 2.g., The contribution to the final report for this subtask was completed.

For Subtask 3.a., The final report contribution for this subtask was completed. The first draft of the user's manual was completed at BYU and sent to METC and AFR for review.

For Subtask 3.b., The development and validation of the FBED-1 code was completed. Also, the contribution to the final report was completed.

For Subtask 3.c., The contribution to the final report for this subtask was completed.

For Subtask 4.a., The contribution to the final report for this subtask was completed.

For Subtask 4.b., The contribution to the final report was completed. The first draft of the user's manual was completed and reviewed internally. The code was ported to a Silicon Graphics machine but the execution was not successful. Modifications needed for successful execution of the code on a Silicon Graphics machine were initiated. The code was demonstrated at the Seventh Annual ACERC conference. An overview of the fixed-bed code status was presented at the METC/AFR/BYU Contract Review Meeting.

"MEASUREMENT AND MODELING OF COAL CONVERSION PROCESSES"

Contract No. DE-AC21-86MC23075

Table of Contents

SECTION I. INTRODUCTION

I.A. PROGRAM BACKGROUND AND DESCRIPTION

During the past several years, significant advances have been made at Brigham Young University (BYU) in comprehensive two-dimensional computer codes for mechanistic modeling of entrained-bed gasification and pulverized coal combustion. During the same time period, significant advances have been made at Advanced Fuel Research, Inc. (AFR) in the mechanisms and kinetics of coal pyrolysis and secondary reactions of pyrolysis products. This program presents a unique opportunity to merge the technology developed by each organization to provide detailed predictive capability for advanced coal characterization techniques in conjunction with comprehensive computer models to provide accurate process simulations.

The program will streamline submodels existing or under development for coal pyrolysis chemistry, volatile secondary reactions, tar formation, soot formation, char reactivity, and SO_x-NO_x pollutant formation. Submodels for coal viscosity, agglomeration, tar/char secondary reactions, sulfur capture, and ash physics and chemistry will be developed or adapted. The submodels will first be incorporated into the BYU entrained-bed gasification code and subsequently, into a fixed-bed gasification code (to be selected and adapted). These codes will be validated by comparison with small scale laboratory and PDU-scale experiments. The validated code could then be employed to simulate and to develop advanced coal conversion reactors of interest to METC.

I.B. OBJECTIVES

The objectives of this study are to establish the mechanisms and rates of basic steps in coal conversion processes, to integrate and incorporate this information into comprehensive computer models for coal conversion processes, to evaluate these models and to apply them to gasification, mild gasification and combustion in heat engines.

I.C. APPROACH

This program is a closely integrated, cooperative effort between AFR and BYU. The program consists of four tasks: 1) Preparation of Research Plans, 2) Submodel Development and Evaluation, 3) Comprehensive Model Development and Evaluation, and 4) Applications and Implementation.

I.D. CRITICAL TECHNICAL ISSUES

To achieve the goals of the program, the computer models must provide accurate and reliable descriptions of coal conversion processes. This will require the reduction of very complicated and interrelated physical and chemical phenomena to mathematical descriptions and, subsequently, to operational computer codes. To accomplish this objective, a number of technical issues must be addressed as noted below. The status of each of these tasks is also included:

C Separation of Rates for Chemical Reaction, Heat Transfer, and Mass Transfer
C Particle Temperature Measurements Using FT-IR E/T Spectroscopy
C Functional Group Description of Coal, Char and Tar
C Tar Formation Mechanisms
C Char Formation Mechanisms
C Viscosity/Swelling
C Intraparticle Transport
C Pyrolysis of Volatiles and Soot Formation
C Secondary Reaction of Tar
A Particle Ignition
A Char Reactivity
A Ash Chemistry and Physics
C Particle Optical Properties
C Coupling of Submodels with Comprehensive Codes
C Comprehensive Code Efficiency
C Turbulence
C SO_x and NO_x
C Generalized Fuels Models
A Fixed-Bed Model

(o) to be addressed; (I) initiated; (A) almost completed; (C) completed. These technical issues are addressed in the three Tasks as described in Sections II-IV.

I.E. TWENTY-SIXTH QUARTER PROGRESS

Subtask 2.a. Coal to Char Chemistry Submodel Development and Evaluation

Work continued on the reactivity model. Suggestions for the interpretation of the parameter for the mean pore radius/tortuousity ratio were offered during a group meeting. In particular, comments were made that the model should account for not only the overall particle size, but also the wall thickness, since the char contains numerous bubbles. Future studies in that direction are being planned.

Work continued on the swelling submodel to determine the effect of air on coal swelling. A set of drop tube experiments was performed in air and in N_2 at 540 °C using 200 x 325 Pittsburgh #8 seam coal. SEM photographs of the char particles did not show any obvious differences in swelling between the two atmospheres.

Work continued on the sulfur and nitrogen experiments. Previously collected data was organized and current literature was reviewed for the preparation of a manuscript and presentation titled "Sulfur and Nitrogen in the Argonne Coals: Experiment and Modeling." The presentation was made at the 1993 ACERC meeting in Utah and the manuscript will be submitted for publication in "Energy and Fuel."

Subtask 2.b. Fundamental High-Pressure Reaction Rate Data

The contribution to the final report was completed.

Subtask 2.c. Secondary Reaction of Pyrolysis Products and Char Burnout

No work was scheduled.

Subtask 2.d. Ash Physics and Chemistry Submodel

No work was scheduled.

Subtask 2.e. Large Particle Submodels

No work was scheduled.

Subtask 2.f. Large Char Particle Oxidation at High Pressure

The contribution to the final report was completed.

Subtask 2.g. SO_x - NO_x Submodel Development

The contribution to the final report was completed.

Subtask 3.a. Integration of Advanced Submodels into Entrained-Flow Code, with Evaluation and Documentation

Corrections and comments to the user's manual will be considered and incorporated as appropriate based on the reviews by METC and AFR.

Subtask 3.b. Comprehensive Fixed-Bed Modeling Review, Development, Evaluation, and Implementation

The final report contribution for this subtask was prepared. The first draft of the user's manual was prepared and sent to METC and AFR for review. Corrections and comments will be considered and incorporated as appropriate, based on the reviews. All other work on this subtask is complete.

Subtask 3.c. Generalized Fuels Feedstock Submodel

The final report contribution for this subtask was prepared. This subtask is now complete.

Subtask 4.a. Application of Generalized Pulverized Coal Comprehensive Code

The final report contribution for this subtask was prepared.

Subtask 4.b. Application of Fixed-Bed Code

The contribution to the final report was completed. Work on the FBED-1 user's manual was initiated. The contribution on the FG-DVC devolatilization submodel for the FBED-1 user's manual was received from AFR. The AFR contribution was integrated in the FBED-1 user's manual. The first draft of the user's manual was completed and reviewed internally. Recommendations and modifications needed for improving the manual were finalized and are being implemented.

Work on cleaning up of the code was initiated. The description of code variables and the functions of subprograms are being added to the code for improved comprehension. The governing equations were rederived from the basic principles and checked with the ones used in the code. Some modifications in the code may lead to improved predictions. The code was ported to a Silicon Graphics machine but the execution was not successful. Modifications needed for successful execution of the code on a Silicon Graphics machine were initiated. The code was demonstrated at the Seventh Annual ACERC conference which was followed by a question-and-answer session. An overview of the fixed-bed code status was presented at the METC/AFR/BYU Contract Review Meeting. Modifications needed to simulate novel configurations were discussed in this meeting. The Department of Energy's GPIF (Gasification Product Improvement Facility) configuration was selected as an additional test case for application of the FBED-1 code.

SECTION II. TASK 2. SUBMODEL DEVELOPMENT AND EVALUATION

Objectives

The objectives of this task are to develop or adapt advanced physics and chemistry submodels for the reactions of coal in an entrained-bed and a fixed-bed reactor and to validate the submodels by comparison with laboratory scale experiments.

Task Outline

The development of advanced submodels for the entrained-bed and fixed-bed reactor models will be organized into the following categories: a) Coal Chemistry (including coal pyrolysis chemistry, char formation, particle mass transfer, particle thermal properties, and particle physical behavior); b) Char Reaction Chemistry at high pressure; c) Secondary Reactions of Pyrolysis Products (including gas-phase cracking, soot formation, ignition, char burnout, sulfur capture, and tar/gas reactions); d) Ash Physics and Chemistry (including mineral characterization, evolution of volatile, molten and dry particle components, and ash fusion behavior); e) Large Coal Particle Effects (including secondary reactions within the particle and in multiple particle layers; f) Large Char Particle Effects (including oxidation); g) SO_x-NO_x Submodel Development (including the evolution and oxidation of sulfur and nitrogen species); and h) SO_x and NO_x Model Evaluation.

II.A. SUBTASK 2.a. - COAL TO CHAR CHEMISTRY SUBMODEL DEVELOPMENT AND EVALUATION

Senior Investigators - David G. Hamblen and Michael A. Serio
Advanced Fuel Research, Inc.
87 Church Street, East Hartford, CT 06108
(203) 528-9806

Objective

The objective of this subtask is to develop and evaluate, by comparison with laboratory experiments, an integrated and compatible submodel to describe the organic chemistry and physical changes occurring during the transformation from coal to char in coal conversion processes.

Accomplishments

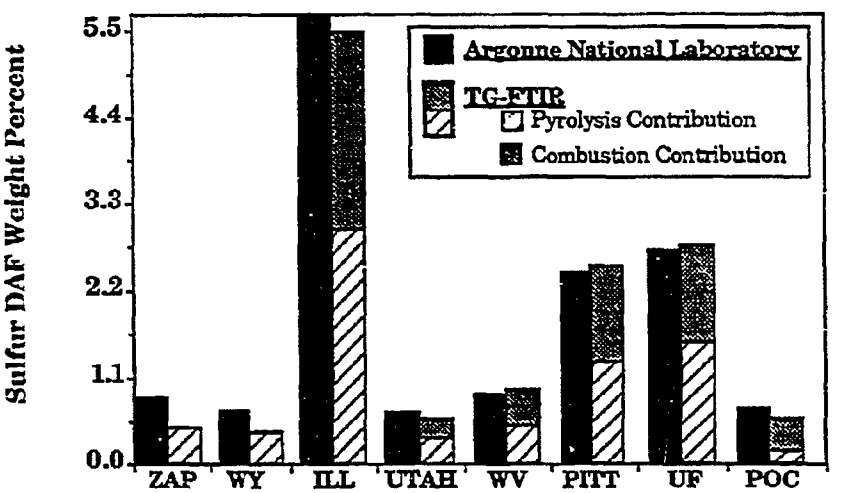
Work continued on the reactivity model. Suggestions for the interpretation of the parameter for the mean pore radius/tortuousity ratio were offered during a group meeting. In particular, comments were made that the model should account for not only the overall particle size, but also the wall thickness, since the char contains numerous bubbles. Future studies in that direction are being planned.

Work continued on the swelling submodel to determine the effect of air on coal swelling. A set of drop tube experiments was performed in air and in N_2 at 540 °C using 200 x 325 Pittsburgh #8 seam coal. SEM photographs of the char particles did not show any obvious differences in swelling between the two atmospheres.

Work continued on the sulfur and nitrogen experiments. Previously collected data was organized and current literature was reviewed for the preparation of a manuscript and presentation titled "Sulfur and Nitrogen in the Argonne Coals: Experiment and Modeling." The presentation was made at the 1993 ACERC meeting in Utah and the manuscript will be submitted for publication in "Energy and Fuel."

During the organization of data, a plot comparing the DAF sulfur weight percent values

determined by the TG-FTIR with those values provided by Argonne National Laboratory was prepared. The plot, which is presented in Fig. II.A-1, shows that, with the exception of Zap lignite and Wyodak coal, the TG-FTIR results are within 16% of the Argonne data. For Zap lignite and Wyodak coal, the TG-FTIR data are 36% and 45%, respectively, lower than the Argonne data. Possible explanations for this large discrepancy are that sulfur is being incorporated in the ash or evolving as gaseous SO_3. The former explanation is more likely since examination of the TG-FTIR absorbance spectra shows no SO_3 evolving during combustion.



As previously reported, Pittsburgh #8 and Illinois #6, when subjected to nitric acid for the removal of pyrite, showed a decrease in the first SO_2 evolution peak in addition to removing the sharp second evolution peak indicative of pyrite. To verify whether this decrease in the first SO_2 peak is actually from the removal of pyrite or whether it could be from the oxidation of aliphatic sulfur forms, a 1.45 density liquid was obtained for float/sink cleaning of Illinois #6 and Pittsburgh #8. The float/sink experiments and TG-FTIR analysis of the float fractions will be done in the next quarter.

Plans

Complete experimental effort for this subtask. Complete contributions for Final Report.

II.B. SUBTASK 2.b. - FUNDAMENTAL HIGH-PRESSURE REACTION RATE DATA

Senior Investigators - Geoffrey J. Germane and Angus U. Blackham
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Student Research Assistants - Charles R. Monson, Ken Bateman and Layne Pincock

Objectives

The overall objectives of this subtask are to measure and correlate fundamental reaction rate coefficients for pulverized-coal char particles as a function of char burnout in oxygen at high temperature. The effect of high pressure will be investigated.

Accomplishments

The contribution to the final report was completed.

Plans

No work is scheduled. This subtask is complete.

II.C. SUBTASK 2.c. - SECONDARY REACTION OF PYROLYSIS PRODUCTS AND CHAR BURNOUT

SUBMODEL DEVELOPMENT AND EVALUATION

Senior Investigators - James R. Markham and Michael A. Serio
Advanced Fuel Research, Inc.
87 Church Street, East Hartford, CT 06108
(203) 528-9806

Objective

The objective of this subtask is to develop and evaluate by comparison with laboratory experiments, an integrated and compatible submodel to describe the secondary reactions of volatile pyrolysis products and char burnout during coal conversion processes. Experiments on tar cracking, soot formation, tar/gas reactions, char burnout, and ignition will continue during Phase II to allow validation of submodels.

Accomplishments

No work was scheduled.

Plans

Complete contribution for Final Report.

II.D. SUBTASK 2.d. - ASH PHYSICS AND CHEMISTRY SUBMODEL

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

Objective

The objective of this task is to develop and validate, by comparison with laboratory experiments, an integrated and compatible submodel to describe the ash physics and chemistry during coal conversion processes. AFR will provide the submodel to BYU together with assistance for its implementation into the BYU PCGC-2 comprehensive code. To accomplish the overall objective, the following specific objectives are: 1) to develop an understanding of the mineral matter phase transformations during ashing and slagging in coal conversion; 2) to investigate the catalytic effect of mineral matter on coal conversion processes.

Accomplishments

No work was scheduled.

Plans

Complete contribution for Final Report.

II.E. SUBTASK 2.e. - LARGE PARTICLE/THICK BED SUBMODELS

Senior Investigator - Michael A. Serio
Advanced Fuel Research, Inc.
87 Church Street
East Hartford, CT 06108
(203) 528-9806

Objective

The objectives of this task are to develop or adapt advanced physics and chemistry submodels for the reactions of "large" coal particles (i.e., particles with significant heat and/or mass transport limitations) as well as thick beds (multiple particle layers) and to validate the submodels by comparison with laboratory scale experiments. The result will be coal chemistry and physics submodels which can be integrated into the fixed-bed (or moving-bed) gasifier code to be developed by BYU in Subtask 3.b. Consequently, this task will be closely coordinated with Subtask 3.b.

Accomplishments

No work was scheduled.

Plans

Complete contribution for Final Report.

II.F. SUBTASK 2.f. - LARGE PARTICLE OXIDATION AT HIGH TEMPERATURES

Senior Investigators - Geoffrey J. Germane and Angus U. Blackham
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Student Research Assistants - Ken Bateman and Parvin Yousefi

Objectives

The overall objective for this subtask is to provide data for the reaction rates of large char particles of interest to fixed-bed coal gasification and combustion systems operating at high pressure.

Accomplishments

The contribution to the final report was completed.

Plans

No work is scheduled. This subtask is complete.

II.G. SUBTASK 2.g. - SO_X/NO_X SUBMODEL DEVELOPMENT

Senior Investigators - L. Douglas Smoot and B. Scott Brewster
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Student Research Assistant - Richard Boardman

Objectives

The objectives of this task are 1) to extend an existing pollutant submodel in PCGC-2 for predicting NO_x formation and destruction to include thermal NO, 2) to extend the submodel to include SO_x reactions and SO_x-sorbent reactions, and 3) to consider the effects of fuel-rich conditions and high pressure on sulfur and nitrogen chemistry in pulverized-fuel systems

Accomplishments

The final report for this subtask was prepared.

Plans

This subtask is complete. No further work is planned.

SECTION III. TASK 3. COMPREHENSIVE MODEL DEVELOPMENT AND EVALUATION

Objectives

The objective of this task is to integrate advanced chemistry and physics submodels into a comprehensive two-dimensional model of entrained-flow reactors (PCGC-2) and to evaluate the model by comparing with data from well-documented experiments. Approaches for the comprehensive modeling of fixed-bed reactors will also be reviewed and evaluated and an initial framework for a comprehensive fixed-bed code will be employed after submission of a detailed test plan (Subtask 3.b).

Task Outline

This task is being performed in three subtasks. The first covers the full 72 months of the program and is devoted to the development of the entrained-bed code. The second subtask is for fixed-bed reactors and is divided into two parts. The first part (12 months) was devoted to reviewing the state-of-the-art in fixed-bed reactors. This led to the development of the research plan for fixed-bed reactors, which was approved. The code development is being done in the remaining 60 months of the program. The third subtask is to generalize the entrained-bed code to fuels other than dry pulverized coal and will be performed during the last 36 months of the program.

III.A. SUBTASK 3.a. - INTEGRATION OF ADVANCED SUBMODELS INTO ENTRAINED-FLOW CODE, WITH EVALUATION AND DOCUMENTATION

Senior Investigators - B. Scott Brewster and L. Douglas Smoot
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Student Research Assistants - Ziaul Huque and Susana K. Berrondo

Objectives

The objectives of this subtask are 1) to integrate the FG-DVC submodel into PCGC-2, 2) incorporate additional submodels and improvements developed Under Task 2, 3) evaluate the improved coad, 4) improve user-friendliness and robustness, and 5) document the code.

Accomplishments

The final report contribution for this subtask was prepared. The first draft of the user's manual was prepared and sent to METC and AFR for review. Corrections and comments will be considered and incorporated as appropriate, based on the reviews. All other work on this subtask is complete.

Plans

Corrections and comments to the user's manual will be considered and incorporated as appropriate based on the reviews by METC and AFR.

III.B. SUBTASK 3.b. - COMPREHENSIVE FIXED-BED MODELING REVIEW, DEVELOPMENT, EVALUATION, AND IMPLEMENTATION

Senior Investigators - Predrag T. Radovic and L. Douglas Smoot
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Student Research Assistants - M. Usman Ghani

Objective

The objective of this subtask is to generalize PCGC-2 to include sorbent injection, as outlined in the Phase II Research Plan.

Accomplishments

The development and validation of the FBED-1 code was completed. Also, the contribution to the final report was completed.

Plans

No work is scheduled. This subtask is complete.

III.C. SUBTASK 3.c. - GENERALIZED FUELS FEEDSTOCK SUBMODEL

Senior Investigators - B. Scott Brewster and L. Douglas Smoot
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Objective

The objective of this subtask is to generalize PCGC-2 to include sorbent injection, as outlined in the Phase II Research Plan.

Accomplishments

The final report contribution for this subtask was prepared. This subtask is now complete.

Plans

No further work is planned on this subtask.

SECTION IV. TASK 4. APPLICATION OF INTEGRATED CODES

Objectives

The objectives of this task are to evaluate the integrated comprehensive codes for pulverized coal and fixed-bed reactors and to apply the codes to selected cases of interest to METC.

Task Outline

This task will be accomplished in two subtasks, one for the entrained-bed lasting 57 months and one for the fixed-bed lasting 48 months. Each of these subtasks will consist of three components: 1) Simulation of demonstration cases on BYU computers; 2) Implementation on a work station at AFR; and 3) Simulations of demonstration cases on the workstation.

IV.A. SUBTASK 4.a. - APPLICATION OF GENERALIZED, PULVERIZED-COAL COMPREHENSIVE CODE

Senior Investigators - B. Scott Brewster and L. Douglas Smoot
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Student Research Assistant - Ziaul Huque

Objectives

The objectives of this subtask are to 1) demonstrate application of the code by simulating reactors of interest to METC and 2) implement the code at METC and conduct training.

Accomplishments

The final report contribution for this subtask was prepared.

Plans

The code will be installed at METC and AFR and training will be conducted at METC.

IV.B. SUBTASK 4.b. - APPLICATION OF FIXED-BED CODE

Senior Investigators - Predrag T. Radulovic and L. Douglas Smoot
Brigham Young University
Provo, Utah 84602
(801) 378-2355 and 6536

Student Research Assistant - M. Usman Ghani

Objective

The objective of this subtask is to apply the advanced fixed-bed code developed in task 3.b. to simulate fixed-bed gasifiers of interest to METC.

Accomplishments

The contribution to the final report was completed. Work on the FBED-1 user's manual was initiated. The contribution on the FG-DVC devolatilization submodel for the FBED-1 user's manual was received from AFR. The AFR contribution was integrated in the FBED-1 user's manual. The first draft of the user's manual was completed and reviewed internally. Recommendations and modifications needed for improving the manual were finalized and are being implemented.

Work on cleaning up of the code was initiated. The description of code variables and the functions of subprograms are being added to the code for improved comprehension. The governing equations were rederived from the basic principles and checked with the ones used in the code. Some modifications in the code may lead to improved predictions. The code was ported to a Silicon Graphics machine but the execution was not successful. Modifications needed for successful execution of the code on a Silicon Graphics machine were initiated. The problem has been narrowed down to a single subroutine which initializes the vector of dependent variables at the start of the each downward integration pass. We expect to resolve the problem shortly.

The FORTRAN programs written for the DISSPLA graphics package and to be distributed with the code were also modified. The improved versions of these programs now label various curves on

the output plots and have eliminated the need for a legend. Figure IV.B-1 shows the typical output generated by the graphics program plot1.

The code was demonstrated at the Seventh Annual ACERC conference which was followed by a question-and-answer session. An overview of the fixed-bed code status was presented at the METC/AFR/BYU Contract Review Meeting. Modifications needed to simulate novel configurations were discussed in this meeting. The Department of Energy's GPIF (Gasification Product Improvement Facility) configuration was selected as an additional test case for application of the FBED-1 code. The GPIF configuration has some similarities with the Foster-Wheeler Pyrolyzer. AFR was contacted for information on this pyrolyzer in order to initiate the modification needed in the code to simulate novel configurations. Discussions were held to provide an interface between the entrained-bed code and the fixed-bed code.

Plans

Test all options provided in the code. Complete modification of the code for successful execution on a Silicon Graphics machine. Complete the user's manual. Apply the FBED-1 code to additional test cases. Complete the modifications in the code to simulate novel configurations and to provide an interface between the entrained-bed and fixed-bed codes. Simulate and document the application of the code to the Department of Energy's GPIF facility. Submit the user's manual to METC and AFR for review and incorporate their recommendations, as appropriate. Deliver the code to METC and AFR and conduct training at METC after completing the user's manual.

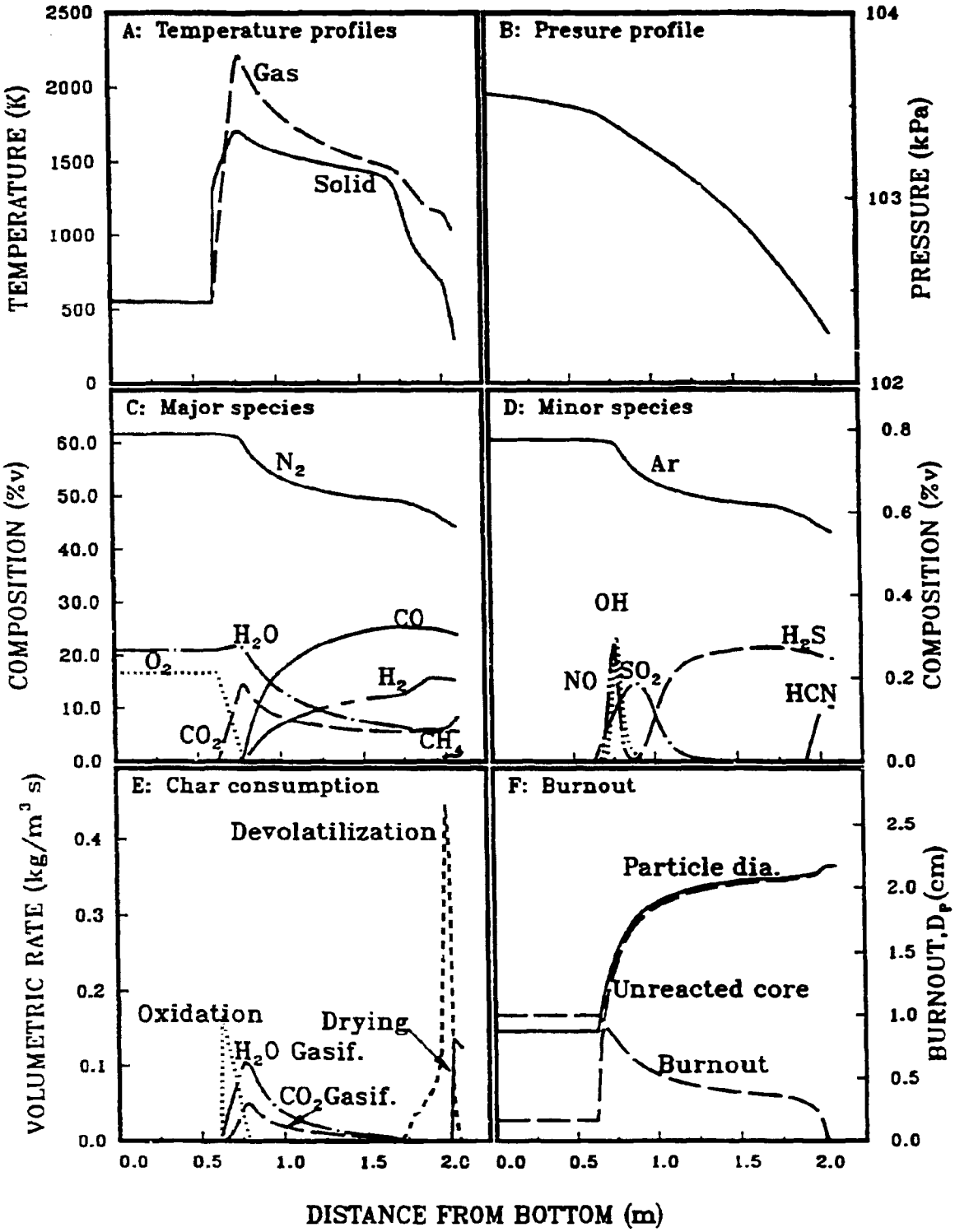


Figure IV.B-1. Typical output generated by the program plotl using the DISSPLA graphics package.

U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161 (703) 605-6000