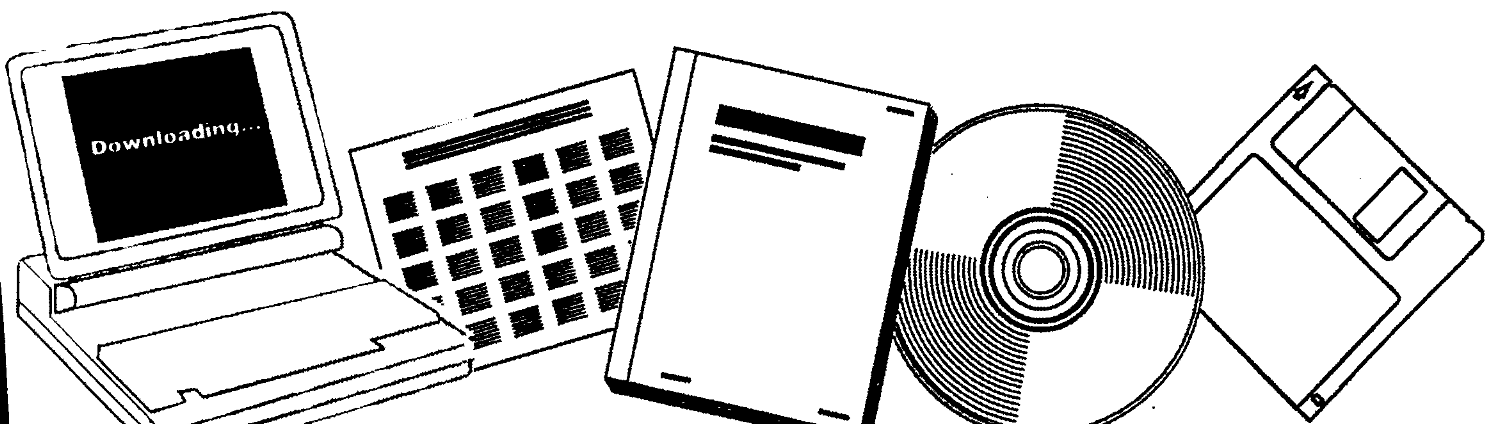
DE92001267

MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES. ANNUAL REPORT, OCTOBER 1990--SEPTEMBER 1991

ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

1991



U.S. Department of Commerce
National Technical Information Service

DE92001267

DOE/MC/23075--3081

DE92 001267

Measurement and Modeling of Advanced Coal Conversion Processes

Annual Report
October 1990 - September 1991

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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
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East Hartford, Connecticut
and
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Provo, Utah

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 fifth year of the program is summarized below.

For Subtask 2.a., During the past year, work was done on using the set of rank dependent kinetic parameters obtained from low heating rate experiments to predict high heating rate data from pyrolysis experiments in our Transparent Wall Reactor (TWR) and Heated Tube Reactor (HTR). Simulations were also done of high heating rate pyrolysis data from the literature.

The process of defining the deliverable FG-DVC submodels was completed during the past year. Under this subtask, submodels will be completed for swelling, sulfur and nitrogen evolution, char reactivity and optical properties.

During the past year, work was also done on using the FG-DVC model to simulate mild gasification processes. The model was modified to include a hydrocarbon cracking routine which describes the cracking of long chain paraffin and olefin species down to smaller hydrocarbons (C_1-C_3's).

Work continued on the swelling model. A single bubble version of the swelling model is now being developed for comparison to data on the Pocahontas coal, which is the most difficult coal to model with respect to the swelling behavior at high heating rates.

Work continued on the sulfur and nitrogen submodel. The first step was to run the series of Argonne coals in the TG-FTIR apparatus with the post-oxidizer attached. This allows detection of species that are not easily detected in the IR, such as H_2S (oxidizes to SO_2). Runs have been done with all eight Argonne coals. The preliminary data suggest that the ratio of NH_3/HCN is much higher than what is observed in pyrolysis at higher temperatures.

Work continued on the char reactivity submodel. The recent progress has been in fitting the reactivity model to both isothermal and non-isothermal data for chars produced from the Argonne coals and developing a set of values for the kinetic rate parameters (A, E_o, σ), the active site concentration (β) and the char structural parameter (Ψ) for the Random Pore Model. A relationship was developed to describe the functional form of the active site concentration, β, with respect to changes in coal rank, mineral content, and the degree of pyrolysis.

For Subtask 2.b., The high-pressure, controlled-profile (HPCP) reactor, including the char, tar and gas separation and collection system, has been successfully operated in coal devolatilization, char preparation and char oxidation experiments. The optical diagnostics for particle temperature, size and velocity were assembled and calibrated, and initial measurements of oxidizing char particles were successfully made. Carefully sized samples of four coals have been prepared and stored for the upcoming char preparation and oxidation tests.

For Subtask 2.c., Discussions were held with BYU on the future direction of the work on modeling the tomography data from the TWR coal flame experiments. Some discrepancies exist in the measured and predicted particle temperatures which could result from problems with the measurements and/or the model.

Under this subtask, models for ignition and soot formation will be delivered. The essential ingredients of the ignition model are already in PCGC-2. What is needed is to refine the assumptions regarding the fraction of CO_2 formed at the surface, as opposed to the gas phase, and the amount of energy feedback to the particle from the oxidation reaction of CO. The soot formation model, to date, is a calculation of the equilibrium amount of condensed carbon. This does a good job of predicting the location of the soot maximum but not the magnitude or the burnout. What is needed is a kinetic model for soot formation and destruction.

During the past year, work was done on developing a radiative model for soot as part of the soot submodel and the results were sent to BYU. The inputs are the volume fraction of soot and the temperature. The output is the average soot emissivity.

Subtask 2.d., Under this subtask, a model for ash chemistry and physics was outlined. The inputs will be the starting mineral concentrations and size distributions while the outputs will be the composition and size distribution of the fly ash. Because of the complexity of this problem and the large amount of DOE and NSF supported work being done elsewhere, this submodel will primarily be an integration of work done outside AFR.

Subtask 2.e., The work on the modified AFR fixed-bed reactor (FBR) system continued. It includes two independently heated stages. The reactor system was assembled and tested and was used for lignin pyrolysis experiments under independent funding. It appears to work as planned.

Under this subtask, a model for the repolymerization of tar in fixed bed gasifiers is being developed. The relatively low yield of tar from these systems is believed to be the result of recondensation of tar in the top of the bed which carries the tars back into the bed where they can be repolymerized into char or cracked into gas. A compilation was made of literature data from laboratory reactors and full-scale moving bed gasifiers that can be used to help validate the model.

Subtask 2.f., Construction of the balance unit for the large-particle insert was initiated. A series of sets of large particles was devolatilized and oxidized in platinum crucibles in air. A run was also made with a large particle pressed from pulverized coal. Smaller particles have a larger mass reactivity. North Dakota lignite and Wyoming subbituminous coal show results similar to Utah bituminous coal.

Subtask 2.g., The NO_x and SO_x/sorbent reactions submodels were incorporated into the final product code versions. Additional insight into the thermal NO submodel was obtained. Evaluation of the SO_x/sorbent reactions submodel was initiated. A benchmark case was used to demonstrate the sorbent capture submodel and to investigate the effects of the Ca/S ratio on SO_2 reduction efficiency.

Subtask 3.a., A new version of the FG-DVC submodel, with rank-dependent kinetics, was incorporated into PCGC-2. The effects of direct enthalpy feedback from volatiles flames to devolatilizing particles and heterogeneous CO_2 formation to oxidizing particles were investigated. Simulations for the base code (without FG-DVC) were performed for the BYU/ACERC controlled-profile reactor, the Imperial College reactor, the BYU gasifier, the ABB Combustion Engineering drop-tube reactor, and the Goudey plant of New York State Electricity and Gas.

Subtask 3.b., Work continued on the fixed-bed model. The first version (MBED-1) was completed and evaluated. A user's manual was written, and the code and user's manual were submitted to METC. Minimum specifications for the final code product (FBED-1) were determined. The present version of FBED-1 includes the properly integrated FG-DVC percolation submodel, and was tested by simulating the Wellman-Galusha gasifier fired with Jetson bituminous coal. The results compare well with predictions from previous versions of the code.

Subtask 3.c., Modifications were completed to allow PCGC-2 to simulate coal and sorbent injection in additional (sidewall) inlets.

Subtask 4.a., Letters were written to representatives of three Clean Coal Technology projects for information. A response was received from Coal Tech Corp., and their cyclone combustor was selected as an application case. The other application case will be the Texaco gasifier (Coolwater project).

Subtask 4.b., Two new cases of potential interest for code application were identified. Both are fixed-bed gasifiers integrated into gasification/combined-cycle systems.

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