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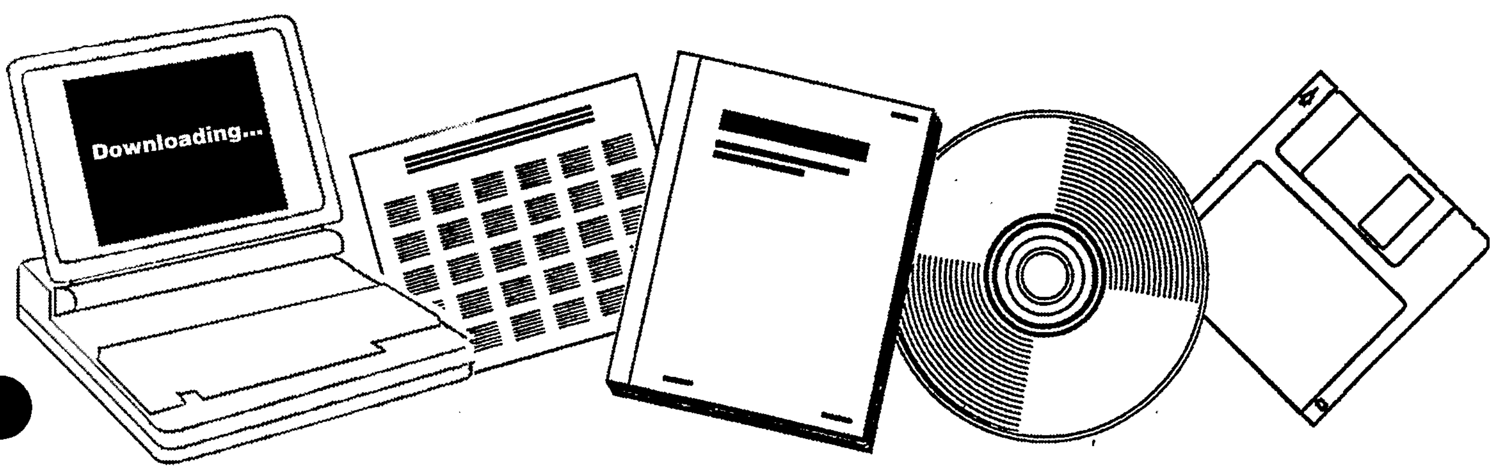
MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES: SECOND ANNUAL REPORT, OCTOBER 1987-SEPTEMBER 1988

ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

OCT 1988



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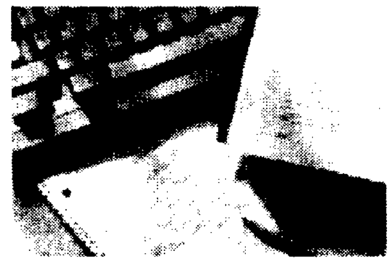

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Measurement and Modeling of Advanced Coal Conversion Processes

Second Annual Report,
October 1987 - September 1988

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

October 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

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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 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.

During the second year of the program, progress was made on nearly all of the tasks, as summarized below.

Under Subtask 2.a, "Coal to Char Chemistry Submodel Development and Evaluation", additional characterization of the coal samples for this program was performed by pyrolysis experiments in a TG-FTIR, in a Field Ionization Mass Spectrometry (FIMS) apparatus, and in an Entrained Flow Reactor (EFR). The FG-DVC model was used to predict baseline pyrolysis data for the eight Argonne coals from these three reactors. In general, the model did a good job in predicting the data for gas, tar and char yields and for the tar molecular weight distributions. Additional improvements were made in the FG-DVC model. Work was also done on comparing the FG-DVC model to the statistical model of Pugmire and Grant at the University of Utah which is based on percolation theory. A review of internal pore transport models was prepared by Professor Eric Suuberg of Brown University. In order to refine the combined kinetic/mass transport submodel used in the FG-DVC model, a search was made of literature pyrolysis data for the Pittsburgh Seam coal, starting with heated grid experiments. To examine the effect of product evolution, char viscosity, and transport on the swelling of char, drop tube experiments have been done with a Pittsburgh coal at temperatures varying from 475-600°C in 25°C intervals. Selected chars were potted and polished for analysis of their morphology by SEM. Finally, preliminary measurements were made of the spectral emissivity for coals of varying particle size and rank. The average emittance increased with increasing rank and particle size.

Under Subtask 2.b, "Fundamental High-Pressure Reaction Rate Data", the design of the high-pressure, controlled-profile (HPCP) reactor was completed, and fabrication of major reactor components was also finished. Assembly of the reactor facility is in progress, with initial char tests planned for next January. Char preparation was continued with the objectives of understanding the experimental details associated with char preparation at elevated pressures as well as at atmospheric pressure and comparing the physical properties of chars prepared with different reactors in anticipation of the availability of the HPCP reactor. Five coals were selected for detailed char oxidation measurements in the HPCP reactor.

Under Subtask 2.c, "Secondary Reaction of Pyrolysis Products and Char Burnout", studies of ignition and soot formation in flames were continued in the transparent wall reactor (TWR) in experiments which include in-situ FT-IR diagnostics. Attention is being focused on what controls ignition (heterogeneous or homogeneous oxidation) and soot formation. Seven additional samples were completed in addition to the four reported in the First Annual Report. Flame properties were compared with characteristics of the samples to determine the factors which control flame behavior. In addition, in order to obtain in-situ data from an actual gasifier, an FT-IR spectrometer was temporarily installed at BYU on their high pressure gasifier.

For Subtask 2.d, "Ash Physics and Chemistry Submodel" 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. Sample collections were performed using these probes from Zap lignite and Montana Rosebud coal flame experiments. SEM/dispersive x-ray analysis was performed on individual ash spheres that were recovered from the preseparator and the eight stages of the cascade impactor for an "in stack" ash collection from 200 x 325 mesh Zap lignite. In order to further understand the role played by ion-exchanged cations on char reactivity, samples of demineralized Zap coal were subjected to ion-exchange experiments with Ca, Na, Mg, and K. The reactivity of the resultant chars was measured in air and CO_2.

For Subtask 2.e, "Large Particle Submodels", a critical evaluation was made of two models from the literature that have been used to describe coupled reaction and transport in large particles. The formulation of our own single particle model was begun. Discussions were also held with BYU on the interface between the single particle model and the advanced fixed bed reactor model. The design and construction of a small scale fixed-bed reactor was completed. This reactor will have on-line analysis of evolved volatile products and on-line measurement of char functional group composition and particle temperature.

Under Subtask 2.g, "SO_x/NO_x Submodel Development", incorporation of the Zeldovich thermal NO_x mechanism into the existing NO_x submodel has been completed. The revised NO_x submodel can now predict the joint contribution of fuel and thermal NO. Evaluation of this submodel is in progress. A sorbent-particle reaction model is currently being incorporated in PCGC-2, under independent funding. Prediction of the gaseous sulfur species has also been studied and a reaction mechanism has been identified.

For Subtask 2.h, "NO_x/SO_x Submodel Evaluation", modifications were completed on the cold-flow facility designed to replicate the geometry of the entrained-flow gasifier, and mixing data were obtained for the cross-flow injection of sorbent. The cold-flow testing was completed, and analysis of the data is nearly complete. Photographs of injected smoke illustrate the deflection of the jet plume as it was entrained in the free stream. The jets can be made to penetrate to any desired distance by adjusting the diameter of the jet and the momentum flux ratio. Contour maps of normalized tracer gas concentration were obtained to quantify the mixing patterns of the cross-flow jets. Based on the results obtained in the cold-flow study, modifications to allow sorbent injection in the entrained flow gasifier were completed, and testing was initiated. Tests were conducted with four coals of varying sulfur content.

For Subtask 3.a, "Integration of Advanced Submodels into Entrained-Flow Code, with Evaluation and Documentation", work continued on incorporating the FG-DVC devolatilization submodel being developed under Subtask 2.a and the SO_x/NO_x submodel being developed under Subtask 2.g into PCGC-2, implementing the advanced code on computers, and evaluating the comprehensive code. Modifications were made in PCGC-2 to test the Multiple Solids Progress Variables (MSPV) method with two solids progress variables independently tracking coal offgas, and converged solutions were obtained for a swirling combustion case and a non-swirling gasification case. The results clearly show the importance of accounting for variability in coal offgas composition, enthalpy, or both. The FG-DVC submodel was integrated into PCGC-2 assuming constant coal offgas composition and enthalpy, and work is continuing to investigate the effects of variability in the offgas. A laminar option in the code is being developed for submodel validation in the comprehensive code in the absence of turbulence effects. A method for evaluating the comprehensive code has been outlined.

For Subtask 3.b, "Comprehensive Fixed-Bed Modeling Review, Development, Evaluation, and Implementation", a detailed review of existing fixed-bed coal gasification codes was accomplished previously and described in the First Annual Report. The proposed features of the advanced model were reviewed by external consultants and, based on their written comments, an extensive plan for developing the model was formulated. Evaluation of existing models continued during the second year. Predictions were compared with experimental values and a sensitivity analysis was performed. Preliminary reviews of flow, mass, and heat transfer processes in fixed beds as well as fixed-bed technology were completed. A comprehensive review of fixed-bed combustion and gasification was initiated. Development of the advanced fixed-bed model was also initiated and the key model assumptions were determined.

Under Subtask 4.a, "Application of Generalized Pulverized Coal Comprehensive Code", the FG-DVC model was successfully integrated with PCGC-2. This work is summarized under Subtask 3.a.

No work was scheduled for Subtask 4.b and Subtask 2.f was not initiated yet due to a reduced funding level.

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Contract No. DE-AC21-86MC23075

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