MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES: QUARTERLY REPORT, APRIL-JUNE 1988

ADVANCED FUEL RESEARCH, INC.
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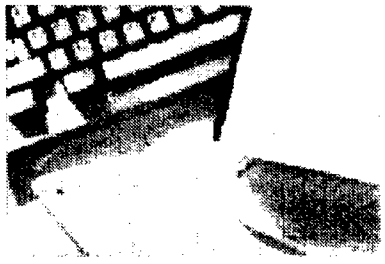

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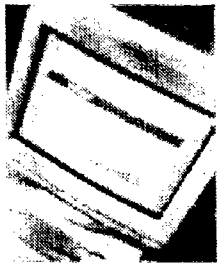

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L.D. Smoot
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June 1988

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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87 Church Street
East Hartford, Connecticut 06108

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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 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 seventh quarter of the program, progress was made in several areas, as summarized below.

For Subtask 2.a, additional improvements were made in the FG-DVC model. The FG-DVC model was also used to predict baseline pyrolysis data for the eight Argonne coals from three different 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.

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. When a comparison was made of data produced by heating at 1000 K/s to various peak temperatures, it was found that the results of different investigators did not agree, even when obtained from the same laboratory. We begin an experimental and theoretical study into possible reasons for these variations.

For Subtask 2.b, several char samples were prepared with the simple hot-tube reactor, and a char sample was collected from the BYU gasifier. These samples have been analyzed by a CH analyzer and SEM. Hydrogen content generally decreases as residence time increases. Some samples, however, showed the opposite effect, probably due to a buildup of tar on the walls of the reactor tube which effectively decreased the residence time. Particles with longer residence times were more

porous. The gasifier char, however, was non-porous. Construction of the high-pressure, controlled-profile reactor continued.

For Subtask 2.c, data collection was temporarily suspended as the FT-IR spectrometer was needed for a different project.

For Subtask 2.d, 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, and K. Ca exhibited a saturation effect, while Na and K exhibited a maximum in reactivity with increased loading.

For Subtask 2.e, the construction of the fixed-bed reactor was nearly completed. Discussions were held with Dr. Radulovic (from BYU) on the relationship between the fixed-bed reactor model and the large particle pyrolysis model.

For Subtask 2.g, development of the combined thermal- and fuel-NO_x submodel has proceeded with two computer simulations being made to evaluate the theory and code. The first case was for an entrained-flow coal/oxygen gasifier. Predictions for this case were favorable, showing improvement of the predicted NO concentrations from inclusion of thermal NO. The second case was for a propane/air turbulent diffusion flame. This prediction was also favorable, showing that the Zeldovich mechanism, assuming equilibrium of molecular and atomic oxygen, correctly predicts NO concentrations in post-flame regions, provided the temperature and oxygen concentration are correctly predicted.

For Subtask 2.h, the cold-flow facility was modified with a flow straightener to eliminate recirculation and replicate the flow patterns in the aft-region of the gasifier. Tracer gas and smoke visualization tests are in progress. The gasifier was recast and a flash tank was installed. Several checkout tests were conducted, including one with sorbent mixed with the coal. A new gas-quenched sample system was developed. Improvements were made to the chemical analysis procedures to better analyze the sulfur capture, and pulverized samples of coal and limestone were prepared.

For Subtask 3.a, the FG-DVC model was integrated into a more recent version of PCGC-2 and the new version was transferred to AFR. The new code was tested for Pittsburgh seam coal, and FG-DVC submodel predictions were compared with predictions obtained with the two-step devolatilization model using the rate constants of Kobayashi et al. (1977). Development of a graphics interface using the UNIRAS software package was initiated. A review of the FG-DVC submodel was initiated, and potential improvements were identified. The review of advanced devolatilization models continued, and a laminar code was identified for investigating the relative effects of various devolatilization models in the absence of turbulence effects. Plans were initiated for developing a new approach to chemistry/turbulence modeling based on a Lagrangian description of the gas phase.

For Subtask 3.b, the computer code development for the improved fixed-bed gasifier model was continued. The development of the advanced fixed-bed gasifier model was initiated. The collection of fixed-bed reactor design and test data was continued. A comprehensive review of fixed-bed combustion and gasification was initiated.

For Subtasks 4.a and 4.b, no work was scheduled.

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TABLE OF CONTENTS