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MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES: 11TH QUARTERLY REPORT, APRIL 1, 1989-JUNE 30, 1989

ADVANCED FUEL RESEARCH, INC.
EAST HARTFORD, CT

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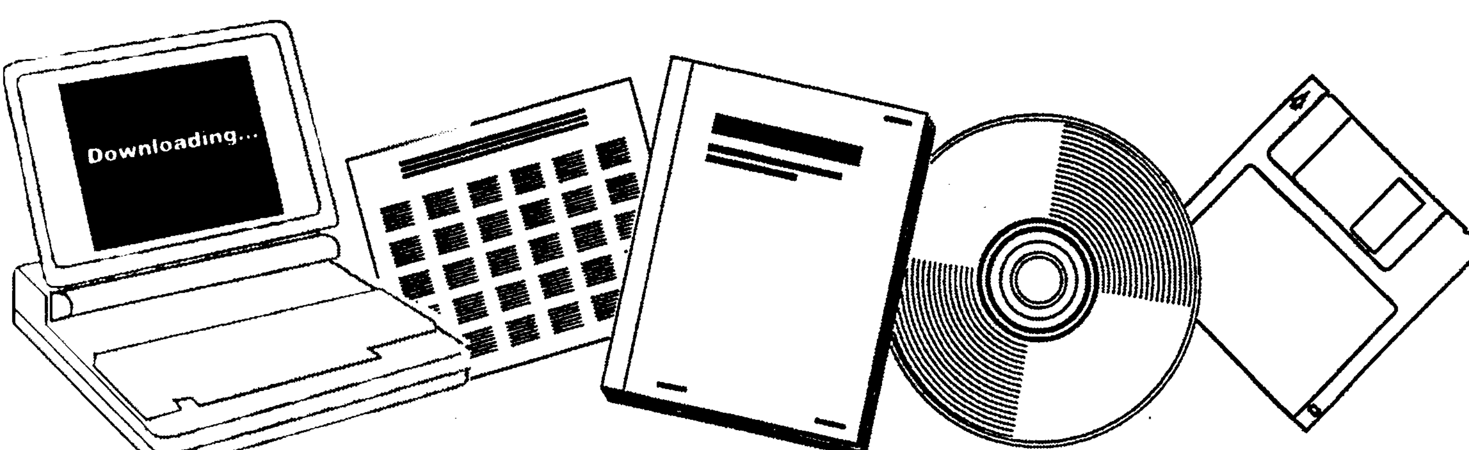

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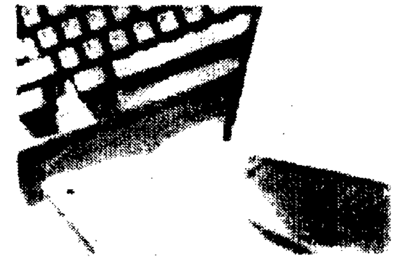

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MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES

11th Quarterly Report #523043-36
April 1, 1989 to June 30, 1989

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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 eleventh quarter of the program, progress was made on nearly all of the tasks, as summarized below.

For Subtask 2.a., work continued on the coal viscosity (fluidity) model. During the past quarter, the effects of different maceral groups on viscosity were addressed. The sensitivity of the model to the activation energy for the temperature dependence of the viscosity was also investigated. We have also obtained additional fluidity data on coals in the Exxon sample bank which will be used to test the model.

In view of the importance of macromolecular network models to the accurate predictions of coal processing behavior, we have assessed the assumptions and limitations of the proposed models. We are considering using percolation theory instead of Monte Carlo methods as the basis of our network decomposition model in order to reduce the computation time for running the FG-DVC model.

An independent investigation was made of the rank dependence of the pyrolysis kinetics by doing experiments in a TG-FTIR reactor over a series of heating rates (3, 30, 50, 100°C/min) with three coals (Pocahontas, Pittsburgh, No. 8, and Zap lignite) from the Argonne set. The results indicated that the rates for tar evolution or bridge breaking vary by about a factor of 10 if the

Pocahontas coal is excluded, which is consistent with previous results for coals from the same range of ranks. This corresponds to a difference in T_{max} for tar evolution of - 40°C at a heating rate of 30°C/min. If the Pocahontas coal is included, the rank variation for the tar evolution/bridge breaking rate is about a factor of 50. This corresponds to a difference in T_{max} for the tar evolution of - 65°C at a heating rate of 30°C/min.

Work also began on adding the polymethylene species to the FG-DVC model. These are long chain aliphatic species which are important components of the tar in low rank coals.

For Subtask 2.b., work continued on the instrumentation and testing of the high-pressure, controlled-profile (HPCP) reactor, preparation and characterization of char, and kinetics of char oxidation at high pressure. The reactor was tested by producing char from Pittsburgh No. 8 bituminous coal. Chars from this coal were prepared in the hot-tube reactor at pressures ranging from 1-10 atm and 1275-1530 K. SEM's were taken of all the samples for comparison with previous samples from other coals, and for comparison with chars produced in the HPCP.

For Subtask 2.c., discussions continued with BYU on the modeling of the Transparent Wall Reactor (TWR) experiments with the Montana Rosebud Coal. This work is being reported under subtask 3.a.

Work was also done to modify the TWR experiment to do pyrolysis and combustion experiments with FT-IR measurements of particle temperatures. During the past quarter, a series of pyrolysis experiments was done with Zap lignite and Pittsburgh seam bituminous coal. These experiments included FT-IR gas and particle temperature measurements, thermocouple measurements of the gas temperature and collection of char samples with a probe at six different heights. The particle temperature measurements were used to reconstruct the particle temperature-time history. The pyrolysis yields were then simulated with the FG-DVC model and the results were consistent with the kinetic rates measured previously at high heating rates at AFR and Sandia for experiments where particle temperature measurements were made.

For Subtask 2.d., work continued on improving the collection of ash from the entrained flow reactor experiments with the eight Argonne coals. It appears that most of the problem for the Upper Freeport coal, where low collections were obtained, was due to particles and ash sticking in the collection probe. This appears to be solved by rinsing the probe with acetone.

Work on the effects of minerals on char reactivity continued. As discussed in the previous quarterly, a particular area of interest is the investigation of the effects of Na on the reactivity of demineralized Zap coal. Surface area analyses were done of the chars produced from coals with high Na loadings during the past quarter. It appears that a significant reduction in the CO_2 surface area can explain the low reactivity of the 2.0 wt.% Na char. The reason for this has not yet been determined. SEM photographs do not reveal anything unusual about the char morphology.

For Subtask 2.e., the main modeling activity during the past quarter was to develop a revised version of the FG-DVC model which does not have a lot of extraneous variables which have accumulated over many years of development. This new version will be used by BYU in the Fixed-Bed Reactor Model and will eventually replace the version which is now in the Entrained Bed Model (PCGC-2).

Work continued on testing the AFR fixed-bed reactor system. Some preliminary coal pyrolysis experiments were done with Zap lignite coal. The system appears to function properly except for an air leak that needs to be fixed.

For Subtask 2.f., this subtask has not been initiated and no work was conducted during the past quarter.

For Subtask 2.g., an experimental program (independently funded) is currently in progress to collect data for evaluating the thermal NO mechanism of the revised NO_x submodel. PCGC-2 simulations of the reactor system are also in progress. One simulation was completed to compare an alternative empirical NO_x mechanism with the original fuel NO mechanism of PCGC-2 and experimental data.

For Subtask 3.a., work continued on the integration and evaluation of the FG-DVC submodel in PCGC-2. The relative effects of variability in coal offgas and enthalpy are being evaluated to assess the need for multiple solids progress variables. A previous case was repeated with the FG-DVC submodel and solving the full energy equation. A converged solution was obtained. Work also continued on the simulation of the transparent-wall reactor for submodel evaluation, and parametric calculations were carried out for inlet turbulence intensity varying from 5 to 15 percent. The code calculations are sensitive to the assumed value of intensity. Work was also initiated on developing a graphical user interface for the code.

For Subtask 3.b., work continued on reviewing numerical techniques used in comprehensive fixed-bed models, obtaining validation data from the literature, and coding the chemical submodels. Three equilibrium-based, moving-bed submodel component codes were written, debugged, and partially validated. The three codes are based on total equilibrium, 1-zone partial equilibrium, and 2-zone partial equilibrium.

For Subtask 4.a., no work was planned or conducted on this subtask during the past quarter.

For Subtask 4.b., this subtask was initiated during the past quarter. Fixed-bed technology and data were reviewed, and fixed-bed gasifiers of potential interest for simulation were identified. Design and test data were obtained for these gasifiers. Particular attention was paid to mild gasification data reported at the recent METC Ninth Annual Gasification and Gas Stream Cleanup Systems Contractors Review Meeting.

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MEASUREMENT AND MODELING OF COAL CONVERSION PROCESSES

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