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# MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES. 15TH QUARTERLY REPORT, APRIL 1, 1990-JUNE 30, 1990

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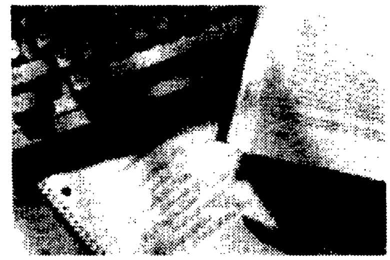

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FOSSIL ENERGY

# MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES

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April 1, 1990 to June 30, 1990

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## PATENT STATUS

## 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 fifteenth quarterly of the program is summarized below.

**For Subtask 2.a.**, work continued on the improvements to the FG-DVC model. A set of rank dependent kinetic parameters has been developed for tar, $CH_4$, CO, $H_2O$, and $CO_2$ for each of the Argonne coals. The predictions of the model are being compared to pyrolysis kinetic data from the TG-FTIR system at four heating rates. For a given coal, it is being assumed that the pre-exponential factors are similar for the evolution of the components of a given species (e.g., $CO_2$-Extra Loose, $CO_2$-Loose, and $CO_2$-Tight), but that the activation energies increase in the order Loose ---> Tight. It is also being assumed that for a given species pool, the frequency factor is fixed (independent of rank) and that the activation energies for each functional group pool increase in the rank order. This approach has been successfully used for the component pools of the major volatile species (CO, $CO_2$, $H_2O$, $CH_4$) for four of the eight Argonne Premium coals, to date (Utah, Pittsburgh, Upper Freeport, Pocohontas). Work on the remaining coals is in progress.

This complete set of kinetic parameters were tested in both Monte Carlo and the 2-$\sigma$ percolation theory versions of the FG-DVC model. Results for three of the eight coals indicate that only small adjustments are required in the

kinetic parameters between the two models.

The kinetic parameters are also being validated indirectly through the application of the fluidity model to the Geissler fluidity data for six of the eight Argonne coals. Comparisons are being made to the NMR data of Lynch obtained at CSIRO on the Argonne premium coals. The changes in the fluid fraction predicted from the fluidity model are in good agreement with the change in hydrogen mobility observed in the NMR experiment. We are rechecking the current version of the model with the latest kinetic parameters against van Krevelen's data for fluidity as a function of heating rate and against the isothermal data of Oxley and Pitt.

Work also continued on the swelling model. By using an adjustable parameter for either the diffusion distance or bubble wall thickness in the model, we were able to obtain good predictions for swelling ratio, porosity, and surface area over a range of pyrolysis heating rates.

**For Subtask 2.b.**, during the last quarter, significant progress in developing the optical particle imaging system and the reactor collection system was made. The optical stands and brackets were designed and fabricated for the HPCP facility. The time required for size classification of pulverized coal was considerably reduced and the quality of the classification was improved significantly. Sufficient quantities of narrow size ranges of two of the test coals were produced for upcoming char preparation and oxidation tests. Analytical techniques to determine tar composition directly from tar filters were also developed and improved accuracy of char weight loss analysis through the use of four simultaneous tracers was investigated. Previously collected char and tar from Pittsburgh No. 8 bituminous coal was analyzed and compared using the new procedures.

**For Subtask 2.c.**, additional work was done on the coal flame experiments in the TWR using the FT-IR Emission/ Transmission Tomography technique. Two cases have now been completed for the Montana Rosebud coal (low velocity and high velocity). A low velocity case for the Pittsburgh Seam coal is about 50% complete.

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

**For Subtask 2.e.**, the work on the AFR fixed-bed reactor (FBR) system continued. A redesign of the experiment has been proposed and approved which will allow better quantitation of the tar yields and independent control of the temperature of the second bed. Assembly has begun on a redesign of the experiment. Samples of large particles for each of the eight premium coals have been ordered from Argonne and should be received by July 1, 1990.

Discussions continued with BYU about the single particle FG-DVC model for use in the fixed bed reactor. For this purpose, AFR is developing an ordinary different equation (ODE) version of the 2-$\sigma$ percolation FG-DVC model. Additional refinements were done to the model to improve its speed. The code was sent to BYU for integration into the Advanced Fixed-Bed Model. A meeting was scheduled at AFR to discuss the single particle model which will involve members of both teams.

**For Subtask 2.f.**, work continued on designing a large-particle insert to be placed in the HPCP reactor and evaluating analytical procedures for monitoring the rates of large-particle oxidation. A second set of preliminary oxidation experiments were carried out with large char particles made from Utah Bituminous coal, and mass reactivities were determined. The average value of 0.0358 $min^{-1}$ compares favorably with the value of 0.0475 $min^{-1}$ reported previously. Some problems with temperature measurement were experienced.

**For Subtask 2.g.**, pollutant predictions for coal combustion and gasification cases were completed to verify the extended and alternative fuel NO mechanisms of the submodel. The ability to predict NO formation during gasification of North Dakota lignite was given special consideration. Joint fuel and thermal NO predictions were also completed for combustion and gasification cases. The revised submodel has been fully integrated into PCGC-2 and a user's guideline has been prepared. Work is in progress to complete a sorbent reactions submodel.

**For Subtask 3.a.**, work was nearly completed on modeling the transparent wall reactor for code validation and on developing a graphical, user-friendly interface. After modifying for up-firing, gas buoyancy, and laminarization, reasonable results were achieved for the simulation of the non-reacting flow case and the "fast-flow" Rosebud coal flame. Key flame properties, such as ignition point, burnout profile, and gas and particle temperature, have been reasonably well predicted. Complex flow patterns at the nozzle promote particle dispersion, and have not been adequately resolved with current grid spacing. Code predictions are sensitive to inlet boundary conditions for the coal stream at the nozzle exit, and detailed characterization of this boundary condition is needed. Soot formation seems to correlate with equilibrium concentration of condensed carbon, but decays more slowly than predicted from equilibrium. The energy feedback to particles or the $CO_2$/CO ratio produced at the particle is not adequately predicted.

A window was added to the graphical user interface (GUI) on the Sun workstation for specifying the composition and temperature of the inlet streams. The thermodynamic input file can now be generated automatically using information in the main data file and a chemical species database. Work was also initiated to apply two graphical programs that have been developed under independent funding, a pre- and a post-processor, to PCGC-2. The preprocessor generates a grid file and the post-processor presents computational results. The format of the grid file used by PCGC-2 differs from that used by the pre-processor, and a program was written for converting files between the two formats. A subroutine was modified and added to PCGC-2 for writing the plotting file needed by the post-processor. Both the pre- and post-processors were applied to the TWR simulation described above.

**For Subtask 3.b.**, work continued on reviewing, coding, and validating submodels. To enhance user-friendliness, the input file was rewritten to segregate input parameters for the two-zone and one-dimensional submodels. Also, the fixed-bed code was rewritten in a modular fashion with extensive comment statements. The two-zone submodel was improved to accommodate user-specified burnout. Also, two heat transfer zones were added to the well-mixed model to account for heat loss in the freeboard and heat transfer between solid and gas in the ash zone of the reactor. The ash enthalpy calculation was improved.

The fixed-bed code was evaluated by parametric sensitivity analysis. Sensitivity runs were divided into model options, model parameters and operational parameters. Model options include tar vapor reaction equilibrium, volatile mass transport, char ash layer formation, and combustion product distribution. Model parameters include the solid-to-gas heat transfer correction factor, effective diffusivity, bed-to-wall heat transfer, potential tar forming fraction, functional group composition (coal rank), oxidation and gasification kinetics. Operational parameters include the temperature of the feed gas, reactor pressure, coal mass flow rate, steam mass flow rate, air mass flow rate, proximate ash content of the feed coal, proximate moisture content of the feed coal, particle diameter , and bed void fraction.

**For Subtask 3.c.**, work was initiated on modifying PCGC-2 to allow sorbent injection.

**For Subtask 4.a.**, this subtask has not been initiated.

**For Subtask 4.b.**, during the last quarter, work continued on collecting fixed-bed design and test data. The advanced fixed-bed code was applied to seven new test cases, including the dry-ash Lurgi gasifier, the Wellman-Galusha gasifier, the METC gasifier, and the slagging BGC-Lurgi gasifier. A presentation was given at the joint METC/AFR/BYU project review meeting, and discussions were held with AFR concerning code development.

Four different gasifier types were simulated: the high pressure, oxygen-fired Lurgi gasifier; the low pressure, air-fired Wellman-Galusha gasifier; the medium pressure, air-fired METC gasifier; and the high pressure oxygen-fired BGC-Lurgi slagging gasifier. Twelve coal types were simulated, which range from lignite to bituminous.

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