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MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES. FOURTEENTH QUARTERLY REPORT, JANUARY 1-MARCH 31, 1990

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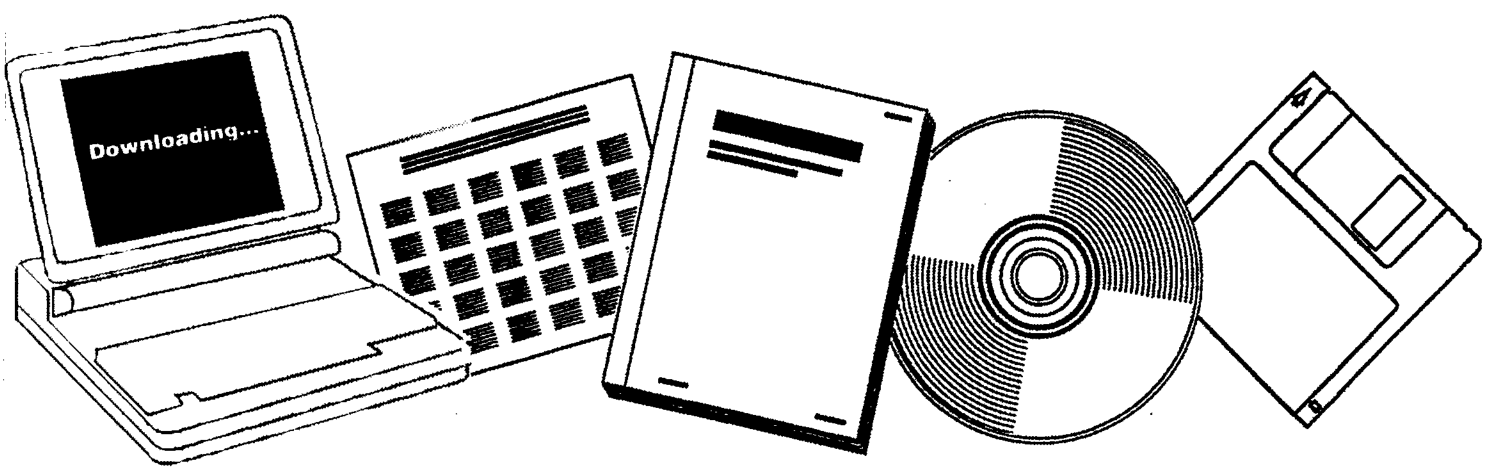

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ABSTRACT

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 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 fourteenth quarterly of the program is summarized below.

For Subtask 2.a., work continued on examining a percolation theory approach instead of Monte Carlo for doing the network decomposition calculations in order to increase computational speed. Using percolation theory, we can get comparable predictions of the tar and gas rates. For the same set of bridge breaking parameters, there are some slight differences in the shape of the tar peak and in the fluidity predictions. The fluidity predictions appear to be the most sensitive to the choice of percolation theory over the Monte Carlo approach, as the definition of the fluid fraction is model dependent.

Work also continued on the incorporation of rank dependent pyrolysis kinetic rates. We have completed a first round of fits to the TG-FTIR data obtained from all eight Argonne coals at four different heating rates and the fluidity data obtained for six of the coals at one heating rate. This procedure provides a set of rank dependent kinetic parameters for gas evolution (CH_4, CO_2) and the breaking of weak bridges (required for tar evolution). The next step is to try this set of kinetic parameters in the percolation theory version of the model in order to arrive at a consistent set and to complete the work on the

other major gas species (CO, H_2O, H_2).

Work continued on the particle swelling model. Additional sets of equations were examined to describe the driving force for swelling and one was chosed which we feel is the most consistent with the physics. It is planned to obtain additional swelling data, to find more relevant data on the gas diffusivity and to make some measurements of pore wall thickness.

For Subtask 2.b., the suction pyrometer for reactor centerline temperature characterization was fabricated and temperature profiles for the HPCP facility were measured. Also, the smaller diameter injection probe was installed, and development of the optical particle imaging system was continued.

Significant improvement was made in particle size classification and characterization by using aerodynamic and screen separation, along with an optical particle sizer. Devolatilization runs were made with North Dakota lignite, at atmospheric and elevated pressure, to continue evaluation of the effectiveness of reaction quenching and of the separation of the char and tar in the collection system during devolatilization runs.

For Subtask 2.c., additional work was done on the coal flame experiments in the TWR using the FT-IR Emission/Transmission Tomography technique. It has been found that the preheated air velocity has a significant effect on the shape of the flame. At low velocities, the ignition point of the flame has a donut-shaped ring of ignition with a cooler center. At high velocities, there appears to be a solid ball of ignited particles. Two cases are being done for the Montana Rosebud coal (low velocity and high velocity) and a low velocity case for the Pittsburgh Seam coal is also being done. The three flames showed both coal and flow dependent phenomena. The slow flow cases showed reduced mixing (more soot and more variations in flame properties with radius) compared to the fast flow case. The Pittsburgh Seam coal showed higher soot, higher swelling, lower particle temperatures, lower char reactivity, and higher volatility compared to the Rosebud coal.

For Subtask 2.d., work began on characterizing the reactivity of chars collected from the coal flame experiments. These chars have been analyzed by the standard TG-FTIR analysis which directly provides information on the reactivity index ($T_{critical}$) and the active site concentration (based on the amount of oxygen chemisorbed). A correlation was found between these two measurements. In order to apply this technique on high ash chars from the coal flame, a method was developed to correct the $T_{critical}$ for the char ash content.

For Subtask 2.e., the experimental work on the AFR fixed-bed reactor (FBR) system continued with the Pittsburgh Seam bituminous and Zap lignite coals. For both coals, we have not observed a strong effect of bed depth on tar yield over the range of conditions studied. A second series of pyrolysis experiments was done with the FBR using Pittsburgh Seam bituminous coal. The reactor was modified so that the coal could be held in two separate layers on top of each other with a gap in between. The lower bed is at a lower temperature which depends on the geometry and flow rate. The experiments were done at two different flow rates. The higher flow rate resulted in an increase in tar and a decrease in CH_4 and char yields in both the single and dual bed experiments.

Discussions were held with BYU about the single particle FG-DVC model. Work was completed on a percolation theory version which is based on a system of ordinary differential equations which describes the creation and loss of n-oligomers. This version will be the basis for the single particle FG-DVC model which will be input into the Advanced Fixed Bed Model being developed at BYU.

For Subtask 2.f., design of a large-particle insert for the HPCP reactor was continued. Analytical procedures for monitoring the rates of large particle oxidation are being evaluated. Preliminary oxidation experiments were conducted with a set of large particles of Utah bituminous coal, and mass reactivities were determined.

For Subtask 2.g., thermal NO predictions were found to be sensitive to the method of estimating radical oxygen concentration, wall temperature, chemistry/ turbulence interactions, swirl number, and overall equivalence ratio. A scheme was developed to allow the code to check the local equivalence ratio at each node in the computational domain and choose either of two expressions to estimate the radical oxygen concentration. Thermal NO increased with increasing wall temperature due to a proportional increase in local gas flame temperature. The strong sensitivity of the model to wall temperature may lead to erroneous predictions and the inability to match trends when inadequate wall temperature data are available. As with fuel NO formation, predicted thermal NO was considerably higher when chemistry/ turbulence interactions were taken into account.

For Subtask 3.a., work continued on simulating the transparent wall reactor (TWR). The calculational grid was refined and gas buoyancy and laminarization effects were investigated. Both were found to be definitely important in the TWR. The ignition point is extremely sensitive to inlet coal stream diameter, with a diameter of 3 mm giving good agreement with measured burnout and visual observation of the flame. The observed convergence of the particle stream after ignition has not been predicted in the simulations, but may be due to the dampening effect of particles on gas turbulence. This effect is being investigated. Work continued on the development of a graphical user interface (GUI) for PCGC-2 on the Sun workstation, and a window was added for specifying inlet stream composition and temperature.

For Subtask 3.b., work continued on reviewing, coding, and validating the well-mixed, partial-equilibrium submodel used for estimating effluent composition and temperature for the 1-D fixed-bed code. Predictions were compared with measured effluent temperatures and compositions from fixed-bed reactors, and quantitative agreement was obtained for a wide range of coal types. The interface between the fixed-bed code and FG-DVC submodel was considered, and a plan was formulated for incorporating the percolation theory version of the DVC model while retaining the current implementation of the FG model.

For Subtask 4.b., work continued on collecting fixed-bed design and test data, and on testing and validating the 1-D code.

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