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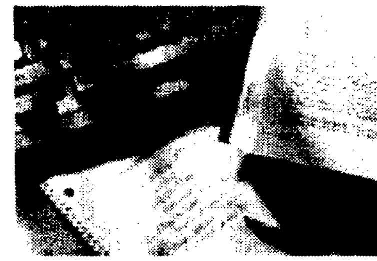

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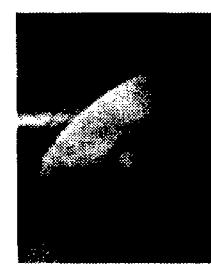

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MEASUREMENT AND MODELING OF ADVANCED COAL CONVERSION PROCESSES

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October 1, 1990 to December 31, 1990

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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 seventeenth quarter of the program is summarized below.

For Subtask 2.a., most of the effort was on using the set of rank dependent kinetic parameters obtained from low heating rate experiments to predict high heating rate data from pyrolysis experiments in our Transparent Wall Reactor (TWR) and Heated Tube Reactor (HTR). We also did simulations of high heating rate pyrolysis data from the literature, such as the heated grid experiments of Gibbins, the wire grid experiments of Fong and coworkers of MIT, and the TWR experiments of Fletcher at Sandia.

Some problems were obtained in predicting the changes in the tar yield and tar molecular weight distributions with heating rate for low rank coals using the current version of the model. It was decided to re-examine the assumptions on the model input parameters, such as 1) the crosslinking efficiencies, 2) the tar vaporization law, and 3) the ΔP parameter. Changes in the crosslinking efficiencies were thoroughly evaluated and found to be largely unnecessary.

The effects of the tar vaporization law and the ΔP parameter were found to be very important. The change in the original vaporization law from the expression proposed by Suuberg to a factor of 10 higher was found to be mainly responsible for the inability to predict the high heating rate Zap data. By changing to Suuberg X1, and allowing ΔP to be the sole adjustable parameter, the predictions are much better. The main unresolved question is the appropriate choice for ΔP and how this could be functionalized. It appears that the model predictions of the FIMS data are very sensitive to the choice of this parameter. Possible solutions would be to: 1) parameterize ΔP; 2) improve the description of the external transport of tar to resolve the problem of the higher molecular weight tars coming out earlier than expected.

For Subtask 2.b., progress was made in increasing the signal-to-noise ratio of the optical particle imaging system so that small particles at low temperature can be measured. The modified reactor collection system was operated successfully under devolatilization conditions. Under independent funding, coal devolatilization tests were successfully conducted using the modified reactor collection system. Computer software was written to support the data acquisition and heater control hardware that was previously interfaced to the reactor instrumentation and heaters, and was successfully used during the devolatilization tests.

For Subtask 2.c., discussions were held with BYU on the future direction of the work on modeling the tomography data from the TWR coal flame experiments. Some discrepancies exist in the measured and predicted particle temperatures which could result from problems with the measurements and/or the model. A rate limiting step in comparing the model with the data is the generation of suitable plots. A new approach which involves output of the predictions of the model into a spreadsheet format was agreed upon.

For Subtask 2.d., no work was scheduled during the past quarter.

For Subtask 2.e., the work on the modified AFR fixed-bed reactor (FBR) system continued. It includes two independently heated stages. The reactor system was assembled and tested and is now being used for lignin pyrolysis experiments under independent funding. It appears to work as planned. As expected, the quantitation of gas and tar is much better than in the old system and a wider range of sample sizes and flow rates can be used.

For Subtask 2.f., the decision was made previously to construct an experimental facility that would connect to the HPCP reactor of Subtask 2b. Of the two experimental approaches considered in the previous reports, the decision has been made to develop the "cantilever beam insert." In this approach the sample will be mounted horizontally to one or two of the optical access ports of the HPCP reactor. A summary of the design of this facility was prepared and sent to a few principal investigators active in fields of closely related research for their comments and criticisms. The suggestions received have been included in the details for the design of this facility. Construction of this "cantilever beam insert" will start during this next quarter. Analytical procedures for monitoring rates of oxidation of large particles continue to be evaluated. Further data analysis of large particle oxidation in air in platinum crucibles shows a marked dependence of mass reactivity on the initial mass of the large particles. This is in contrast to a dependance on temperature, which was expected.

For Subtask 2.g., the method used to determine atomic oxygen concentrations in the NO_x submodel was revisited. Further insight into the best quasi-equilibrium expression to use for predicting atomic oxygen concentrations in lean, swirling-flow, natural gas flames was gained. Work continued on the integration and evaluation of a SO_x/sorbent reaction computerized submodel. This submodel has been integrated into PCGC-2 and is currently being evaluated. Experimental data are being sought to determine H_2S capture rates to use in an H_2S sulfation subroutine.

For Subtask 3.a., work continued on code evaluation and user-friendliness. Data from four reactors were identified for code evaluation. Simulations were performed for a natural gas flame in the BYU controlled-profile reactor and for the near-burner field of a full-scale industrial boiler. Two-dimensional combustor data were requested from Imperial College. A set of minimum specifications for a foundational, entrained-bed code that will satisfy the terms of the contract was identified. These specifications were documented in a letter to AFR and METC. Two menu-driven post-processors were developed for converting PCGC-2 plotting files for gas and particle properties into a format that can be used by spreadsheet programs.

For Subtask 3.b., work continued on developing and evaluating the one-dimensional fixed-bed model. The model response to variations in operating conditions was validated by simulating several such test cases. Predicted temperature profiles were compared to measurements for the atmospheric, air-blown Wellman-Galusha gasifier fired with Elkhorn bituminous, Jetson bituminous, Leucite Hills subituminous, and Utah Blind Canyon bituminous coals. These test cases included temperature profiles at different operating conditions. Discussions with AFR, about the single particle FG-DVC submodel for integration into the fixed-bed code, continued. Development of the user's manual for the fixed-bed code was initiated. The first draft of the manual was prepared.

For Subtask 3.c., PCGC-2 was modified to allow sorbent injection in the primary stream.

For Subtask 4.a., potential application cases for demonstrating the entrained-bed code were identified. A post-doctoral research associate was recruited to work on this subtask.

For Subtask 4.b., work continued on collecting fixed-bed design and test data from the open literature as well as by direct contact of the individuals and the organizations active in the field. No new data sets have been obtained. No new test cases were identified or simulated.

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