SECTION III. TASK 3. COMPREHENSIVE MODEL DEVELOPMENT AND EVALUATION

OBJECTIVE

The objective of this task is to integrate advanced chemistry and physics submodels into a comprehensive two-dimensional model of entrained-flow reactors (PCGC-2) and to evaluate the model by comparing with data from well-documented experiments. Approaches for the comprehensive modeling of fixed-bed reactors will also be reviewed and evaluated and an initial framework for a comprehensive fixed-bed code will be employed after submission of a detailed test plan (Subtask 3.b).

OUTLINE

This task will be performed in three subtasks. The first covering the full 60 months of the program will be devoted to the development of the entrained-bed code. The second subtask for fixed-bed reactors will be divided into two parts. The first part of 12 months will be devoted to reviewing the state-of-the-art in fixed-bed reactors. This will lead to the development of the research plan for fixed-bed reactors. After approval of the research plan, the code development would occupy the remaining 45 months of the program. The third subtask to generalize the entrained-bed code to fuels other than dry pulverized coal would be performed during the last 24 months of the program.

III.A. Subtask 3.a. - Integration of Advanced Submodels into Entrained-Flow Code, with Evaluation and Documentation

Senior Investigators - B. Scott Brewster and L. Douglas Smoot
Brigham Young University
Provo, Utah 84602
(801) 378-6240 and (801) 378-4326

OBJECTIVES

The objectives of this subtask are 1) to improve an existing 2-dimensional code for entrained coal combustion/gasification to be more generally applicable to a variety of coals by incorporating advanced coal chemistry submodels, advanced numerical methods, and an advanced pollutant submodel for both sulfur and nitrogen species, and 2) to validate the advanced submodels in the comprehensive code. The comprehensive code into which the advanced submodels will be incorporated is PCGC-2 (Pulverized Coal Gasification and Combustion-2 dimensional).

ACCOMPLISHMENTS

An effort to recruit a graduate student was initiated. A literature review and code calculations were initiated to better understand the FG/DVC models and how they might best be incorporated into PCGC-2. A contract review meeting was conducted at BYU.

Student Recruiting and Hiring

Work on this subtask was initiated after the first month of the quarter. Letters were mailed to many recent graduates of Chemical Engineering at BYU and to several other universities. Several responses were received and evaluated. At this point, a Ph.D. candidate has been identified to work on this subtask. Mr. Michael Hobbs is prepared to begin work approximately July 1, if he is accepted for doctoral study in Chemical Engineering. In addition, another student, Mr. Larry Baxter, who has a strong background in the structure of PCGC-2 and pyrolysis modeling, has been hired on a part-time basis while he completes his Ph.D. degree later this summer. After that, he will begin work at the Sandia Laboratories in Livermore, where he will likely continue to assist this work in a consulting capacity.

Literature Review of AFR Models

A literature review of current pyrolysis models, particularly the functional group (FG) and depolymerization/vaporization/ crosslinking (DVC) models developed by AFR, has begun. The goal of this review is to understand these models and how they might best be incorporated into PCGC-2.

Presentation at ACERC Annual Review Meeting

The Advanced Combustion Engineering Research Center (ACERC) at BYU hosted its first annual technical review meeting on March 5 and 6. This meeting was attended by all of the faculty and students working in the center as well as representatives from approximately 20 supporting industrial organizations and the National Science Foundation. A presentation on the work being performed for this subtask was given by Dr. Scott Brewster.

Review Meeting at BYU with AFR and METC Personnel

The second technical review and planning meeting between AFR and BYU personnel was conducted at BYU on March 13. This meeting was attended by all of the BYU research team, as well as Dr. Peter Solomon and Mr. David Hamblen from AFR, and Dr. Tom O'Brien and Mr. Justin Beeson from METC. Based on discussions at this meeting, it was decided that a simple approach to incorporate the advanced pyrolysis model into PCGC-2 would be to allow for varying heating value of the volatiles while keeping constant volatiles composition. Possibly, the composition effect may be second order compared with the heating value effect. This simple approach will be compared to more rigorous approaches being developed. A decision was also made to use the Merrick heat capacity model which takes the temperature dependence of coal and char heat capacity on temperature into account.

Effects of Turbulence

One of the major questions associated with integrating an advanced submodel for pyrolysis into PCGC-2 is the relative importance of turbulent fluctuations of the coal gas mixture fraction. If coal offgas composition is to be varied, and if the interaction of chemistry/turbulence is to be taken into account, the volatiles will need to be divided into several discrete groups, with a separate mixture fraction variable defined for each group to represent the mixture composition. In addition, the statistical variance of each mixture fraction will need to be calculated throughout the reactor, and instantaneous properties will need to be convoluted over the joint probability density function for all mixture fraction variables to obtain time-mean values. If the effect of the turbulent fluctuations of one or more of the mixture fractions can be shown to be insignificant, that mixture fraction will not need to be included in the integration, and the complexity of the problem will be significantly reduced.

A plan has been formulated for investigating the effects of varying offgas composition and turbulent fluctuations on the code predictions. According to this plan, a few test cases will be identified, and then a series of simulations will be performed for each test case, where the offgas composition is allowed to be constant or to vary, and the turbulent fluctuations are taken into account or ignored. The test cases will include a fuel-lean combustion case, a fuel-rich gasification case, and a high-pressure case. The fuel-lean combustion case has been selected, and simulations have been performed looking at the effect of ignoring the turbulent fluctuations when the offgas composition is assumed constant. A summary of the main input parameters for this test case is given in Table III.A-1.

Figures III.A-1a-III.A-1d show the effect of ignoring turbulent fluctuations in the inlet gas and coal gas mixture fractions on typical code predictions for the combustion test cases. In this case, the primary and secondary gas consisted of air at 300 K and 589 K, respectively. As seen in the figures, the effects of ignoring the turbulent fluctuations in the inlet gas mixture fraction (f) appear negligible, even with the small difference in inlet temperature, while the effects of ignoring the fluctuations in the coal gas mixture fraction are significant.

The effect of ignoring turbulent fluctuations on centerline NO_x concentration for p.c. combustion is shown in Figure III.A-2. Here, the fluctuations were ignored for both the solution of the major variables and species and for the minor species (e.g. NO_x) predictions. The prediction of the latter is assumed independent of and decoupled from the calculation of the former. As shown, the effect is much more dramatic, since the nonequilibrium NO_x predictions are dependent on and very sensitive to the predicted values of major variables and species.

Comparison of Devolatilization Rates

There is considerable variation in the rates of coal pyrolysis reported in the literature. Since the Functional Group model under consideration for incorporation into PCGC-2 predicts similar rates as the single-step model of Solomon et al. (1986), a comparison was made between code predictions using the Solomon kinetics and the kinetics of Ubhayakar et al. (1977). The centerline temperature profile predicted by both methods is shown in Fig. III.A-3. As shown, the differences are observable, but not extraordinary. Total burnout (not shown) differed at the out let by only 2-3%. The temperature is higher, as expected, using the Solomon kinetics, at least in the aft region of the reactor. However, the fast rate of the Solomon kinetics did not produce a more rapid devolatilization. The comparison is undoubtedly complicated by the fact that the Ubhayakar model is a two-step model, whereas the Solomon model is single-step. At any rate, the comparison shows that code predictions using the single Solomon kinetic rate for devolatilization, are not drastically different than those obtained with the two-step rates of Ubhayakar, et al.

PLANS

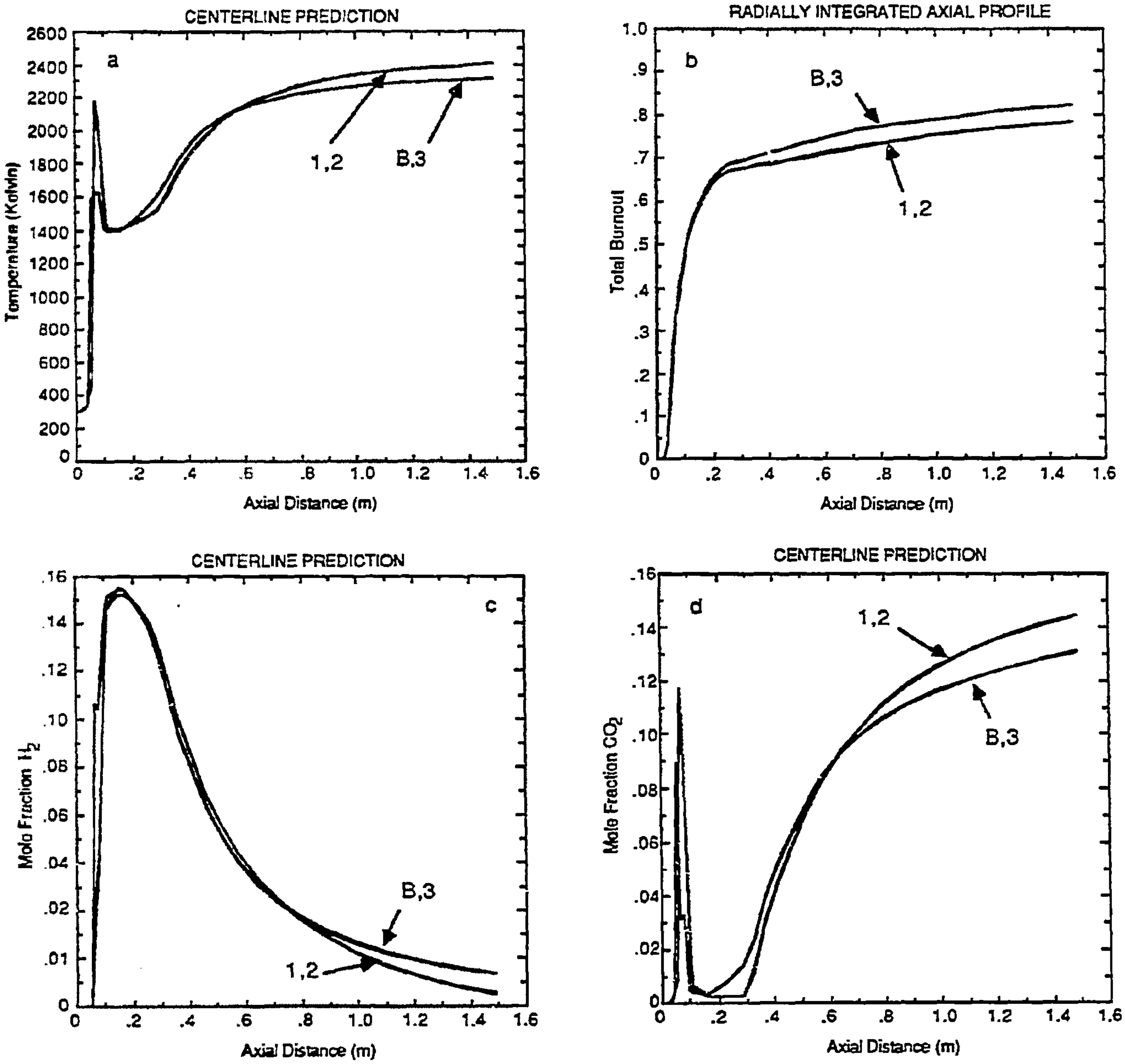
During the next three months, work will continue to understand the FG/DVC model and the best way of incorporating it into PCGC-2. The effect of varying heating value of the volatiles will be investigated, as will the effect of neglecting turbulent fluctuations in fuel-rich systems (i.e. gasification). The Merrick heat capacity model will be incorporated into the code to allow for the dependence of coal and char heat capacity on temperature. The addition of another progress variable to the code and an investigation of the effect of changing volatiles composition will be considered. In addition, a paper based on the work being conducted under this subtask will be prepared for the ACS Conference on Coal Pyrolysis being held in New Orleans next September.

TABLE III.A-1.

INPUT DATA FOR COAL COMBUSTION CASE

GEOMETRY	
Primary tube diameter (m)	0.022
Secondary tube diameter (m)	0.084
Chamber diameter (m)	0.203
Chamber length (m)	1.561
FEED RATES	
Primary gas (kg/s)	6.228E-03
Secondary gas (kg/s)	0.019
Coal in primary (kg/s)	2.835E-03
INLET GAS PROPERTIES	
Primary swirl number	0.000
Primary turbulent intensity (%)	15.0
Primary temperature (K)	300.0
Primary mole fractions:	
AR	0.046
H2O	0.035
N2	0.725
O2	0.194
Secondary swirl number	2.000
Secondary turbulent intensity (%)	18.0
Secondary temperature (K)	589.0
Secondary mole fractions:	
AR	0.009
N2	0.781
O2	0.210
REACTOR PARAMETERS	
Reactor pressure (N/sq.m)	8.600E-04
Side wall temperature (K)	1000.0
PARTICLE PARAMETERS	
Particle solid density (kg/cu.m)	1340.0
Heat of Formation, daf (J/kg)	-1.504E-07
Mass mean particle diameter* (m)	5.025E-05
Initial analysis:	
raw coal	0.931
Elemental analysis (daf):	
C	0.724
H	0.047
O	0.218
N	0.012

* continuous distribution simulated with 5 discrete sizes



‾ure III.A-1. Effect of ignoring turbulent fluctuations of inlet gas and coal gas mixture fractions on typical code predictions for pulverized coal combustion.

B-Base case
1-Ignore η fluctuations
2-Ignore f and η fluctuations
3-Ignore f fluctuations

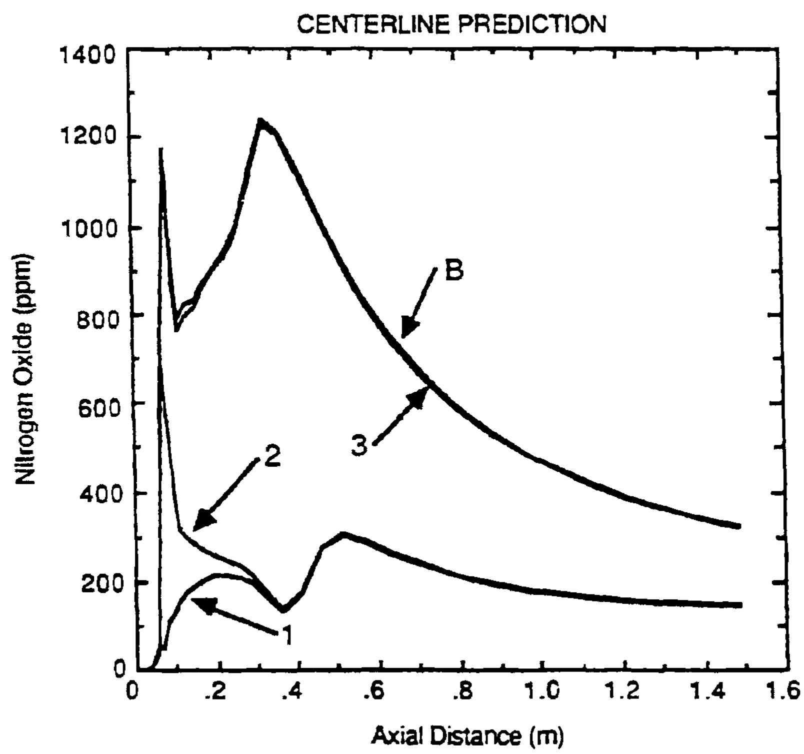


Figure III.A-2. Effect of ignoring turbulent fluctuations on centerline NO_x concentrations for pulverized coal combustion.

B - Base case
1 - Ignore η fluctuations
2 - Ignore f and η fluctuations
3 - Ignore f fluctuations

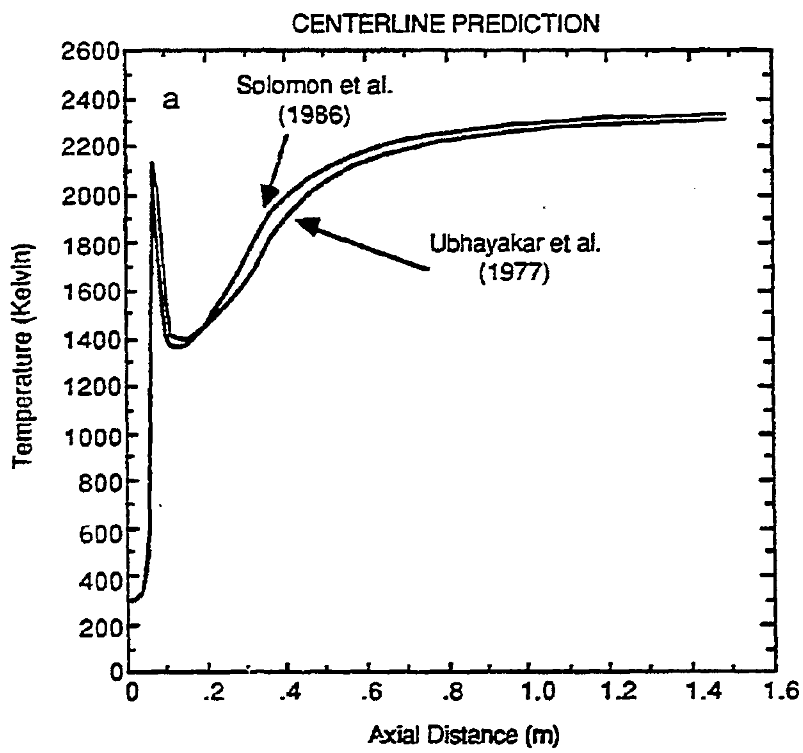


Figure III.A-3. Comparison of Predicted Centerline Temperature for the Two-Step Pyrolysis Model of Ubhayakar et al. (1977) and the Single-Step Model of Solomon et al. (1986).

III.B. Subtask 3.b. - Comprehensive Fixed-Bed Modeling Review, Development, Evaluation, and Implementation

Senior Investigators - B. Scott Brewster and L. Douglas Smoot
Brigham Young University
Provo, Utah 84602
(801) 378-6240 and (801) 378-4326

OBJECTIVES

The objectives of this subtask are: 1) to provide a framework for an improved fixed-bed model that can incorporate coal chemistry submodels, improved boundary conditions, and pollutant formation processes; and 2) to provide a basis for evaluating the model.

ACCOMPLISHMENTS

Recruiting

During the past two months, efforts were initiated to recruit a post-doctoral research associate to work on this subtask. A research associate, Mr. Sung-Chul Yi, has been hired and will begin work on approximately April 15. Mr. Yi is presently completing his Ph.D. degree in Chemical Engineering at BYU.

List of Models and Evaluation Criteria

A list of potential models to be evaluated and criteria for evaluation were identified as shown in Table III.B-1. These models and criteria were taken from a review conducted by Rinard and Benjamin (1985).

Evaluation Criteria

Possible criteria for evaluating the models include complexity, solution method, validation, and availability and detail provided. The complexity (e.g. 1-D vs. 2-D) should be sufficient to justify including an advanced pyrolysis model. The numerical methods should be robust. The code should be well-validated, and it must necessarily be available for use in this contract and well-documented.

PLANS

Early in the next quarter, technical work will begin on the review of existing fixed-bed models.

TABLE III.B-1.

EXISTING FIXED-BED CODES AND CRITERIA FOR EVALUATING

Fixed-Bed Models (Rinard and Benjamin, 1985)

University of Delaware Models

West Virginia University Model

General Electric Model

IBM Model

Washington University Model

University of Minnesota Model

ASPEN RGAS Model

Others

Criteria for Evaluation

Complexity

Solution method

Validation

Availability and Detail Provided