SECTION IV. TASK 4. APPLICATION OF INTEGRATED CODES

Objective

The objectives of this task are to evaluate the integrated comprehensive codes for pulverized coal and fixed-bed reactors and to apply the codes to selected cases of interest to METC.

Task Outline

This task will be accomplished in two subtasks, one for the entrained-bed lasting 45 months and one for the fixed-bed lasting 36 months. Each of these subtasks will consists of three components: 1) Simulation of demonstration cases on BYU computers; 2) Implementation on a work station at AFR; and 3) Simulation of demonstration cases on the workstation.

IV.A. SUBTASK 4.A. - APPLICATION OF GENERALIZED, PULVERIZED-COAL COMPREHENSIVE CODE

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Objectives

The objectives of this subtask are 1) to simulate reactors of interest to METC and 2) to implement the comprehensive entrained-bed code at METC.

Accomplishments

This subtask has not been initiated.

Plans

No work is planned on this subtask during the next quarter.

IV.B. SUBTASK 4.B. - APPLICATION OF FIXED-BED CODE

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Objective

The objective of this subtask is to apply the advanced fixed-bed code developed in Subtask 3.b. to simulate fixed-bed gasifiers of interest to METC.

Accomplishments

During the last quarter, work continued on collecting fixed-bed design and test data from organizations and individuals involved in fixed- or moving-bed gasification or combustion research or in research on non-reacting fixed- or moving-beds. Work also continued on collecting fixed-bed experimental data from the open literature.

Fixed-bed code application

The advanced fixed-bed code, developed, tested and validated under Subtask III.B, was applied to seven new test cases under this subtask. The test cases included 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 the 1-D fixed-bed code development.

Lurgi Dry Ash Gasifier - Predicted temperature, pressure drop, gas concentration, carbon consumption, burnout, and particle diameter for gasification of Illinois #5, Pittsburgh #8, and Rosebud coals in a high-pressure, oxygen-fired Lurgi gasifier at Westfield, Scotland are shown in Figures IV.B-1 through 3. Complete input files for these cases are presented in Hobbs (1990).

The sensitivity analysis was presented previously for a low-pressure, air-fired Wellman-Galusha gasifier. The most obvious differences between the

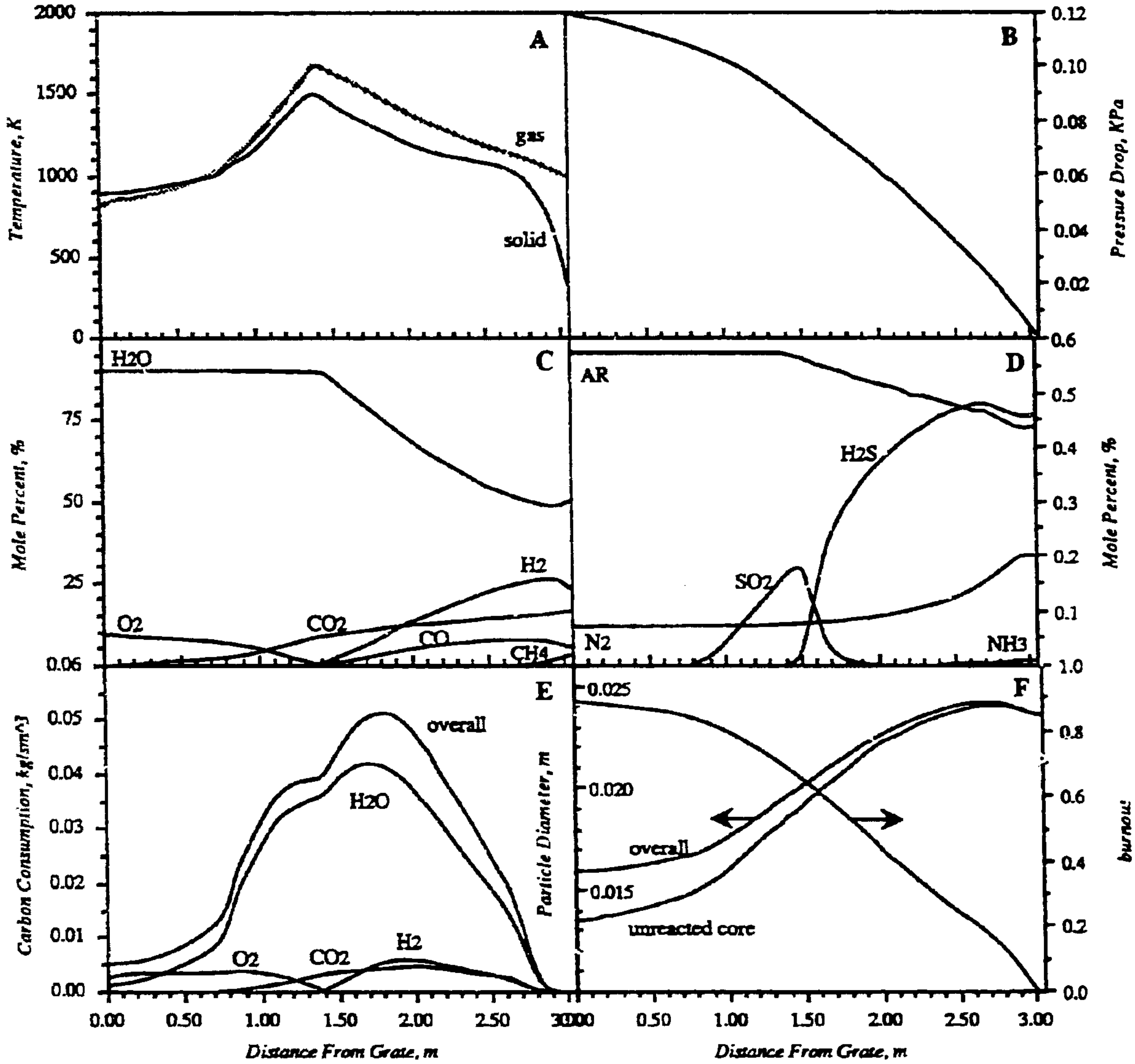

Figure IV.B-1 Predicted temperature, pressure drop, gas concentration, carbon consumption due to oxidation and gasification, burnout, and particle diameter for gasification of Illinois #5 bituminous coal in high pressure gasifier with oxygen (Elgin and Perks, 1974): **A)** solid and gas temperature profile, **B)** pressure drop, **C)** major species concentration profile, **D)** minor gas species concentration profile, **E)** volumetric solid carbon consumption rate due to oxidation and gasification reactions, and **F)** burnout, overall and unreacted particle diameter throughout reactor. Input conditions can be found in Hobbs (1990).

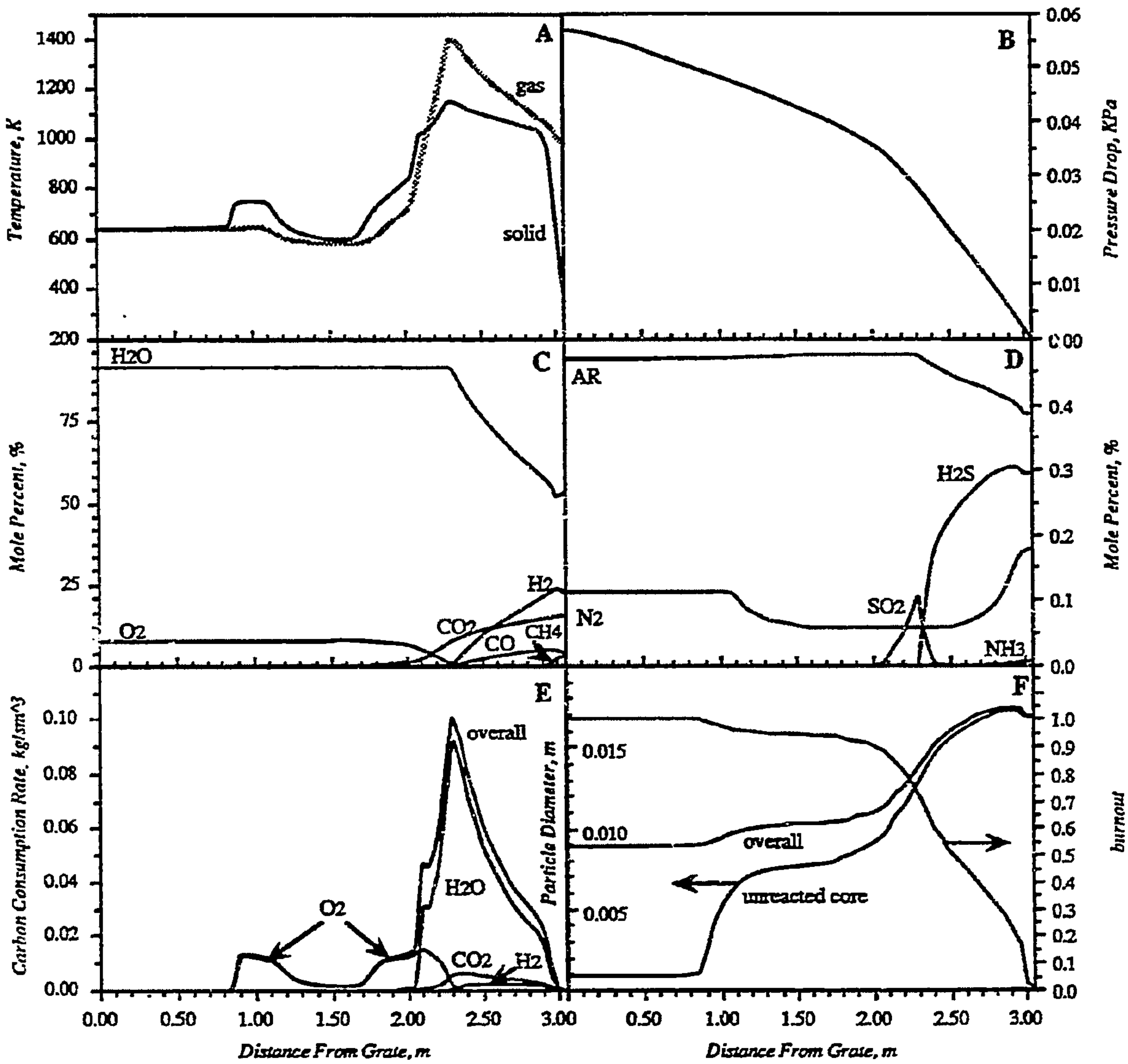

Figure IV.B-2 Predicted temperature, pressure drop, gas concentration, carbon consumption due to oxidation and gasification, burnout, and particle diameter for gasification of Pittsburgh #8 bituminous coal in high pressure gasifier with oxygen (Elgin and Perks, 1974): **A)** solid and gas temperature profile, **B)** pressure drop, **C)** major species concentration profile, **D)** minor gas species concentration profile, **E)** volumetric solid carbon consumption rate due to oxidation and gasification reactions, and **F)** burnout and overall and unreacted particle diameter throughout reactor. Input conditions can be found in Hobbs (1990).

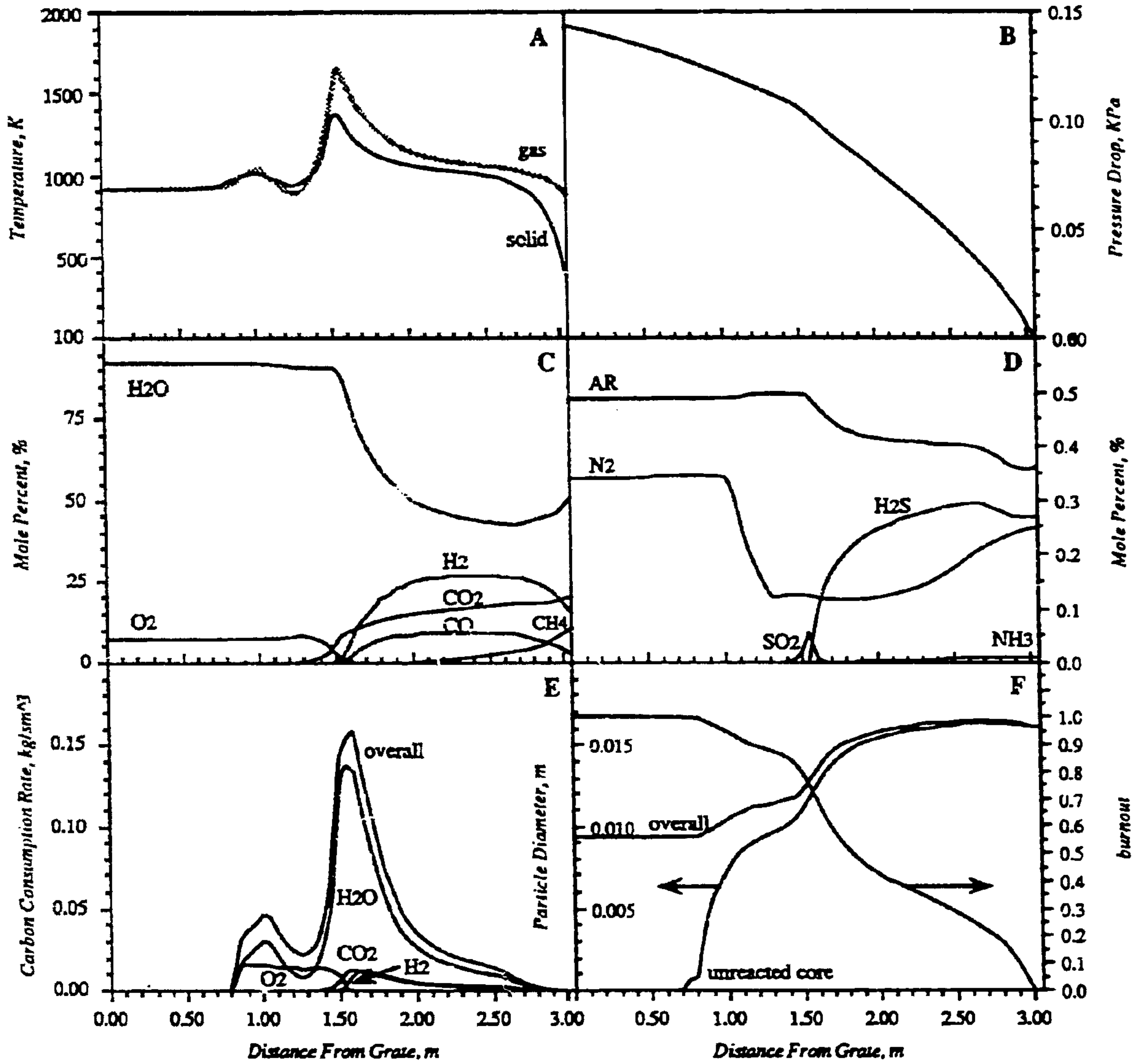

Figure IV.B-3 Predicted temperature, pressure drop, gas concentration, carbon consumption due to oxidation and gasification, burnout, and particle diameter for gasification of Rosebud subbituminous coal in a high pressure gasifier with oxygen (Elgin and Perks, 1974): A) solid and gas temperature profile, B) pressure drop, C) major species concentration profile, D) minor gas species concentration profile, E) volumetric solid carbon consumption rate due to oxidation and gasification reactions, and F) burnout, overall and unreacted particle diameter throughout reactor. Input conditions can be found in Hobbs (1990).

Wellman-Galusha cases and the Westfield cases are the absence of the carbon dioxide peak during high pressure gasification and the appearance of dual temperature peaks in the Pittsburgh and Rosebud Westfield simulations as shown in Figure IV.B-2 and IV.B-3. The dual peaks may be attributed to high pressure operation as discussed in detail in Section III.B.

The simulations of Illinois #5 bituminous, Pittsburgh #8 bituminous, and Rosebud subbituminous coals in the Lurgi gasifier are shown in Figures IV.B-1 through IV.B-3, respectively. No experimental temperature or pressure profiles were reported for these cases. The predicted profiles seem reasonable and similar to the Illinois #6 bituminous case, which has been discussed in Section III.B.

<u>Wellman-Galusha Dry Ash Gasifier</u> - Predicted temperature, pressure drop, gas concentration, carbon consumption, burnout, and particle diameter for gasification of Illinois #6 bituminous and Rosebud subbituminous (weathered) coals in an atmospheric, air-fired Wellman-Galusha gasifier (Thimsen et al., 1984) are shown in Figures IV.B-4 and IV.B-5. Complete input files for these cases can also be found in (Hobbs, 1990).

Experimental data from runs that gasified poorly were difficult to simulate. Poor gasification refers to significant distribution problems such as channeling or clinker formation which leads to questionable reported operational conditions. The one-dimensional code is very sensitive to input conditions as discussed in the sensitivity analysis. For example, if the selected values for the bed void fraction were significantly in error, the devolatilization zone could potentially exist throughout the entire reactor with no gasification or oxidation taking place. The Illinois #6 bituminous case was easy to simulate while the weathered Rosebud subbituminous case was difficult. The low-rank coal cases required more adjustment of parameters such as the bed void fraction, the solid-to-gas heat transfer coefficient, and the effective diffusivity, to match experimental data.

The simulation of Illinois #6 bituminous coal in the Wellman-Galusha gasifier is shown in Figure IV.B-4. No experimental temperature profiles or pressure profiles were reported for this case. The predicted profiles seem reasonable and similar to the Jetson bituminous coal case, which has experimental data and has been discussed in Chapter III.B.

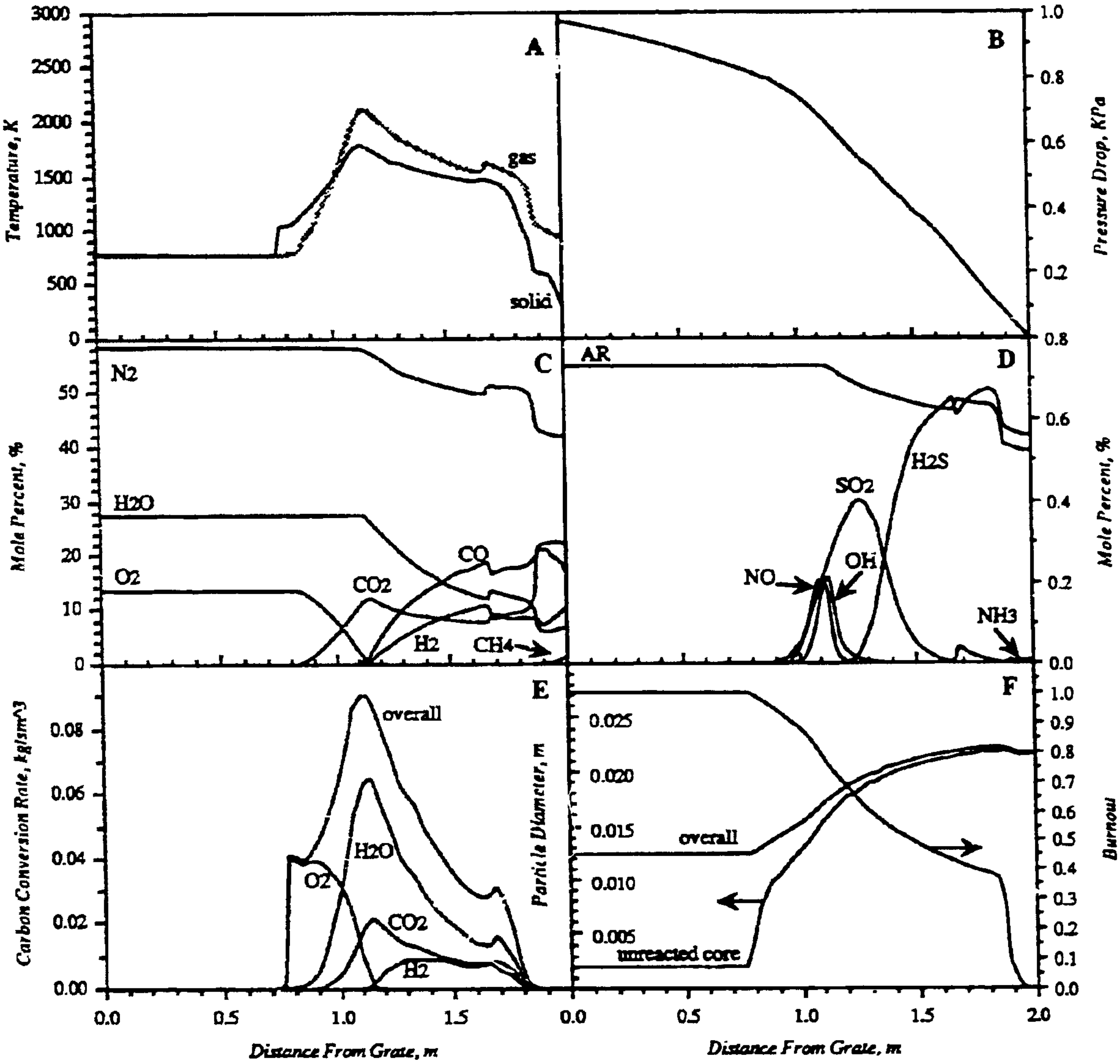

Figure IV.B-4 Predicted temperature, pressure drop, gas concentration, carbon consumption due to oxidation and gasification, burnout, and particle diameter for gasification of Illinois #6 bituminous coal in an atmospheric gasifier with air (Thimson et al., 1984; Vol 8, page 68): **A)** predicted gas and solid temperature profile, **B)** predicted pressure drop, **C)** predicted major species concentration profile, **D)** predicted minor gas species concentration profile, **E)** predicted volumetric solid carbon consumption rate due to oxidation and gasification reactions **F)** predicted burnout, overall and unreacted particle diameter throughout reactor. Input conditions can be found in Hobbs (1990).

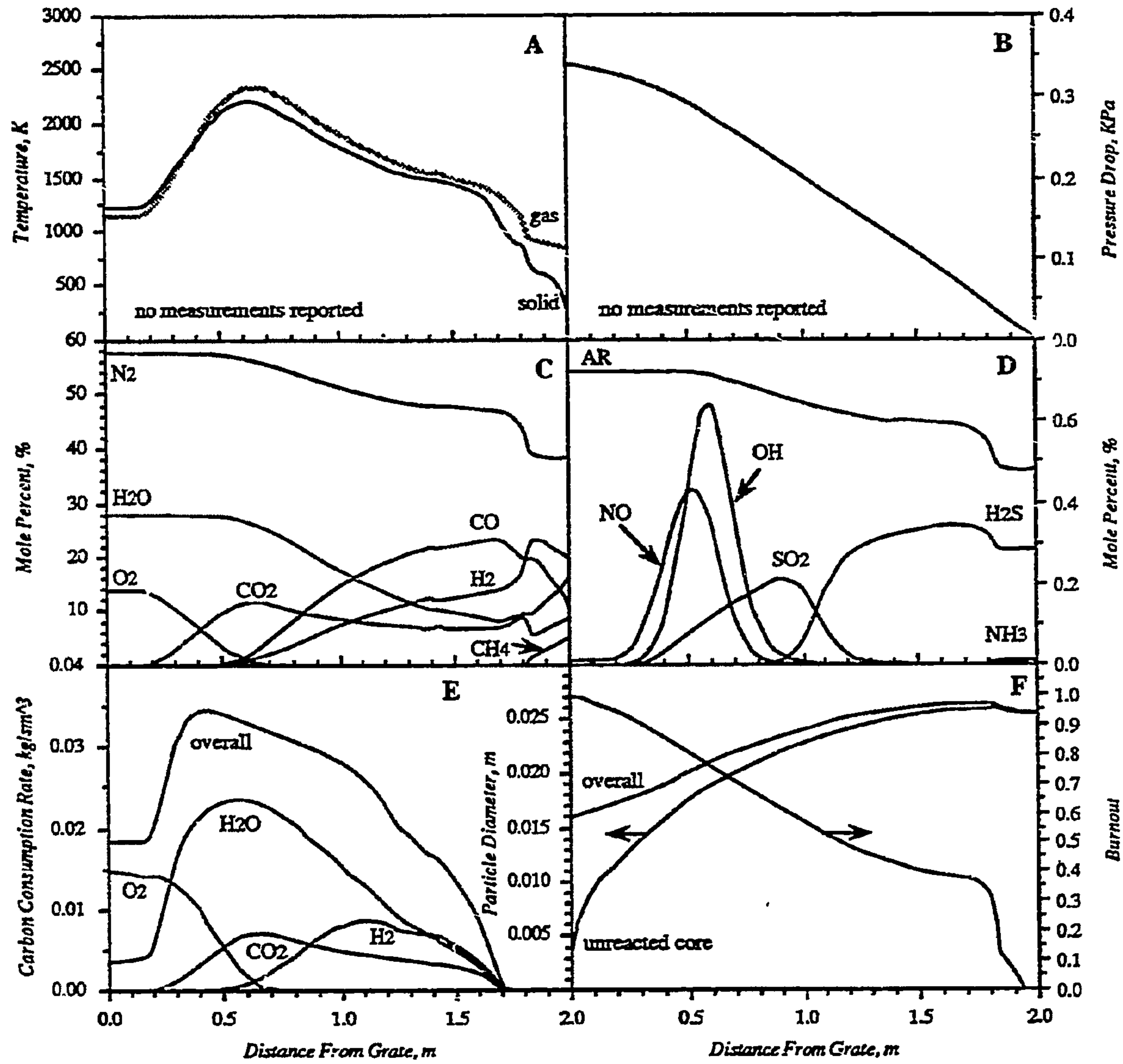

Figure IV.B-5 Predicted temperature, pressure drop, gas concentration, carbon consumption due to oxidation and gasification, burnout, and particle diameter for gasification of Rosebud subbituminous coal in an atmospheric gasifier with air (Thimson et al., 1985: Vol 3, page 63): A) predicted gas and solid temperature profile, B) predicted pressure drop, C) predicted major species concentration profile, D) predicted minor gas species concentration profile, E) predicted volumetric solid carbon consumption rate due to oxidation and gasification reactions F) predicted burnout, overall and unreacted particle diameter throughout reactor. Input conditions can be found in Hobbs (1990).

The simulation of the weathered Roseoud subbituminous coal in the Wellman-Galusha gasifier is shown in Figure IV.B-5. This simulation was similar to the fresh Rosebud case, which has experimental data (Hobbs, 1990).

METC Gasifier - A comparison of solid and gas temperature profiles and selected gas species profiles for gasification of Arkwright bituminous coal in the air-fired, METC gasifier operated at 6.4 atmospheres (absolute) is shown in Figure IV.B-6. The input conditions for this case were found in Desai and Wen (1978). The solid and gas temperature profiles predicted by Desai and Wen are indistinguishable. Desai and Wen believed that the prediction was the average of the gas and solid temperature. However, the sample calculation in the Appendix of Desai and Wen (1978) indicates that the solid and gas temperatures were indeed equal. It is assumed that Desai and Wen did not account for the difference between the nonreacting solid-to-gas heat transfer coefficients and the reacting solid-to-gas heat transfer coefficients. In other words, they assumed that ζ was equal to 1, which would give equal solid and gas temperatures as indicated by the sensitivity analysis on ζ. The concentration profiles show the instantaneous devolatilization assumption made by Desai and Wen. Also the lack of a peak in the CO_2 profile indicates simplified assumptions regarding the gas-phase chemistry.

BGC-Lurgi Slagging Gasifier - Predicted temperature, pressure drop, gas concentration, carbon consumption, burnout, and particle diameter for gasification of Pittsburgh #8 bituminous coal in a high-pressure, slagging gasifier with oxygen (Scott, 1981) are shown in Figure IV.B-7. The coal flow rate is 2-3 times larger than for dry-ash gasifiers. The temperature is higher to promote slagging of the ash. The predicted temperature of the ash zone is low. A possible explanation could be inadequacy of the plug flow assumption for the ash flow rate. The BGC-Lurgi slagging case is presented to show the possibility of simulating the slagging gasifier.

Plans

During the next quarter, work will continue on collecting fixed-bed design and test data. The fixed-bed design and test data will be collected both from the open literature and from organizations and individuals involved in fixed- or moving-bed gasification or combustion research or in research on non-reacting fixed- or moving-beds. Efforts will continue to identify additional test cases for simulation. The code will be applied to these additional test cases.

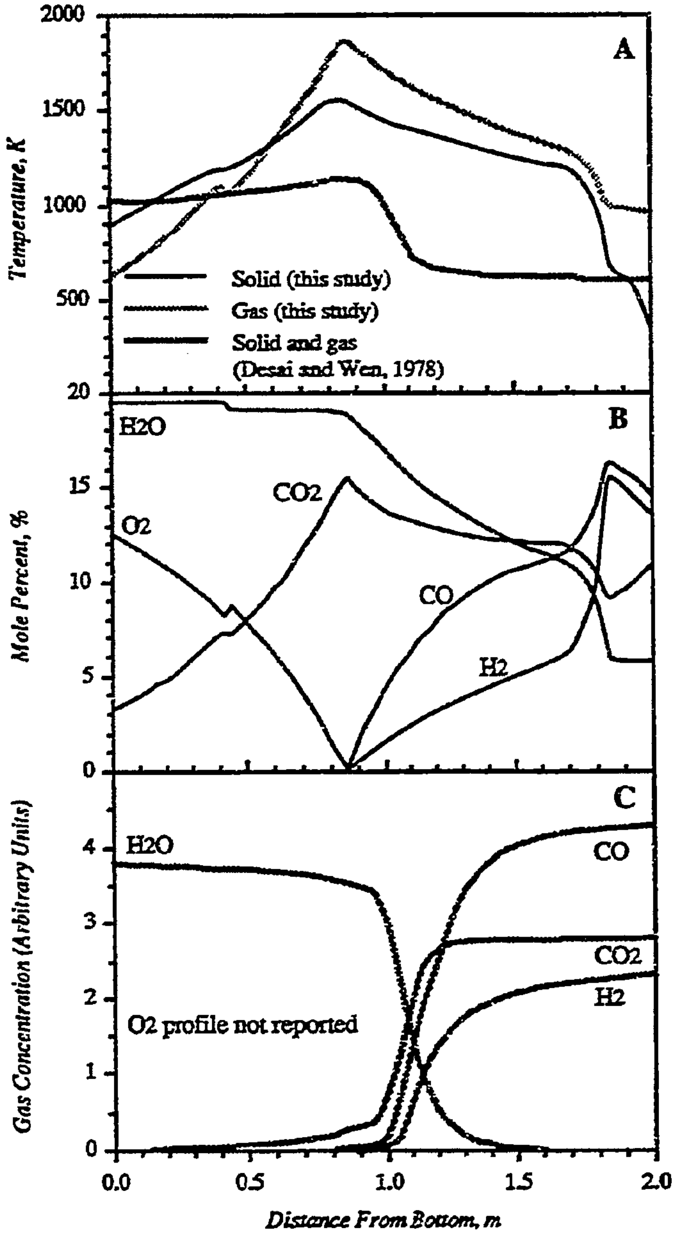

Figure IV.B-6 Comparison of A) solid and gas temperature profiles, and B) selected gas species profiles for gasification from this study and C) Desai and Wen (1978) of Arkwright bituminous coal in the air-fired METC gasifier operated at 6.4 atmospheres (absolute). Input conditions and model predictions from Desai and Wen (1978). Input file for MBED-1D can be found in Hobbs (1990). Coal, air, and steam mass flow rate are 0.138, 0.518, and 0.0631 kg/s, respectively.

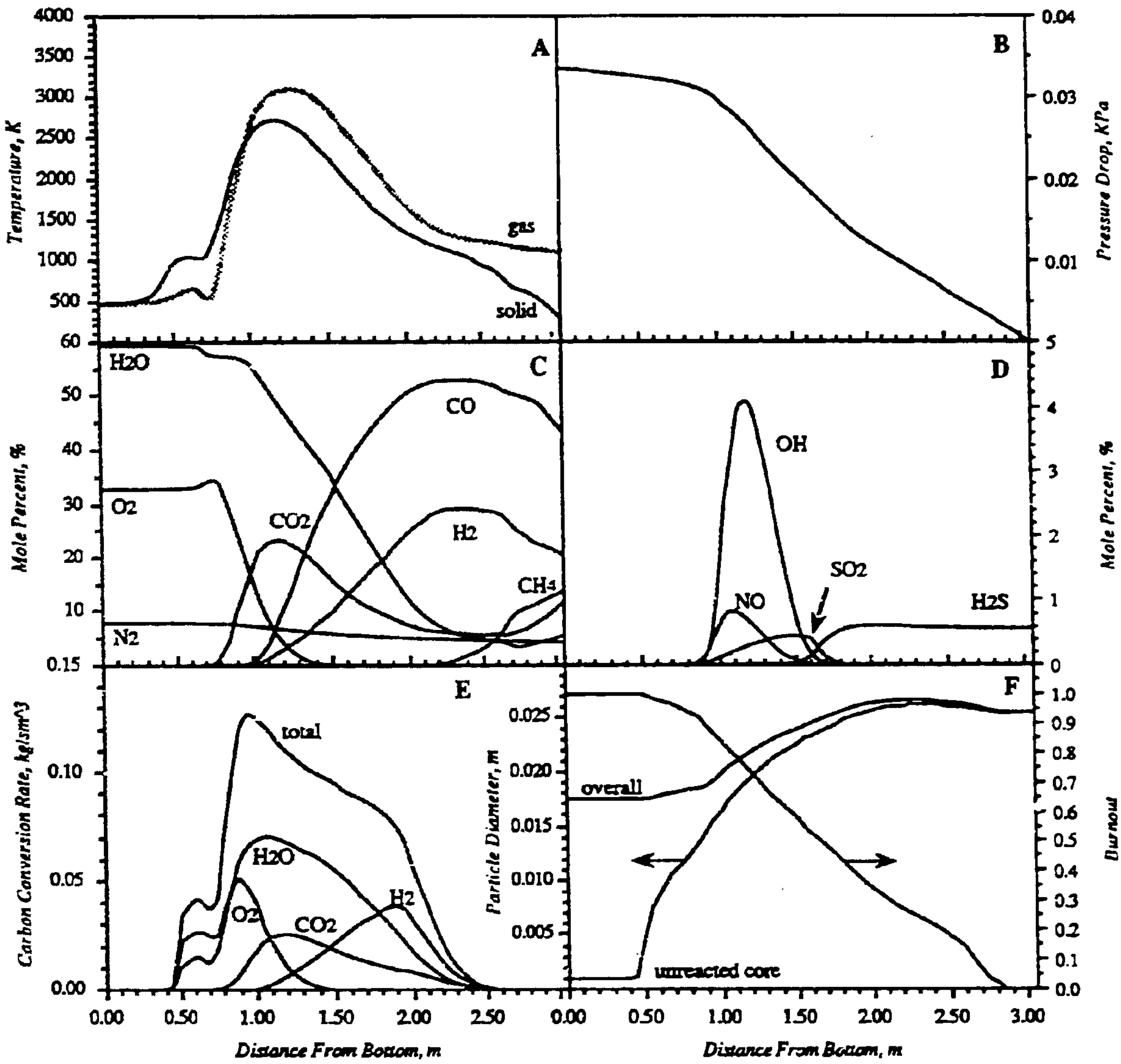

Figure IV.B-7 Predicted temperature, pressure drop, gas concentration, carbon consumption due to oxidation and gasification, burnout, particle diameter for gasification of Pittsburgh #8 bituminous coal in a high-pressure slagging gasifier with oxygen (Scott, 1981; page E-50): A) predicted solid and gas temperature profile, B) predicted pressure drop, C) predicted major species concentration profile, D) predicted minor gas specie concentration profile, E) predicted volumetric solid carbon consumption rate due to oxidation and gasification reactions, and F) predicted burnout, overall and unreacted particle diameter throughout the reactor. Reactor geometry is the same as the Westfield Lurgi cases. Coal, oxidizer and steam mass flow rates are 2.793, 1.6329, and 0.9464 kg/s, respectively. Complete input file can be found in Hobbs (1990).

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