SECTION III. TASK 3. COMPREHENSIVE MODEL DEVELOPMENT AND EVALUATION

Objectives

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).

Task Outline

This task is being performed in three subtasks. The first covers the full 60 months of the program and is devoted to the development of the entrained-bed code. The second subtask is for fixed-bed reactors and is divided into two parts. The first part (12 months) was devoted to reviewing the state-of-the-art in fixed-bed reactors. This led to the development of the research plan for fixed-bed reactors, which was approved. The code development is being done in the remaining 45 months of the program. The third subtask is to generalize the entrained-bed code to fuels other than dry pulverized coal and will 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

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Objectives

The objectives of this subtask are 1) to integrate the FG-DVC submodel into PCGC-2, 2) incorporate additional submodels and improvements developed under Task 2, 3) evaluate the improved code, 4) improve user-friendliness and robustness, and 5) document the code.

Accomplishments

Work continued on code evaluation and user-friendliness. Minimum specifications for a foundational, entrained-bed code that will satisfy the terms of the contract were identified. Other desirable features that could be considered were also identified. A post-processor was developed to convert PCGC-2 plotting files to spreadsheet-compatible format.

Code Evaluation

Data from four reactors have been identified for code evaluation: the AFR transparent wall reactor (TWR), the BYU/ACERC controlled-profile reactor (CPR), the 2-D furnace at Imperial College, and the near-burner test data from the 80 MWe Goudey Station at Johnson City, New York, operated by New York State Electricity and Gas (NYSEG). Simulations of the TWR flames were described in the 4th Annual Report (Brewster et al., 1990). No further work was conducted on the TWR simulations during the past quarter. Simulations were performed during the past quarter for a natural gas flame in the CPR and for the near-burner field of the NYSEG Goudey plant. The Goudey simulations were performed under independent funding. Also, 2-D data with coal combustion were requested from Imperial College for code evaluation.

Controlled-Profile Reactor (CPR) - A diagram of the CPR reactor is shown in Figure III.A-1. The reactor is referred to as "controlled-profile" because of its computer-controlled wall temperature profile. Using the reactor's access windows, gas temperature, composition, and three velocity components were measured with independent funding in a swirling natural gas flame. (Eatough, 1990). Gas temperature, measured with a suction pyrometer, is compared with code predictions in Figure III.A-2. The effect of soot on radiation was investigated theoretically by injecting carbon particles of 1 μm diameter with the primary gas. A loading of 0.1 lb solids/lb gas was assumed. The effect of radiation model type (Varma six-flux or discrete ordinates) was also investigated (Smoot et al., 1988).

The effect of radiation model type was insignificant, except at large axial distances. Both models underpredicted the gas temperature at the outlet, with the underprediction by the flux model being more significant. The underprediction seems unreasonable, since the temperature boundary conditions were higher (1300 K) than the predicted outlet temperature (1150 K for the flux model and 1275 K for the discrete ordinates method). Only the "no soot" simulations underpredicted the temperature. The predicted outlet temperature with soot was 1375 K. The problem is being investigated but has not been resolved.

Particle trajectories for the soot case are shown in Fig. III.A-3. The 1-μm particles were injected at 10 starting locations in the primary duct. The presence of soot particles causes smoother radial temperature profiles. The gas is hotter than otherwise predicted near the centerline and near the wall. The shape of the predicted profile agrees much better with the shape of the measured data at axial locations of 0.26, 0.31, 0.36, 0.46, 0.66, and 0.76 m. The effect of the soot particles, which were considered inert, is thought to occur primarily through radiation. Particles in cold areas of the reactor receive radiation and act as heat sources to the gas. Particles in hot areas radiate heat away and act as heat sinks. These effects can be seen in the comparisons in Fig. III.A-2. In general, however, the temperature is predicted too high, and this investigation is continuing.

Near-Burner Goudey Data - The near-burner region of the Goudey NYSEG plant is being simulated with PCGC-2 under independent funding to see whether 2-D code predictions can be applied to this zone. The plant is located in Johnson City, New York. A schematic of the furnace is shown in Fig. III.A-4a. Near-burner measurements were taken at Level 2, following the probe paths

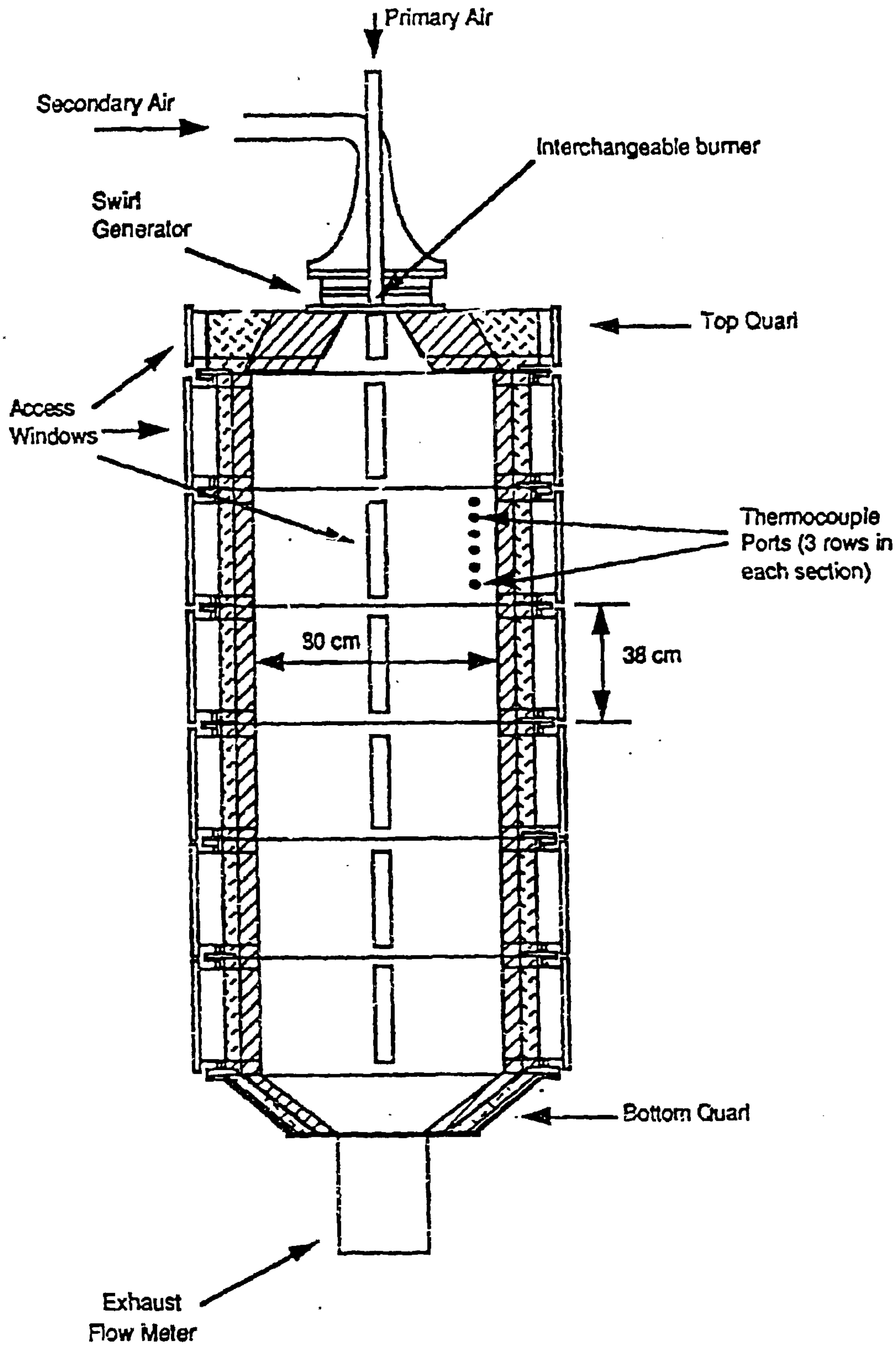

Figure III. A-1. Cross-section diagram of BYU-ACERC controlled profile reactor.

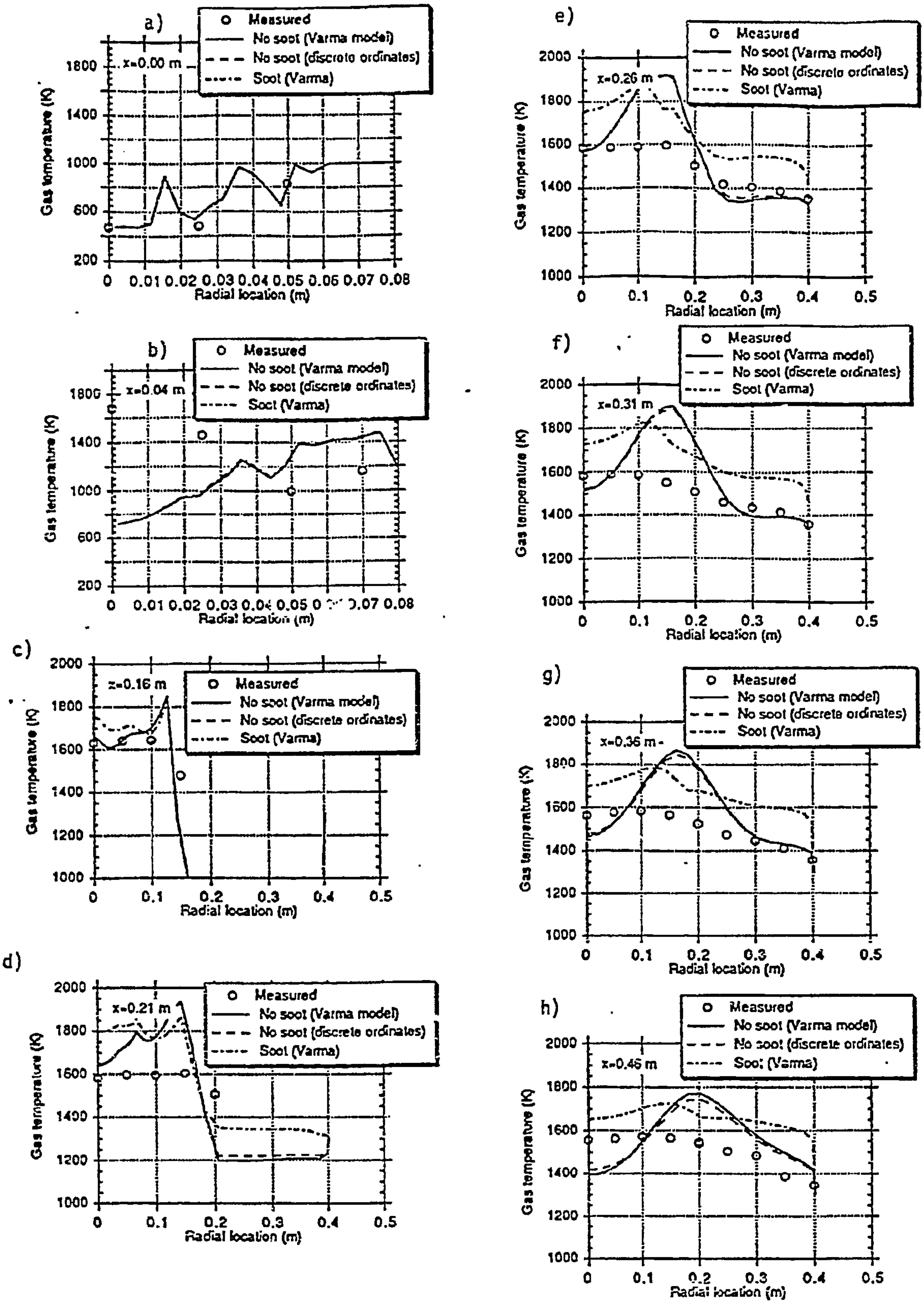

Figure III. A-2. Predicted gas temperature compared with experimental data (Eatough, 1990) for a natural gas flame in the CPR (continued on following page).

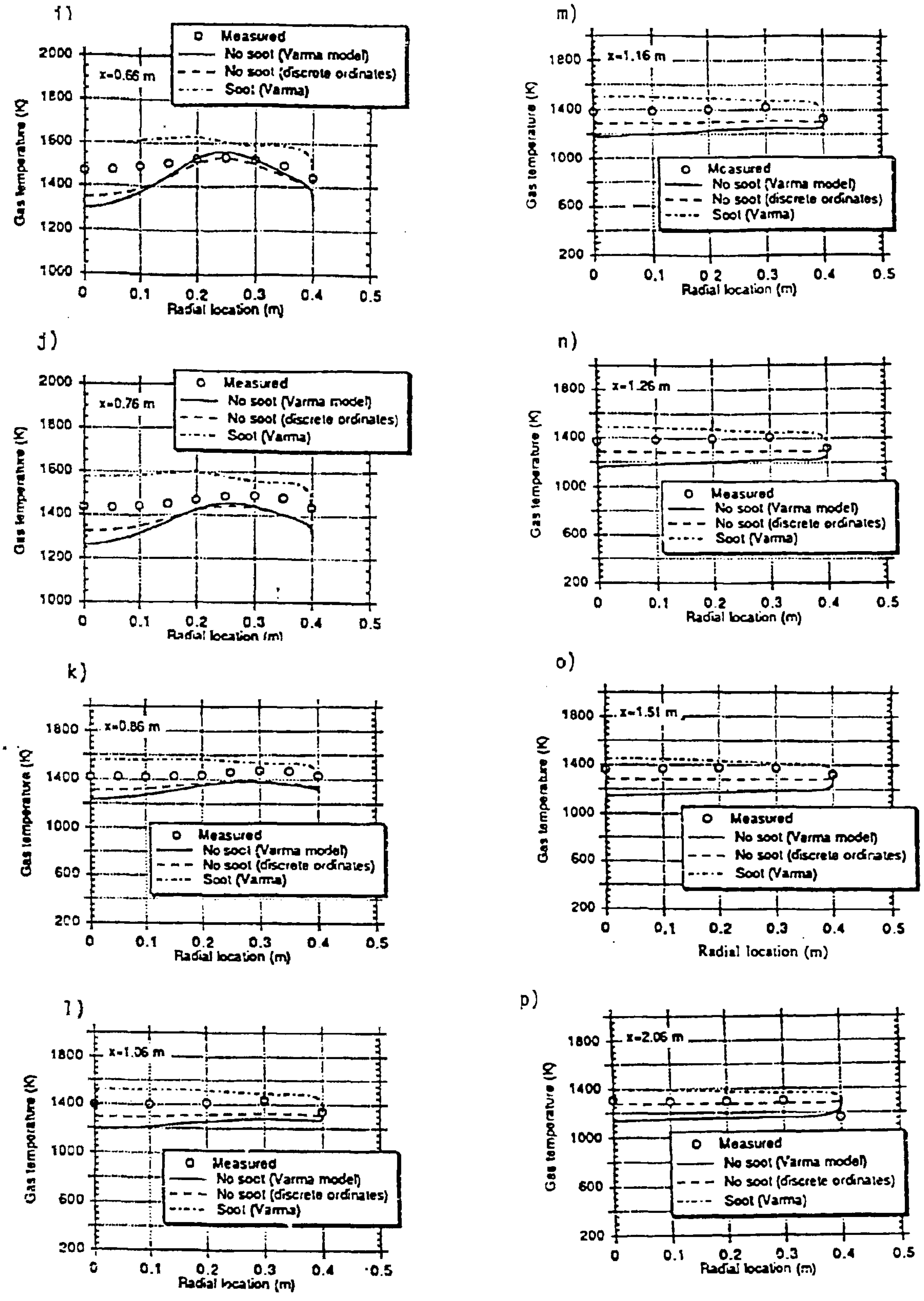

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Figure III. A-2. Predicted gas temperature compared with experimental data (Eatough, 1990) for a natural gas flame in the CPR.

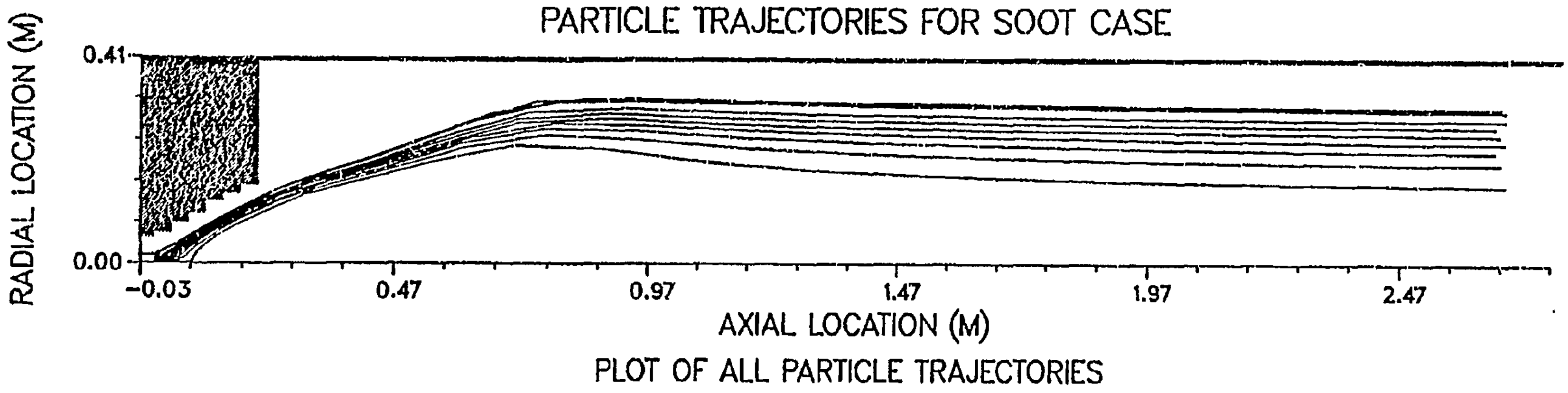


Figure III. A-3 Predicted soot particle trajectories for simulation of natural gas flame in the CPR.

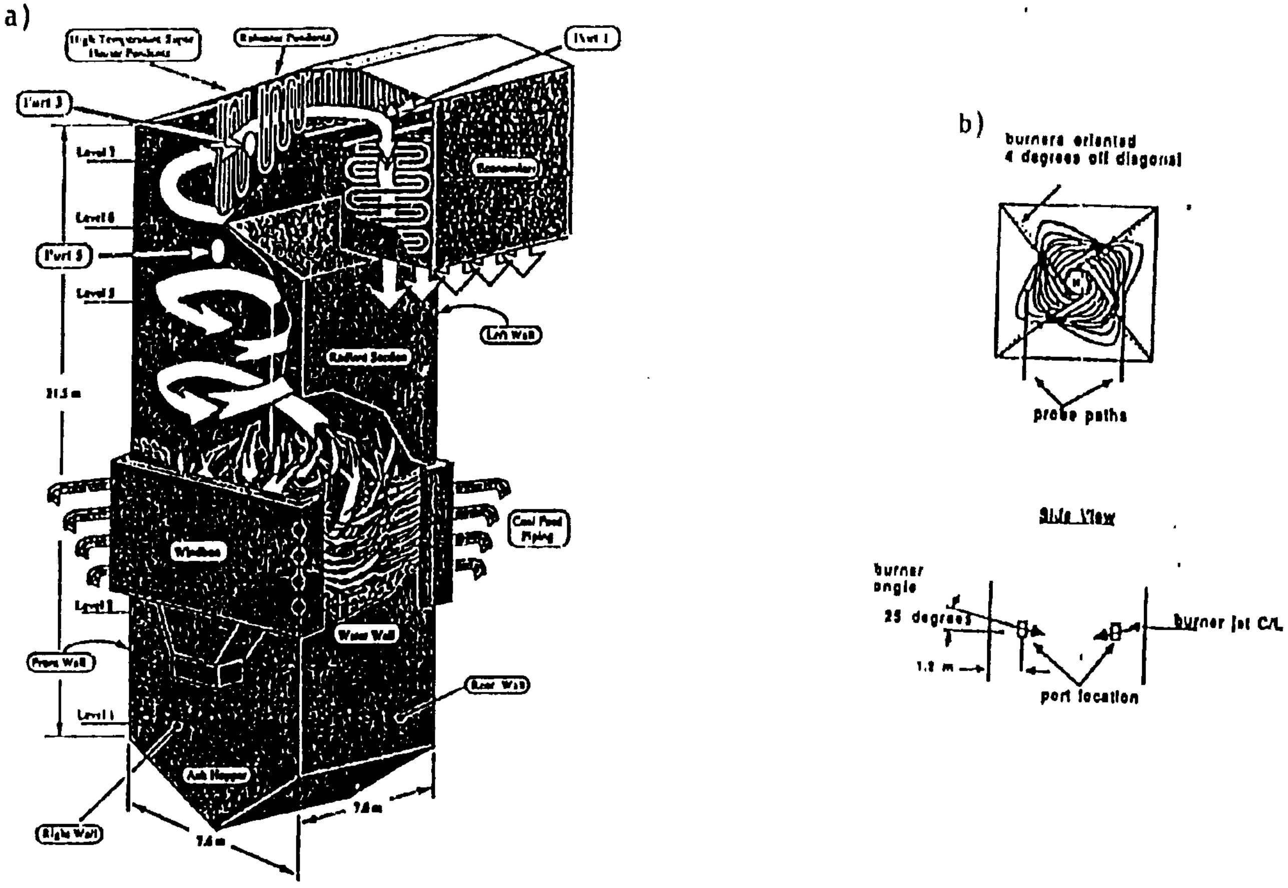


Figure 6D-3. Schematic of Goudey Station Configuration

Figure III. A-4. Schematic of the Goudey NYSEG combustor (taken from Cannon et al., 1990).

shown in Fig. III.A-4b. The data were compared with predictions of the 2-D, axisymmetric code, assuming the axis of symmetry coincides with the centerline of the burner jet. As shown in the figure, the furnace is corner-fired, and the centerline is offset from the 45-degree diagonal by 4 degrees and tilted downward. The equations for coordinate transformation from the Goudey reactor coordinates to the axisymmetric coordinate system with axis corresponding to the burner centerline and origin corresponding the burner inlet are given in the appendix.

A plot of the predicted particle trajectories and assumed geometry for the simulation is shown in Fig. III.A-5. The angle between the reactor wall and burner centerline was assumed to be 45 degrees (i.e. the 4-degree offset was neglected). After a distance equal to half the width of the reactor, the wall was assumed to converge back toward the reactor centerline, in order to prevent recirculation at the exit plane and achieve convergence over a relatively short axial length. Otherwise, the reactor length would have needed to be increased by a factor of 3 or more in order to provide enough distance so as to not have any recirculation at the reactor exit plane. The code cannot converge if there is recirculation at the reactor exit plane. Since it is only the near-burner region of the calculation that is of interest, the modified geometry to achieve convergence for a shorter total axial distance of simulation has no adverse effect. In fact, it allows for more detailed simulation of the near-burner region with the same number of total grid points.

A contour plot of predicted temperature is shown in Fig. III.A-6. The probe path with measurement locations is also shown. Temperature was measured at most, but not all, of the indicated locations. Due to the uncertainty in the burner tilt angle, two values were tried. A plot of predicted and measured temperature along the probe path is shown in Fig. III.A-7. The initial trough in predicted temperature near the wall does not agree with the measurements. The results shown in the figure are very preliminary, and the investigation is continuing. It is not clear at this time whether the 2-D code can be successfully applied to the near-burner field in this 3-D reactor.

Imperial College Data - Costa et al. (1990) recently presented new coal combustion data for gas phase species concentration, temperature, and char burnout for two swirl numbers, obtained in an axisymmetric reactor. The data contain near-field measurements that have brought to light a deficiency in the Imperial College 2-D model (Lockwood et al., 1980, 1984; Lockwood and Salooja,

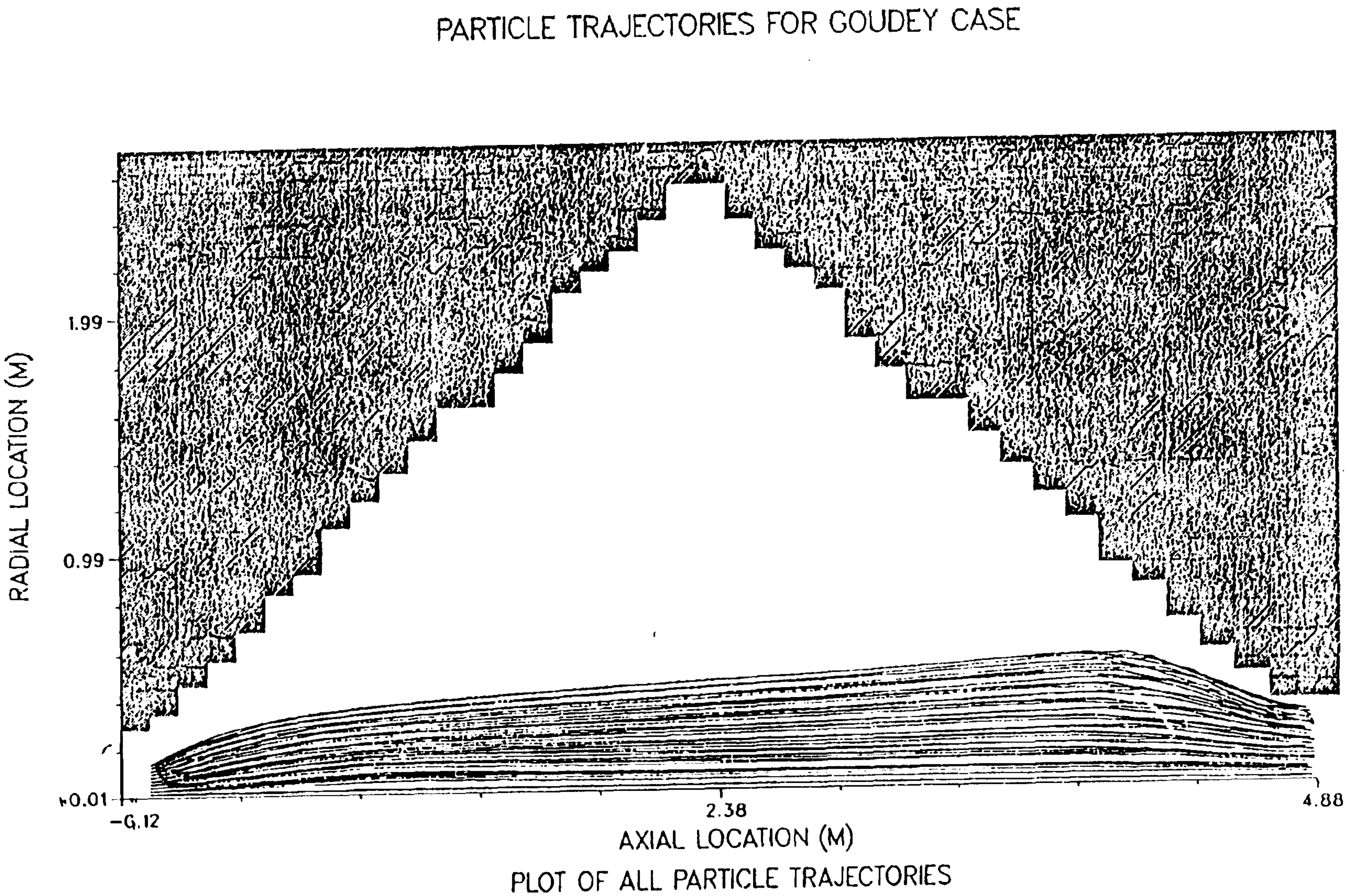


Figure III.A-5. Predicted particle trajectories for Goudey simulation.

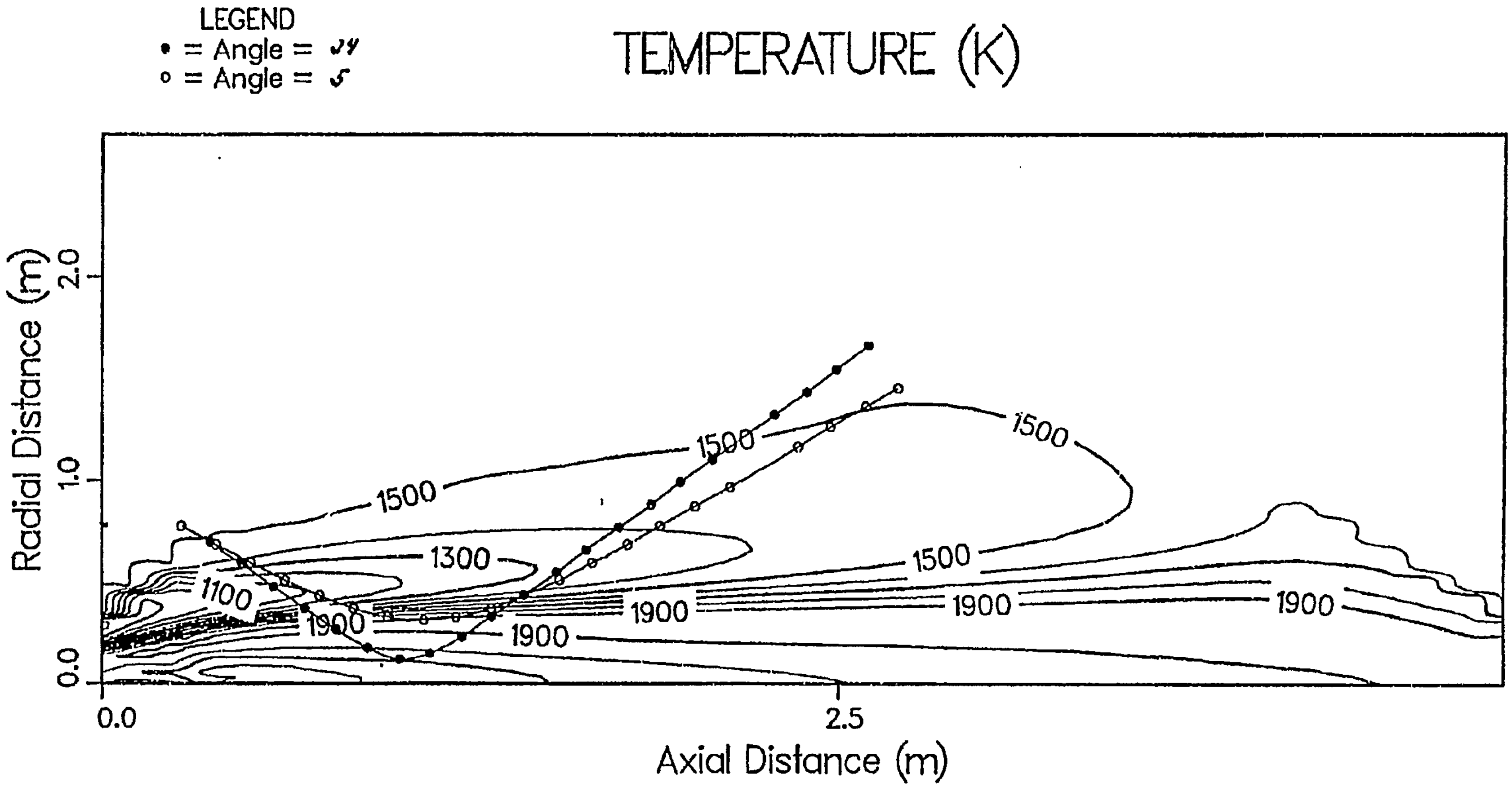


Figure III.A-6. Predicted particle temperature and probe path for two burner tilt angles for Goudey simulation.

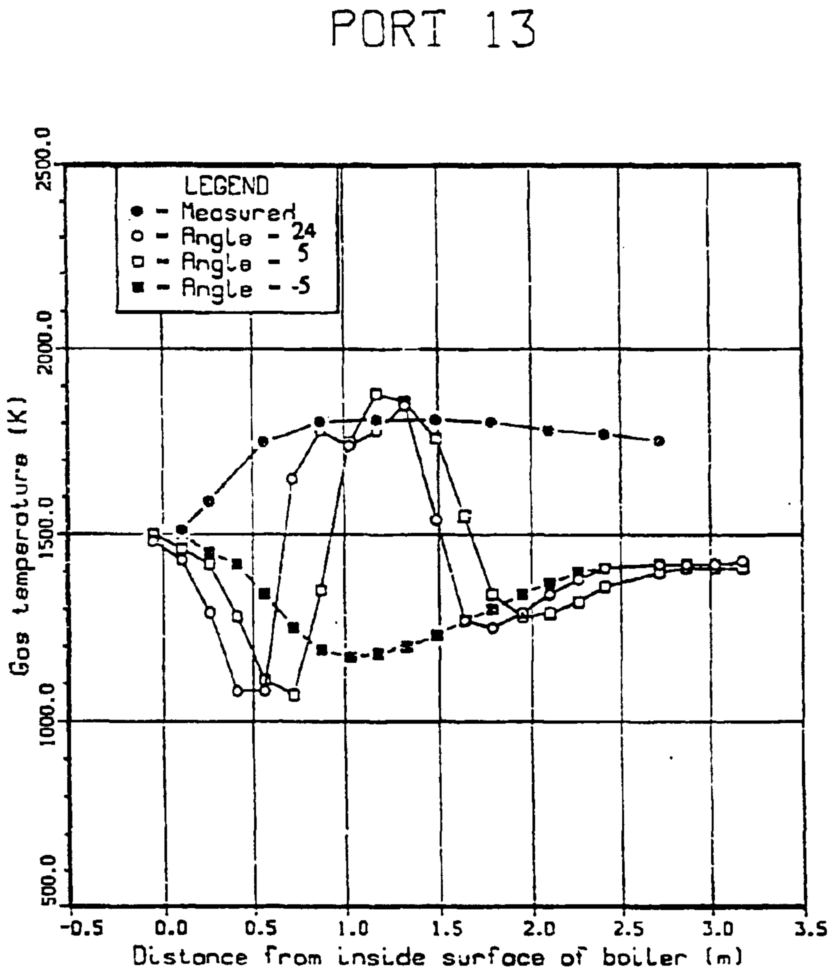


Figure III. A-7. Predicted and measured gas temperature along probe path in Goudey reactor.

1983; Lockwood and Mahmud, 1988), in that the ignition distance is significantly underpredicted. The quality of the data appears to be quite good, e.g. the radial oxygen concentration profiles are quite symmetric around the centerline. Since one of the potential benefits of detailed coal chemistry submodeling is more accurate prediction of particle ignition, these data are significant interest to this study. A copy of the data on computer-readable media has been requested from the Imperial College investigators.

User-Friendliness

Improving code user-friendliness is an on-going activity. During the past quarter, the graphical user interface (GUI) for editing input files was extended to particle combustion cases, and diagnostic messages were added to assist the user in detecting errors in code input. The GUI currently runs under the OPEN LOOK™ windowing system developed by Sun Microsystems. Although it has only been tested on Sun workstations, it should work on any machine with OPEN LOOK. The particle data window is shown in Figure III.A-8. The top part of the window contains logical variables which toggle between their true and false states by clicking the mouse on the arrow. A brief text string by the side of the arrow explains the meaning of the current setting. Below the logical variables are numeric fields for specifying the number of trajectories, particle sizes, etc. These values are changed by using the mouse to position the cursor in the appropriate numeric field and entering the data from the keyboard. Directly below the numeric field for specifying the maximum number of particle iterations for convergence is a stack button for selecting the option for interpolating gas properties. Again, the user can cycle through the available options by clicking the mouse on the box with the arrow. Below the stack button for the gas properties interpolation index is an array of numeric fields for specifying the particle diameters. A stack button for cycling through available unit options is also provided. At the bottom of the window, numeric fields are provided for specifying particle properties. Stack buttons allow the user to select from several unit options.

Diagnostic messages are continually added to the code when problems with code input are encountered. During the past quarter, a problem was encountered in the Goudey plant simulation when the gas stream flowrates were mistakenly input in kg/hr rather than kg/s. This error resulted in the simulation not converging because of extremely high gas velocities at the inlet, far in excess of the speed of sound. Diagnostic messages were therefore added to warn the user when the inlet velocities, calculated from input flowrate values, exceed a reasonable value. A value greater than 200 m/s is considered unreasonable. Diagnostics were also added to aid the user in selecting the upper temperature limit for the physical properties table. The lower limit is fairly easy to select; it is commonly set equal to the lowest inlet stream temperature entering the reactor. The upper temperature limit is difficult to specify because some regions of the reactor may exchange significant heat through radiation with other regions of the reactor. Therefore, the code was modified to print a message whenever the upper temperature limit specified by the user is inadequate and needs to be modified. The message also suggests what the new value should be.

Foundational Code Specifications

Minimum specifications for a foundational, entrained-bed code that will satisfy the terms of the contract were identified. These specifications are as follows:

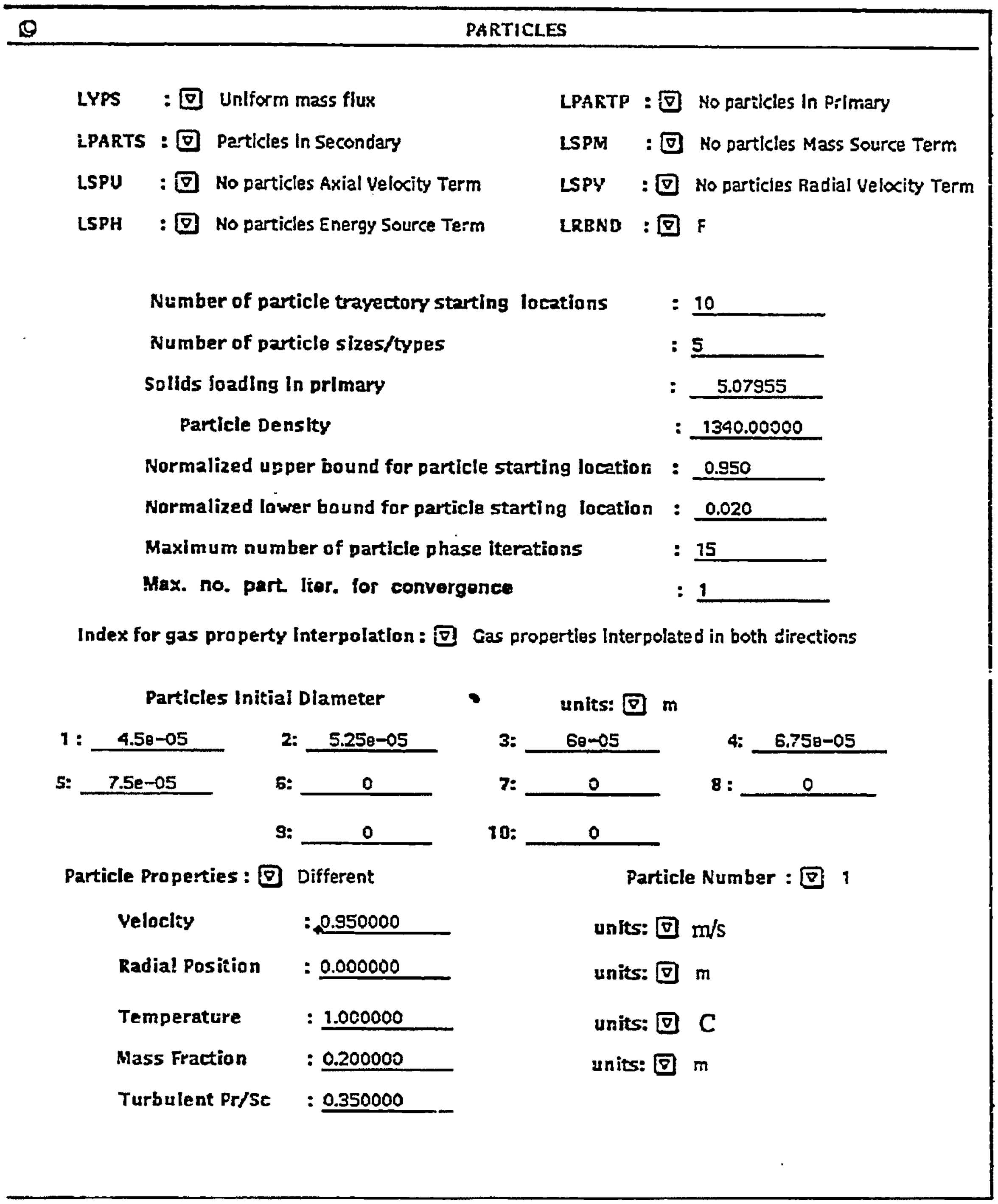
1. The percolation version of FG-DVC with rank-dependent kinetics will be included, if available. Additional submodels from AFR will also be included based on availability.

2. The code will operate with a single solids progress variable. Coal offgas composition and enthalpy will be assumed constant.

3. Code output will be provided in a format suitable for hardcopy printout. In addition, electronic data files suitable for use with independent computer graphics programs (e.g. spreadsheets and/or more advanced, commercial software) for plotting will be provided, and experiences with such graphics programs will be documented. Any software (i.e. driver programs) developed under this program in connection with the use of such graphics programs will also be provided.

4. Sorbent injection will be allowable with the coal or through an additional, sidewall inlet.

This list of specifications was presented at the Contract Review Meeting held at METC on October 25th, 1990, and documented in a letter to AFR and METC on November 28th. In order to insure adequate time for code integration, it was requested that the final submodel versions be made available by December 31st,



PARTICLES

LYPS : ▽ Uniform mass flux

LPARTS : ▽ Particles In Secondary

LSPU : ▽ No particles Axial Velocity Term

LSPH : ▽ No particles Energy Source Term

LPARTP : ▽ No particles In Primary

LSPM : ▽ No particles Mass Source Term

LSPV : ▽ No particles Radial Velocity Term

LRBND : ▽ F

Number of particle trayectory starting locations : 10

Number of particle sizes/types : 5

Solids loading in primary : 5.07955

Particle Density : 1340.00000

Normalized upper bound for particle starting location : 0.950

Normalized lower bound for particle starting location : 0.020

Maximum number of particle phase iterations : 15

Max. no. part. iter. for convergence : 1

Index for gas property interpolation : ▽ Gas properties interpolated in both directions

Particles Initial Diameter units: ▽ m

1 : 4.5e-05
2: 5.25e-05
3: 6e-05
4: 6.75e-05
5: 7.5e-05
6: 0
7: 0
8 : 0
9: 0
10: 0

Particle Properties : ▽ Different

Particle Number : ▽ 1

Velocity : 0.950000 units: ▽ m/s

Radial Position : 0.000000 units: ▽ m

Temperature : 1.000000 units: ▽ C

Mass Fraction : 0.200000 units: ▽ m

Turbulent Pr/Sc : 0.350000

Figure III.A-8. Particle data window for the OPENLOOK GUI.

1990, in the case of FG-DVC, and by March 31st, 1991, in the case of all other submodels.

In addition to identifying a set of minimum specifications for compliance with the contract, additional features that would further enhance code performance were identified. These additional features will be considered once the delivery of a code with the minimum specifications is insured, based on availability of resources and technology. The additional features include additional submodels (these will be difficult to incorporate if unavailable until after March 31st, 1991), an additional solids progress variable for tracking coal offgas (this would greatly increase the code computational burden and introduce technical uncertainties in the turbulent statistics), and aft injection of coal.

Spreadsheet Plotting

As indicated above, it was proposed at the Contract Review Meeting held at METC during the last quarter on October 25th, that an option be provided for plotting PCGC-2 output using spreadsheet programs. Accordingly, post-processors were developed during the past quarter for converting the PCGC-2 plotting files for gas and particle properties to spreadsheet format. These "spreadsheet" post-processors are menu-driven and similar in look and feel to the driver programs that already exist for DISSPLA plotting.

Plans

During the next quarter, work will continue on code evaluation and user-friendliness. The Goudey reactor simulations will be concluded. A coal flame in the CPR reactor will be simulated. Based on availability of data, simulation of the Imperial College reactor will be initiated. If available, integration of the final FG-DVC submodel code version with rank-dependent kinetics will be initiated.

III. B. SUBTASK 3.B. - COMPREHENSIVE FIXED-BED MODELING REVIEW, DEVELOPMENT, EVALUATION, AND IMPLEMENTATION

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Objectives

The objectives of this subtask are: 1) to develop an advanced fixed-bed model incorporating the advanced submodels being developed under Task 2, particularly the large-particle submodel (Subtask 2.e), and 2) to evaluate the advanced model.

Accomplishments

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 subbituminous, and Utah Blind Canyon bituminous coals. These test cases included temperature profiles at different operating conditions. Discussions with AFR, about the large-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. A progress report on fixed-bed model development was presented at the Peer Review Meeting in Pittsburgh and the Project Review Meeting in Morgantown. An article on fixed-bed model development was prepared and published in ACERC's Burning Issues.

Comparison of Temperature Profiles at Different Conditions

Several of the Wellman-Galusha experimental test cases included temperature profiles at different operating conditions. Predicted temperature profiles were compared with measurements for the Elkhorn bituminous, Jetson bituminous, Leucite Hills subbituminous, and Utah Blind Canyon bituminous coal cases as shown in Figure III.B-1.

Elkhorn Bituminous Coal Case - A shift in the measured temperature profile due to changing reactant feed rates during gasification of Elkhorn bituminous coal was shown in Figure III.B-1A. The predictive trends were in agreement with the direction of the measured temperature shifts in each case. From the sensitivity analysis, an increase in coal flow rate caused the location of the maximum temperature to move closer to the bottom of the reactor. In general, an increase in either the steam flow rate or air flow rate caused the location of the maximum temperature to move closer to the top of the reactor. In this case the coal and the air flow rates were increased, the steam flow rate was decreased, and the location of the maximum temperature moved toward the reactor bottom. Although the increased air flow rate should have caused the location of the maximum temperature to move toward the reactor top, changes in coal and steam flow rates were more significant for the Elkhorn case.

Jetson Bituminous Coal Case - The effect of varying operational parameters on the location of the maximum temperature was shown in Figure III. B-1B for gasification of Jetson bituminous coal. The direction of the temperature shift was predicted adequately by the one-dimensional model. An increase in the coal, air and steam mass flow rates caused the location of the maximum temperature to move toward the top of the reactor. For the Jetson case, the increase in steam and air mass flow rates was more significant than the increase in the coal mass flow rate.

Leucite Hills Subbituminous Coal Case - Although gasification of low-rank coals seems to be more difficult to simulate, predictions from the one-dimensional model were in agreement with the experimental data for the Leucite Hills subbituminous coal as shown in Figure III.B-1C. The increase in coal flow rate and decrease in steam flow rate caused the location of the maximum temperature to shift toward the bottom of the reactor for the Leucite Hills case.

Utah Blind Canyon Bituminous Coal Case - The Utah Blind Canyon case depicted in Figure III. B-10 also showed the effect of increased coal and gas throughputs. Trends in measured and predicted profiles do not agree for this case. The uncertainty in the experimental measurements may explain the discrepancy. The temperature measurements were taken for two time periods. For the first time period, the measurements were repeated on two separate days, but only one set of operational data set was reported for this time period (Thimsen et al., 1984). The spread in experimental data indicates the variability in the experimental data.

User's Manual

Development of a user's manual for the one-dimensional fixed-bed model was initiated. The first draft of the manual was prepared. The manual consists of two parts. The first part includes a model formulation and a solution method while the second part includes user's and implementation guides as well as sample problems. The model formulation and the solution method have been discussed to some extent in previous reports and thus will not be presented here. The table of contents and the user's guide are included in the appendix.

Plans

During the next quarter, work will continue on developing and evaluating the fixed-bed code. Work to integrate the new version of the FG-DVC model in the fixed-bed code will be initiated. After integration, the fixed-bed code will be validated and a sensitivity analysis will be performed. The iteration method will be further modified to improve the convergence and the robustness of the code. Development of the user's manual will continue.

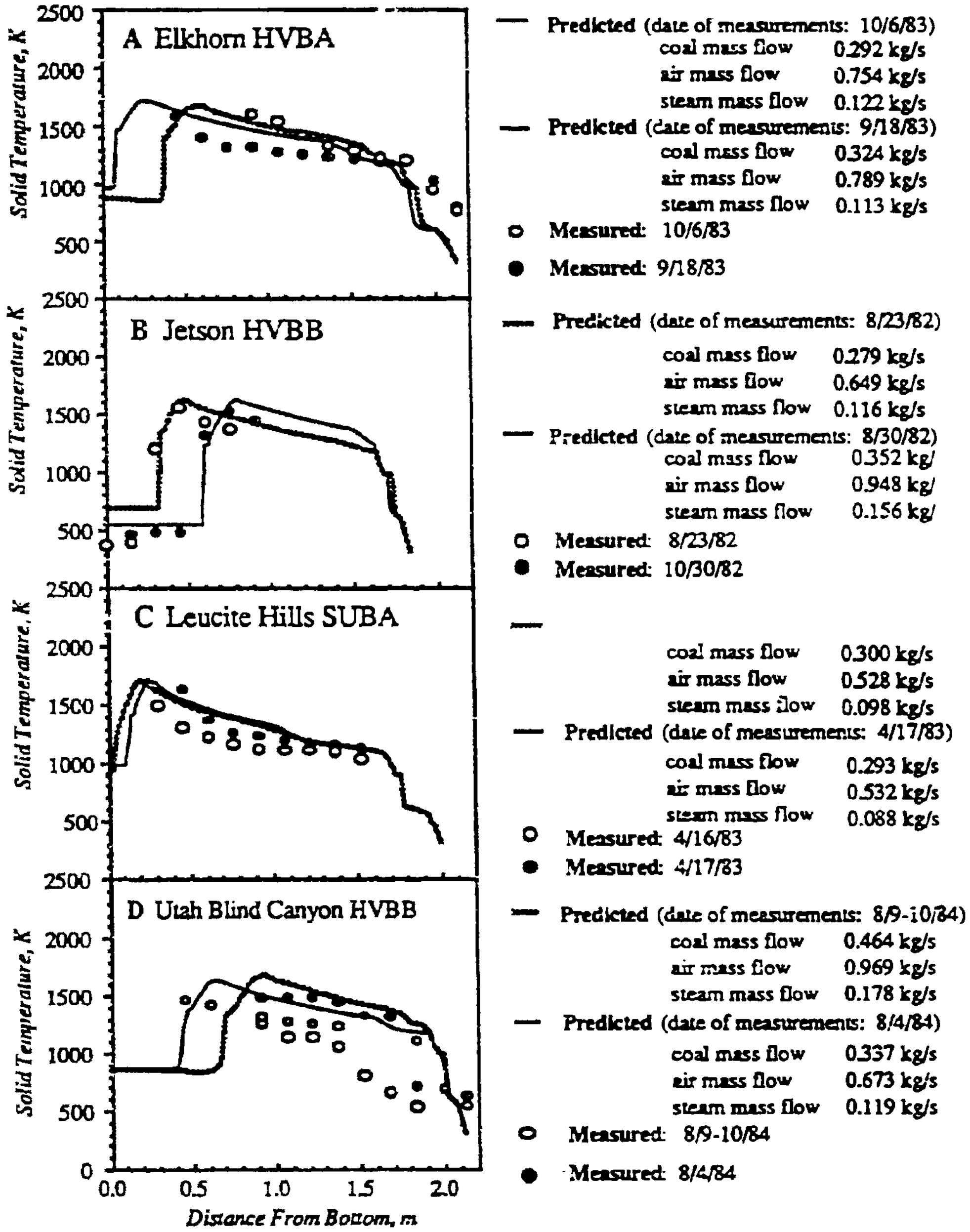

Figure III. B-1.Comparison of measured temperature and predicted solid temperature for gasification of several coals in an air-fired, low pressure Wellman-Galusha gasifier. Experimental data can be found in Thimsen et al. (1984).

III.C. SUBTASK 3.C. - GENERALIZED FUELS FEEDSTOCK SUBMODEL

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Objective

The objective of this subtask is to generalize PCGC-2 to include sorbent injection, as outlined in the Phase II Research Plan.

Accomplishments

PCGC-2 was modified to allow sorbent injection in the primary stream.

Plans

Evaluate sorbent injection submodel. Extend to additional inlets (aft sorbent injection).