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 is devoted to the development of the entrained-bed code. The second subtask is for fixed-bed reactors 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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Objective

The objective of this subtask is to improve and validate an existing 2-D code (PCGC-2) for entrained coal gasification and combustion to be more generally applicable to variation in coal rank and operating conditions. The approach being followed is to 1) incorporate detailed, coal-chemistry submodels being developed under Task 2 into PCGC-2, 2) validate the code with carefully chosen experimental data, 3) improve robustness for a wide range of operating conditions, and 4) improve user-friendliness by implementing the improved code on a workstation with a graphical user interface. The code will be applied to systems of practical interest in Task 4.a.

Accomplishments

Several improvements were made in PCGC-2 during the last quarter. A major error was discovered and corrected in the radiation submodel. This correction apparently resolved the previously reported problem with unreasonably high temperature predictions in some cases. A new option was also added to the code for solving the radiation submodel for gaseous combustion (no particles). Other improvements were made in the full energy equation option, the SIMPLE-based numerical algorithm used for solving the fluid flowfield, and the tri-diagonal matrix solver used by SIMPLE. Converged solutions were then obtained for several cases being used in Subtask 2.g to evaluate the extended NO_x submodel, and for the gasification case chosen previously as a standard test case. Additional model validation data were also obtained from AFR, and work continued on modeling the TWR reactor facility. Development of a user-friendly, graphical interface on the Sun workstation was also continued.

PCGC-2 Improvements

During the past quarter, PCGC-2 was applied to several cases being used to evaluate the extended NO_x submodel (see Subtask 2.g). In these cases, maximum and effluent gas temperatures known to be as much as 1000 degrees higher than the actual temperatures were predicted. In the detailed investigation that followed, a new option was added to code to solve the radiation submodel in gaseous combustion cases (no particles). Several errors were also discovered and corrected in the code, and several minor improvements were made to make the code more user-friendly. The most significant error was found in the radiation submodel and was apparently responsible for the unreasonable temperature predictions. This error involved calculating the blackbody emissive power (E_b) as $2\sigma T^4$ rather than $4\sigma T^4$. In addition to correcting this factor-of-two error, the code was changed to calculate E_b for the particle phase from gas temperature rather than particle temperature. This latter change makes the calculation of E_b consistent with the calculation of the radiation flux field, which substitutes gas temperature for the particle temperature since Eulerian particle temperature information is not available.

Other corrections and improvements were made in the full energy equation option, the SIMPLE-based numerical algorithm used for solving the fluid flowfield, and the tri-diagonal matrix solver used by SIMPLE. In the full energy equation option, a counter counts the number of times properties are requested at enthalpy levels that are outside the table limits. The user must insure that the limits are wide enough to cover the necessary range. During the past quarter, it was discovered that this feature was not working properly at the low end. The user was being told that physical properties were being requested from the table at enthalpies that corresponded to temperatures less than the lowest inlet temperature to the reactor, which was true due to the nature of the interpolation algorithm, but these properties were not being used in the interpolation process (e.g. their weighting factors were zero). Hence, the code was modified to not include these requests in the total number of requests (if any) outside the table limits.

Also, it was discovered that the code had been inadvertantly modified in recent history to under-relax the pressure corrections in the SIMPLE algorithm. Since this procedure is not standard practice, it was removed. Also, it was found that the convergence acceleration parameter recommended by Van Doormaal and Raithby (1984) for the tri-diagonal matrix solver used in SIMPLE, and which was incorporated into PCGC-2 during the past year, was causing instability in the solution algorithm in some cases. It was found that a more conservative implementation of this feature is desirable for code robustness, and the code was modified appropriately. This modification led to the ability to converge several cases that previously would not converge. At least two of these cases are being applied to validate the extended NO_x submodel (Subtask 2.g).

<u>PCGC-2 Validation</u>

Work continued on validating the code for selected cases. Results for a gaseous combustion case being used to validate the thermal NO_x submodel are shown in Figure III.A-1. For this validation, it is critical to correctly predict the gas temperature. Predicted centerline temperature is shown for the simulation of natural gas combustion in the laboratory-scale BYU-ACERC reactor. These results illustrate the importance of including the radiation submodel in gaseous combustion cases and the effect of the corrections to the radiation submodel described above. In addition to the results without radiation and the corrected and uncorrected results with radiation, results are shown assuming no local heat losses (adiabatic assumption). Experimental data are shown for comparison. Radiation plays a significant role in the predictions for this gaseous combustion case. The prediction with the corrected radiation submodel is up to 700 K lower than the prediction without the correction, and agrees closely with the data.

During the last quarter, additional data obtained from the TWR facility were received from AFR. These data include thermocouple measurements of gas temperature (with and without coal), video camera measurements of particle velocity, and tomography measurements of a Montana Rosebud subbituminous coal flame. The tomography measurements were obtained by FT-IR and include particle and gas temperature, particle and soot concentration (percent blockage), and CO_2 concentration (absorbance). The TWR simulation for gas only (no coal) and

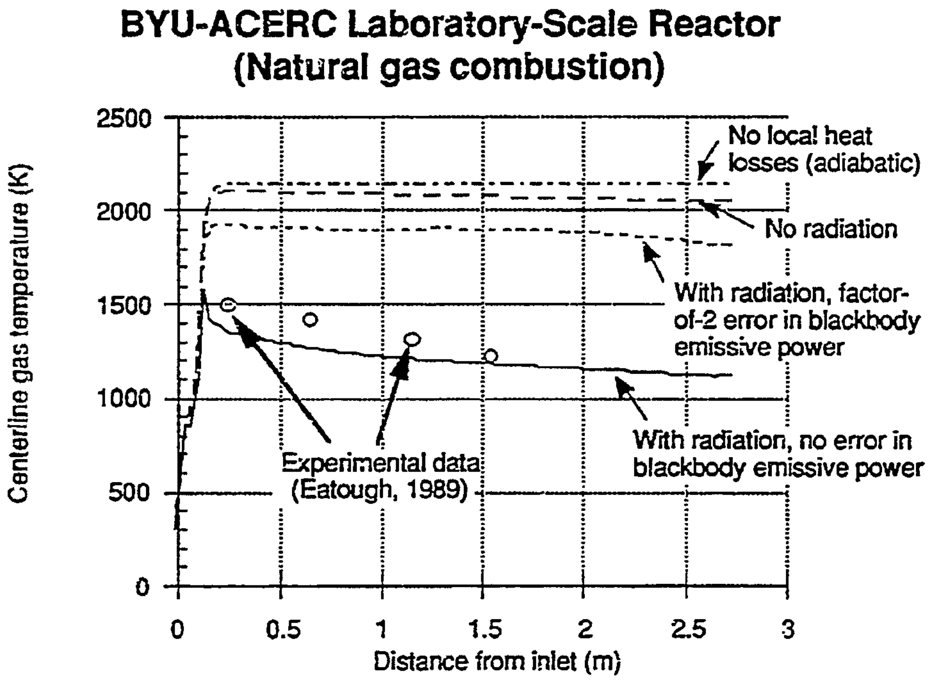

Figure III.A-1. Predicted centerline temperature profiles for combustion of natural gas in the BYU-ACERC laboratory-scale reactor compared with experimental data.

Montana Rosebud coal combustion were repeated with the corrections that have been made to the code during the past quarter.

Figure III.A-2 shows radial temperature profiles for air only (no coal). A similar figure was presented in the 3rd Annual Report (Brewster and Smoot, 1989); however, the experimental data shown previously had not been corrected for radiative heat loss from the thermocouple. The data in Figure III.A-2 are corrected for two assumed values of thermocouple emissivity. The values for ϵ=0.5 are thought to be more accurate, since the thermocouples were oxidized. As shown before, the predicted values agree reasonably well with the experimental data, with predictions accounting for both laminar and turbulent viscosities.

Figure III.A-3 shows a similar plot for combustion of Montana Rosebud subbituminous coal. Again, the measurements were corrected for radiation loss from the thermocouple, assuming two values of emissivity. The values for the higher emissivity (in this case, ϵ=0.9) are again thought to be more accurate. The assumed emissivity is higher in the case of particle combustion due to tar depositing on the thermocouple. Two predictions are shown for alternative geometries simulating the coal injection nozzle. These two geometries may be thought of as limiting cases. In the first case, the nozzle was modeled as a non-protruding 1-mm-i.d. tube with a 2.45-mm wall thickness. In the second case, the nozzle was modeled as a 4.9-mm-i.d. tube with a 0.5-mm wall thickness. A flat profile was assumed for the particles and gas in both cases. The first model geometry is consistent with the physical dimensions of the nozzle duct. The latter model geometry is consistent with the observed diameter of the particle stream as it exits the nozzle. As shown by the dotted lines in the figure, the code predictions are sensitive to the nozzle geometry. The effects of the cold carrier gas persist to a height of 5 cm for the 1-mm nozzle prediction, whereas no effects are seen at that height for the 4.9-mm nozzle prediction.

There are two major discrepancies between the predictions and data in Figure III.A-3. First, ignition is predicted too early as shown in Figure III.A-3b. The observed ignition point is 10 cm above the nozzle (Serio, 1987). However, the fact that the predicted gas temperature exceeds the hot air temperature at a height of 5 cm indicates that ignition has occurred prior to

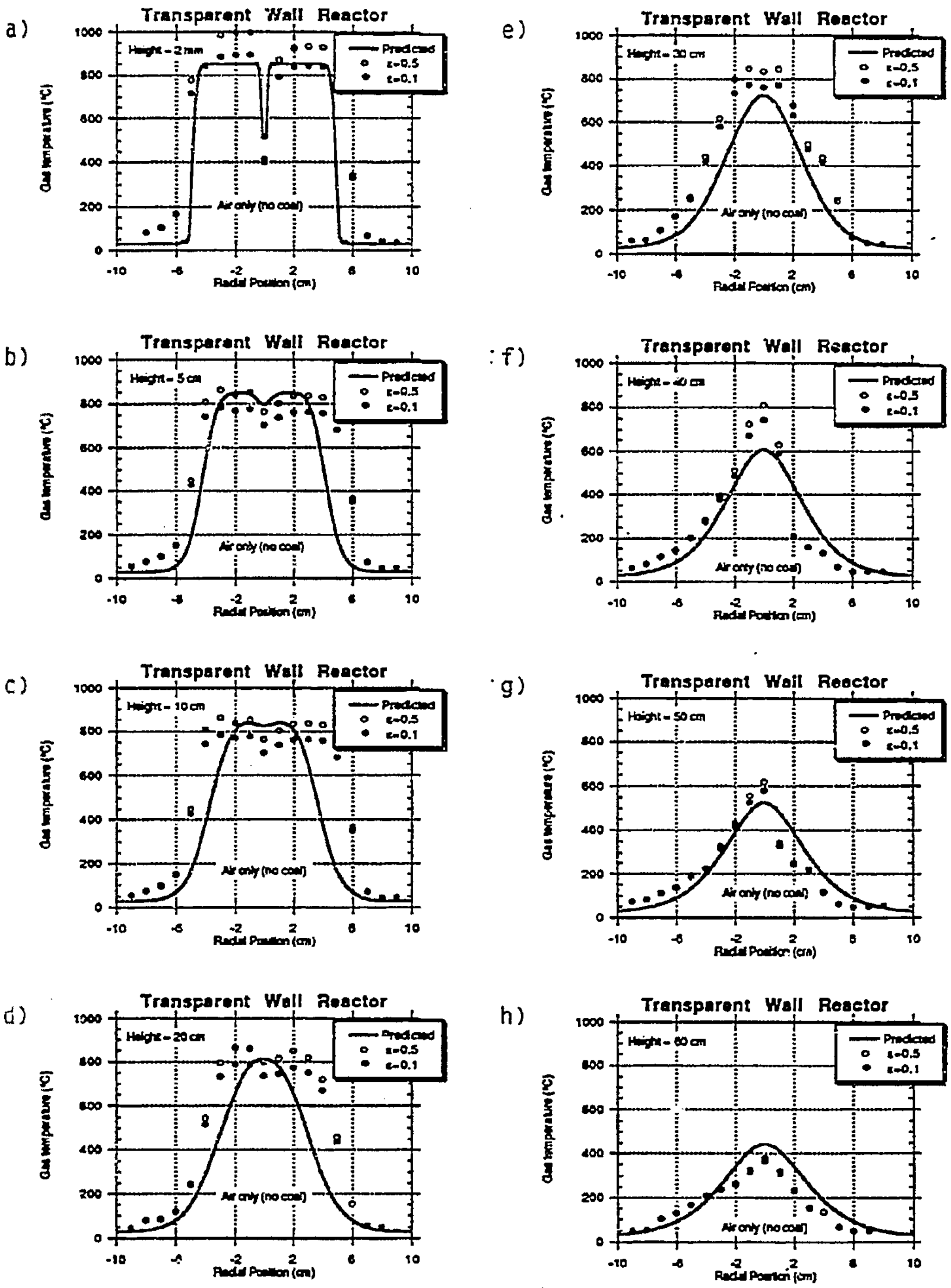

Figure III.A-2. Predicted radial temperature profiles for transparent wall reactor with no coal in primary stream compared with measured values, corrected for radiation loss from the thermocouple (Markham et al., 1990).

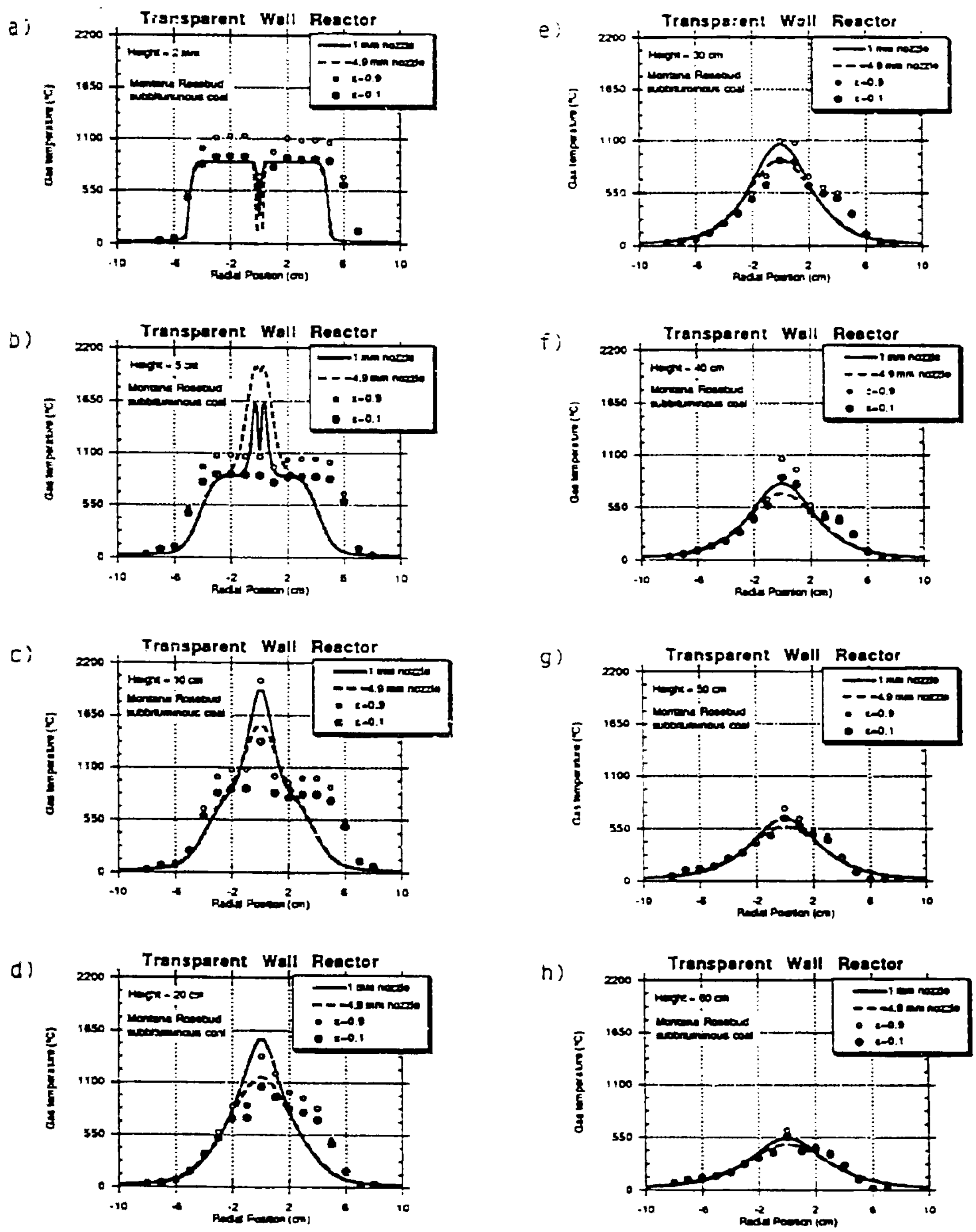

Figure III.A-3. Predicted radial temperature profiles for combustion of Montana Rosebud subbituminous coal in transparent wall reactor compared with measured values, corrected for radiation loss from the thermocouple (Markham et al., 1990).

5 cm in the predictions. The second major discrepancy is that the mixing rate between the hot and cold air at a radial location of approximately 5 cm is overpredicted (see Figures III.A-3b, c, and d). Neither of these discrepancies appears correctable by the nozzle geometry assumed for the model.

Other factors that might be responsible for the discrepancies between the predictions and data in Figure III.A-3 include inaccurate knowledge of the boundary (inlet) conditions for turbulence intensity, neglecting the effects of turbulence on gas-phase chemistry, neglecting the effects of gas buoyancy in laminar flow, using the standard k-ϵ turbulence model which is designed for fully turbulent flows, and neglecting the effects of local composition, temperature, and pressure on laminar viscosity. Inlet turbulence intensity could be determined by making calculations using a literature correlation for screen-generated turbulence and confirming the results with measurements from a hot-wire anemometer in the TWR. The effects of turbulence on local gas properties can be investigated by simply turning on a flag in the code. Buoyancy effects can be included by modifying the gas momentum source terms. The k-ϵ model could be extended to include re-laminarization by including the appropriate additional terms. It is not clear at this point whether these terms could all be lumped into the source terms, or whether the solution procedure for the k and ϵ equations would need to be modified. The effects of local composition, temperature, and pressure on viscosity could be included by modifying a flag already in the code.

The transparent wall reactor was designed to operate in the laminar regime. As shown in the 3rd Annual Report, the Reynolds numbers of the cold carrier gas and hot air stream are in the laminar range. The flowrate of the cold air entering from the room is not accurately known, but its inlet velocity has been assumed to be equal to that of the hot air (1.4 m/s). At the assumed flowrate, the Reynolds number was in the turbulent regime (10,000). Recent measurements have indicated that the inlet velocity may be significantly higher (2.3 m/s). A higher inlet velocity of room air may alter the previous conclusions about the relative importance of laminar and turbulent mixing. At any rate, the flowrate of room air needs to be accurately known for the simulation, and the laminar option should be reinvestigated, especially with the modifications described above. Based on the inlet Reynolds numbers, it is likely that the reactor is operating in transitional flow. It may be desirable to adjust the velocity of the room air in future experiments to match that of the hot air by varying the velocity of the exhaust fan which draws the room air into the reactor.

Graphical User Interface

Work continued on developing a graphical user interface (GUI) for PCGC-2. Menus associated with the panel buttons were added to allow the user to browse through the available options without having to open a window. The menus also allow the user to jump directly to the desired option. A multiple units options has been added which allows the user to provide the required data in several choices of units. The data are then automatically converted to SI units and written to the main data file to be read by PCGC-2.

Work continued on the grid generation option to make it more user-friendly. Input data consistency checks and helpful error messages were added. The windows created by the grid generation option are shown in Figure III.A-4. The GUI reads the main PCGC-2 data file, allows the user to make any changes, and then generates a grid based on the data in the main data file. The user can review the grid data file thus generated in a scrollable window, change the data, and create a new grid. After creating a suitable grid, it can be saved for use by PCGC-2.

Plans

The evaluation of the full energy equation option in PCGC-2 will continue during the next quarter. Both gaseous and particle combustion cases will be checked for enthalpy conservation. Simulation of the TWR will continue and the following possible actions will be considered: Increasing the room air flowrate in the simulation to match the measured velocity, calculating the laminar viscosity locally, incorporating buoyancy effects in the gas phase, locating a correlation for screen-generated turbulence in the literature and using it to predict the turbulence intensity boundary condition, and incorporating an extension to the k-ϵ model to handle re-laminarization. Work will also continue on the graphical interface to extend it to a network-based windowing system. The interface will also be extended to include a database of thermodynamic data which the user can use to modify the thermo file.

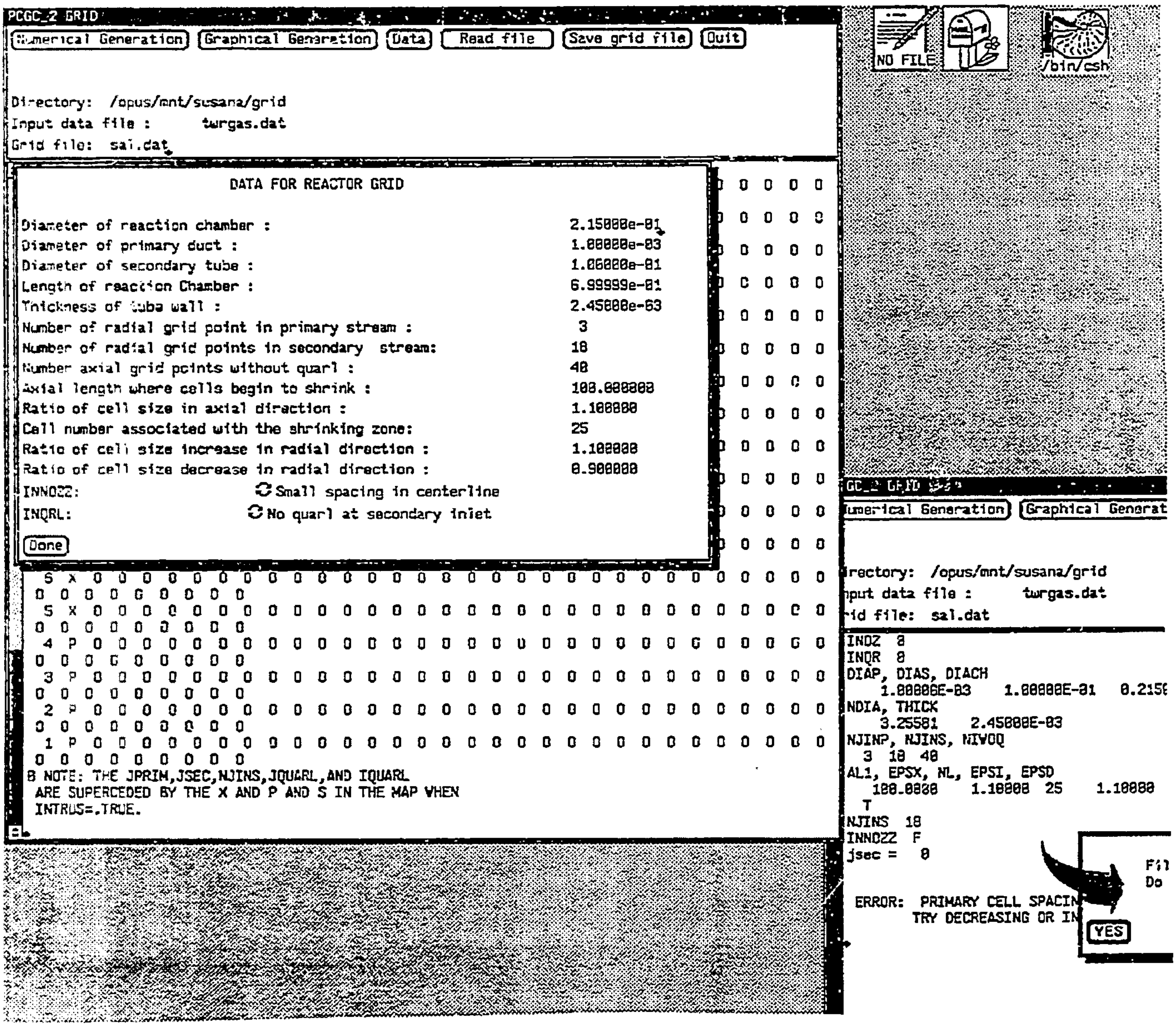

Figure III.A-4. Windows created by grid generation option in graphical user interface for PCGC-2 on Sun-4 workstation computer.

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

During the last quarter. work continued on coding chemical and physical submodels and on model validation. Improved temperature profiles and pressure profiles have been obtained from the one-dimensional fixed-bed code. The fixed-bed model considers separate gas and solid temperatures. partial equilibrium in the gas phase. variable bed void fraction. coal drying. devolatilization based on chemical functional group composition. oxidation and gasification of residual char with an ash layer. and axially variable solid and gas flow rates. Predictions and comparisons to experimental data include effluent gas compositions and temperatures. temperature profiles. and axial pressure variation. Additional predictions with comparison to limited data include carbon conversion. particle size effects. and species concentration profiles. The relative importance of char oxidation resistances to bulk film diffusion. ash diffusion. and chemical reaction are identified. For the cases examined. chemical resistance dominates in the cool regions at the bottom and top of the reactor while ash diffusion resistance competes with chemical resistance through most of the reactor. The importance of adequate treatment of devolatilization. gas phase chemistry. and variable bed void fraction is identified. A paper describing the one-dimensional model and the model validation was submitted to the 23rd International Symposium on Combustion. This paper is included in Appendix B.

A review meeting was held in order to specify final features of the one-dimensional model. Further work was performed on the well-mixed, partial-equilibrium model. This model provides an initial estimate of the effluent composition and temperature for the one-dimensional model. A draft of a paper describing the well-mixed, partial-equilibrium model was prepared. Work continued on a review paper on fixed-bed gasification and combustion.

Plans

The development of the fixed-bed code will continue next quarter with emphasis on integrating the large-particle, FG-DVC devolatilization submodel. The equations describing devolatilization need to be solved simultaneously with the conservation equations. AFR's assistance will be needed in understanding all of the comprehensive model equations as well as the submodel equations and solution algorithm.