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COMPUTATIONAL TOOLS FOR PULVERIZED-COAL
COMBUSTION

Third Quarterly Report, October—December 1981

By
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January 1982

Work Performed Under Contract No. AC22-81PC40265

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U. S. DEPARTMENT OF ENERGY

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DOE/PC/40265--3

DE82 011211

COMPUTATIONAL TOOLS FOR PULVERIZED-COAL COMBUSTION

Third Quarterly Report for the
Period October 1981 through December 1981

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Work Performed Under Contract DE-AC22-81PC40265

Prepared for the
Department of Energy
Pittsburgh Energy Technology Center
Under Contract DE-AC22-81PC40265

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ABSTRACT

This report summarizes the work conducted during the third quarter of a 30-month contract with the Department of Energy's Pittsburgh Energy Technology Center (DOE PETC). The general objective is to develop and verify a computer code capable of modeling the major aspects of pulverized-coal combustion. Achieving this objective will lead to design methods applicable to industrial and utility furnaces.

The combustion model (COMO) consists of a number of relatively independent modules that represent the major processes involved in pulverized-coal combustion. These modules will be continually upgraded over the course of the contract. Three distinct versions of the COMO will be developed over the duration of the contract.

Version 1 of COMO will model all of the major features of pulverized-coal combustion but with a number of simplifying assumptions. It will be used primarily to determine a satisfactory means of integrating the numerical models of the combustion processes into an overall combustion model, since this is perhaps the major challenge. Later versions will relax these assumptions and incorporate state-of-the-art combustion information.

During the first quarter, detailed life-of-the-project task descriptions were prepared, literature searches were conducted, and process models were selected for Version 1. Code development guidelines were prepared and reviewed with each task leader; the guidelines present the information required to allow process modules to be developed relatively independently, while providing for the subsequent integration of these modules into COMO.

During the second quarter, the formulation and coding of the Version 1 gas-phase turbulence, chemistry and radiation models were completed. Test cases were run for each model, and good agreement was obtained with other analyses and with data when available. A formal method for documenting COMO was investigated, and preliminary specifications were developed.

During this quarter, several models were documented and reviewed. This documentation will serve as an example for the remainder of the models.

A set of isothermal and gas-phase combustion data was selected for comparison with COMO. The isothermal flow runs were completed and are discussed in this report; the combustion run was also initiated. Results from both runs will be compared with available data and reported next quarter.

The definition of the solid-phase combustion model was initiated and will be completed during the next quarter; coding the model will also begin next quarter.

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1. INTRODUCTION

1.1 REPORT ORGANIZATION

This report summarizes progress during the third quarter of a 30-month contract to develop a pulverized-coal combustion model. The overall perspective of the project is briefly presented in the abstract. This introduction outlines the project objectives and the general approach for achieving them.

The approach is reviewed in Section 2 to provide a framework for understanding the objectives and progress for each part of the task. Those readers familiar with the project may wish to proceed directly to the task reports, starting with Section 3 (Integration and Validation of COMO).

1.2 PROJECT OBJECTIVE

The objective of this project is to develop a computer code capable of modeling the major aspects of pulverized-coal combustion. The mathematical representation of each significant process will be based on fundamental physical laws. The use of empirical models will be minimized as much as possible. An axisymmetric, cylindrical combustion chamber will be modeled. Multiple air and fuel inlets may be located anywhere in the inlet plane or along the cylindrical enclosure. The predictions of the computer code will be systematically compared to experimental data so that the validity of each process model can be evaluated.

Once physically realistic process models are available, along with a numerical method to solve the resulting equations, the method can be applied to more complex combustion problems. Therefore, achieving the objective of this project is the first step in the development of verified design methods applicable to industrial furnaces. The models will, of course, also be applicable to utility boiler furnaces and will have the potential of reducing the amount of empiricism presently incorporated in the design process.

1.3 GENERAL APPROACH

Computational methods in heat transfer and fluid flow have been advanced to the point that such methods are being applied to the simulation of complex -- yet practical -- combustion systems. These computational tools will ultimately be used by the designer to accurately determine the performance in the conceptual design stage.

The simulation of a pulverized-fuel combustion system involves modeling a number of complex, simultaneous, interdependent processes. The model must account for fluid flow, radiation heat transfer, particle transport, turbulence, chemistry, combustion, etc. Gas-fired combustion processes have been modeled with reasonable success by a number of investigators over the previous five to 10 years, such as Gosman et al., (1969) or Abou Ellai et al., (1978). However, pulverized-coal combustion has received less attention, partly because of the significant increase in complexity required to model the behavior of the coal particles and their effect on the gas phase. Although the physics of solid-phase combustion is not as well understood as gas-phase combustion, models are being developed that will permit a numerical simulation of the coal combustion process (Lockwood et al., 1980; Smith et al., 1980). Furthermore, there is a worldwide research effort to develop better physical models.

This project has been planned so that as new models become available, they can be readily incorporated in the overall combustion model. In addition, predictions will be compared to data in the literature to identify the adequacy of each of the individual process models, as well as the overall combustion model. Areas where additional data or improved models are required will be identified.

B&W has had considerable success with the numerical heat transfer and fluid flow techniques developed at the Imperial College of London and summarized by Patankar (1980). Computer programs based on these techniques have been developed by B&W to analyze two-phase flow and heat transfer in a pressurized water reactor (PWR) steam generator (Fortino et al., 1980; Promey et al., 1980) and to predict the efficiency of pulverized-coal classifiers (Sharma et al., 1980). Gas-phase combustion has also been modeled. The FORCE code, which employs these techniques, will be used as the basis for the coal combustion model, called COMO.

The objective of this project is to be achieved by upgrading existing numerical models of the physical processes involved in pulverized-coal combustion. These numerical models, or process modules, will be integrated to form the comprehensive combustion model, COMO. In many cases, because the modifications to the existing models will be extensive, the modules have been renamed to avoid confusion. The processes being modeled and the module names are:

Gas flow field	- FLOW	Heterogeneous chemistry	- COAL
Particle flow field	- SFLOW	Radiation heat transfer	- RAD
Homogeneous chemistry	- CHEM		

Two procedures have been defined to aid the demanding task of developing and integrating five complex process models to achieve a practical pulverized-coal model. First, code development guidelines were prepared; the guidelines define how the process models are to be independently developed and then integrated with the remainder of COMO. The guidelines were presented in the first quarterly report. Secondly, preliminary specifications for code documentation have been developed. Two of the process models are being documented on a test basis and the experience gained will be used to refine the final specifications. The remainder of COMO will then be documented. The final procedures will be presented in a subsequent quarterly report.

The development of each of the process modules is carried out in a separate project task. In addition, there is a specific task for the integration of the process modules and the validation of the combustion code. The remaining sections of this report describe the specific problem being addressed and the technical approach being taken to solve the problem (Section 2), and the progress made on each of the individual tasks during the third quarter:

Section 3 -- Integration and	Section 5 -- Chemistry
Validation of COMO	Section 6 -- Particle Flow Field
Section 4 -- Gas Flow Field	Section 7 -- Radiation Heat Transfer

Sections 3 through 7 each begin with a summary, which presents the task objectives for the current quarter, the technical accomplishments for the quarter and the objectives for the next quarter. Technical accomplishments are then discussed in detail.

2. PROBLEM DEFINITION

This section briefly describes the combustion-chamber geometry and boundary conditions; the simplifying assumptions are also presented. The governing equations and the modeling approach were presented in the first quarterly report and are not repeated here.

2.1 GEOMETRY AND BOUNDARY CONDITIONS

Specifically, numerical methods will be developed to model the geometry of a cylindrical, axisymmetric furnace (Figure 2-1). Though shown in the figure as an axial-fired unit, the numerical model will also be applicable to axisymmetric geometries with radial inlet ports. Also, the numerical model is not limited to modeling geometries with a constricted exit.

The simulated furnace is fired with pulverized coal. However the model is general enough that any well characterized gaseous or pulverized solid fuel may be analyzed. The optical and chemical properties including rate constants for the decomposition of the fuel and its intermediate products must be provided.

The boundary conditions for the furnace in Figure 2-1 vary for the different physical processes modeled. The furnace has no-slip walls, specified fuel and gas injection velocities and a fully developed, nonrecirculating outlet flow. The gas and particle composition and the particle mass and size distribution must be specified at the inlet. The furnace wall emissivity and temperature or heat flux must be provided.

With this data as input, the pulverized-coal-fired furnace model will produce results displayed in both tabular and graphical form. The pressure and velocity fields will define the gas flow. The history of the solid particles will be

represented by their trajectories, composition, temperature, size and mass. From the gas composition and temperature, the ignition delay and heat release can be established. Finally, the radiative heat fluxes seen by the furnace wall will be presented.

2.2 MODELING ASSUMPTIONS

COMO will evolve in three versions; each succeeding version will be more complex, requiring fewer simplifying assumptions than the preceding one. In general, these assumptions will affect more than one process module. The assumptions for Version 1 of COMO have been established and are listed in Table 2-1. Note that some of these assumptions considerably simplify the model, but the primary goal of Version 1 is to gain early experience in integrating the five modules of COMO and to obtain a converged solution of reasonable accuracy. The initial version will provide guidance for the development of subsequent versions of COMO.

In Version 2, some of these assumptions will be relaxed. An attempt will be made to incorporate in the homogeneous chemistry module a simplified method of considering all of the associated rate-limiting processes. This improvement will relax Assumption 3 somewhat. For this version, slip between particles and the gas will be modeled (Assumption 4). More complex solid chemistry models will be incorporated, along with a separate particle-energy equation affecting only Assumptions 5, 7, and 8.

Version 3 of COMO will extend the relaxation of these assumptions by considering several particle sizes which may vary throughout the furnace (Assumption 6). Further, other coal types will be considered (Assumption 11). Models for the formation of soot and particle fragmentation will be examined. In general, all of the modules will be upgraded by the incorporation of appropriate state-of-the-art, numerical modeling techniques.

Figure 2-1. Model furnace geometry.

Table 2-1. Assumptions for Version 1 of COMO.

- 1) Two-dimensional, axisymmetric furnace.
- 2) An energy-dissipation, turbulent-viscosity model can be used to model the fluctuating terms in the time-averaged governing equations.
- 3) One of three different gas phase chemistry models can be selected:
 - a) Infinite-rate micromixing and infinite-rate kinetics for homogeneous chemistry.
 - b) Infinite-rate micromixing and finite-rate kinetics for homogeneous chemistry.
 - c) Finite-rate micromixing and infinite-rate kinetics for homogeneous chemistry.
- 4) Solid particles are in dynamic equilibrium with gas phase; no slip.
- 5) Solid particles are in thermodynamic equilibrium with gas phase; particle temperature = gas temperature.
- 6) Particle size is constant; only one size considered.
- 7) Coal devolatilizes to a single, gaseous, hydrocarbon species.
- 8) Char oxidation occurs at particle surface.
- 9) No soot is formed.
- 10) Particle fragmentation can be neglected.
- 11) Coal type is bituminous Pittsburgh No. 8.
- 12) Volume of particles is neglected.

3. INTEGRATION AND VALIDATION OF COMO (TASK 5)

3.1 SUMMARY

As described previously, COMO is organized in a modular structure. The modules which comprise COMO are:

- FLOW - gas flow-field calculations
- SFLOW - particle flow calculations
- CHEM - gas-phase chemistry calculations
- COAL - heterogeneous chemistry calculations
- RAD - radiation heat transfer calculations

Version 1 of COMO will contain each of these modules in their initial form. Later versions will improve the physical models used by the modules. One of the objectives of this task is to conduct a smooth integration of these modules.

In the last quarter, the gas-phase modules (FLOW and CHEM), along with the Version-1 radiation module (RAD), were integrated with COMO. The resulting code will be referred to as COMO - Version 1 - Gas-Phase Combustion. During the current quarter, the validation run for this code was initiated. The results of this run will be compared to the experimental data identified last quarter (Hutchinson, et al., 1976). Also during this quarter, the documentation of the COMO code and the integration of the solid flow and chemistry modules (SFLOW and COAL) into COMO were initiated.

3.2 OBJECTIVES FOR CURRENT QUARTER

- 1) Begin process of integration of solid flow and chemistry modules into COMO.
- 2) Initiate documentation of COMO computer code.
- 3) Verify COMO - Version 1 - Gas-Phase Combustion.

3.3 TECHNICAL ACCOMPLISHMENTS

Through discussions with the various task leaders, the overall design of the solid-flow and chemistry modules (SFLOW and COAL) has been established. This design defines the flow of information between the SFLOW and COAL modules and COMO, along with the mode of transfer. The description of both modules, including effects on other modules in COMO, is currently being compiled in the respective module documentation. Actual coding of the modules and the physical integration of SFLOW and COAL into COMO will be initiated next quarter.

Documentation is an essential feature of an efficient computer-code development program. Many programming errors could be eliminated with the use of suitable documentation. The Task 5 leaders are conducting the documentation effort for COMO. In this quarter, an outline of the documentation was established and distributed with sample code documentation to the task leaders. In addition, the overall COMO program and the program's utility routines will be documented under this task. Some of this documentation has been completed and filed. This will be an ongoing effort as later versions of COMO are developed.

As discussed in the first quarterly report, each version of COMO will be verified by comparisons to measured data, if available. This verification effort is being carried a step further; both the gas-phase and final versions of each code will be validated in this manner. This dual-step validation eliminates some uncertainties regarding sources of discrepancies during comparisons. Following this plan, the gas-phase version of COMO is currently being verified. The data set identified in the last quarterly report (Hutchinson, et al., 1976) is being used for this purpose. The input data files have been created for use by COMO, and runs are currently being made. This validation effort will be completed next quarter.

3.4 OBJECTIVES FOR NEXT QUARTER

- Complete verification of COMO - Version 1 - Gas-Phase Combustion.
- Continue integration of SFLOW and COAL in COMO.

3.5 VERIFICATION OF COMO - VERSION 1 - GAS-PHASE COMBUSTION

The gas-phase validation run is an analysis of the furnace described in Hutchinson, et al., (1976) and shown in Figure 3-1. The furnace is axisymmetric with a single burner located on the centerline. The burner consists of two coaxial pipes: the inner pipe is the fuel inlet; the outer is the air inlet with adjustable swirl vanes. For the current run, these vanes were set for a swirl number of 0.52. The actual dimensions and arrangement of the burner are shown in Figure 3-1. Sections of water-cooled walls were used to maintain a constant wall temperature near 400°K. More details of the furnace and burner are provided by Hutchinson, et al., (1976).

The grid arrangement used for the validation run is shown in Figure 3-2. The grid is comprised of 43 axial nodes and 30 radial nodes, including the boundaries. Due to the resolution of the plotter, the very small grid spacing near the burner cannot be seen. As discussed in Section 4, it was found that the amount of detail in this region was necessary to obtain grid independent solutions for swirling flow.

The fuel is natural gas (composition = 94.4% CH₄-1.4% N₂-3.1% C₂H₆) and supplied at room temperature through the central jet. The oxidant is air (78% N₂-22% O₂) supplied at room temperature through the outer annulus.

The walls are assumed to be oxidized carbon steel with an emissivity of 0.8. The principal absorbing gas species are assumed to be CH₄, CO₂ and H₂O. Hottel charts are used to determine the absorption coefficient for a particular gas composition and temperature.

The measurements that were taken include isothermal and combustng flow measurements, temperatures and wall heat flux. The results from COMO will be tabulated and plotted for comparison to this data. Isothermal flow predictions are reported in Section 4. The combustion run was initiated and will be run to convergence next quarter; the comparison data and predictions will also be completed.

Figure 3-1. Furnace analyzed by COMO.

COMO - VERSION 1 - GAS
2-D GEOMETRY

NODE . C

Figure 3-2. Furnace control volumes.

4. FLUID MECHANICS MODULE (TASK 1)

4.1 SUMMARY

The purpose of Task 1 is to provide the gas-phase fluid-mechanics model for COMO. The fluid-mechanics model includes a turbulence model and the conservation equations for mass and momentum.

During the current quarter, isothermal swirling and nonswirling flow in an axisymmetric furnace has been studied extensively, and the results are presented in this report.

4.2 OBJECTIVE FOR CURRENT QUARTER

The objective for the current quarter was to evaluate the turbulence model by comparing predicted and measured flow patterns for isothermal flow in an axisymmetric furnace with and without swirl.

4.3 TECHNICAL ACCOMPLISHMENTS

The effect of swirling flow on the furnace flow patterns was studied using the $k-\epsilon$ two-equation model discussed in the first quarterly report. The dependence of the numerical results on the grid system was also considered.

4.4 OBJECTIVES FOR NEXT QUARTER

- Compare the present predictions with experimental data.
- Study the dependence of flow patterns on the turbulence intensity profile at the inlet.

4.5 TURBULENCE MODEL EVALUATION FOR ISOTHERMAL FLOW

During the past quarter, COMO was applied to study the isothermal flow patterns in the furnace shown in Figure 4-1. This particular geometry was chosen because experimental and numerical data are available for comparison to both isothermal and combusting flows. The effect of changing grid size and swirl velocity was examined. From this study, the convergence rate and accuracy of the two-equation turbulence model can be evaluated before the combustion model is added.

The swirl number (S) is defined as: tangential momentum/axial momentum / r_2 , where the momentum is determined at the burner exit plane, and r_2 is the burner exit radius. In this study, a coarse (16 x 16 or 17 x 15) grid system was first applied to make a preliminary study of the overall isothermal flow pattern. Then, a 31 x 29 system (Figure 4-2) was used to study the cases for $S = 0$ and $S = 0.85$. This grid system is essentially the same as a test case from a proprietary code similar to TEACH-T. It was felt that for the computation of combustion flows in Task 2, the grid size next to the furnace exit must be reduced to obtain more accurate results. Therefore, 12 more grid points were added in the axial direction for the third test case: a 43 x 30 grid system (Figure 4-3) was used to study the flow with $S = 0.5$ (also chosen for the study of combustion flows).

Figures 4-4 and 4-5 show streamlines for a nonswirling flow ($S = 0$) with 16 x 16 and 31 x 29 grid systems, respectively. The spacing between two adjacent contours is 5×10^{-4} . The secondary-inlet airflow velocity is approximately 15 m/sec, and the primary inlet is blocked. The turbulent inlet intensity is taken as:

$$K = 0.01(U^2 + W^2) ; \text{ and } \epsilon = K^{1.5}/(0.33R_0)$$

where U and W are the inlet axial and tangential velocity, respectively (note $W = 0$ for $S = 0$); R_0 is the internal furnace radius.

These figures indicate that without swirl, the flow pattern in the furnace is very similar to that of a cavity and is represented by one large recirculating flow zone around the furnace wall. A very small recirculating bubble is noted at the inlet corner next to the axis. Since the flow patterns predicted by both grid systems are nearly identical, it demonstrates that this particular flow is predicted adequately using a 16 x 16 grid system.

Both Figures 4-6 (with a grid of 17 x 15) and Figure 4-7 (with a grid of 31 x 29) display the flow patterns for $S = 0.85$. It is seen that after one furnace radius downstream of the burner, the flow patterns predicted by these two grid systems are similar. However, in the vicinity of the burner, the flow patterns are completely different. This is due to the fact that the flow there changes direction rapidly. As a result, a coarse grid system cannot pick up a detailed flow pattern next to the burner. It is interesting to note that for nonswirling flow, the velocity gradient is not as steep there and a 16 x 16 grid system gives reasonable results.

At this swirl number, there are two recirculating zones of interest: one is located next to the axis of the furnace, while the other is at the corner of the furnace. Since present predictions with a 31 x 29 grid system agree fairly well with the proprietary computer code and proprietary experimental data, no further refinement of the grid system for flows with $S = 0$ and 0.85 is necessary.

Figure 4-8 depicts the flow pattern for $S = 0.5$. The Reynolds number of the flow in the annulus is 4.7×10^4 , corresponding to a mean axial velocity of 12.85 m/sec, and that of the center jet flow is 0.55×10^4 . In comparison to Figure 4-7, one sees that as the swirl number decreases, the center recirculating zone diminishes as the one at the corner expands.

Figures 4-9 through 4-11 show the flow velocity vectors in the furnace for $S = 0$, 0.85 and 0.5, respectively. For $S = 0$, the flow velocity next to the center is much higher than other parts of the furnace. The flow velocity in the center recirculating zone is very large, although it occupies only a very small area. With swirl velocity, the radial distribution of flow velocity is much more uniform, except for the recirculation zone next to the furnace wall. The effect of increasing swirl on the flow patterns can be seen easily in these figures.

Figures 4-12 and 4-13 display the distribution of swirl velocity in the furnace. It is seen that the swirl velocity decays rapidly next to the burner, but in the vicinity of the furnace center, the swirl velocity remains fairly constant along the axis.

Figure 4-14 shows the contour of turbulent kinetic energy for $S = 0$. This pattern is very similar to that of a sudden-expansion pipe flow (presented in the first quarterly report). Figures 4-15 and 4-16 demonstrate that turbulent intensity is high next to the burner and at the furnace exit, where the velocity gradient is steep.

The flow axial velocity along the furnace radius and at different axial locations for $S = 0, 0.85, 0.5$ is shown in Figures 4-17 through 4-19, while the turbulent kinetic energy is shown on Figures 4-20 through 4-22. The decay of swirl velocity for $S = 0.85$ and 0.5 is shown clearly in Figures 4-23 and 4-24.

The centerline axial velocity for these three flow cases is displayed in Figures 4-25 through 4-27. It can be seen that with $S = 0$, the maximum centerline axial velocity is 10 m/sec, at $x = 0.2$ m. The maximum reverse flow is -5 m/sec. As S increases, this curve changes its shape accordingly. The curves for $S = 0$ and 0.85 agree with the results from the previously mentioned proprietary code with a maximum discrepancy of 10%.

The results for $S = 0.5$ will be compared to the data of Hutchinson, et al., (1976) in the next quarterly report. It is noted that in Hutchinson's report, the definitions for the Reynolds number and Swirl number differ from those presented in this report. Also, the flow inlet condition is not completely reported in their paper; some trial and error must be performed to obtain the inlet condition.

4.6 CONCLUSIONS

From these discussions of the three isothermal-flow test runs, the following conclusions may be obtained:

- 1) The present two-equation turbulence model in Version 1 of COMO is able to predict the flow field in a furnace geometry. The results agree reasonably well with some proprietary numerical and experimental results.
- 2) For the present furnace model considered, swirl velocity has a significant effect on overall flow patterns. This effect is demonstrated by the previous analysis.
- 3) For nonswirling flow, the flow patterns are not sensitive to the grid size and a relatively coarse grid system can be used. But, for swirling flow, the grid size has a profound effect on the flow patterns. In the vicinity of the burner exit (where the velocity gradient is steep) the grid size must be refined to give correct flow patterns.

Figure 4-1. Schematic of furnace geometry.

Figure 4-2. 31 x 29 grid system.

Figure 4-3. 43 x 30 grid system.

Figure 4-4. Stream function (16 x 16) - $S = 0$, spacing = 5×10^{-4} .

Figure 4-5. Stream function (31 x 29) —
 $S = 0$, spacing = 5×10^{-4} .

Figure 4-6. Stream function (17 x 15) —
 $S = 0.85$, spacing = 5×10^{-4} .

Figure 4-7. Stream function (31 x 29) —
 $S = 0.85$, spacing = 5×10^{-4} .

Figure 4-8. Stream function (43 x 30) —
 $S = 0.5$, spacing = 5×10^{-4} .

Figure 4-9. Velocity vectors (31 x 29) —
 $S = 0$, (1" = 6.67 m/sec).

Figure 4-10. Velocity vectors (31 x 29) —
 $S = 0.85$, (1" = 6.67 m/sec).

Figure 4-11. Velocity vectors (31 x 29) –
 $S = 0.5$, ($1' = 6.67$ m/sec).

Figure 4-12. Swirl velocity (31 x 29) –
 $S = 0.85$, spacing = 0.5 m/sec.

Figure 4-13. Swirl velocity (43 x 30) —
 $S = 0.5$, spacing = 0.5 m/sec.

Figure 4-14. Turbulent kinetic energy (31 x 29) —
 $S = 0$, spacing = $0.3 \text{ m}^2/\text{sec}^2$.

Figure 4-15. Turbulent kinetic energy (31 x 29) –
 $S = 0.85$, spacing = $0.3 \text{ m}^2/\text{sec}^2$.

Figure 4-16. Turbulent kinetic energy (43 x 30) –
 $S = 0.5$, spacing = $0.2 \text{ m}^2/\text{sec}^2$.

Figure 4-17. Axial velocity profile – $S = 0$ (axial locations in meters downstream of inlet).

Figure 4-18. Axial velocity profile – $S = 0.85$ (axial locations in meters downstream of inlet).

Figure 4-19. Axial velocity profile — $S = 0.5$ (axial locations in meters downstream of inlet).

Figure 4-20. Turbulent kinetic energy profile — $S = 0$ (axial locations in meters downstream of inlet).

Figure 4-21. Turbulent kinetic energy profile – $S = 0.85$ (axial locations in meters downstream of inlet).

Figure 4-22. Turbulent kinetic energy profile – $S = 0.5$ (axial locations in meters downstream of inlet).

Figure 4-23. Tangential velocity profile – $S = 0.85$ (axial locations in meters downstream of inlet).

Figure 4-24. Tangential velocity profile – $S = 0.5$ (axial locations in meters downstream of inlet).

Figure 4-25. Centerline axial velocity profile – $S = 0$.

Figure 4-26. Centerline axial velocity profile – $S = 0.85$.

Figure 4-27. Centerline axial velocity profile – $S = 0.5$.

5. CHEMISTRY MODULES (TASK 2)

5.1 SUMMARY

The purpose of this task is to develop models for chemical reactions and heat transfer in a combustion environment. There are two program modules: CHEM models gas-phase chemistry and heat transfer; and COAL models solid-phase chemistry and heat transfer.

Specifically, the CHEM module solves the conservation equations for gas species and energy for laminar or turbulent flows. In keeping with the modularization of COMO (discussed in the first quarterly report), other modules provide input required by CHEM, such as velocities and pressure (FLOW), source of gas due to solid fuel decomposition (COAL) and radiant heat transfer (RAD). With this information, CHEM calculates gas species concentrations and temperature, which are then used to determine gas properties (such as density, viscosity, conductivity, etc.). As discussed in the second quarterly report, three models have been coded and integrated with COMO. They are the perfectly stirred equilibrium model (PSE), the perfectly stirred kinetics model (PSK) and the fast-kinetics micromixing model (FKM).

Similarly, the COAL module will solve the conservation equations for particle mass and energy. The solution of these equations also depends upon information supplied by other modules. Particularly, the SFLOW module must provide the particle's initial conditions (temperature, composition and mass). Gas properties are calculated by CHEM, and RAD provides the radiative heat transfer to the particle. Using this data, COAL calculates particle properties, which are then used by other modules. For example, SFLOW requires particle properties to determine trajectories. The design of the Version 1 COAL module was outlined this quarter and is currently being documented. Programming the Version 1 model of COAL will be initiated during the next quarter.

5.2 OBJECTIVES FOR CURRENT QUARTER

- Continue documentation of the gas-phase chemistry module.
- Begin development of solid-phase chemistry module.

5.3 TECHNICAL ACCOMPLISHMENTS

During this quarter, documentation guidelines were refined and several examples were distributed. These guidelines include a detailed outline for documenting the module and its overall purpose and operation, as well as an outline for the subroutines contained in the module. In this quarter, the gas phase chemistry module documentation was initiated according to these guidelines. Specifically, the module description of the energy equation was completed and the module description of the conservation of chemical species was begun.

Along with this documentation effort, the solid phase chemistry module design was outlined. This design was formulated from the results of the literature survey reported in the first quarterly report and through discussions with the other task leaders. The latter discussions were held to ensure integration of this module with the other COMO modules. The design of this module is discussed in Section 5.5.

5.4 OBJECTIVES FOR NEXT QUARTER

- Continue documentation of the gas-phase chemistry module.
- Evaluate the fast-kinetics micromixing model by comparison with experimental data.
- Program solid-phase chemistry module.

5.5 COAL MODULE DESIGN

As recommended in the first quarterly report, the devolatilization scheme proposed by Ubhayakar, et al., (1976) will be used by Version 1 of COMO. The measurements taken by these researchers were done using a Pittsburgh No. 8 bituminous coal. The mechanism which they proposed included two steps:

where $0 < \alpha < 1$. α is determined by the hydrogen-to-carbon ratios (H/C) of the raw coal and the volatiles. The reaction rate constants (k) were assumed to have an Arrhenius form:

$$K_n = B_n \exp (-E_n/RT)$$

From the measurements, Ubhayakar, et al., (1976) obtained values for α and k . In addition, the fraction of volatiles which crack to soot was also considered, and an empirical expression based on the amount of dry ash-free coal was given. According to the authors, this expression compared well to experimental data over a wide range of conditions. This two-step devolatilization mechanism, along with the soot-formation expression, will be used in Version 1 of COAL.

The char-oxidation mechanism used in Version 1 of COAL will be the one recommended by Skinner and Smoot (1979). This mechanism includes the oxidation of char by oxygen, carbon dioxide and steam. The implementation of these kinetic parameters follows the recommendations of Smith (1979). Smith derives an expression for char reactivity which depends upon the kinetics discussed in Skinner and Smoot (1979) and mass transfer of the oxidant and oxidation products through the boundary layer surrounding the coal particle.

Both the reaction rate of the coal (devolatilization) and the char (oxidation) represent source terms to the particle mass-conservation equation. This equation is solved in the solid flow module (SFLOW). Hence, SFLOW calls COAL to get these source terms. After SFLOW solves the equations necessary to determine the number and location of particles, COAL is again called to calculate the source terms to the gas-phase conservation equations -- specifically, the equations for gas-phase species and energy. In addition, COAL calculates and stores the variables needed by the radiation module (RAD) to calculate radiation properties. The variables required by COAL have been defined so that it can be used with either an Eulerian or Lagrangian description of the particle flow.

6. PARTICLE FLOW FIELD (TASK 3)

6.1 SUMMARY

The purpose of Task 3 is to develop a process module that solves the conservation-of-mass and momentum equations for coal particles and that also provides the following information to other process modules: number of particles of each type, particle velocity for each type, and the change in momentum due to particle acceleration.

6.2 OBJECTIVE FOR CURRENT QUARTER

The objective for this quarter was to formulate and code a Eulerian, homogeneous-equilibrium, multiphase flow module for Version 1 of COMO.

6.3 TECHNICAL ACCOMPLISHMENTS

During this quarter, it was decided not to formulate and code the particle flow module until the solid-phase chemistry module is well defined. Therefore, there was no activity for this task.

6.4 OBJECTIVE FOR NEXT QUARTER

To formulate and code the solid-phase flow module for Version 1 of COMO.

7. RADIATION HEAT TRANSFER (TASK 4)

7.1 SUMMARY

This section addresses the work on the radiation heat transfer module for the last quarter. The purpose of this task is to integrate a radiation model into the overall COMO computer program and to determine the radiative properties for the radiation model. The radiation heat transfer module will be developed during the life of the project, with increasingly more realistic models being integrated into subsequent versions of COMO.

7.2 OBJECTIVES FOR THIS QUARTER

- Begin work on optimizing the numerical scheme for later versions of COMO.
- Initiate property predictions for Version 2.
- Continue to compare the discrete-ordinates method against experimental data.

7.3 TECHNICAL ACCOMPLISHMENTS

During this quarter, work began on optimizing the numerical scheme. The point-by-point iteration scheme currently in use is quite time consuming when particles are included because of the laborious calculations required for in-scattering source terms. Alternate solution schemes are now being examined; a line-by-line solution scheme may be more efficient than the point-by-point method. A detailed report will be made upon completion of the work.

Property predictions were initiated for Version 2 of COMO. Using the Mie scattering programs, together with the refractive indices of coal, char and ash, (refer to the second quarterly report), absorption and scattering cross sections were predicted. This work will be completed and detailed next quarter.

The discrete-ordinates method was compared to additional test data; the effect of increasing the ordinate directions was also investigated. This work is summarized in Section 7.5. Some of the discussion from last quarter's report is repeated to provide background. The S_n approximations were examined (that is, S_2 , S_4 , S_6 and S_8). The S_2 approximations represent solutions quite well, while solutions seem to converge to an S_4 approximation for the cases tested. No improvement in the solutions was observed for S_6 and S_8 . Since solutions to COMO are iterative in nature, early iterations should use S_2 approximations (four fluxes). Consequently, COMO was formulated to allow the user to change the S_n approximation for a range of iterations. This option is currently available in COMO with the S_2 , S_4 and S_6 approximations.

7.4 OBJECTIVES FOR NEXT QUARTER

Next quarter's work will include:

- Continuing work on optimizing the numerical scheme for Versions 2 and 3 of COMO.
- Completing property predictions for Version 2.
- Begin recoding Version 1 of COMO to reflect Version 2 improvements.

7.5 THE DISCRETE-ORDINATES METHOD

7.5.1 Results

The discrete-ordinates method covered in the previous quarterly reports is compared to a number of exact solutions and data. Solutions were found using the S_n method, which generally requires $n(n+2)$ ordinate directions. But because there is geometrical symmetry, only half of these ordinate directions are required. The S_2 , S_4 , S_6 and S_8 approximations were investigated for several examples presented here. Accuracy did not improve noticeably beyond S_4 by increasing the number of directional fluxes, while computer storage and computational time increased significantly. Tabulations for the S_2 , S_4 and S_6 approximations may be found in Tables 7-1 through 7-3, respectively. Results are presented using the S_2 and S_4 methods, in which four and 12 fluxes are required, respectively.

Consider the geometry shown in Figure 7-1. Predictions for wall heat flux are depicted in Figure 7-2 for heat transfer in an emitting, absorbing and isotropically scattering medium in a one-dimensional cylindrical geometry with radiatively black walls. All calculations were performed assuming a single scattering albedo of 0.5. In this case, the distance (L) is assumed to be much larger than the radius (R). Numerical solutions were obtained using six radial nodes and 10 axial nodes.

Figure 7-2 shows the wall heat flux normalized to the emissive power at the centerline for three different temperature profiles. Profile A represents a constant temperature medium with a tube wall at a different temperature, T_w . Profiles B and C simulate turbulent and laminar temperature profiles in the tube, respectively. For all numerical calculations, the value $T_G/T_w = 5$ was used. Nondimensional wall flux is plotted versus the optical thickness of the medium. For optically thin conditions ($\tau \rightarrow 0$), the agreement between the discrete-ordinates numerical solution and the exact solution presented by Azad and Modest (1980) is excellent. At large optical thicknesses ($\tau \rightarrow \infty$), the wall flux is overpredicted by <2% with the S_4 discrete ordinate solution and <6% with the S_2 approximation. The S_4 solution is the limiting S_n solution; that is, S_6 and S_8 provide no better accuracy. Azad and Modest (1980)] have shown that differential and kernel approximations overpredict the exact solution.

The behavior of the wall flux is linked to the form of the temperature profile. For example, a jump in temperature exists near the wall for Profile A, and wall flux continuously increases with increasing optical thickness. No jump in temperature at the wall exists for Profiles B and C. Wall flux increases continuously to a maximum value at some critical optical thickness beyond which wall flux decreases. This trend is consistent, because radiative flux must vanish in the limits of small and large optical thicknesses, respectively.

Wu and Fricker (1971) have collected data on a water-cooled cylindrical furnace (0.9 m-diameter, 5 m-length) positioned vertically with the burner at the bottom. Data were collected from a nonswirling natural-gas flame with a total heat release of 1060 KW. Measurements of gas temperature and wall heat flux have been documented by Wu and Fricker. In accordance with the predictions of Fields (1981) on the same furnace, a wall emissivity of 0.8, inlet and exit-plenum

emissivities of 1.0, and an absorption coefficient of 0.3 m^{-1} were assumed. Numerical solutions were obtained using a grid of six radial nodes and 19 axial nodes, together with the input information used by Fields (1981) and the measured gas temperatures documented by Wu and Fricker.

Figure 7-3 displays radiant wall heat flux predictions using the S_2 and S_4 discrete-ordinates approximations versus experimental data from Wu and Fricker (1971) and the predictions of Fields (1981). The data in Figure 7-3 represent furnace conditions for a peak heat flux positioned 1.4 diameters downstream from the burner exit. The proposed discrete-ordinates method not only predicts the magnitude of the radiative flux but the proper location of the peak heat flux. The S_4 discrete-ordinates approximation clearly agrees with the data better than Fields' four-flux method and predicts the trend of data more consistently.

Detailed test data have been collected by Michelfelder and Lowes (1973) in a furnace with an approximately square cross section ($2.0 \text{ m} \times 2.0 \text{ m}$) and a length of 6.25 m. Experimentally determined gas temperatures, wall temperatures and wall emittances documented by Michelfelder and Lowes (1973, flame trial-29) were used together with a gray-gas absorption coefficient of $K = 0.2 \text{ m}^{-1}$ reported by Lowes, et al. (1974). Since the proposed model is axisymmetric, an equivalent diameter was chosen to equate the cross-sectional area of the actual furnace with the modeled one. Numerical solutions were obtained using a grid of five radial nodes and 19 axial nodes. Incident radiant heat flux was predicted using the discrete-ordinates S_4 method and is shown in Figure 7-4 along with experimental data reported by Michelfelder, et al. (1973) and predictions published by Lowes, et al. (1974). As shown, the discrete-ordinate S_4 solution compares favorably with the data and the predictions of Lowes, et. al., [1974].

7.5.2 Summary and Conclusion

A discrete-ordinates method has been presented and can be applied to predict radiant heat transfer in a cylindrical enclosure. Solutions have been found by using the S_n approximations and by using a point-by-point iterative scheme developed by Carlson and Lathrop (1968). The method accurately predicts radiant heat transfer for several, simple, one-dimensional configurations involving absorption and scattering. Furnace heat transfer was predicted for two test

furnaces: the Delft furnace and the Ijmuiden furnace. For the Delft furnace, the S_4 and S_2 discrete-ordinate solutions compared well with the data and less favorably with predictions of the Fields' [1981] four flux model. For the Ijmuiden furnace, the S_4 method, the data from Michelfelder, et al. (1973), the zonal and four-flux method from Lowes, et al. (1974) all compared within 15%.

Figure 7-1. Model of cylindrical geometry.

Figure 7-2. Wall heat fluxes for an infinite cylinder bounding an absorbing/isotropically scattering medium.

Figure 7-3. Wall heat flux predictions and data for the Delft furnace.

Figure 7-4. Prediction of test-flame 29 M2 trials (Wu). comparison of data with several prediction methods.

Table 7-1. Ordinates and weights for S_2 approximation.

Direction Number	Ordinates			Weight
n^*	ν	ξ	η	w
1	-.81649658	0	-.57735026	0
2	-.57735026	.57735026	-.57735026	π
3	+.57735026	.57735026	-.57735026	π
4	-.81649658	0	+.57735026	0
5	-.57735026	.57735026	+.57735026	π
6	+.57735026	.57735026	+.57735026	π

*The ordinates include the two special directions in which $\eta = 0$. Ordinate values taken from: Lee, C. E., "The Discrete S_n Approximation to Transport Theory," Lawrence Livermore Report LA2595, 1962.

Table 7-2. Ordinates and weights for S_4 approximation.

Direction Number	Ordinates			Weights
n^*	ν	ξ	η	w
1	-.47140452	-.88191710	0	0
2	-.33333333	-.88191710	.33333333	$\pi/3$
3	+.33333333	-.88191710	.33333333	$\pi/3$
4	-.94280904	-.33333333	0	0
5	-.88191710	-.33333333	.33333333	$\pi/3$
6	-.33333333	-.33333333	.88191710	$\pi/3$
7	+.33333333	-.33333333	.88191710	$\pi/3$
8	+.88191710	-.33333333	.33333333	$\pi/3$
9	-.94280904	.33333333	0	0
10	-.88191710	.33333333	.33333333	$\pi/3$
11	-.33333333	.33333333	.88191710	$\pi/3$
12	+.33333333	.33333333	.88191710	$\pi/3$
13	+.88191710	.33333333	.33333333	$\pi/3$
14	-.47140452	.88191710	0	0
15	-.33333333	.88191710	.33333333	$\pi/3$
16	+.33333333	.88191710	.33333333	$\pi/3$

*The ordinates include the four special directions in which $\eta = 0$. Ordinate values taken from: Lee, C. E., "The Discrete S_n Approximation to Transport Theory," Lawrence Livermore Report LA2595, 1962.

Table 7-3. Ordinates and weights for S_6 approximation.

Direction Number	Ordinates			Weights
n	μ	ξ	η	w/π
1	-.36514835	-.93094934	0	0
2	-.25819889	-.93094934	+.25819889	.16086125
3	+.25819889	-.93094934	.25819889	.16086125
4	-.73029674	-.68313005	0	0
5	-.68313005	-.68313005	.25819889	.17247209
6	-.25819889	-.68313005	.68313005	.17247209
7	+.25819889	-.68313005	.68313005	.17247209
8	+.68313005	-.68313005	.25819889	.17247209
9	-.96609178	-.25819889	0	0
10	-.93094934	-.25819889	.25819889	.16086125
11	-.68313005	-.25819889	.68313005	.17247204
12	-.25819889	-.25819889	.93094934	.16086125
13	.25819889	-.25819889	.93094934	.16086125
14	.68313005	-.25819889	.68313005	.17247204
15	.93094934	-.25819889	.25819889	.16086125
16	-.96609178	.25819889	0	0
17	-.93094934	.25819889	.25819889	.16086125
18	-.68313005	.25819889	.68313005	.17247204
19	-.25819889	.25819889	.93094934	.16086125
20	+.25819889	.25819889	.93094934	.16086125
21	.68313005	.25819889	.68313005	.17247209
22	.93094934	.25819889	.25819889	.16086125
23	-.73029674	.68313005	0	0
24	-.68313005	.68313005	.25819889	.17247209
25	-.25819889	.68313005	.68313005	.17247209
26	+.25819889	.68313005	.68313005	.17247209
27	+.68313005	.68313005	.25819889	.17247209
28	-.36514835	.93094934	0	0
29	-.25819889	.93094934	.25819889	.16086125
30	+.25819889	.93094934	.25819889	.16086125

*The ordinates include the six special directions in which $\eta = 0$. Ordinate values taken from: Lee, C. E., "The Discrete S_N Approximation to Transport Theory," Lawrence Livermore Report LA2595, 1962.

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