ADVANCED PULVERIZED COAL COMBUSTOR FOR
CONTROL OF NO_x EMISSIONS

FIRST QUARTERLY REPORT

for the period

24 September 1980 to 24 December 1980

R. Pam, E. K. Chu, J. T. Kelly

January 30, 1981

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Work Performed Under Contract

DE-AC22-80PC30296

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ABSTRACT

The first quarter results under the Advanced Pulverized Coal Combustor for Control of NO_x Emissions Program (DOE Contract DE-AC22-80PC30296) are reported. A preliminary gas phase reaction model for predicting fuel NO_x formation during combustion of methane fuel has been constructed. Predictions of NO_x formation under stirred reactor conditions agree with existing experimental data. Thermal NO_x and coal reaction data will be developed and verified during the next reporting period.

Progress has been made in formulating the changes necessary to upgrade the Acurex PROF code for use as the comprehensive data analysis tool in this program. The radiation modeling and the incorporation of the needed modifications into the PROF code will occur during the next reporting period.

During this reporting period, the idealized combustor was designed, and requests for bids to fabricate the combustor were submitted. Combustor fabrication will be completed during the next reporting period.

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TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
Abstract	iii
1 CONTRACT OBJECTIVES	1
2 CONTRACT TASKS	1
2.1 Analytical Model (Task 1.1).	1
2.1.1 Base Model Selection (Task 1.1.2)	2
2.1.2 Data Analysis Model Formulation (Task 1.1.2)	9
2.1.3 Kinetic Modeling (Task 1.1.1)	17
2.2 Combustor Design and Fabrication (Task 1.2)	32
REFERENCES	44

1. CONTRACT OBJECTIVES

The objective of the proposed program is to quantify and define, in terms of kinetic mechanisms and rates, the pulverized coal NO_x emission control benefits of fuel staging. A well defined experimental combustor, incorporating fuel staging, will be built and a comprehensive computer model constructed to allow mechanisms and rates to be extracted from the experimental data. Experiments are proposed in which fuel and air injection parameters will be varied to determine the effect of first and second stage fuel loading ratio on NO_x emissions and combustion.

The computer analysis of the resulting data will yield quasi-global kinetic rates and mechanisms for the process. These rates can ultimately be used in a realistic engineering model to help guide industrial combustor designers.

The characterization of the fuel staging NO_x reduction process in pulverized coal combustion will allow more flexibility in designing low NO_x combustors. The increased flexibility will help overcome industrial combustor configurational, volumetric, and material constraints limiting present NO_x control techniques.

2. CONTRACT TASKS

During the first quarter of this project, progress was made in data analysis model formulation and combustor design. This progress is discussed in the following subsections.

2.1 Analytical Model (Task 1.1)

The objective of this task is to create a comprehensive data analysis tool to develop pulverized coal combustion and NO_x formation kinetic mechanisms and rates from the idealized combustor data.

During the first quarter of this program, the computer model used as the base for the comprehensive data analysis model was defined. In addition, progress was made in formulating the modifications needed to upgrade the base model for use in this program. The following subsections will describe the base computer model selection and the progress made in formulating the base model upgrades.

2.1.1 Base Model Selection (Task 1.1.2)

During this reporting period, a brief review of previous coal combustion and pollutant formation analytical models was undertaken to define a model which could be used as a base for the comprehensive data analysis tool. At the beginning of the review, all of the important processes needed to accurately model the idealized combustor coal combustion and pollutant formation events were identified. These processes are listed in Table 1. The number and complexity of these processes requires that a detailed computer code be applied to model these processes.

Examining the combustor design, as given in Figure 1, it can be seen that the overall combustion process consists of (1) an initial premixed fuel/air combustion in stage 1, (2) the mixing of fuel, air, and combustion products at station 2, (3) combustion of this mixture in stage 2, (4) addition of the air required to complete combustion at station 3, and (5) completion of combustion of this mixture in stage 3. Therefore, we have mixing processes at stations 2 and 3 with essentially plug flow occurring between mixing stations.

Based on simple calculations made in the combustor design task, it was concluded that fuel/air combustion product mixing at the staging locations along the combustor length would be rapid compared to chemical event times between stage locations. Therefore, it was concluded that the three stages of the idealized combustor could be modeled by assuming premixed initial conditions in each stage followed by a plug flow reacting section until the next stage is reached.

Figure 1. Combustor breakdown.

TABLE 1. COAL COMBUSTION AND POLLUTANT FORMATION PROCESSES

- Heat and Mass Transfer
 - Upstream diffusion of heat and reactive species in the gas phase
 - Particle to particle radiative heat transfer
 - Heat convection and radiation to combustor walls
 - Particle/gas heat and mass transfer for groups of different particle sizes
- Thermal Decomposition of Particles
 - Coal volatiles evolution and char formation
 - Fast secondary reactions
 - Products of secondary reactions
- Char Oxidation
 - Surface Reactions
- Gas Phase Reactions
 - Combustion — pyrolysis, partial oxidation, burnout
 - Pollutant formation/reduction — nitrogen intermediates, terminal paths to NO_x/N_2
- Heterogeneous Pollutant Reduction
 - NO char reduction
 - NO, CO catalysis by solid

Given the processes needed to be modeled, and the plug flow nature of the processes, the main requirements of an adequate model were identified. These are:

- Detailed treatment of chemical and physical events
- Particle and gas property treatment, including several particle size groups
- Upstream feedback of heat and species

These model requirements necessitate the application of a comprehensive computer model, including gas and particle phases, which can treat a multivariable boundary value problem.

With these requirements established, a brief review of existing models was undertaken. The review had the dual purpose of finding an available base model and getting information on how detailed coal combustion chemical and physical processes are modeled by various investigators.

Table 2 lists a number of coal dust flame propagation models. This table was partially excerpted from a publication by Smoot (Reference 1) in which a comprehensive review of these models was undertaken. Propagating flame models are relevant to the idealized combustor since a coordinate transformation to the flame front and inclusion of proper wall and upstream boundary conditions allows application of these methods to the current problem of interest.

Another candidate model for use in the program is the Acurex-developed and delivered PROF code (Reference 2). As explained in the program proposal, this code satisfies the detailed chemistry and physical events and upstream heat and mass transfer modeling requirements of the comprehensive model. However, the code does not presently include particle/gas effects. The lack of treatment of particle/gas effects in the PROF code was evaluated relative to the modeling deficiencies of other potentially applicable models to determine the best base model upon which to build the comprehensive data analysis tool.

TABLE 2. SUMMARY OF SELECTED THEORIES FOR PREMIXED LAMINAR PROPAGATING COAL-AIR FLAMES

No.	Reference	Date	Assumptions/Basis	Advances	Evaluation/Limitations
1.	Nusselt (a) Traustel (b)	1924 1941	Plane flame radiation to premixed system	First theory	No comparisons with measurements
2.	Cassell et al. (c,d)	1949 1956	Radiation and conduction to incoming gas; modified gaseous theory	Added conductive heat transfer	Not readily usable for quantitative predictions
3.	Essenhigh and Csaba (e,f)	1964	Radiative transfer to incoming mixture, equal gas-solid velocities; specified coal ignition temperatures; no combustion during preheat	Different gas and particle temperature; finite ignition distance	Predicts higher v_f for smaller coal, increased O_2 and larger ignition distance, but predicts thick flames not observed
4.	Bhaduri, Bandyopadhyay (g)	1971	Radiative transfer with reaction; for low volatile coals or chars; no heat conduction or scattering	Heat generation due to char oxidation	Predicts little dependence of particle size on v_f which is not observed; no direct comparisons with measurements.
5.	Palmer, Seery Marshall (h,i)	1962 1964	Radiative and conductive effects both considered together with coal devolatilization	Approximate treatment of coal devolatilization and gas phase reaction	Requires coal ignition temperature; predicts about correct effect of % O_2 on v_f .
6.	Smoot, et al. (j,k)	1974 1976 1979	Unsteady state, radiation, conduction, diffusion, volatiles combustion, char oxidation; equal gas-particle velocities, no scattering or gas radiation	Multiple particle sizes, generalized treatment of coal kinetics, molecular diffusion, gaseous combustion	Predicts observed effects of coal concentration, size & size distribution; difficult convergence for very lean or very rich flames; of questionable applicability to thick flames
7.	Krier and Krazinski (l)	1974	Generalized formulation of steady-state equations	Gas-particle drag	No solution reported and no comparison with data
8.	Krazinski,* et al., (m)	1977	Radiation, conduction, char oxidation; no devolatilization, equal gas-particle velocity.	Radiative scattering	Limited to low volatile coals; no available measurements to confirm predictions; predicts very small dependence of v_f on d_p .
9.	Kansa and Perlee	1980	Unsteady state, microscopic treatment of a single particle combustion; no macro-physical process between particles except for radiation, equal gas-particle velocity	Added radiative heat exchange while maintaining detailed treatment of single particle combustion	Not applicable to flames near stoichiometric ratios, i.e., only applicable to thick flame

*Additional work by these authors was recently published in Comb. Sci. Tech. 5, 31 (1979), which includes code predictions for high and low volatile coals and comparisons with thin and thick coal dust flames.

REFERENCES FOR TABLE 2

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- m. Krazinski, J. L., Backius, R. O., and Krier, H., "Modeling Coal-Dust-Air Flames with Radiative Transport," Spring Meeting Central States Section, Combustion Institute, Cleveland, Ohio (March 1977).

Examination of the existing models listed in Table 2 indicated that Smoot's model, with some modification, could be applied to the case of interest. The other models did not include sufficient detail to model combustion and pollutant formation events.

Comparing Smoot's model to the PROF code model, it was found that gas phase chemical reaction and transport treatments were not significantly different. Smoot's model does include particle effects, including radiation, whereas the PROF code does not presently include these effects. Since Smoot's model is for propagating flames, it utilizes a time dependent formulation which relaxes to a steady state. Also, the model does not fully include all of the needed wall boundary and flameholder effects.

The PROF code is a steady state combustion procedure which does include all of the wall and flameholder effects of interest. Also, because PROF is a steady state combustion procedure, a very rapid predictor-corrector convergence scheme has been built into the code. This results in solution computer times much lower than unsteady relaxation methods. Therefore, the PROF code should be more efficient of computer time than Smoot's time-dependent model.

Besides these efficiency and wall effects modeling advantages of the PROF code, the use of this model in this program also has the advantages of (1) sophisticated chemical kinetic rescue logic procedures to ensure solution convergence, (2) generalized chemistry solver to handle any number of chemical reactions, (3) plug and stirred as well as flame modeling options, and (4) Acurex personnel experienced in the modification and use of the code on complex combustion problems. In addition, particle/gas effects and radiation should be fairly straightforward to integrate into PROF since Acurex personnel have performed a similar function in developing the FRCOL code. The FRCOL code has been described in the program proposal.

Based on the above arguments, the PROF code has been selected for use as the base model for the comprehensive data analysis tool.

2.1.2 Data Analysis Model Formulation (Task 1.1.2)

During this reporting period, progress was made in formulating the comprehensive data analysis model. As discussed above, the Acurex PROF code will be used as a base for this model. The modifications necessary to upgrade the PROF code for use in this program have been formulated. During the next reporting period, these modifications will be incorporated into the code.

The data analysis model must include all of the processes listed in Table 1. In addition, in order for the describing equations to be amenable to numerical solution, several additional simplifying assumptions are required. These are given in Table 3.

It should be noted that, if needed, turbulent flow transport properties could be easily substituted for laminar properties in the model. Also of special note is the assumption of transport coefficients for radial heat and mass transfer. Radial transport, for this essentially one-dimensional problem, should not be dominant. To include a detailed treatment of radial transport would complicate the solution procedure tremendously (i.e., problem would require partial rather than ordinary differential equation treatment. Therefore, the transport coefficient approach was selected as a best compromise to give adequate modeling for a minimum of computational effort. With this approach the describing equations remain one dimensional.

TABLE 3. DATA ANALYSIS MODEL ASSUMPTIONS

- Steady State
- Laminar Flow (could be modified if needed)
- Particle/Gas Dynamic Equilibrium
- Initial uniform Mixture
- Negligible gravity effects
- Spherical Particles
- Continuum of Gases and Particles
- Constant Pressure
- Radial Heat and Mass Transfer by Transport Coefficient Approach

Given the processes and the assumptions in Tables 1 and 3 respectively, the governing equations for the data analysis model can be written as follows. The symbols used in these equations are described in Table 4.

Gas Phase Energy Conservation

$$\dot{m} \frac{dh}{dx} = A\dot{Q} - \frac{d}{dx} \left(\sum_i A J_i h_i + A k \frac{dT}{dx} \right) - C_w \dot{Q}_w$$

$$\left[- A \sum_j \dot{Q}_{c_j} - \sum_j \frac{d\dot{m}_{p_j}}{dx} (h_{p_j} - h) \right] \leftarrow \text{New terms}$$

Gas Phase Species Conservation

$$\dot{m} \frac{dY_i}{dx} = A W_i - \frac{d(A J_i)}{dx} - C_w J_{w_i}$$

$$\left[\sum_j \frac{d\dot{m}_{p_j}}{dx} (Y_{p_{ij}} - Y_i) - A J_{p_i} \right] \leftarrow \text{New terms}$$

The gas thermal and transport properties for these equations are identical to those used in the PROF code. The details of these property calculations are given in Reference 2. The form of the gas and wall heat and mass flux terms and gas phase reactions are also identical to those in the PROF code and are given in Reference 2.

TABLE 4. LIST OF SYMBOLS

A	combustor cross sectional area	cm^2
A_p	particle surface area	cm^2
C_p	specific heat	cal/gm
d_j	particle diameter	cm
h	enthalpy of bulk gas	cal/gm
h_i	enthalpy of bulk gas species i	cal/gm
h_{p_j}	gas enthalpy at particle j surface	cal/gm
$h_{p_j}^*$	condensed phase enthalpy of particle j	cal/gm
J_i	axial species flux	gm/sec cm^3
$J_{p_{ij}}$	species flux to particles	gm/sec cm^3
J_w	wall species flux	gm/sec cm^2
k	thermal conductivity of bulk gas	cal/sec cm K
$\dot{m}$	mass rate of gas	gm/sec
$\dot{m}_{p_j}$	mass rate of particles j	gm/sec
n_j	number of particles per volume	cm^{-3}
$\dot{Q}$	gas volumetric heat loss	$\text{cal/cm}^3\text{sec}$
$\dot{Q}_{c_j}$	particle/gas heat transfer	$\text{cal/cm}^3\text{sec}$
$\dot{Q}_{r_j}$	particle to particle radiative transfer	$\text{cal/cm}^3\text{sec}$
$\dot{Q}_w$	combustor wall heat transfer	$\text{cal/cm}^2\text{sec}$
$\dot{r}_j'''$	mass rate of gas from particles	$\text{gm/cm}^3\text{sec}$
$\dot{R}_c''$	heterogeneous oxidation rate	$\text{g/cm}^2\text{-s}$
$\dot{R}_v$	devolatilization rate	g/s
$\dot{R}_w^*$	moisture vaporization rate	$\text{g/cm}^2\text{-s}$

T	temperature of gas	K
T_{p_j}	temperature of particle	K
W_i	gas phase reaction contribution to species i	gm/cm ³ sec
$W_{p_{mj}}$	particle reaction rate of mth reaction	gm/cm ³ sec
x	axial distance	cm
Y_i	mass fraction of species i	

Particle Energy Conservation

$$\dot{m}_{p_j} \frac{dh_{p_j}^*}{dx} = \dot{Q}_{c_j} A + \frac{d\dot{m}_{p_j}}{dx} (h_{p_j} - h_{p_j}^*) + \dot{Q}_{r_j} A \quad \leftarrow \text{New terms}$$

Particle Mass Conservation

$$\frac{d\dot{m}_{p_j}}{dx} = -\dot{A}r_j''' \quad \leftarrow \text{New terms}$$

In calculating particle properties, particle groups will be tracked individually in the combustor. The number of particles will not change unless a total group of particles becomes fully consumed. These particles will then disappear as a group.

In addition to the PROF auxiliary equations, described in Reference 2, a number of additional auxiliary equations are needed to complete the model definition. These are given below.

Particle Reaction Model

$$\frac{\dot{r}_j'''}{\dot{n}_j} = \dot{R}_c A_p + \dot{R}_v + \dot{R}_w A_p$$

In the particle reaction model, heterogeneous and volatilization reactions are generalized and can include reactions with CO_2 , H_2O , O_2 , NO

and volatilization of C, H, O, N, S elements. This generalization permits inclusion of all important reactions into the data analysis procedure.

Convective Heat/Mass Transfer Model (Gas-Particle)

Heat transfer

$$Nu = 2 = \frac{h_{c,j} d_j}{k} \quad - \text{small spherical particle assumption}$$

Blowing correction $B'_j / (\exp B'_j - 1)$

$$\begin{aligned} \dot{Q}_{c,j} &= h_{c,j} A_{p,j} n_j (T - T_{p,j}) \frac{B'_j}{\exp B'_j - 1} \\ &= 2k\pi d_j n_j (T - T_{p,j}) \frac{B'_j}{\exp B'_j - 1} \end{aligned}$$

where the blowing parameter is defined as:

$$B'_j \equiv \frac{\frac{\dot{m}_j}{A_{p,j} n_j}}{\rho_e u_e C_{m,j}}$$

$$\rho_e u_e C_{m,j} = h_{c,j} / C_p (Le)^{2/3} \quad - \text{heat to mass transfer analogy}$$

Mass transfer

$$\begin{aligned} J_{p_{i,j}} &= \rho_e u_e C_{m,j} A_{p,j} n_j (Y_i - Y_{p_{i,j}}) \frac{B'_j}{\exp B'_j - 1} \\ J_{p_{i,j}} &= \frac{2k}{C_p} (Le)^{2/3} \pi d_j n_j (Y_i - Y_{p_{i,j}}) \frac{B'_j}{\exp B'_j - 1} \end{aligned}$$

In the convective particle heat and mass transfer equations, the small spherical particle assumption is used giving a Nusselt number of two. This coefficient is modified by a correction term for surface blowing. This correction accounts for the effect of volatile evolution on heat and mass transfer to the particle surface. For coal in which volatiles form discrete jets from the particle rather than a uniform outgassing, this blowing correction can be deactivated.

An analogy between heat and mass transfer is used to develop mass transfer coefficients from known heat transfer coefficients.

Species Equation on Particle Surface

$$J_{p_{ij}} - \dot{r}_j'' Y_{p_{ij}} + n_j \sum_m (\nu_{m,i}^P - \nu_{m,i}^R) w_{p_{mj}} = 0$$

In the species equation at the particle surface, the surface reaction term, $w_{p_{mj}}$, is general and can accommodate both char consumption and pollutant reduction reactions.

Radiation Model

Presently, there exists three methods for the calculation of radiation heat transfer within an enclosure containing an absorbing medium: zone method,

Monte Carlo method, and flux method. The zone method was first suggested by Hottel and his coworkers (Reference 3), and was typically used when the combustion and flow patterns are given. In principle, a simultaneous solution of all variables is possible, but the computation time required may not be economical. The Monte Carlo method is probably the most sophisticated of the three methods. Like the zone method, however, its computational efficiency is poor. Since we are dealing with a complex chemical kinetic problem, computational efficiency is a prime requirement of the model.

The flux method was initially introduced by Schuster (Reference 4) for astrophysical applications, and was later advocated by Spalding for solving combustion problems. One of the advantages of the flux method is that it replaces the exact integro-differential equations of radiative heat transfer (the main cause of poor computational efficiency) by approximate differential ones. This transformation reduces the required solution matrix into a sparse one. This is compatible with the PROF code sparse matrix formulation and thus allows the use of an efficient block tri-diagonal matrix inversion scheme. In addition, the effects of scattering could also be included without much complication. This method has its limitations for multidimensional and complicated geometry problems. However, for a one-dimensional and simple geometry problem, which is the current application, this method was proved to be adequate (References 5, 6, and 7). Therefore, the flux method was selected for incorporation into the data analysis model. The details of the formulation of this technique will be given in the next progress report.

In the conservation equations, those terms which represent additions to the PROF code formulation have been put in parentheses. In the next reporting period, these terms will be translated into Fortran V and incorporated into the PROF code. It is anticipated that the particle/gas terms will be the first terms incorporated into the PROF code. Once these terms are verified, the radiation terms will then be incorporated into the code and verified. Using this two-step approach will make code debugging easier.

2.1.3 Kinetic Modeling (Task 1.1.1)

The NO formation process from fuel bound nitrogen in coal has been postulated to occur by various homogeneous and heterogeneous pathways as illustrated in Figure 2. Ideally, one would like to model the process in terms of elementary reactions. Unfortunately, such detailed knowledge is still under development and may require some time before a thorough understanding can be achieved. On the other hand, if a one-step global reaction were assumed, it would be so crude that mechanistic information regarding the formation of NO may not be attained.

Since an analytical design tool for low NO_x burner development is desired, the objective of this program is to develop a quasi-global kinetic model. In this model, the volatilization of coal and secondary reactions of volatilization products are assumed to occur in a small number of global steps while the subsequent sequence of reactions of low molecular weight products are expressed in terms of elementary reactions. A schematic of a possible quasi-global kinetic model is that of Figure 2. Here the assumption is made that, as the coal volatilizes into the hot surroundings, the high molecular weight volatile fractions pyrolyze rapidly to form low molecular weight species. There is evidence to show that pyrolysis reactions are very rapid (References 1 and 8) and as a first approximation, we can neglect intermediate steps and postulate that species such as HCN, NH_3 , C_2H_2 , C_2H_4 , CO and H_2 are formed almost instantaneously from the volatilized compounds. Once the volatile components are cast in this form, elementary reaction sets available for the postulated species can be used as a first order model.

The development of the present kinetic model is comprised of four steps:

- Survey study
- Kinetic model formulation
- Model verification
- Final model correlation

Figure 2. Schematic of fuel-N conversion process.

The survey study is designed to:

- Assess the state of the art of kinetic modeling, e.g., global reactions versus elementary reactions
- Compile accepted rate data for pertinent reactions
- Compile experimental data which could be used for model verification purposes

Based on the inputs from the survey study, the second step is to formulate the kinetic model. This entails the following activities:

- Define reaction subsets of the kinetic model
- Prioritize the level of importance for each reaction subset
- Determine the level of analytical approach for each reaction subset based on model requirements

To verify the validity of the kinetic model, the third step is to exercise each reaction subset to predict results that are consistent with existing experimental data. The PROF code (Reference 2) will be used as the base for the data analysis tool. Upon the completion of these verification studies, the final test of the model will be to compare its predictions with the advanced coal combustor data. Good agreement will insure that proper links between reaction subsets have been modeled properly.

Progress in kinetic model formulation is summarized below.

Literature Survey and Formulation of the Kinetic Model

As mentioned earlier, a quasi-global kinetic model approach is applied to model the fuel nitrogen conversion process. It has the following general form.

This approach includes the following assumptions:

- The initial degradation of gaseous volatiles via pyrolysis and oxidation is rapid in comparison to other simultaneously ongoing reactions
- The initial decomposition products may be represented by a relatively small set of light hydrocarbon and nitrogenous species
- Hydrocarbons which could react with nitrogenous species are limited to C_1 and, at most, C_2 type species

The first two assumptions are easily justified. Based on ignition delay experiments (References 9 to 11), it was found that the ignition delay time for both aliphatic and aromatic hydrocarbons is of the order of microseconds. The devolatilization and the NO destruction reactions, on the other hand, are of the order of milliseconds -- orders of magnitude slower than the volatile

degradation reactions. Thus, the rate step for the volatile degradation reactions may not be of great importance. In addition, some references cited, although inconclusive, indicate that the fuel nitrogen in these devolatilization products appear rapidly and nearly completely as HCN and NH_3 intermediates (Reference 12). The third assumption, however, is uncertain at present because of the complexities involved when higher order hydrocarbons are considered. Furthermore, reaction mechanisms involving C_2 hydrocarbons are still under development. The compilation of rate data for the formulation of the kinetic model will be completed in the second quarter. The current status is summarized in Table 5.

Coal reactions include evolution of products (gases and tar) from rapid particle heating and heterogeneous combustion of coal particles. These two processes typically occur in sequence, but may occur simultaneously or even in reverse order under some conditions (References 13 and 14). In addition, these two processes are dependent on each other. Heterogeneous combustion requires oxidants on the particle surface. Volatiles evolving from the surface not only reduce the mass transfer rate of oxidants to the surface, but also consume the oxidants if gas phase combustion occurs, thereby depleting the availability of oxidant to the surface. Recently, the occurrence of gas phase volatile combustion has been confirmed through direct observations (References 15 and 16). On the other hand, heterogeneous combustion produces heat for the devolatilization process during the early stage. Thus, for the completeness of the model, heterogeneous combustion of coal particles as well as the mutual influences of the two processes must be included. Models to account for these effects are in existence and are described in References 7, 13 and 17.

A recent review on the modeling of devolatilization was given by Anthony (Reference 18). The two most common techniques for predicting devolatilization rates are (1) a method based on a simple rate equation with a distribution of activation energies, and (2) the two-component model:

where α_1 and α_2 are stoichiometric coefficients, V's are volatiles, S is residue solid, and k_1 and k_2 are reaction rates represented by Arrhenius expressions. The two-component model accounts for the impact of heating rate and final temperature on the rate and extent of devolatilization. This model is generally adequate for pulverized coal combustion at moderate and high temperatures. This model, or a modification for multicomponent devolatilization, will be used in the present model.

Regarding the formation of NO, the evolution of fuel nitrogen relative to hydrocarbons from the coal requires special attention. Existing data show that nitrogen evolution is somewhat more temperature sensitive than the liberation of carbon. It evolves more slowly than carbon at low temperatures and more rapidly at high temperatures (References 19 to 21). This behavior is believed to be related to the coal structure. The nitrogen in coal is mostly incorporated in the ring structures (References 22 to 30) with possibly small amounts of nitrogen contained in side chains (References 31 to 33). Based on this coal structure, the following speculative picture for the behavior of coal nitrogen was postulated:

- At low temperatures, pyrolysis of coal is expected to be dominated by the release of nitrogen from side chains, and thus nitrogen is emitted more slowly than carbon
- At moderate or high temperatures, the aromatic rings will decompose and release nitrogen. However, secondary cracking reactions will also occur leading to char formation. Very small or negligible amounts of nitrogen are expected to remain with the char.

Model Verification

As shown in Table 5, elementary reaction sets are available for a reactive system of C_7 hydrocarbons, nitrogen, and oxygen species. In fact, a comprehensive elementary reaction set has been formulated by Energy and Environmental Research Corporation under EPA's funding (Reference 34). The reaction set, shown in Table 6, consists of 136 elementary reactions, and has been applied successfully in predicting NO formation of simple model fuel nitrogen, e.g., NH_3 . To take advantage of this effort, this reaction set is used as our baseline set. The baseline will be expanded to incorporate other reaction mechanisms occurring during gas phase volatiles combustion.

A preliminary evaluation of the baseline reaction set was performed during the quarter by predicting jet-stirred reactor data for methane/air doped with ammonia, nitric oxide, and cyanogen (Reference 35). The comparisons are shown in Figures 3 to 6. Good agreement has been obtained with ammonia and cyanogen as the additive. With NO, however, the agreement was not as good under fuel-rich conditions. The model tends to underpredict NO emissions. Figure 6 shows the comparison of measured and predicted flame temperatures. Again, good agreement was obtained. As a preliminary evaluation, the results are encouraging. To further improve this reaction set, the following efforts are required:

- Identify the dominant reactions for NO formation and adjust the rate data (if necessary)
- Check the accuracy of the thermochemical data
- Introduce additional reactions (if needed)

This work will be completed during the second quarter.

During the next reporting period and subsequent data analysis tasks, the above kinetic model formulation will be further developed and refined to produce a valid data analysis kinetic model.

TABLE 5. FORMULATION OF PRELIMINARY KINETICS MODEL

Class of Reactions	Description of Reactions	Modeling Approach	Existence of Data
Coal devolatilization	Coal $\xrightarrow{\text{heat}}$ char + volatiles	One/two step global reactions	Lots
Volatile combustion	Volatiles + O ₂ → CO + CO ₂ + H ₂ + HC's + H ₂ O	One step global reactions	Some
Coal heterogeneous combustion	Coal + O ₂ → CO + CO ₂ + H ₂ + HC's + H ₂ O	One step global reaction	Some
Simple HC's combustion	Simple HC's + O ₂ → CO + H ₂	One step global reaction (C _n), Elementary reactions (C ₁)	C ₁ -Lots C ₂ , C _n -scarce
H ₂ , CO combustion	H ₂ , CO + O ₂ → CO ₂ + H ₂ O	Elementary reactions	Lots
NO formation and destruction	Fuel-N → HCN + ...	One step global reaction	Scarce
	HCN → NH _i + ...	Elementary reactions	Some
	NH _i + O ₂ → NO + N ₂ + ...	Elementary reactions	Some
	NO + CO $\xrightarrow{\text{char}}$ N ₂ + ...	One step global reactions	Some
	NO + HC's → HCN + ...	Elementary reactions	C ₁ -Lots C _n -Scarce

TABLE 6. KINETIC REACTION DATA (REFERENCE 35)

NUMBER OF REACTIONS=136										INDIVIDUAL THIRD BODY EFFIC.			
M	REACTION			PRL EXP FACTOR (MOLE-CM-S)	TEMP EXP	ACTIVATION (KCAL/MOLE)	NAME1	ETH1	NAME2	ETH2			
1	CH4 +	+M	---	CH3 +H	.1000+18+ 0.	.000	48.4000	.000	.000	.000			
2	CH3O+	+M	---	CH2O+H	.4000+01+40.	-7.500	22.6000	.000	.000	.000			
3	CH2O+	+M	---	CHO +H	.3160+18+ 0.	.000	87.0000	.000	.000	.000			
4	CHO +	+M	---	CO +H	.2500+21+ 0.	-1.500	16.0000	.000	.000	.000			
5	CO2 +	+M	---	CO +O	.1000+18+ 0.	.000	100.0000	.000	.000	.000			
6	H +O	+M	---	OH +	.1000+19+ 0.	-1.000	.0000	.000	.000	.000			
7	H +O2	+M	---	HO2 +	.3000+18+ 0.	.000	-1.0000	.000	.000	.000			
8	OH +O	+M	---	HO2 +	.1600+21+ 0.	-1.500	.0000	.000	.000	.000			
9	H2 +	+M	---	H +H	.2000+16+ 0.	.070	103.0000	.000	.000	.000			
10	H2O +	+M	---	OH +H	.2300+23+ 0.	-2.000	122.6000	.000	.000	.000			
11	NO +O	+M	---	NO2 +	.1380+22+ 0.	-1.820	.0000	.000	.000	.000			
12	N2 +	+M	---	N +N	.4000+22+ 0.	-1.600	225.0000	.000	.000	.000			
13	O +O	+M	---	O2 +	.1000+19+ 0.	-1.000	.0000	.000	.000	.000			
14	CH4 +CH2 +	---	---	CH3 +CH3	.1260+13+ 0.	.700	20.0000	.000	.000	.000			
15	CH4 +H +	---	---	CH3 +H2	.5000+11+ 0.	1.000	10.0000	.000	.000	.000			
16	CH4 +OH +	---	---	CH3 +H2O	.3000+14+ 0.	.000	5.0000	.000	.000	.000			
17	CH4 +O +	---	---	CH3 +OH	.1900+15+ 0.	.000	11.7000	.000	.000	.000			
18	CH3 +CH2O+	---	---	CH4 +CHO	.2000+12+ 0.	.000	6.5000	.000	.000	.000			
19	CH3 +OH +	---	---	CH2 +H2O	.2000+12+ 0.	.700	2.0000	.000	.000	.000			
20	CH3 +OH +	---	---	CH3O+H	.6310+12+ 0.	.000	.0000	.000	.000	.000			
21	CH3 +HO2 +	---	---	CH4 +O2	.1000+12+ 0.	.500	6.0000	.000	.000	.000			
22	CH3 +O +	---	---	CH2O+H	.2600+15+ 0.	.000	2.0000	.000	.000	.000			
23	CH3 +O2 +	---	---	CH2 +HO2	.3160+13+ 0.	.000	69.5000	.000	.000	.000			
24	CH3 +O2 +	---	---	CH2O+OH	.9000+12+ 0.	.000	12.0000	.000	.000	.000			
25	CH3 +O2 +	---	---	CH3O+O	.3500+14+ 0.	.000	28.8000	.000	.000	.000			
26	CH2 +CH2O+	---	---	CH3 +CHO	.2000+12+ 0.	.000	6.5000	.000	.000	.000			
27	CH2 +H +	---	---	CH +H2	.3160+12+ 0.	.700	5.0000	.000	.000	.000			
28	CH2 +OH +	---	---	CH +H2O	.5000+12+ 0.	.500	6.0000	.000	.000	.000			
29	CH2 +OH +	---	---	CH3 +O	.5000+12+ 0.	.500	6.0000	.000	.000	.000			
30	CH2 +OH +	---	---	CH2O+H	.1000+14+ 0.	.000	5.0000	.000	.000	.000			
31	CH2 +H2 +	---	---	CH3 +H	.3000+13+ 0.	.000	7.0000	.000	.000	.000			
32	CH2 +NO +	---	---	CH2O+N	.1600+13+ 0.	.000	7.0000	.000	.000	.000			
33	CH2 +O +	---	---	CHO +H	.5000+12+ 0.	.500	4.0000	.000	.000	.000			
34	CH2 +O2 +	---	---	CH2O+O	.5000+12+ 0.	.500	7.0000	.000	.000	.000			
35	CH +CH4 +	---	---	CH2 +CH3	.1000+13+ 0.	.000	17.1000	.000	.000	.000			
36	CH +CO2 +	---	---	CHO +CO	.1000+11+ 0.	.500	6.0000	.000	.000	.000			
37	CH +OH +	---	---	CHO +H	.5000+12+ 0.	.500	10.0000	.000	.000	.000			
38	CH +HO2 +	---	---	CH2 +O2	.1000+11+ 0.	.500	15.0000	.000	.000	.000			
39	CH +O +	---	---	CO +H	.5000+12+ 0.	.500	.0000	.000	.000	.000			
40	CH +O2 +	---	---	CHO +O	.5000+12+ 0.	.500	6.0000	.000	.000	.000			
41	CH3O+H +	---	---	CH2O+H2	.1000+15+ 0.	.000	.0000	.000	.000	.000			
42	CH3O+OH +	---	---	CH2O+H2O	.3160+14+ 0.	.000	.0000	.000	.000	.000			
43	CH3 +O +	---	---	CH2O+OH	.1000+13+ 0.	.000	.0000	.000	.000	.000			
44	CH3+O2 +	---	---	CH2O+HO2	.1000+13+ 0.	.000	8.0000	.000	.000	.000			
45	CH2O+H +	---	---	CHO +H2	.1260+11+ 0.	1.000	3.2000	.000	.000	.000			
46	CH2O+OH +	---	---	CHO +H2O	.3160+11+ 0.	1.000	.0000	.000	.000	.000			
47	CH2O+O +	---	---	CHO +OH	.2000+12+ 0.	1.000	4.4000	.000	.000	.000			
48	CHO +CHO +	---	---	CH2O+CO	.1600+12+ 0.	.500	.0000	.000	.000	.000			
49	CHO +CH2 +	---	---	CHO +CO	.1600+11+ 0.	.700	1.0000	.000	.000	.000			
50	CHO +CH3 +	---	---	CHO +CO	.3160+12+ 0.	.700	.0000	.000	.000	.000			

TABLE 6. CONTINUED

51	CHO +H +	---	CO +H2	.3000+11+ 0.	1.000	.0000	.000	.000
52	CHO +OH +	---	CO +H2O	.3000+11+ 0.	1.000	.0000	.000	.000
53	CHO +H2 +	---	CH2O +O2	.1000+15+ 0.	.000	3.0000	.000	.000
54	CHO +H +	---	CH +NO	.1000+15+ 0.	.000	4.6000	.000	.000
55	CHO +O +	---	CO +OH	.6310+12+ 0.	1.000	.5000	.000	.000
56	CHO +O +	---	CO2 +H	.3160+12+ 0.	.000	.0000	.000	.000
57	CO +OH +	---	CO2 +H	.1510+08+ 0.	1.500	-.7650	.000	.000
58	CO +H2O2 +	---	CO +O2	.3000+13+ 0.	.000	37.1000	.000	.000
59	CO +O2 +	---	CO2 +O	.3160+13+ 0.	.000	50.0000	.000	.000
60	CO2 +H +	---	CO +NO	.2000+12+ 0.	.500	25.0000	.000	.000
61	H +OH +	---	H2 +O	.2710+18+ 0.	-.990	14.6000	.000	.000
62	H +H2O2 +	---	OH +OH	.2500+15+ 0.	.000	1.0000	.000	.000
63	H +H2O2 +	---	OH +NO	.3160+15+ 0.	.000	1.5000	.000	.000
64	OH +H2 +	---	H +H2O	.2500+14+ 0.	.000	5.2000	.000	.000
65	OH +OH +	---	H2O +O	.6000+13+ 0.	.000	1.0000	.000	.000
66	OH +O +	---	H +O2	.6310+12+ 0.	.500	.0000	.000	.000
67	H2O2 +H +	---	O2 +H2	.2500+14+ 0.	.000	.7000	.000	.000
68	H2O2 +OH +	---	H2O +O2	.5000+14+ 0.	.000	1.0000	.000	.000
69	H2O2 +O +	---	OH +O2	.5000+14+ 0.	.000	1.0000	.000	.000
70	N +OH +	---	NO +H	.6310+12+ 0.	.500	.0000	.000	.000
71	N +NO +	---	N2 +O	.3100+14+ 0.	.000	.3340	.000	.000
72	N +H2O2 +	---	N2 +O2	.1000+13+ 0.	.000	.0000	.000	.000
73	N +H2O2 +	---	NO +NO	.4000+13+ 0.	.000	.0000	.000	.000
74	N +O2 +	---	NO +O	.6000+10+ 0.	1.000	6.3000	.000	.000
75	NO +OH +	---	H2O2 +N	.5000+11+ 0.	.500	96.5000	.000	.000
76	NO +H2O2 +	---	NO2 +OH	.5000+12+ 0.	.500	3.5200	.000	.000
77	NO2 +O +	---	NO +O2	.1000+14+ 0.	.000	1.0000	.000	.000
78	CH +CH3 +	---	CH2 +CH2	.3200+13+ 0.	.000	8.0000	.000	.000
79	H +NO +H	---	HNO +	.2000+17+ 0.	.000	.0000	.000	.000
80	N2O +H	---	N2 +O	.4000+15+ 0.	.000	51.4000	.000	.000
81	CH4 +CN +	---	HCN +CH3	.3160+12+ 0.	.700	5.0000	.000	.000
82	CH3 +CN +	---	HCN +CH2	.1000+12+ 0.	.700	3.0000	.000	.000
83	CH3 +HNO +	---	CH4 +NO	.5000+12+ 0.	.500	.0000	.000	.000
84	CH2 +CN +	---	CH +HCN	.3160+13+ 0.	.000	5.0000	.000	.000
85	CH2 +N2 +	---	HCN +NH	.1000+15+ 0.	.000	60.0000	.000	.000
86	CH3O+N +	---	CH2O+NH	.1000+15+ 0.	.000	.0000	.000	.000
87	CH3O+NO +	---	HNO +CH2O	.5000+12+ 0.	.500	4.2300	.000	.000
88	CHO +HNO +	---	CH2O+NO	.3160+12+ 0.	.500	.0000	.000	.000
89	CHO +N +	---	HCN +O	.1000+15+ 0.	.000	.0000	.000	.000
90	CHO +N +	---	CO +NH	.2000+12+ 0.	.500	2.0000	.000	.000
91	CHO +NO +	---	CO +HNO	.2000+12+ 0.	.500	2.0000	.000	.000
92	HCN +OH +	---	CN +H2O	.2000+12+ 0.	.600	5.0000	.000	.000
93	HCH +H +	---	CH +H2	.2500+12+ 0.	.000	16.0000	.000	.000
94	HCH +O +	---	CH +NO	.1000+15+ 0.	.000	72.0000	.000	.000
95	CH +CO2 +	---	NCO +CO	.3720+13+ 0.	.000	.0000	.000	.000
96	CH +OH +	---	HCN +O	.3160+13+ 0.	.000	3.0000	.000	.000
97	CH +OH +	---	HCO +H	.6200+14+ 0.	.000	.0000	.000	.000
98	CH +H2 +	---	HCO +H	.6200+13+ 0.	.000	5.3000	.000	.000
99	CH +H +	---	CH +H2	.1000+15+ 0.	.000	46.0000	.000	.000
100	CH +H2 +	---	CO +H2	.3000+12+ 0.	.000	.0000	.000	.000
101	CH +O +	---	CO +H	.6310+12+ 0.	.500	.0000	.000	.000
102	CH +H2 +	---	CO +H2	.3000+12+ 0.	.000	.0000	.000	.000
103	CH +O +	---	CH +H	.5000+12+ 0.	.500	6.2700	.000	.000
104	CH +H2O +	---	CH2 +H2O	.1000+12+ 0.	.500	7.0000	.000	.000
105	CH +H2O +	---	H2 +H2O	.1000+12+ 0.	.000	2.5000	.000	.000
106	CH +H2O +	---	OH +H2O	.2000+12+ 0.	.500	25.0000	.000	.000
107	CH +H2O +	---	OH +H2O	.2000+12+ 0.	.000	15.0000	.000	.000

TABLE 6. CONCLUDED

108	H	+N2O	+	---	NH	+NO	.1000+12+ 0.	.500	30.0000	.000	.000
109	HNO	+HNO	+	---	N2O	+H2O	.1000+11+ 0.	.500	41.5500	.000	.000
110	HNO	+OH	+	---	H2O	+NO	.1000+13+ 0.	.000	1.0000	.000	.000
111	HNO	+NO	+	---	OH	+N2O	.2000+13+ 0.	.000	26.0000	.000	.000
112	HNO	+O	+	---	OH	+NO	.5000+12+ 0.	.500	.0000	.000	.000
113	HNO	+O	+	---	NH	+O2	.1000+12+ 0.	.500	7.0000	.000	.000
114	OH	+N2O	+	---	H02	+N2	.5160+14+ 0.	.000	15.0000	.000	.000
115	NH	+H	+	---	N	+H2	.5310+12+ 0.	.500	8.0000	.000	.000
116	NH	+OH	+	---	H2O	+N	.5000+12+ 0.	.500	2.0000	.000	.000
117	NH	+OH	+	---	NO	+H2	.5000+12+ 0.	.500	2.0000	.000	.000
118	NH	+O	+	---	N	+OH	.1700+11+ 0.	.700	.1000	.000	.000
119	NH	+O	+	---	NO	+H	.6310+12+ 0.	.500	.0000	.000	.000
120	OH	+N	+	---	H	+N2	.6000+12+ 0.	.500	.0000	.000	.000
121	OH	+NH	+	---	N2	+H2	.5600+12+ 0.	.550	1.9500	.000	.000
122	NH	+NO	+	---	N2	+OH	.2400+13+ 0.	.000	.0000	.000	.000
123	H02	+H	+	---	NH	+H2	.1400+12+ 0.	.670	4.3500	.000	.000
124	H02	+OH	+	---	NH	+H2O	.5000+11+ 0.	.680	1.5000	.000	.000
125	H02	+O	+	---	NH	+OH	.9200+12+ 0.	.500	.0000	.000	.000
126	H02	+O2	+	---	NH	+H02	.1000+14+ 0.	.000	50.5000	.000	.000
127	H02	+NH2	+	---	NH3	+NH	.1700+12+ 0.	.650	3.6000	.000	.000
128	NH2	+NO	+	---	N2	+H2O	.5000+13+ 0.	.000	.0000	.000	.000
129	NH3	+OH	+	---	NH2	+H2O	.1260+11+ 0.	.680	1.1000	.000	.000
130	NH3	+H	+	---	NH2	+H2	.1900+12+ 0.	.670	3.4000	.000	.000
131	NH3	+O	+	---	NH2	+OH	.1500+13+ 0.	.000	6.0000	.000	.000
132	NH3	+O2	+	---	NH2	+H02	.5000+12+ 0.	.500	56.0000	.000	.000
133	N2O	+O	+	---	N2	+O2	.1000+15+ 0.	.000	28.0000	.000	.000
134	N2O	+O	+	---	NO	+NO	.1000+15+ 0.	.000	28.0000	.000	.000
135	NO	+N2O	+	---	NO2	+N2	.2000+15+ 0.	.000	50.0000	.000	.000
136	NO	+NO2	+	---	N2O	+O2	.1000+13+ 0.	.000	60.0000	.000	.000

Figure 3. Conversion of NH_3 to NO_x .

Figure 4. Conversion of $(CN)_2$ to NO_x .

Figure 5. Retention of added NO.

Figure 6. Temperature versus mixture ratio in jet-stirred combustor.

2.2 Combustor Design and Fabrication (Task 1.2)

During this reporting period, the idealized plug flow combustor was designed, and fabrication begun. The principal components include the combustor housing with refractory lining; premixed burner; water-cooled, water-quenched sample probe; suction pyrometer; backfire burner system; and Acurex-supplied ancillary air, fuel, exhaust and cooling water systems. Figure 7 shows the combustor assembly and feed systems. A description of the combustor follows.

Combustor

The combustor is a down-fired, cylindrical chamber 8 inches in internal diameter and 72 inches long. The refractory lining is composed of an 8-inch layer of 3400°F, high conductivity castable refractory, 4 inches of a medium conductivity, 3000°F castable refractory, and 2 inches of fiber insulating blanket. This arrangement provides hot walls in the combustion zone, while maintaining the outer steel shell at safe temperatures. The outer shell is 36 inches in diameter.

Figure 1 shows the combustor details. The backfire burner ports can be seen located within the refractory, centered at a radius of 7-1/2 inches from the combustor centerline. These ports will contain the hot combustion products from the gas fired backfire burners and will be used to help reduce heat losses and maintain high combustor temperature.

One and three-quarter inch ports for the sample probe, suction pyrometer and thermocouples start 6 inches from the burner exit, which is the zero time point, and are spaced every 4 inches along the combustor length as shown in Figure 8. Each location will define a residence time along the flow path. The last port, a distance of 72 inches from the burner exit, will be used to determine "stack" emissions.

Figure 7. Fuel/air delivery systems.

Figure 8. Assembled combustor.

The secondary air/fuel and tertiary air will also be injected through a selected number of these ports, providing a means of varying 1st, 2nd, and 3rd stage lengths and thereby residence times. Injection of secondary air/fuel or tertiary air at each level is provided by four 1/4-inch jets equally spaced around the circumference of the combustor, pointed perpendicularly into the main flow stream. In order to ensure complete mixing before the injected jet is swept downstream, the jets are sized for high entry velocities relative to the main flow velocity ($V_{\text{injection}} \gg V_{\text{main}}$). Typical $V_{\text{injection}}/V_{\text{main}}$ velocity ratios will be on the order of 5 to 10.

Each coal feeder can provide up to 60,000 Btu/hr of coal at a maximum 5 lbm/hr feed rate. The lower limit of feeder operation is ~20,000 Btu/hr, and is determined by the necessity to keep velocities above the typical flame speed range of 1.5 to 4.5 ft/sec, both in the burner and in the combustor itself. With both feeders in operation, this will allow a turndown from 120,000 to 40,000 Btu/hr. Residence times for a typical arrangement of an 8-inch long 1st stage and a 16-inch long 2nd stage are shown in Figure 9.

Premixed Burner

Figure 10 shows the burner design. A fuel tube with a spreader-type nozzle carries the fuel and transport air vertically downward into the burner mixing chamber. The remainder of the primary air (no fuel) is injected in four locations around the burner circumference as shown in Figure 10. This impinging jet arrangement will provide a well-stirred fuel and air mixture. The mixture will then move down past the cooling coil (used to prevent flashback) and through a flow straightener (to provide axial flow), and will then enter the combustor. The outlet of the flow straightener will thus define the zero time point. Total mass flows through the burner will be from 15 to 65 lbm/hr. The lower limit is set by the need to keep velocity above the flame speed for additional flashback protection, while the upper limit is set

First Stage

- Length = 8 inches, diameter = 8 inches
- Temperature = 2400°F

$\begin{array}{c} Q \\ \text{(Btu/hr)} \\ \text{SR}_1 \end{array}$	τ (sec)		
	20,000	40,000	60,000
1.15	0.53	0.29	0.19
0.80	0.78	0.39	0.26

Second Stage

- Length = 16 inches, diameter = 8 inches
- Temperature = 2100°F

$\begin{array}{c} Q \\ \text{(Btu/hr)} \\ \text{SR}_1 \end{array}$	τ (sec)				
	40,000	60,000	80,000	100,000	120,000
1.15	0.63	0.41	0.31	0.25	0.21
0.80	0.87	0.58	0.43	0.35	0.29

Third Stage

Same as $\text{SR}_2 = 1.15$ case.

Figure 9. Variation of residence time.

Figure 10. Premixed burner.

by the maximum projected fuel flow rate of 5 lbm/hr at 15 percent excess air (assuming a typical bituminous coal requires 10 pounds of air for each pound of fuel).

The transport air and "burner mixing" air (transport air and burner mixing air equals primary air) will be controlled by two separate valves. The fuel/air supply tube will be sized for 50 to 100 ft/sec transport velocity to prevent coal dropout in the tube for the given transport air flow. To minimize coal feed variations, this transport velocity will remain fixed during the tests and only the burner mixing air and fuel feed rate will be varied.

Ancillary Systems

Air/Coal

Four independent air flows will be supplied: primary transport air, burner mixing air, second stage air, and third stage air. Each flow will be instrumented with its own rotameter, pressure regulator and flow control valve. Preheated tertiary air, while not required, will be available. Flow sensors and interlocks will prevent each coal feeder from operating without its associated air flow. Each coal feeder will be manually and independently controllable.

Exhaust

The combustion chamber exhausts downward to a refractory-lined elbow; a side access door can be used to remove ash buildup. The elbow turns the flow upward and out the exhaust stack through an I.D. fan; a bypass damper can be used for air dilution of the exhaust gases.

Gas/Ignition

A main natural gas line is provided for warming up the combustor until the walls are hot enough to ensure stable combustion (~1300°F). This line is

interlocked with a gas/air pilot which is manually inserted into the combustor. A UV flame sensor is used to detect unsafe flameout conditions, and to shut down the gas and coal systems.

Emissions Sampling

The sampling probe is water cooled and uses a quench water spray as shown in Figure 11. From experience with various orientations of quench water spray on other probes, the orientation shown in Figure 11 will give best results. Spraying across the sample gas will provide good mixing of sample and water for rapid quenching. The probe can be pointed either directly into or away from the main combustor flow for particulate and gas sampling or gas sampling only, respectively.

The sampling system can be seen in Figure 12. This gas and quench water will travel through a vapor-liquid separator; the gas can then be routed to the emissions console for O_2 , CO, CO_2 , NO/ NO_x , and UHC measurements to a GC or bubbled through impinger solutions for other species measurements (the types of species to be measured will be determined in the next reporting period, in conjunction with the analytic model effort). The particulate in the quench water can be separated from the water, and ultimate and proximate analyses of the particulate can be performed.

Suction Pyrometer

The Acurex suction pyrometer is shown in Figure 13. A platinum/platinum-rhodium thermocouple will be housed in a 1/4-inch ceramic tube, concentric inside a larger 5/8-inch ceramic tube. Only the ceramic portion of the probe will enter the combustion chamber. The two layers of ceramic surrounding the thermocouple should provide an adequate radiation shield.

The pyrometer was designed to have gas flowing over the thermocouple at 650 ft/sec (200 m/sec). This requires a mass flow of ~3.9 lbm/hr. For low total combustor mass flows, this may influence the main flow stream. For these low flow cases, the suction flow may have to be proportionally decreased

Figure 11. Water cooled, water quench sample probe.

Figure 12. Sampling system.

Figure 13. Suction pyrometer.

Testing during combustor verification will include testing of the pyrometer to determine optimal flow rate.

Backfire Burner

The backfire burner system for reducing energy loss through the refractory walls will have its own premixed burner and flame safeguard system. It will be possible to run the system overnight to minimize warm-up time before each test.

Cooling

Cooling water will be used only for the water cooled sample probe and suction pyrometer. No active water cooling is needed for the combustor.

3. SUMMARY

The Acurex Prof code has been defined as the base model to be upgraded for use in this program as the comprehensive data analysis model. Considerable progress has been made in formulating the required upgrades for the PROF code. Only the radiation model remains to be formulated.

A reasonable methane combustion and fuel NO_x formation kinetic mechanism has been activated on the PROF code. Predictions of NH_3 , NO , and C_2N_2 doped gas stirred reactor NO_x emissions have been favorably compared with data.

The idealized combustor has been fully designed and fabrication has been initiated.

4. PLANS FOR THE NEXT REPORTING PERIOD

During the next reporting period the following activities will be accomplished:

- In the analytic modeling task, the radiation model will be formulated and all of the upgrade formulations will be translated into Fortran V and integrated into the PROF code. Also, coal reaction mechanisms and rates, for use in the data analysis task, will be developed.

- In the combustion facility task, the combustor will be fabricated and installation will be initiated.

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