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**FUNDAMENTAL STUDY OF ASH FORMATION AND DEPOSITION:
EFFECT OF REDUCING STOICHIOMETRY**

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SECTION 1
EXECUTIVE SUMMARY

1. EXECUTIVE SUMMARY

The technical objectives of this project are:

- a. To identify the partitioning of inorganic coal constituents among vapor, submicron fume, and fly ash products generated during the combustion of pulverized coal under a variety of combustion conditions. Fuel lean and fuel rich combustion conditions will be considered.
- b. To identify and quantify the fundamental processes by which the transformations of minerals and organically-associated inorganic species occur. Emphasis will be placed on identifying any changes that occur as a result of combustion under sub-stoichiometric combustion conditions.
- c. To incorporate the effects of combustion stoichiometry into an Engineering Model for Ash Formation based upon the understanding developed in (a) and (b). When completed, this model will predict the particle size and chemical composition distributions of ash formed during the combustion of pulverized coal under a broad range of conditions.

A description of the work plan for accomplishing these objectives is presented in Section 2 of this report.

The work discussed in this report highlights the accomplishments of the seventh quarter of this two year project. This includes University of Arizona efforts to minimize periodicity in the coal feeder for the drop tube furnace, and MIT efforts to calculate the concentrations of CO, CO₂, and O₂ surrounding a burning char particle.

In Section 3, the use of a pulsed gas flow to maintain a smooth coal feed to the drop tube furnace is discussed. Addition of pulsing action, driven by a peristaltic pump, has eliminated the coal feeder pluggage problems that had been occurring.

In Section 4, the development of a single particle char combustion model by MIT is discussed. The model is then used for calculating oxygen, CO, and CO₂ concentrations on the char particle surface as a function of char particle diameter. This information can then be used to interpret results of ash formation experiments conducted as a function of particle size and combustion stoichiometric ratio.

SECTION 2

OVERVIEW OF PROGRAM TASKS (PSI Technologies)

2. OVERVIEW OF PROGRAM TASKS

This project is designed to examine the effects of combustion stoichiometry on the fundamental aspects of ash formation and ash deposit initiation. Emphasis will be placed on reducing stoichiometries associated with low-NO_x combustion, although a range of oxidant/fuel ratios will be considered. Previous work has demonstrated that ash formation depends strongly upon coal mineralogy, including mineral type, size, amount, and the presence of organically associated inorganic species. Combustion temperature and the oxidation state of iron will also play a significant role. As these latter items will vary with changes in stoichiometry, research to determine the net effect on deposition is required.

To achieve these goals, a research program with the following technical objectives will be pursued:

- (1) identify the partitioning of inorganic coal constituents among vapor, submicron fume, and fly ash products generated from the combustion of pulverized coal under a variety of combustion stoichiometries. Fuel-lean and fuel-rich combustion conditions will be considered.
- (2) identify and quantify the fundamental processes by which the transformation of minerals and organically-associated inorganic species occur. Identify any differences from standard pulverized coal combustion conditions.
- (3) modify, to incorporate the effects of combustion stoichiometry and based on the understanding developed in (1) and (2) above, an Engineering Model for Ash Formation. The previously developed model is capable of predicting the size and chemical composition distributions of the final ash products under standard pulverized coal combustion conditions of 20% excess air. These modifications will extend the model to include phenomena that may be dominant under a broad range of stoichiometries.

Experiments, sample analyses, and modeling will be conducted at several facilities as part of this program. Detailed coal and ash sample analysis using Mössbauer spectroscopy, x-ray absorption fine structure spectroscopy (XAFS), and computer controlled scanning electron microscopy will be carried out at the University of Kentucky (UKy). Small-scale drop tube combustion tests using size and density classified coal samples and possibly synthetic char samples will be carried out at the MIT to determine the extent of mineral coalescence and inorganic vaporization as a function of combustion stoichiometry. Combustion experiments utilizing utility grind coals will be conducted at PSI to examine the effects of stoichiometry on mineral interactions. Deposition experiments using ash generated from combustion experiments and using pure minerals will also be conducted to investigate deposit initiation as a function of combustion conditions. The engineering model for ash formation (EMAF) will be modified to include effects of combustion stoichiometry as part of this effort. Self-sustained pilot scale combustion experiments will be conducted in the University of Arizona (UA) 100,000 Btu/h facility to address

issues of scaling in combustion processes. The interaction of iron with aluminosilicates as a function of changing combustion conditions will be the focus of this effort. Modeling of the iron-aluminosilicate interaction process will be conducted as part of the UA study. Finally, interaction with an integrated program led by the utility PowerGen will be used to address issues of deposit formation at full scale for comparison with the bench and laboratory scale results of this program. A work breakdown structure containing a brief description of each task follows. The relationship among the participants is illustrated schematically in Figure 2-1.

Task 1 - Program Planning, Management, Reporting, and Peer Review

This task, to be performed by PSI Technologies, consists of: (1) preparing and annually updating a program plan; (2) coordinating, managing, and integrating the subcontracts and project results; (3) preparing project monthly reports; (4) integrating and preparing project quarterly reports; (5) integrating and preparing the program final report; (6) conducting annual peer review and project coordination meetings with the project principal investigators, either as a separate meeting or in conjunction with a technical conference, and including when appropriate the principal investigators of other DoE-supported ash formation research programs identified by the DoE project manager; and (8) acquiring and distributing coals to all of the project principal investigators.

Task 2 - Fundamental Study of Ash Formation and Deposit Initiation Under Reducing Conditions (PSI Technologies)

PSI will study the effect of combustion stoichiometry on mineral matter and inorganic species transformations with an emphasis on sub-stoichiometric combustion. This will occur through a series of experiments to be conducted in a well-characterized laboratory flow reactor on a minimum of two coals. Coal blends may also be examined if of benefit to the program and of mutual interest to PSI and DoE/PETC. One or more of the coals studied in this task may be coals previously studied at PSI under DoE contract number DE-AC22-86PC90751 to permit a direct comparison with results obtained under oxidizing conditions. Model mineral compounds will also be examined as necessary to identify the importance of the oxidation state of iron in determining mineral coalescence and ash deposition. Selection of any coal samples will be coordinated with the DoE/PETC program manager.

PSI will also conduct limited experiments to determine the effect of pyrite weathering on the evolution of an iron oxide fume. These experiments will be coordinated with a similar study at Sandia National Laboratories.

PSI will also conduct in-situ combustion experiments in conjunction with the University of Kentucky and Brookhaven National Laboratories using an in-situ combustion reactor at beamline X19-A of the National Synchrotron Light Source.

Activities under this task will include collection and examination of ash samples at varying combustion temperatures and/or oxidant concentrations. Ash samples will be collected using extractive sampling. In-situ deposit collection techniques will be used to measure ash particle

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Figure 2-1. Program structure.

collection efficiencies as a function of temperature and stoichiometric ratio. Extracted ash and deposit samples will be characterized as necessary to determine particle size and chemical composition distributions as well as the chemical state of key components such as iron and calcium.

Task 3 - PowerGen Collaboration (PSI)

In order to understand the effects of combustion scale on ash formation and deposition under reducing conditions, PSI will interact with a government and industrial program currently underway in Great Britain. Led by the utility PowerGen, this program includes experiments at scales ranging from fundamental bench reactors to operating power plants. As part of a collaborative effort, PSI hopes to conduct laboratory experiments either at PSI, at BNL on the in-situ XAFS combustor, or in both reactors under a range of combustion conditions using a coal provided by PowerGen. If deemed appropriate by PSI, UA, and the DoE/PETC Program Manager, UA may also conduct combustion experiments with one of these coals. These experiments will permit direct comparison of results obtained in this project with those obtained at full scale in the PowerGen program. This interchange will also add to the database used in the modifications of the engineering model for ash formation described under Task 4.

Task 4 - Engineering Model for Ash Formation (PSI)

The results obtained by the organizations participating in this project will be applied by PSI to revise, test, and validate the EMAF developed previously. The work on this subtask includes analyzing the experimental results and identifying data and technical information related to extending EMAF. Specific areas of interest include the formation of ash under reducing stoichiometries, the formation (particularly the chemical composition) of the submicron ash fume, and the influence of char fragmentation on ash formation. As part of this task, PSI will also coordinate modeling activities to be conducted by the MIT and UA subcontractors.

Task 5.1 - Advanced Techniques for Coal and Ash Characterization Including In-situ XAFS Measurements (UKy)

The University of Kentucky will apply advanced analytical techniques such as computer-controlled scanning electron microscopy (CCSEM), Mössbauer spectroscopy, and x-ray absorption fine structure spectroscopy (XAFS) to characterize coal and ash samples from this program as needed by the individual principal investigators. If agreed upon by PSI, UKy, and the DoE program manager, UKy will also analyze selected coal and/or ash samples obtained from the PowerGen program in Great Britain.

As part of this task, UKy will conduct dynamic in-situ XAFS experiments at the Brookhaven National Laboratories (BNL) National Synchrotron Light Source (NSLS) with PSI and BNL using an in-situ drop tube furnace previously constructed by PSI. Static in-situ measurements at elevated temperatures will also be conducted using a cell previously built by UKy. The in-situ measurements will be used to investigate phenomena such as the transformation of pyrite under various conditions, the formation of iron aluminosilicate compositions as a

function of combustion conditions, the formation of calcium aluminosilicate ash compositions as a function of combustion conditions, and the composition and oxidation state of key components in sticky, depositing ash particles as a function of combustion conditions.

Task 5.2 - Pulverized Coal Combustion Studies Under Reducing Conditions in a Continuous, Self-sustained Laboratory Scale Reactor (UA)

UA will conduct experiments to assess the interaction of iron and aluminosilicate minerals under reducing combustion conditions. UA will also examine the amount and chemical composition of the submicron fume generated under reducing conditions. This study will be conducted in the UA self-sustained 100,000 Btu/h combustion facility. UA will conduct this study using at least one of the coals studied by PSI and MIT under this program and including at least one coal studied previously under oxidizing conditions. As part of the experimental effort, UA will conduct Auger analyses for samples provided by other principal investigators on an as-needed basis. UA will also conduct Mössbauer analysis on selected ash samples generated at UA.

Based upon the results generated in this program, UA will modify the previously developed model for iron aluminosilicate formation to incorporate additional coals and/or combustion conditions.

Task 5.3 - Fundamental Study of Mineral Interactions and Ash Vaporization Under Reducing Conditions (MIT)

MIT will conduct drop tube experiments to study the fundamental aspects of ash formation under sub-stoichiometric conditions using narrowly sized and density classified coal samples and/or synthetic char samples. Size segregated chemical composition measurements will be conducted to assess the release of inorganic species to the vapor phase under sub-stoichiometric conditions. MIT will also conduct fundamental coalescence experiments under reducing conditions to elucidate the mechanism and rate of interaction of key mineral pairs. MIT will assist in the EMAF model testing and validation as described under Task 4.

SECTION 3

TASK 5.2: PULVERIZED COAL COMBUSTION STUDIES IN A CONTINUOUS SELF-SUSTAINED LABORATORY REACTOR

(University of Arizona)

3. THE EFFECT OF REDUCING STOICHIOMETRY ON FE PARTITIONING DURING COAL COMBUSTION

One of the main objectives for the last quarter was to improve the operation of the coal feed system. The old design of the feed system had two major problems associated with it: pulsing of the coal feed would occur, and the syringe pump used in the feed system would occasionally jam. The old design consisted of a piston and cylinder arrangement, with the coal outlet and an entrainment gas inlet at one end. (See Figure 1.) The gas entered at the top of the cylinder, entraining the coal and carrying it into the furnace. This setup caused the feed system to occasionally jam, since the coal in the middle of the cylinder would be removed, leaving the coal along the walls. (See Figure 2.) This coal would then jam the piston, either by lodging between the piston and the cylinder walls, or the coal would be compressed until the syringe pump could no longer provide sufficient force to move the coal. This problem was overcome by the addition of two more inlets for the entraining gas. (See Figure 3.) This removed the coal along the walls of the cylinder, preventing the feed system from being jammed.

The problem of the pulsing coal feed has been a major design concern since the feed system was developed. One method of overcoming this problem was to use a large amount of entraining gas. This would remove most of the pulses, giving a smooth coal feed. However, this led to other problems. The main problem was that the entraining gas (in our case, nitrogen) would be in such large quantities, that the oxygen concentration would be too low to maintain combustion.

When observing the feed system in operation with a low entraining gas flow rate (<2.0 SLPM), it was noticed that the pressure would build up inside of the feed system cylinder. When the pressure became too great, it would be released. When the pressure was released, a pulse of coal would then be fed into the furnace. This would happen on a very periodic basis.

Figure 3-1. Old feed system design.

Figure 3-2. Schematic of coal removal problem.

Figure 3-3. New entraining gas setup for the feed system.

nitrogen flow indicates a continuous flow and does not detect the pulses.

Another aspect of the furnace that was changed was the section between the feed system and the inlet of the furnace. In the past, 1/4 inch diameter tubing was used in this section. It was decided that larger diameter tubing should be used in this section to prevent clogging of the tubing if the coal particles adhered to the walls of the tubing. All of the tubing in this section has been replaced with 3/8 inch diameter tubing. These three changes to the feed system have combined to provide a much smoother coal feed to the furnace.

Runs were conducted using this new feed system arrangement. The Illinois #6 coal, sieved to 38 to 44 μm , was used, and nitrogen was used as the entraining gas. The coal feed rate was set to 4.0 grams per hour and pure oxygen was fed to obtain a target stoichiometric ratio of 1.2. Most of these experiments had similar results. The total filter samples at the exhaust indicated that incomplete combustion was occurring. A visual inspection showed that the outside layers of the filter particles were reacted. The filter particles were covered with a layer of ash, but, upon crushing of the particles, it was evident that the inside of the particles remained unreacted. This indicates that there is either a problem with oxygen transport to the uncombusted core or that the coal particles do not have sufficient residence time in the furnace for complete combustion to occur.

This led us to examine what would happen if the entraining gas was fed into the cylinder in a pulsed manner, instead of being a continuous flow. This was done using a peristaltic pump. The entraining gas was fed through the peristaltic pump prior to going to the feed system. The peristaltic pump that was used was variable speed, with a maximum speed of 100 revolutions per minute. Since the pump head consisted of three rollers, the gas could be pulsed up to 300 times per minute (five times per second). A series of experiments was conducted to examine the effects of this arrangement on the coal feed. It was determined that a 2.0 SLPM flow rate, with the peristaltic pump running at its maximum speed (100 rpm) would feed the coal to the furnace with the minimum number of pulses. Since the gas flow is being pulsed at such a high frequency, it can be considered to be continuous. The flow meter used to monitor the

In the past, experiments were done using the unsieved Illinois #6 coal. The unsieved coal contains larger particles than the sieved coal. The unsieved coal contains a large fraction of particles that are greater than 74 μm . When this coal was burned, the same amount of combustion occurs. Since the residence time for the two particle sizes are different, and this seems to have no effect on the amount of combustion, this leads us to believe that the transport of oxygen to the unreacted core is the limiting factor in the combustion process. The next thing to do is overcome this problem.

There also has been some work done on the large scale furnace. At the present time, the large furnace is being used by another student, who has done a lot of work to get it up and running. All of the sampling ports have been redone, fixing most of the leaks. The gas and the temperature sampling systems have also been redone, and a computer system has been added to automate the data collection. The coal burner and the particle sampling systems still need to be redesigned and rebuilt. Hopefully, it will be ready for use by the end of February.

SECTION 4

TASK 5.3: FUNDAMENTAL COMBUSTION STUDIES UNDER REDUCING CONDITIONS

(Massachusetts Institute of Technology)

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4. FUNDAMENTAL COMBUSTION STUDIES UNDER REDUCING CONDITION

In the previous report, it was shown that the fate of iron during coal combustion depends upon the combustion environment, namely the concentration of CO and O₂, and the combustion temperature. Therefore in the past quarter, calculations were carried out to obtain the concentrations of CO, CO₂ and O₂ surrounding a burning char particle, and the combustion temperature of the particle.

4.1 Transport Properties of Reacting Gases

It is well known that the combustion of the char particle can be classified into three regions: region I – kinetically controlled combustion, in this region char reacts with oxygen in the whole particle, region II – kinetically and diffusively controlled combustion, in this region oxygen penetrates into the particle to some depth, and region III – diffusively controlled combustion, in this region reactions occur only on the particle surface. Under general combustion condition, the char combustion is in region III. The determination of oxygen transport properties is therefore essential to this study.

- The diffusion coefficient for O₂ - N₂

The main compositions of the reacting gases surrounding the particle are CO, CO₂, O₂ and N₂. The dominant gases in this system are O₂ and N₂. So the diffusion between the gases can be taken as O₂ - N₂. We can calculate the diffusion coefficient according to Eq. (1):

$$D_{O_2-N_2} = \frac{(1.83583 \times 10^{-7}) T^{3/2}}{p \sigma_{AB}^2 \Omega_D} \sqrt{\frac{1}{M_A} + \frac{1}{M_B}} \quad (1)$$

where $p = 1$ atm, σ_{AB} and Ω_D are Lennard-Jones parameters, with $\sigma_{AB} = 3.5785$, $\Omega_D = 0.6558$, M_A is the molecular weight of oxygen (32), M_B is the molecular weight of nitrogen (28).

At $T = 2000$ K, $D_{O_2-N_2} = 5.024 \times 10^{-4}$ m/s

At other temperatures:

$$\frac{D(T)}{D(2000)} = \left(\frac{T}{2000} \right)^{\frac{3}{2}} \quad (2)$$

- Density of reacting gas

We take the gas to be an ideal gas, so

$$P = \rho R T$$

or

$$\rho = \frac{P}{RT} \quad (3)$$

4.2 Estimation for Reaction Time

The momentum equation for char particle in gas can be written as

$$m \frac{dV}{dt} = mg - 3\pi\mu d(V - V_g) - \frac{m}{\rho} \rho_a g \quad (4)$$

or

$$\frac{dV}{dt} = g - \frac{3\pi\mu d(V - V_g)}{m} - \frac{\rho_a}{\rho} g \quad (5)$$

The pathway of the particle is composed by two sections: the first one is the vertical path from the coal feeder to the reaction zone, and the second one is in the reaction zone. For the first section, the vertical (feeder) length is 0.57 m, the section-area of the feed pipe is

$$S = \frac{\pi}{4} D^2 = \frac{\pi}{4} (0.3175 \times 10^{-2})^2 = 7.9168 \times 10^{-6} \text{ m}^2 \quad (6)$$

and the feed flow rate is

$$\begin{aligned} Q &= 150 \text{ ml/min} \\ &= 2.5 \times 10^{-6} \text{ m}^3 / \text{s} \end{aligned}$$

So the velocity of gas is

$$V_g = Q/S = 0.31578 \text{ m/s}$$

The initial condition for particle is

$$V(t=0) = V_g$$

By using MAPLE, an interactive computational program, we can easily calculate

$$V(z=0.57 \text{ m}) = 0.5224 \text{ m/s for } d_p = 75 \text{ }\mu\text{m}$$

For the second section in reaction zone, the flow rate of the main gas is

$$Q = 6 \text{ l / min} = 0.1 \times 10^{-3} \text{ m}^3 / \text{s}$$

The section-area of the furnace is

$$S = \frac{\pi}{4} (2 \times 2.54 \times 10^{-2})^2 = 2.0268 \times 10^{-3} \text{ m}^2 \quad (7)$$

The furnace temperature is 1650 K, so

$$V_g = \bar{V}_{\text{gas}} = \frac{(0.1 \times 10^{-3}) \times \frac{1650}{300}}{2.0268} = 0.271 \text{ m/s} \quad (8)$$

The length with $T_{\text{wall}} = 1650 \text{ K}$ is 3.5 inches or 0.0889 m.

- When the particle is very small, it will follow the main gases in the furnace, then the reacting time for the particle is $\frac{L}{\bar{V}_{\text{gas}}} = 0.33 \text{ s}$
- When the mass of the particle does not change or decreases slightly (corresponding to low carbon conversion), we can simply integrate equation (5) to obtain $V(t)$. Then we can calculate $\bar{V}_p = 0.518$, so the reaction time for the particle is $\frac{L}{\bar{V}_p} = 0.17 \text{ s}$.

4.3 Estimation of Chemical Kinetics for Char Combustion

To determine the reaction rates of char oxidation is always the core of coal combustion research. There are numerous articles and methods on this topic. However, acknowledging that the char combustion is essentially carbon reaction, we can greatly simplify the combustion analysis. The reactions for carbon oxidation are as follows:

The reaction rates for these reactions can be written as:

$$\frac{dm(a)}{dt} = K_{\text{oa}} (\rho_s Y_{\text{o,s}})^{n_a} \exp \left(- \frac{E_a}{RT_p} \right) \frac{M_{\text{co}_2}}{M_{\text{o}_2}} \quad (9)$$

$$\frac{dm(b)}{dt} = K_{ob}(\rho_s Y_{o,s})^{n_b} \exp\left(-\frac{E_b}{RT_p}\right) \frac{M_{co}}{\frac{1}{2}M_{o_2}} \quad (10)$$

$$\frac{dm(c)}{dt} = K_{oc}(\rho_s Y_{co_2,s}) \exp\left(-\frac{E_c}{RT_p}\right) \quad (11)$$

In a previous study, the kinetic parameters have been determined for solid pure carbon particle²:

$$K_{oa} = 3500, n_a = 0.88, E_a = 113000$$

$$K_{ob} = 1.05 \times 10^6, n_b = 0.64, E_b = 18000$$

$$K_{oc} = 10^8, E_c = 270000$$

The difference between the solid pure carbon particle and the coal particle is that the coal particle has porosity within the particle. As mentioned in section 4.1, when the coal combustion is region I and II, the porosity may increase the reaction area, while in region III, the porosity may not have effects on reaction area or decrease the reaction area. For example, Hecker et al.³ found that the intrinsic rates of char partially burned out at high temperatures decrease with burnout level. For simplification we take the kinetic parameters as constants. This can be achieved by multiplying a constant K to the expressions for reaction rates of solid pure carbon particle, i.e.

$$\frac{dm_{char}}{dt} = K \left[K_{oa}(\rho_s Y_{o,s})^{n_a} \exp\left(-\frac{E_a}{RT_p}\right) + K_{ob}(\rho_s Y_{o,s})^{n_b} \exp\left(-\frac{E_b}{RT_p}\right) + K_{oc}(\rho_s Y_{co_2,s}) \exp\left(-\frac{E_c}{RT_p}\right) \right] \quad (12)$$

Measurements on solid pure particle² and pulverized coal particle⁴ showed that the combustion temperature of particles kept constant during most of char combustion. So we can take the combustion processes to be quasi-steady. Then we can write the energy equation for the particle as follows:

$$Q_a K \frac{dm_a}{dt} + Q_b K \frac{dm_b}{dt} - Q_c K \frac{dm_c}{dt} = -\lambda_a \frac{dT}{dr} + \epsilon \sigma (T_p^4 - T_g^4) \quad (13)$$

The particle diameter can be computed from:

$$\frac{d\left(\rho \frac{4}{3}\pi r^3\right)}{dt} = -\frac{dm}{dt} \quad (14)$$

By solving the mass conservation equations and the energy conservation equations governing the species and temperature distributions surrounding the particle, we can obtain the oxygen concentration on the particle surface in terms of the combustion temperature.^{2,5} Thus we can predict mass loss of the particle. Take the following experimental results into consideration:

Furnace temperature (T_g) = 1650 K	Bulk oxygen concentration (Y_{O_∞}) = 10 %
Particle diameter (d_p) = 75 μ m	Reaction time = 0.2 s (from Section 4.2)
Carbon conversion = 41 %	Coal type = Pittsburgh #8 (cleaned)

By adjusting K, we can make the prediction consistent with the experimental results. Therefore we obtain

$$K = 0.2$$

4.4 Prediction of Combustion Processes

In the same method in section 4.3 and with $K = 0.2$, we can predict the combustion processes under other combustion conditions (the combustion is still in region III). A typical result is shown in Figures 1 through 4. Knowing the combustion processes, we can predict the vaporization rates of mineral matter and reactions of iron between CO and O_2 , which will be the task of next quarter.

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Figure 4-1. Char mass as a function of time.

Figure 4-2. Oxygen concentration on char surface as a function of particle size.

Figure 4-3. CO₂ concentration on char surface as a function of diameter.

Figure 4-4. CO concentration on char surface as a function of diameter.