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ABSTRACT

The principal activities in the quarter involved the global experiments. These were resumed at the beginning to December. The results completed in this quarter include an analysis of the effects of oxygen concentration on one of the bituminous coals. Also, two of the bituminous coals were compared under identical conditions. These results have been correlated by use of the breakup model and the pertinent deviations noted.

The engineering analysis activities have been held in abeyance during this quarter. This is per the revised program plan, and is a direct result of the fact that the analysis activities have progressed to a greater degree than the experimental work. The engineering analysis work will restart when a larger data base becomes available.
1.0 INTRODUCTION

The overall objectives of this project are to provide a basic understanding of the principal processes that govern fine particulate formation in pulverized coal flames. This understanding is to be used to develop a model (or models) which will predict the yield and size distribution of fine particulate as a function of coal type, coal processing, and combustion conditions. The goal of the model is to provide an engineering tool that will enable the practitioner to estimate the consequences of design decisions and fuel selection on the fine particulate yield. The practitioner can then make rational decisions regarding the required technology and costs associated with effluent cleanup while still in the design phase.

Long term work is presently supported by PETC that will develop detailed models of the entire mineral transformation process. The present work is directed toward global models of behavior which will become available on a shorter timeframe, and will be immediately usable in engineering activities.

Another goal of the work is to extend the capabilities for the characterization of fine particulate. Present technology for characterizing size distributions usually involves manual impactor techniques for sizes down to 0.2 μm. The EAA analyzer is used for aerosols. Although the impactor covers the size range of interest, it is a very time consuming procedure. Another difficulty is that the impactor and EAA overlap only over a small size band. The results of the comparison of the two techniques are not always consistent within the region of overlap. The goal is a single instrument that will characterize the fine particulate size band rapidly and accurately.

Particles in the 0.5-10.0 μm size band are of interest for several reasons. First, a considerable portion of the flyash generated in pulverized coal combustion falls within this size range. Particulate control devices, in particular electrostatic precipitators, are at their least efficient in this size band. Also, particles in this size range are most efficiently
collected within the alveolar passages of the human lung. In coal combustion, a considerable portion of the heavy, toxic metals are vaporized within the flame. As the furnace gases cool, these metals will condense, and the fine particulate size band forms a convenient condensation surface. Thus, the particles that are deposited in the alveoli may be coated with toxic compounds and provide an exposure that is well beyond their proportion in the original mineral matter.

Finally, the mechanism by which this fine flyash is formed is not yet clear. Obviously, predicting the yield will require some definition of the dominant mechanisms. Also, the manner in which these mechanisms respond to differing coal types and combustion conditions will have to be understood to make predictions.

The project objective is being accomplished through a combination of literature research, experimentation, and model development activities. The program tasks include:

Task 1. Literature review and program plan.

Task 2. Engineering analysis.

Task 3. Experimental program.

Task 4. Reporting.

This report describes work performed during the period from October 1, 1988 through December 31, 1988. The principal activity during this period involved the isothermal experimental system. Specifically, the influence of coal type and free oxygen concentration was investigated within the global experimental tests.
2.0 ENGINEERING ANALYSIS

The objective of this task is to modify an existing model that predicts the yield of fine particulate from pulverized coal flames. This objective is organized onto three subtasks:

- Initial Definition, in which a review of the current state-of-the-art of modeling fine particulate formation was conducted and the requirements for the improved model defined.

- Model Adaptation and Development, in which the model outlined in the initial definition subtask is to be assembled.

- Data Interpretation and Scaling, in which the model will be exercised against data generated in the experimental program to help interpret the data, to refine the model, and to project the full-scale implications of the findings.

Presently, the initial definition task has been completed. A modified breakup mechanism has been completed and an element that treats the fate of extraneous ash has been added to the model. The pending task is the development of a model that handles both the breakup of coke cenospheres, and the breakup of ash bubbles. The status of these activities is reported in detail in the last quarterly report.

Due to the fact that the engineering analysis task is ahead of the experimental tasks in terms of schedule, the decision was made to suspend activities on engineering analysis until the April/May timeframe. The reason for this was to allow the experimental tasks to "catch up" so that further model development would have the advantage of a more complete data base.
3.0 EXPERIMENTAL PROGRAM

3.1 Introduction

The experimental portion of this project consists of a study of the fundamental mechanisms at laboratory scale, followed by a process simulation study conducted at bench-scale. One of the main features of the program is the correlation of the process simulation data with corresponding data obtained at three full-scale boilers (one cyclone-fired, one tangentially-fired, and one wall-fired) to be obtained under EER's Clean Coal program.

Within the fundamental task, the work has been organized into three subtasks. The first dealt with the modification of a laser diffraction particle sizer to provide analysis in the 0.5-10.0 μm size range. This task has been completed and is reported in detail in the previous quarterly progress report.

The second major task involves the global experiments. These are designed to provide a view of how coal type and combustion parameters influence fine particle yield. As such, no special coal preparation is performed. The idea is to evaluate how the fine particle yield changes due to all of the mechanisms present. This test series is presently underway.

The final subtask includes the mechanistic experiments. These are focused on a quantitative evaluation of the various candidate mechanisms for fine particulate formation. As such, special fuels and firing conditions will be used. These tests are outlined in the program plan.

3.2 Results

Figure 3-1 shows the Isothermal Reactor (ITR) used in the global experiments. It consists of a 10 cm diameter ceramic tube mounted in a three-zone electric furnace. The furnace is capable of operating to 1500°C. The reacting gas is supplied by a gas flame, as shown on the figure. The flame is designed to be fired at temperatures above the target furnace
Figure 3-1. The Isothermal Reactor.
temperature. Since the gas generator chimney is not insulated, the gases cool as they approach the furnace; the temperatures are selected such that the gases reach the furnace target temperature at the point where they enter the furnace. The role of the electric furnace is then to simply maintain the desired isothermal temperature for the desired residence time.

Coal is fed from a screw feeder into a two-phase transport line. From here it is fed to a single water-cooled injector that is set just before the throat of the venturi shown in the figure. The high shear rates present in the venturi throat provide rapid dispersion to uniformly spread the coal over the reactor cross-section.

The flat flame is fired on lean methane/air. High oxygen levels in the post-flame gas are obtained by use of oxygen enrichment at the burner.

As shown on the figure, samples are collected by a water-cooled probe at the bottom of the reactor. The particulate matter is removed by filtration, and resuspended in a liquid for laser diffraction analysis. The previous quarterly outlines the general approach.

Table 3-1 lists the coals selected for this study. The first three of the coals were selected from the suite of coals that have been characterized under DOE's mineral matter transformation program. These have been supplied through the courtesy of Physical Science Technology Corporation. These coals have undergone what is probably the most extensive mineral characterization ever performed, and thus they provide a unique opportunity for correlating behavior against mineral properties.

The Illinois/Kentucky bituminous blend is the baseline coal used in certain of the Clean Coal boilers. The rationale for selecting this coal is to allow comparison between the small-scale results, the engineering analysis prediction of these results, and full-scale performance. The Utah bituminous coal was selected because EER has an extensive data base on the behavior of this particular coal, including some information on fine particulate formation at pilot-scale.
Table 3-1. Coals Selected for this Study.

<table>
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<th>COAL</th>
<th>MINERAL CONTENT</th>
<th>MINERAL ANALYSIS</th>
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<tr>
<td>Beulah Lignite</td>
<td>9.6%</td>
<td>High Ca, Na</td>
</tr>
<tr>
<td>Eagle Butte Subbituminous</td>
<td>4.8%</td>
<td>High Ca, Low Na</td>
</tr>
<tr>
<td>Illinois Bituminous</td>
<td>9.3%</td>
<td>High Ca, Pyrite</td>
</tr>
<tr>
<td>Illinois/Kentucky Bituminous Blend</td>
<td>6.2%</td>
<td>Low Ca, Na</td>
</tr>
<tr>
<td>Utah</td>
<td>8.8%</td>
<td>Low Ca, Na, Pyrite, High Si</td>
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Figure 3-2 outlines results on the influence of firing condition on the fine particulate matter yield. The left panel shows the original size distribution of the parent Utah coal. The two dashed lines show measured particle size distributions for firing under 20 and 30% oxygen atmospheres. The results suggest a fair amount of similarity between the two conditions. However, the data suggest that the 30% oxygen case produces more particles below 3 μm.

Also shown on the left panel of Figure 3-2 are lines representing the size distribution that would result if one coal particle yielded 1 ash particle, and 2.4 ash particles, respectively. This is essentially the breakup model in its original form. Note that the data are best matched by the assumption that each coal particle, independent of size, yields 2.4 ash particles. (In fact the value of 2.4 was selected to yield the best fit.) Note also that the measured size distribution is broader than the simple breakup model. This means that more large particles and more fine particles are generated than would be predicted by the model. Note that the largest ash particles are larger than would be predicted from assuming that all the mineral matter in the largest coal particles is converted into one ash particle. This means that these large ash particles are due to either extraneous minerals that are included with the coal, or they are due the enrichment of some of the larger coal particles with minerals.

The right panel of Figure 3-2 shows similar size distribution results for a bench-scale facility in which the Utah coal was fired through three different burners. The sequence of axial to radial to premixed has the effect of progressively increasing the rate at which the particles are exposed to the high temperature environment. Not only is the effective heating rate increased, but also the peak particle temperature is increased. Note that this has the particular effect of increasing the yield of particles below 10 μm. The left panel of the figure shows that higher oxygen and higher particle temperatures also had the effect of yielding more fine ash.
Figure 3-2. Influence of firing conditions on fine particulate yield.
The dotted line on the right panel of the figure shows the breakup model prediction for each coal particle yielding one ash particle. While this assumption appears most adequate for predicting the mass-mean diameter, it greatly underpredicts the fine particle yield. (Note that on this linear scale, the differences are minimized. In reality, the differences between the data and the model, and between the various data themselves, are all quite significant.)

Figure 3-3 shows a comparison between the ash resulting from Utah and Illinois coal. The dotted lines show the breakup model. The Utah coal most closely matches the one ash particle per coal particle model. The Illinois coal yield a value much closer to 10 ash particles per coal particle. This suggests that coal type may be one of the strongest parameters in influencing fine particulate yield.

These two extremes provide one illustration of a proposed mechanism for the production of multiple ash particles from single coal particles. Figure 3-4 provides an overview of the mechanism. During devolatilization many bituminous coal particles swell into cenospheres. When these cenospheres start to undergo char oxidation, the large pores or blowholes form convenient sites for the reaction. Thus, the cenosphere can break into a number of smaller particles, as shown in the figure. If each of the daughter fragments yields a single ash particle, then the resulting size distribution will be both reduced in size, and broadened. Finally, note that any of the fragments that contain more than one ash inclusions may yield a ash agglomerate rather than a single ash particle. Such a mechanism may explain the marked difference between the behavior of the two bituminous coals noted in Figure 3-3.
Figure 3-3. Influence of coal type on fine particulate yield.
Figure 3-4. Schematic of ash processing during cenosphere oxidation.
4.0 FUTURE WORK

Per the revised program plan, the engineering analysis activities will be held in abeyance during the coming quarter. The experimental work will focus on completing the global experiments and starting the mechanistic studies.
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