QUARTERLY REPORT
FOR
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ENTITLED
"ADVANCED COMBUSTOR DESIGN CONCEPTS TO CONTROL NOX AND AIR TOXICS"
SUBMITTED BY
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1.0 Program Overview

Direct coal combustion must be a primary energy source for the electric utility industry and for heavy manufacturing during the next several decades because of the availability and economic advantage of coal relative to other fuels and because of the time required to produce major market penetration in the energy field. However, the major obstacle to coal utilization is a set of ever-tightening environmental regulations at both the federal and local levels. It is, therefore, critical that fundamental research be conducted to support the development of low-emission, high efficiency pulverized coal power systems.

The University of Utah, Massachusetts Institute of Technology (MIT), Reaction Engineering International (REI) and ABB/Combustion Engineering have joined together in this research proposal to develop fundamental understanding regarding the impact of fuel and combustion changes on ignition stability and flame characteristics because these critically affect: NOx emissions, carbon burnout, and emissions of air toxics. Existing laboratory and bench scale facilities are being used to generate critical missing data which will be used to improve the NOx and carbon burnout submodels in comprehensive combustion simulation tools currently being used by industrial boiler manufacturers. To ensure effective and timely transfer of this technology, a major manufacturer (ABB) and a combustion model supplier (REI) have been included as part of the team from the early conception of the proposal.

ABB/Combustion Engineering is providing needed fundamental data on the extent of volatile evolution from commercial coals as well as background information on current design needs in industrial practice. Since they will ultimately be a recipient of the enhanced design methodology, they are also providing ongoing review of the practical applicability of the tools being developed. MIT is responsible for the development of an improved char nitrogen oxidation model which will ultimately be incorporated into an enhanced NOx submodel. Reaction Engineering International is providing the lead engineering staff for the experimental studies and an overall industrial focus for the work based on their use of the combustion simulation tools for a wide variety of industries. The University of Utah is conducting bench scale experimentation to (1) investigate alternative methods for enhancing flame stability to reduce NOx emissions and (2) characterize air toxic emissions under ultra-low NOx conditions because it is possible that such conditions will alter the fate of volatile and semivolatile metal species and the emission of heavy hydrocarbons. Finally the University of Utah is responsible for the development of the improved NOx and carbon burnout submodels.

2.0 Progress During Last Quarter

2.1 Introduction

The ability to accurately model NOx formation from coal combustion requires an understanding of the mechanisms of volatile-N and char-N oxidation and reduction. This study has focused on NOx formation from the char-N fraction of coal since much less is known about the fate of char-N than that of volatile-N. As stated in earlier reports, chars from five different coals were collected for this study. These chars were subsequently burned in a simulated coal flame (see report for quarter ending 12/95) under a variety of
conditions. The experimental phase of the study is now complete and key results will be included here.

2.2 Char-N Experiments

The char-N experiments were designed with two goals in mind. One, to identify which parameters affect char-N to NO\textsubscript{x} conversion and quantify the results and two, to provide a set of reliable data for use in modeling NO\textsubscript{x} formation in pulverized coal furnaces. The effects of many different parameters were tested including coal char type, degree of char burnout, char preparation method, NO\textsubscript{x} levels in the flame, local oxygen concentration, natural gas and char firing rates in the simulated coal flame, and flame temperature.

Table I lists the parent coals of the chars used in this study, their respective ranks, and the percent nitrogen in both the parent coal and in the chars. Coal rank proves to be an important parameter in char-N to NO\textsubscript{x} conversion as seen in Figure 1. In this experiment, the simulated coal (85,000 BTU/hr of natural gas, 15,000 BTU/hr of char) was burned in a mixture of 64% Ar/15% CO\textsubscript{2}/21% O\textsubscript{2}. Since the only source of nitrogen in this system is char-N, any NO\textsubscript{x} measured in the exhaust results from char-N oxidation. It is clear from Figure 1 that there is a rank dependence of char-N conversion to NO\textsubscript{x}, ranging from 40-50% for two of the bituminous coal chars to 60-70% for the subbituminous and lignite chars.

A second important parameter in this study was the level of NO\textsubscript{x} in the flame zone (also called initial NO\textsubscript{x}). NO\textsubscript{x} levels in pulverized coal furnaces can be significantly reduced using combustion modification techniques such as low-NO\textsubscript{x} burners and staged combustion. These techniques mainly reduce NO\textsubscript{x} formed from volatile-N. But how does the NO\textsubscript{x} level (high or low) in the flame zone affect char-N to NO\textsubscript{x} conversion downstream? Figure 2 shows the results of experiments conducted with six different chars and with a commercially obtained activated carbon called Nuchar (0.13% N). In order to obtain various NO\textsubscript{x} levels, the natural gas used in the simulated coal flame was doped with different amounts of either NH\textsubscript{3} or NO; the NH\textsubscript{3} quickly oxidized to form NO\textsubscript{x} in the flame zone. The results in Figure 2 are reported as percent reduction of NO\textsubscript{x} species. These values are obtained by dividing the total NO\textsubscript{x} measured in the simulated coal system by the total NO\textsubscript{x} possible, which includes the NO\textsubscript{x} from doping, thermal NO\textsubscript{x}, and NO\textsubscript{x} from the char (assuming all the char-N forms NO\textsubscript{x}).

Figure 2 indicates that for Pittsburgh No. 8 and Illinois No. 6 chars, the initial NO\textsubscript{x} level strongly influences the reduction (and thus the formation) of NO\textsubscript{x} species. Of particular interest in this figure is the comparison of the results obtained with the coal chars to those obtained with the very low-nitrogen Nuchar. The Nuchar exhibits very little NO\textsubscript{x} species reduction potential at any NO\textsubscript{x} level. This data may help clarify which of several mechanisms for NO\textsubscript{x} formation and reduction is occurring on or in the char. For example, if NO\textsubscript{x} reduction occurs at carbon sites on the char surface, then Nuchar should be as effective as the coal chars in reducing NO\textsubscript{x} species, and it is not.

Finally, since excess oxygen has such a strong influence on volatile-N to NO\textsubscript{x} conversion, experiments were conducted to determine the effect of excess oxygen on char-N to NO\textsubscript{x} conversion. The results for two chars (Knife River and Pittsburgh No. 8)
are plotted in Figure 3 as apparent percent conversion of char-N to NO\textsubscript{x}. Apparent conversion is calculated by subtracting the total NO\textsubscript{x} measured burning natural gas alone from the total NO\textsubscript{x} measured burning natural gas + char and then dividing by the total char-N (i.e., if all the char-N formed NO\textsubscript{x}). Although there appears to be some rank dependence in these plots, the trend of increasing conversion levels with increasing amounts of excess oxygen is obvious.

### 2.3 Air Toxic Experiments

The redesigned particle sampling train was constructed and tested by both bench experiments and by preliminary furnace experiments. Size-classified samples of fine particles from coal combustion have been collected and the mass distributions have been measured. The samples have been examined by electron microscopy and will be sent for chemical analysis.

A review of the literature on fine particles from coal showed considerable variation both within individual studies and between different investigators. A furnace test series was completed which measured data reproducibility under constant combustion and sampling conditions. A second test series, which is in progress, will measure the variation introduced by modifying the sampling method while maintaining constant combustion conditions. The results of these test series will be used to develop the experimental procedures for future experiments.

During May, John Veranth attended the 2nd Colloquium on Particulate Air Pollution and Health. The technical sessions provided many new ideas for integrating ongoing combustion research on pollutant formation with the results of recent research in the toxicology and epidemiology of particulate air pollution.

### 3.0 Plans for Next Quarter

Although the experimental phase of this study is complete, data analysis still needs to be performed on many of the experimental results. In addition, the question to be resolved in the next quarter is whether or not current NO\textsubscript{x} submodels in CFD codes can accurately predict the results obtained in these experiments. If not, the experimental data discussed here as well as additional results will be used to write an improved NO\textsubscript{x} submodel.

The “shake down” tests on the particulate sampling system will continue and an experimental procedure will be developed. Tests will then be conducted under base and low-NO\textsubscript{x} conditions. Improvements on chemical analysis are also on going.
<table>
<thead>
<tr>
<th>Parent Coal</th>
<th>Rank</th>
<th>%N in coal (dry basis)</th>
<th>%N in chars (dry basis)</th>
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<td>Utah</td>
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<td>1.14</td>
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<tr>
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<tr>
<td>Illinois No. 6</td>
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<td>1.12-1.61</td>
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<tr>
<td>Knife River</td>
<td>lignite</td>
<td>0.92</td>
<td>0.46-0.64</td>
</tr>
</tbody>
</table>

Table I

Figure 1
Figure 2
Initial Exhaust NOx, ppm (as measured)

Figure 3
Apparent % Conversion of Char-N to NOx

Knife River char
Pitt No. 8 char

% Excess O2
% Excess O2