Abstract

Title: **Homogeneous and Heterogeneous Reaction and Transformation of Hg and Trace Metals in Combustion System**

Author: Joseph J. Helble
University: University of Connecticut
c/o Dartmouth College, Thayer School of Engineering
8000 Cummings Hall, Hanover, NH 03755-8000
Contact: Phone: 603-646-2238
Fax: 603-646-2580
Email: joseph.helble@dartmouth.edu
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OBJECTIVE

The objective of this program is to develop improved understanding of the transformations of mercury and other selected trace metals during coal combustion. As part of this effort, models will be developed for different trace metals that can be used to predict metal partitioning between vapor and condensed phase species. It is further expected that for the condensed phase species, these models will provide a dynamic means to predict the distribution between competing surface reactions and condensation as a function of post-combustion conditions. This would represent a significant advance over current models that are interpretive (i.e. that indicate whether condensation or surface reaction was dominant based on a fit to experimental data), and would provide a method for improving predictions of trace metal emissions and trace metal toxicity from a broad range of combustion systems.

The project consists of several experimental and model development tasks. These include:

- measurement of heterogeneous mercury reactions on solid surfaces including ash and synthetic fly ash surfaces to determine the effect of individual constituents in the ash, in a flame-based flow reactor in the presence of important post-flame radical species;

- determination of gas-solid reaction rates between As, Cd, Sb, and Se and reactive fly ash constituents (i.e. calcium oxide and iron oxide) as a function of metal concentration and temperature to obtain fundamental parameters needed for modeling metal partitioning;

- measurement of selected trace metal reactions in the flow reactor in the presence of contaminants such as NOx and SO_2;

- further development of a dynamic model that predicts partitioning by calculating competing rates of condensation and surface reaction for each metal, and thus incorporates boiler temperature profile, fly ash parameters, and gas phase chemistry.

Mercury is being considered as the 2005 announcement of the Clean Air Mercury Rule by the

United States Environmental Protection Agency (EPA) creates a more immediate need for control strategies. Later stages will focus on additional trace metals present in coal.

ACCOMPLISHMENTS TO DATE

Activity for the past year has been distributed among several areas: improving and expanding the partitioning model, continuing to characterize synthetic fly ash, completing a literature search for activation energies of gas-solid reactions, conducting a health risk analysis for the experimental materials involved in the system, determining proper handling and disposal methods, and setting up the thermo-gravimetric analysis (TGA) system to be used in determining reaction rate constants.

The model was expanded to include all six of the coals for which combustion and trace metal concentration data are available in the literature for different sized fly ash particles. Additionally, quench rate was incorporated as another variable in determining the amount of trace metal added to fly ash particles. Characterizing fly ash materials has also continued through this period to verify the success and reproducibility of the particle sizing system. Activation energies of gas-solid reactions were compiled to reveal the bounds for the planned reaction experiments.

In preparation for experiments with trace metals, a health risk analysis associated with proper handling and disposal methods was completed. The health risk analysis was used in determining engineering controls and setting precautions for the experiments, while the handling and disposal methods were used in forming standard operating procedures.

A large effort has been utilized in building and assembling the TGA system. The fittings and tubing in the system are either stainless steel or quartz due to their ability to withstand the operating temperatures of the planned experiments and their chemical stability. In the coming months, it is expected that activity will include initiation of experiments to study the interaction of trace metal compounds with different combinations of synthetic fly ash materials, and conducting initial experiments using flame gases.

FUTURE WORK

Work conducted during the next year of the project is expected to include experiments using aerosolized fly ash for comparison with fixed bed reactor experiments. Initial fixed bed experiments will be completed for trace metals including As, Hg, and other metals, and extraction of heterogeneous and gas-solid reaction rate parameters for these metals under post-combustion conditions.

PAPERS, PATENTS, PRESENTATIONS, STUDENTS SUPPORTED

There are no publications, patents, or presentations at this time.

This project is supporting Ms. Clara Smith, a full-time Ph.D. students at the Thayer School of Engineering at Dartmouth College, respectively. A second Ph.D. student focusing on mercury chemistry will be added during the coming summer.