

**TITLE:**                   **OXIDATION OF MERCURY IN PRODUCTS OF COAL COMBUSTION**

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## **ABSTRACT**

### **Objectives**

The objectives of the work are: (1) to develop catalysts having high activity for both NO<sub>x</sub> reduction and mercury oxidation and (2) to obtain fundamental understanding on mercury reaction kinetics in the flue gas.

### **Accomplishments to Date**

The experimental and theoretical research is making progress. The work plan has three components: catalyst development, catalyst testing and characterization, and development of a chemical kinetic model. New catalysts are being developed at the Center for Surface Chemistry and Catalysis and the Combustion and Emission Laboratory at Clark Atlanta University. Several catalysts, developed at the Gas Technology Institute, were tested at the Catalyst Reactivity Test Facility at the Southern Research Institute. The catalysts are based on iron, vanadium and cerium.

The modeling effort for homogeneous equilibrium calculation and homogeneous kinetic calculation is completed. The results agree with what is published in the literature. The heterogeneous kinetic modeling work is on-going. The chemical kinetic model is currently focused on the reactions of mercury in the presence of HCl and unburned carbon; because the laboratory experimental results indicated that these two components are most important for the mercury oxidation as carbon acts as a catalyst. The model consists of 186 homogeneous reactions, including HCl, NO<sub>x</sub>, SO<sub>x</sub>, and other flue gas species, and several heterogeneous reactions for surface catalytic reactions. Most reaction rate constants were obtained from existing literature. The unknown heterogeneous reaction-rate constants were obtained by interfacing a Simplex Centroid FORTRAN code with the Chemkin software. These rate constants for the heterogeneous model were extracted based on the experimental data from the SRI Catalyst Test Facility.

### **Future Work**

- (1) Continue the catalyst development effort to provide new catalysts for the laboratory evaluation of mercury oxidation.
- (2) Continue the experimental study at the Catalyst Reactivity Test Facility to determine the effect of various factors.
- (3) Continue the development of a chemical kinetic model that is consistent with the results obtained in laboratory, data available in the literature, and data from field tests.

### **List of Papers**

Neelesh S. Bhopatkar, Thomas K. Gale, Peter Walsh and Heng Ban, Prediction of Mercury Speciation in Coal Combustion Systems, Huntsville Simulation Conference, October 26-27, 2005.

T. K. Gale, N. S. Bhopatkar, and H. Ban, Kinetics of Ca-C Synergism During Mercury Adsorption on Fly Ash in Coal-Fired Power Stations, Air Quality V Conference, Arlington, VA. September 18-21, 2005.

### **Students Supported under this Grant**

Rosa Dominguez-Faus, Graduate Student, Environmental Health Engineering  
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