FY05-LIII(53)-139

Investigation of Mercury and Carbon-Based Sorbent Reaction Mechanism – Comparison of Surface Analysis Techniques

Submitted by: Energy & Environmental Research Center
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PARTICIPANTS

Sponsor		Cost Share
SaskPower		$ 19,500
DOE		$ 21,000
NDIC		$ 19,500
	Total Cost	$ 60,000

Project Schedule - 7 Months

Contract Date – 6/10/05
Start Date – 6/15/05
Completion Date – 1/1/06
Time Extension – ~~3/31/06~~
~~Extension Revised to – 1/31/07~~
Extension Revised to – 9/30/07

Project Deliverables

Contract Signed:
Quarterly Reports:
10/31/05(✓); 1/31/06(✓)
Final Report: ~~3/31/06( )~~
~~1/31/07( )~~
9/30/07(✓)

OBJECTIVE / STATEMENT OF WORK:

This project is an extension of LRC-LI (51)-131, Investigation of Mercury and Carbon-Based Sorbent Reaction Mechanisms. Additional fundamental work will focus on bonding on carbon surfaces using two more refined techniques of x-ray photoelectron spectroscopy and x-ray absorption fine structure spectroscopy. The results will define carbon sorbent surface structural features before and after exposure to various treatment methods (chlorine gas levels) flue gas stream, providing direction to improving mercury capture effectiveness.

STATUS

July 1 – September 30, 2005 Quarterly Report

On-going studies indicate that a key surface component that impacts mercury oxidation and retention by activated char result from chemisorption of chloride and sulfur species from flue gas. The char appears to form organically associated chloride on key sites for bonding with oxidized mercury. The key sites thought to impact mercury capture include acidic carboxyl, lactone, hydroxyl, carbonyl functionalities or alkaline pyrone and chromene functionalities. A matrix of activated carbon was pretreated with 3%-5% chlorine to characterize char surface alterations. Analytical characterization methods will employ XPS and XAFS analysis.

October 1 – December 31, 2005 Quarterly Report

Activities during this quarter focused on the analysis of the XAFS data. A preliminary analysis prepared by the University of Kentucky described a surface chemistry consistent with the results of the XPS analysis. These data need further reduction to determine halogen speciation on the carbon surface. The preliminary interpretation of research results as provided by the University of

Kentucky conflicts somewhat with the interpretation of research results obtained previously by the EERC. EERC intends to review the analysis and discuss the interpretation prior to reporting them. Data reduction is ongoing and will be presented in the next report.

Final Report

A comparative study of chlorine and sulfur structures was developed prior to flue gas exposure and after flue gas exposure. X-ray photoelectron spectroscopy (XPS) and x-ray absorption fine structure spectroscopy (XAFS) techniques were used in the analyses. The objectives of the project were to investigate the ability of XPS and XAFS to characterize the chemical bonding of mercury and chlorine on the carbon sorbent surface. Both analytical techniques indicated similar chemical speciation data for chlorine and sulfur bonding on the surface of activated carbon sorbents. The advantage of the XPS over XAFS for chlorine and sulfur analysis is the semi-quantitative nature of the XPS technique. However, XPS does not provide any information for mercury concentration or speciation on most carbon sorbents because of the low levels of mercury present, the spectral interference from silicon, ubiquitous in coal- and biomass-derived activated carbons, and insignificant differences in energy. The results of this study suggest that further research into the behavior of standard compounds under XAFS analysis is needed before the surface of a heterogeneous sample can be characterized accurately. This includes, but is not limited to, the effects of sample preparation and potential interactions among standards on data collection and interpretation.