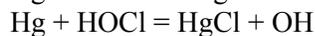
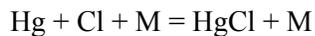
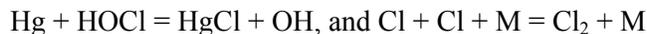


Progress was also made in developing improved rate constants for the homogeneous Hg oxidation model. Several reactions were focused on this year for the identification of basis sets/calculation method combination:



Progress was also made in identification of transition structures and calculation of reaction rate constants using Conventional Transition State Theory (CTST):



using Rice-Ramsperger-Kassel-Marcus (RRKM) theory.

Future Work

Planned work for subsequent periods of this project is detailed as follows:

- Experimental investigation of the effects of NO_x, SO₂ on gas-phase mercury reactions with chlorine in the new drop-tube furnace and the effects of these on the measurement using wet techniques.
- Identification of the effects of particles on mercury oxidation in the entrained-flow reactor at the University of Connecticut.
- Work on other reactions using CTST and RRKM.
- Incorporation of rate constants into overall reaction model for comparison with experimental data

List of Papers Published/Conference Presentations

Balaji Krishnakumar, Joseph J. Helble, "Understanding Mercury Transformations in Coal-Fired Power Plants: Evaluation of Homogeneous Hg Oxidation Mechanisms" (In preparation)

A. Fry, G. Silcox, J. Lighty, C. Senior, "Experimental Evaluation of the Effects of Quench Rate and Quartz Surface Area on Homogeneous Mercury Oxidation" accepted, 31st Symposium (International) on Combustion.

A. Fry, J. Lighty, G. Silcox, and B. Cauch, "Experimental Study of Homogeneous Mercury Oxidation Reactions Designed to Facilitate Model Development and Mechanism Validation," International Conference on Air Quality, Arlington, VA, September 2005.

C. L. Senior, A. Fry, J. S. Lighty, G. D. Silcox, "Detailed kinetic modeling of homogeneous mercury oxidation reactions in a 1000 Btu/hr quartz furnace, presented at 22nd Annual International Pittsburgh Coal Conference, Pittsburgh, PA, September 2005.

Students Supported Under this Grant

- Andrew R. Fry, PhD student, Chemical Engineering, University of Utah (graduating June 2006)
- Brydger Cauch, undergraduate student, Chemical Engineering, University of Utah (will be a BS/MS student)
- Balaji Krishnakumar, graduate student, Chemical Engineering, University of Connecticut

Awards Received

- Air and Waste Management Student Award, B. Cauch and A. Fry
- Barry Goldwater Scholarship, B. Cauch