Themodynamic Equilibrium Modeling of Mercury Speciation in the Environment

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Background

When liquid mercury is present in the environment, it forms compounds with available substances in its surroundings. When dissolved oxygen gas is available in an aqueous environment, liquid mercury will oxidize and form inorganic molecules, such as mercury chloride and mercury hydroxide. When dissolved methane gas is also present, mercury can form especially dangerous organic compounds, such as dimethylmercury ($(CH_3)_2Hg$), methylmercury cation (CH_3Hg^+), and methylmercury chloride (CH_3HgCl). These organic mercury compounds are neurotoxins and can cause serious harm to humans. Therefore, finding methods of removing them from contaminated sites is essential.

Introduction and Problem Statement

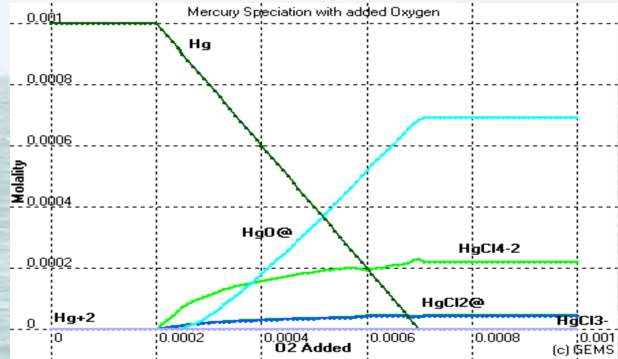
My research is at the Applied Research Center (ARC) at Florida International University (FIU). Along with my colleagues, I am working on the soil and groundwater remediation project under the partnership between FIU and the U.S. Department Of Energy, which focuses on the Oak Ridge National Laboratory (ORNL) site. Throughout the history of ORNL, research on nuclear energy resulted in several major mercury spills at the site. This mercury has since made its way to the soil and groundwater of the area. It is essential now to devise methods of extracting this mercury from the environment.

My Contribution

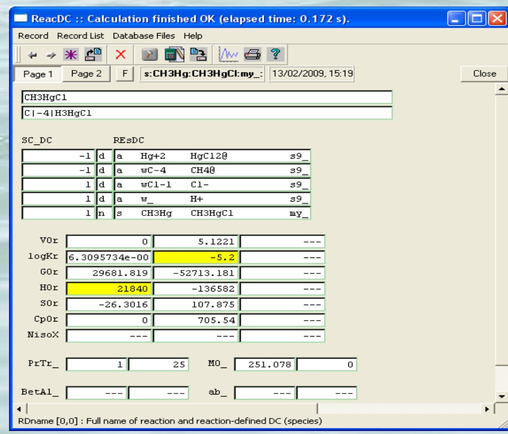
My contribution to the project is the thermodynamic equilibrium modeling of mercury speciation in the soil and groundwater. I am using a computer program called Gibbs Energy Minimization Selektor (GEMS), which models speciation by minimizing the Gibbs free energy of a system such as a lake or an ocean. Although the GEMS database contains much information on mercury compounds, there is very little information in the database on organic mercury compounds.

I am working on adding organic and inorganic mercury compounds to the GEMS database in order to more accurately estimate the speciation of mercury in different environments.

Plotting in GEMS



Speciation of inorganic mercury compounds with addition of O_2 (g)



Adding Methylmercury Chloride to the Database through log(K) and heat of reaction:

$CH_4(aq) + HgCl_2\ (aq) \rightarrow CH_3HgCl + H^+ + Cl^-$

log(K) ~ -5.2, Heat of reaction = 21 840 J/mol

Sources

Dean, John A. Lange's Handbook of Chemistry. 14th ed. McGraw-Hill, Inc. 1992.

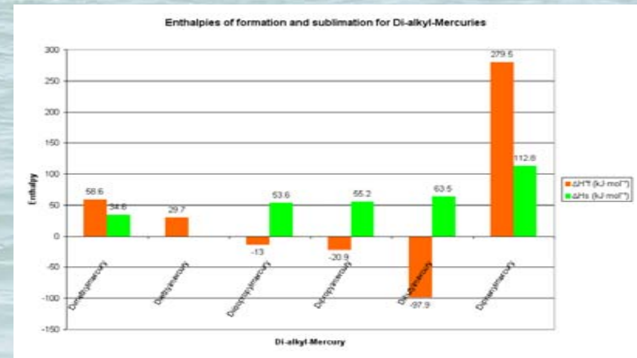
Stumm, Werner, and James J. Morgan. Aquatic Chemistry. 3rd ed. John Wiley and Sons. 1996.

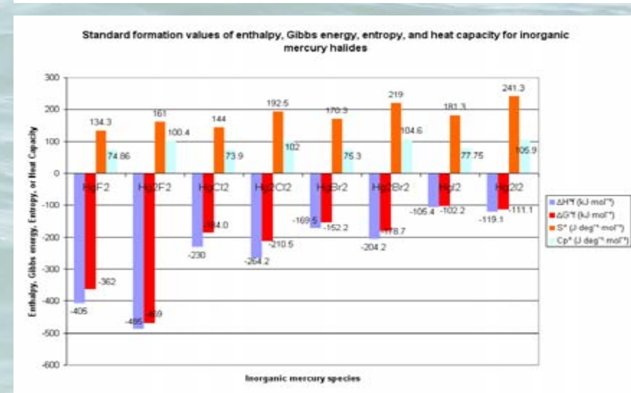
Morel, Francois M. M., et. al. "The Chemical Cycle and Bioaccumulation of Mercury". *Annual Review of Ecology and Systematics*, Vol. 29, 1998. JSTOR.

GEMS website. Paul Scherrer Institut. http://gems.web.psi.ch

Trends Between Mercury Species

Understanding trends in thermodynamic values for similar mercury species, such as mercury halides, can help determine whether or not output from the program seems reliable. The two graphs below are trends among organic mercury species and mercury halide species.





Future Work

My plans are to continue researching the chemistry of organic mercury compounds. I will focus on the different environmental conditions in which organic mercury species form. I will use this information to enhance the GEMS thermodynamic database. Most importantly, this will help in devising methods of extracting mercury from contaminated sites.