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Mercury in natural gas and hydrothermal fluids: insights from molecular dynamics simulations

DR. YUAN MEI[1], WEIHUA LIU[1] AND JULIEN BOURDET[2]

[1]CSIRO Mineral Resources
[2]CSIRO

Presenting Author: yuan.mei@csiro.au

Mercury is a contaminant in natural gas that poses health and safety risks and can cause equipment corrosion. Understanding the behaviour of mercury, including its speciation, transport, and partitioning during fluid-rock interactions, is crucial for predicting its mobility in natural gas, petroleum systems and ore-forming processes. However, the behaviour of mercury, especially its association with other elements such as S and Cl at high temperature and pressure conditions remains unclear, and experimental studies are challenging due to the toxicity of the element and the extreme conditions. Recently, ab initio molecular dynamics (MD) simulations have advanced our understanding of chemical processes under extreme conditions, allowing for the theoretical prediction of metal speciation and thermodynamic properties with high accuracy. The MD simulation complements experimental studies to provide a more complete picture of the elemental behaviour in geological fluids[1-2].

In this presentation, we showcase the MD simulations of mercury speciation in natural gas systems and hydrothermal fluid systems. We calculated the speciation of mercury in natural gas systems rich in H_2S and CO_2 to understand the distribution and association of Hg, H_2S, and CO_2 (as demonstrated in Figure.1). To quantify mercury speciation and solubility in hydrothermal fluids, we performed *ab initio* thermodynamic integration to calculate the thermodynamic properties of Hg^{2+} complexation with HS^- and Cl^- ligands in hydrothermal brines up to 350ºC. The obtained speciation models and thermodynamic data of mercury behaviour in high temperature-pressure fluids help understand the source and mobility of mercury in host rocks and reservoirs of natural gas, facilitating the improvement of mitigation techniques to remove mercury in natural gas products and reducing potential hazards during production. By combining experimental studies, this research can contribute to the compilation of a self-consistent database of mercury geochemistry, which can be used to model mercury sources and mobility in natural gas systems[3].

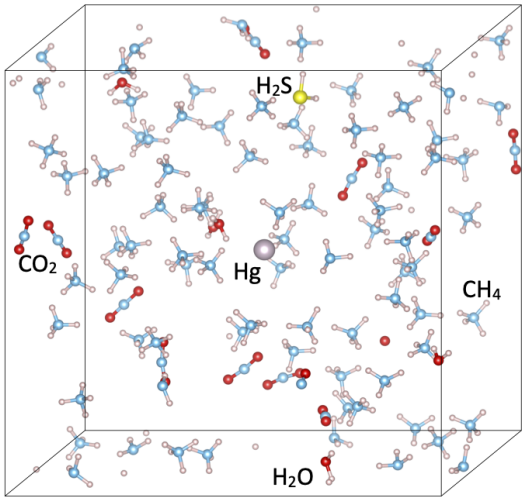

Figure 1. Simulation box of Hg in natural gas at 200ºC, 400 bar (0.19 g/cm^3). Silver = Hg; Red = O; yellow = S; blue = C; light pink = H.

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