Investigating the structural characterization of amorphous mineral precursors for enhanced understanding of contaminant adsorption and incorporation.

SAMANGI ABEYSINGHE AND TORI Z. FORBES*

Department of Chemistry, University of Iowa, Iowa City, IA, USA
tori-forbes@uiowa.edu

Metal oxyhydroxide mineral phases, particularly those containing Fe(III) or Al(III), play an important role in determining the long fate and transport of heavy metals and radionuclides in environmental systems. During rapid hydrolysis of the metal in solution, an amorphous or poorly crystalline precipitate initial forms, which can further transform into a thermodynamically stable mineral phase. During aggregation and flocculation processes, contaminants can adsorb to the surface of the particles, leading to co-precipitation and incorporation. Therefore, understanding the relationship between the soluble molecular precursor species present in solution and the amorphous precipitate is vital for gaining a molecular-level understanding of contaminant uptake by mineral species.

To investigate the structural relationship between the soluble precursors and the amorphous phase, we have begun synthesizing geochemical model compounds to compare to X-ray scattering of the amorphous phase. These model phases are metal oxyhydroxide nanoclusters that are 1-2 nm in diameter that can be packed into an ordered lattice for structure determination via single-crystal X-ray diffraction. The Pair Distribution Function (PDF) analysis of the module compounds can be calculated and compared to experimentally derived spectra. In this presentation we will focus on the relationship between aluminum based nanoclusters and amorphous aluminum hydroxide. In addition, geochemical model compounds with adsorbed contaminants will also be discussed that may provide information regarding possible adsorptions sites within amorphous materials.

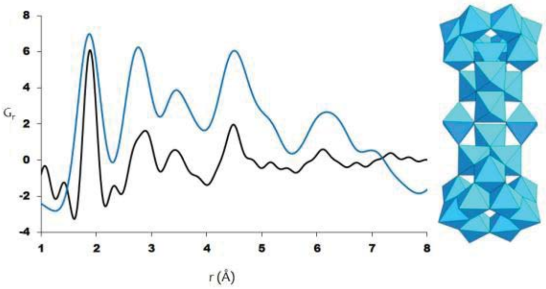

Figure 1. Comparision of the PDF spectra of amorphous metal oxyhydroxide material and the structurally characterized geochemical model compound.

Methane and dissolved inorganic carbon biogeochemistry in the Argentine Basin

M.FORMOLO[1*], N. RIEDINGER[2], J.M. MOGOLLÓN [3], S. HENKEL[4], J. TOMASINI[5], M. STRASSER[6], A. VOßMEYER[7], AND S.KASTEN[3]

[1]Dept. of Geosciences, University of Tulsa, Tulsa, OK 74104, USA, michael-formolo@utulsa.edu (* presenting author)
[2]Dept. of Earth Sciences, Univ. of California, Riverside, CA 92521, USA
[3]Alfred Wegener Institute for Polar and Marine Research, Bremerhaven, Germany
[4]Instit. Geology and Mineralogy, Univ. of Cologne, Cologne, Germany
[5]ANCAP, Montevideo, Uruguay
[6]Geological Institute, ETH, Zürich, Switzerland
[7]Center for Geomicrobiology, Aarhus Univ., Aarhus, Denmark

The Argentine Basin, located on the continental margin and slope of Uruguay and Argentina, has been well documented as a region susceptible to mass sediment transport processes and high sedimentation rates. These dynamic conditions impact the pore water and dissolved methane biogeochemistry. During Expedition M78/3 (May - June 2009) aboard the RV Meteor sediment and corresponding pore water samples were collected. The methane and pore water constituents provide a unique opportunity to address how sensitive methane and dissolved inorganic carbon (DIC) biogeochemistry are to environmental perturbations in these dynamic continental margin settings.

Adopting the definitions from Hensen et al. [1], for pore water profiles from this region, we have subdivided the sample locations into four profile categories; linear, concave-up, kink, and s-type. Comparisons among these categories allow us to address how methane biogeochemistry responds to sediment movements and variable methane fluxes. Within the Argentine Basin the observed sulfate and methane geochemistry are transitory in nature following mass-flow deposition or variations in methane fluxes. Over time the pore water profiles are constantly returning to a more steady-state situation and information regarding these transient periods can be lost. However, these end member steady-state, transient and non-steady conditions provide an opportunity to model the biogeochemical conditions during these phases. This will provide more detailed information regarding natural biogeochemical response to similar events in marine systems. Integrating pore water CH_4, DIC, and SO_4^{2-} concentrations with $\delta^{13}C$-CH_4 and $\delta^{13}C$-DIC into isotope and reactive-transport models will allow us to address what are the naturally occurring dominant biogeochemical pathways in these sediments and how they respond to perturbations from variable methane fluxes or sediment mass transport events.

[1] Hensen et al. (2003) *Geochim. Cosmochim. Acta* **67(14)**, 2631-2647.