



Fall 2009 Environmental Engineering seminar series



Presenting:

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Natural Organic Matter and Metal-NOM Aggregation in the Environment: Challenges and Opportunities for a Molecular Scale Understanding

Abstract

Natural organic matter (NOM) is ubiquitous in the environment and plays many important geochemical roles by forming aqueous complexes of widely differing chemical and biological stabilities with various inorganic and organic species. Metal-NOM interaction induces strong correlations between the concentration of natural organic matter and the speciation, solubility and toxicity of many metals in the environment. In water purification and desalination, NOM is also implicated in being the major foulant of nanofiltration and reverse osmosis membranes, either directly or by forming a surface conditioning layer for microbial attachment (“biofouling”). Despite significant geochemical, environmental and technological interest, the molecular-level mechanisms and dynamics of the physical and chemical processes involving NOM are not yet well understood. Computational molecular modeling can be an ideal tool to study these phenomena in true atomistic detail at nano-scale in both space and time. Yet, this route presents significant challenges due to the extraordinary compositional and structural diversity of NOM which preclude a unique definition of its molecular structure.

This talk will give a brief overview of the challenges and opportunities for the application of molecular modeling to NOM-related problems with specific focus on developing quantitative tools for structural, dynamic, and energetic characterization of metal-NOM ion complexation, hydration, hydrogen bonding, hydrophobic interactions, and supramolecular aggregation based on our on-going molecular dynamics (MD) computer simulations using relatively simple, but reasonably realistic model fragments of NOM in aqueous solutions. The modeling predictions from large-scale MD simulations of the effects of various metal cations on NOM aggregation in aqueous solutions will be compared with experimental data on dynamic light scattering (DLS) and small angle neutron scattering (SANS) using Suwannee River NOM (SRNOM). The DLS data for Ca^{2+} -NOM suggest the formation of a wide range of supramolecular structures with sizes between 100 and 1,000 nm. In contrast, Mg^{2+} and Na^+ do not seem to affect the aggregation of SRNOM as strongly. SANS data are inconclusive, but also indicate the presence of quite large (>50 nm) fractal particles formed presumably through a cluster-cluster aggregation. The results of MD simulations qualitatively agree with these observations, but also point out to the need for simulations at much larger time and length scales with more complex NOM models in order to fully capture the diversity of molecular processes involving NOM.

Thursday, October 22, 2009

4:10– 5:00pm

**3400 Engineering Building
Refreshments Provided**

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