SPP 1315 Biogeochemical Interfaces in Soil

ADVANCED SPECTROSCOPIC AND MICROSCOPIC CHARACTERISATION TECHNIQUES - TOOLS TO ENLIGHTEN BIOGEOCHEMICAL INTERFACES IN SOIL

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The Use of Q-XAS and ATR-FTIR Techniques to Elucidate Reaction Mechanisms at Biogeochemical Interfaces in Soil

Donald L. Sparks

Delaware Environmental Institute, University of Delaware, Newark, DE 19716, USA
dlsparks@udel.edu

The rates of important geochemical processes at biogeochemical interfaces including ion exchange, sorption, and redox can occur over wide time scales. Ex- situ batch and flow techniques offer high elemental sensitivity, but their time resolution is not adequate to capture rapid reaction rates that often comprise a significant portion of many processes such as sorption and oxidation-reduction. Measurement of rapid, initial rates of environmentally important reactions at the mineral/water interface is critical in determining reaction mechanisms. Until recently, experimental techniques with sufficient time resolution and elemental sensitivity to measure initial rates were very limited. Some techniques such as pressure-jump methods can capture rapid reactions on millisecond time scales but the rate parameters are indirectly measured and reaction mechanisms can only be inferred. Ideally, one would prefer to follow reaction rates in real-time, in-situ, and at the molecular scale to definitively determine reaction mechanisms. In this presentation the use of in-situ synchrotron-based, quick scanning X-ray absorption spectroscopy (Q-XAS) and attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), at sub-second time scales, are applied to measure the initial oxidation of As(III) and Cr(III) by hydrous manganese oxide. Results indicate that with these techniques, chemical kinetics are being measured. The rapid kinetic techniques are coupled with synchrotron-based XAS and XRD, and a stirred-flow technique, to provide a comprehensive assessment of As(III) oxidation kinetics and mechanisms on hydrous manganese oxide.