

Quantifying nitrate migration and natural attenuation in a shale/saprolite pathway from a former waste disposal site

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Understanding and quantification of contaminant transport in preferential pathways are important for long-term stewardship of contaminated sites. Characterization, monitoring and research results over the past several decades show contaminant migration through a transition zone between saprolite and shale bedrock along strike for over 3000 ft from the former S-3 Ponds in Oak Ridge Tennessee during a 32-year operation period. The cross-bedding migration appears limited at least after the primary source was removed. Contaminant concentration decreases slowly due to natural attenuation (dilution and/or denitrification) in the past 27 years since the capping of the ponds. The contaminant concentration near the S-3 ponds remains very high, suggesting strong nonequilibrium processes, i.e. either diffusion between the highly permeable transition zone and the less permeable saprolite and shale, or between matrix and fractures, or a combination of both.

A numerical model is constructed to quantify the diffusion processes, assess the natural attenuation rates, and evaluate the influence of recharge on the nitrate transport that has occurred for over half a century. Model results show that an equivalent porous medium model, with the transition zone as the fast flow pathway, and low permeable saprolite and shale as sink during plume emplacement and source after the primary source was removed, is sufficient in describing the major characteristics of the plume dynamics; the mass transfer between fractures and matrix in saprolite and shale may not be significant at this time scale of decades; dilution by recharge is the major mechanism that reduces nitrate concentration with natural attenuation rate not differentiable from dilution.

These results help us improve our understanding of the controlling processes and provides a foundation for further investigation on the fate and transport of co-contaminants such as uranium, technetium, and mercury at the site.

Nanoparticle surface properties deduced from single crystal mineral/water interface studies

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Nanoparticle properties are often controlled by their surface structure, and this can in-turn be affected by the detailed nature of surface ligands and surface functional groups. However determination of this structure even for synthetic analogs presents major experimental difficulties, and is also not readily accomplished with current simulation methods. One approach to understanding nanoparticle surfaces is afforded by the study of analogous or related single crystal mineral/water interfaces. In one such study we have analyzed the hydrogen bonding on the surfaces of C-plane and R-plane sapphire using nonlinear optical laser spectroscopy, and from such work can show why nanoparticles may have different acid-base properties from their single crystal analogs. In another study we have evaluated the overall details of the surface hydrogen bonding of R-plane sapphire and determined how this relates to surface structure as determined from x-ray reflectivity or crystal truncation rod diffraction. The technique is found to be highly complementary to the x-ray methods, and can be used as a test of model assumptions and type of surface termination.

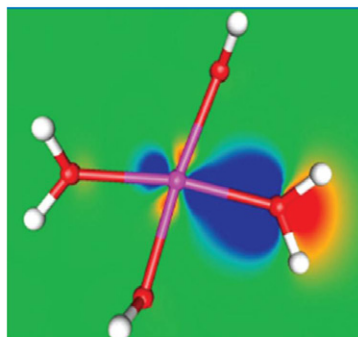


Figure 1: Electron density of 1st shell H₂O lone pair interacting with Fe³⁺(aq)[1]