Synergistic use of ZVI and SRB in groundwater remediation: Impact on metal removal and stability

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Groundwater bioremediation has emerged as a potential research interest in recent years. Moreover, different metallic particles has been tested as possible tool in groundwater treatment. ZVI (Zero Valent Iron) has already been proved highly efficient in treating contaminant like arsenic and chlorinated compounds but not much explored with metal removal, for which SRB (Sulfate Reducing Bacteria) is widely studied and trusted option. Redox potential and pH always play an important role in success of any in situ bioremediation process. In most cases extra substrate and considerable time is needed to start biological reduction. ZVI can play an important role in stimulating anaerobic degradation faster by depleting O2 and producing H2 during anaerobic corrosion, which marks an increase in pH and decrease in redox potential. Both of these technologies (ZVI and SRB) can possibly lead to new developments in groundwater remediation if used synergistically, the option which is very less explored yet.

In this study we used different ZVIs to stimulate SRB in low pH groundwater. Molecular tools were used to identify microbial communities, precipitates were characterized using different techniques like SEM and XRD. Stability of precipitates was compared in different pH and redox conditions. Our results indicate that bioaugumentation of ZVI can be very effective in wide range of contaminant removal and forming more stable precipitates, which is always a key parameter while dealing with groundwater remediation processes.

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Comparison of vibrations of water on rutile and cassiterite surface

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The vibrational spectrum of water is modified by the interface with oxides. This variation in the vibrational properties of the liquid serves as a probe of the interactions at play. We use large scale ab-initio molecular dynamics (AIMD) simulations to study the vibrational density of states (VDOS) of water on rutile (110) surface (titanium dioxide) and cassiterite (110) surface (tin dioxide). The velocityvelocity auto correlation function, calculated from the long trajectories of AIMD simulations, is used to extract the VDOS of water for these systems. The calculated total VDOS of water from our simulation (Figure 1) is in good agreement [1] with Inelastic Neutron Scattering (INS) experiment [2, 3]. The stretching band of the total VDOS of water shifts to a lower frequency for cassiterite surface in comparison to rutile surface. We will show that the microscopic analysis of our simulation reveals that this red shift in stretching band frequency is due to the stronger hydrogen bond formation on the cassiterite surface. This also causes the water on cassiterite to be closer to the surface than on rutile.



Figure 1: Computed total VDOS of water on cassiterite (in gray) and rutile (in black) surface.

[1] Kumar *et al.* (2009) JPC C **113**, 13732–13740. [2] Spencer *et al.* (2009) JPC A **113**, 2796–2800. [3] Private Communication with Levchenko *et al.*