Controlled Sulfidation to Optimize the Remediation Performance of Zerovalent Iron and Related Materials

Dimin Fan (fan.dimin@epa.gov) (ORISE Fellow, U.S. Environmental Protection Agency, Arlington, VA)
Ying Lan (lany@ohsu.edu), Paul G. Tratnyek (tratnyek@ohsu.edu), and Richard L. Johnson (rick.johnson.phd@gmail.com) (Oregon Health & Science University, Portland, OR)
Ariel Nunez Garcia (anunezga@uwo.ca) (Western University, London, ON, Canada)
Denis M. O'Carroll (d.ocarroll@unsw.edu.au) (University of New South Wales, Sydney, Australia)
Jan Filip (jan.filip@upol.cz) (Palacký University Olomouc, Czech Republic)
Abinash Agrawal (abinash.agrawal@wright.edu) (Wright State University, Dayton, OH)

Background/Objectives. Controlled sulfidation of iron-based materials, especially nano zerovalent iron (nZVI), has been shown in recent laboratory studies to be an effective approach for improving their remediation performance. The benefits can include favoring less reversible sequestration pathways, improving reactivity with chlorinated compounds, and enhancing selectivity for contaminant degradation. However, given the diversity of sulfidation methods and conditions that have been employed in these studies, the underlying factors that control the apparent benefits of sulfidation remain unclear, which creates uncertainties for the design and selection of these materials at large scale for field remediation applications. The objective of this study is to compare sulfidated materials prepared by various methods in terms of their properties and reactivity and to identify the controlling factors that need to be considered for optimizing the remediation performance of sulfidated materials.

Approach/Activities. Building on our experience in preparing and characterizing sulfidated iron-based materials in the laboratory, we compiled and compared the results reported in other sulfidation studies. Preparation methods and sulfidation conditions were used to categorize the sulfidated materials, and were further employed to catalogue the results of material and reactivity characterizations. By doing so, the effects of preparation methods and sulfidation conditions on properties and reactivity of sulfidated materials became evident, which we then used to develop a conceptual model that explains the dynamic and complex effects of sulfidation and that helps in predicting performance in future applications.

Results/Lesson Learned. We found that different sulfidation approaches result in materials with distinct surface, structural, and compositional characteristics. The aqueous-solid sulfidation method was of particular interest because it represents a major anticipated approach to modify the existing iron-based remediation products. For this method, S/Fe ratio and sulfidation duration are two key variables in affecting the property and reactivity of the sulfidated materials. The process is analogous to extensively-studied sulfur induced corrosion, and the structural evolution and reactivity trend of the materials can also be explained by models proposed in corrosion literature. Overall, we showed that the effects of sulfidation shift from kinetic enhancement to capacity preservation with increasing S/Fe ratio and sulfidation duration. This indicates the property and reactivity of sulfidated materials can be tuned by varying these operational variables to optimize their utility for different field application requirements.