

Reactive Nanoparticles for In Situ Groundwater Remediation: Effect of Surface Coatings on Reactivity, Transport, and Emplacement

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Novel reactive nanomaterials, such as Fe⁰ nanoparticles (NZVI), offer the potential for highly efficient targeted delivery of remedial agents to subsurface contaminants. The primary challenge to application is selecting appropriate surface modifiers that enable emplacement in the contamination zone, but do not adversely impact the particle's reactivity with the contaminant. Appropriate injection conditions are also needed. Concomitant optimization of mobility and reactivity requires a fundamental molecular level understanding of the surface modifiers properties along with their effect on mobility and reactivity. Dynamic light scattering and electrophoretic mobility measurements, along with Ohshimas's analysis are used to characterize the layer conformation and properties of different types of common synthetic and natural polyelectrolytes adsorbed onto NZVI. Batch reactivity studies and column and 2-D flow cell studies under a variety of hydrogeochemical conditions and heterogeneities were then conducted on polyelectrolyte-modified NZVI to determine the effect of the adsorbed layer properties on reactivity and mobility. Surface coatings decreased particle reactivity with TCE by up to a factor of 20. The magnitude of the effect depended on the adsorbed layer conformation of the polyelectrolyte as explained using the Scheutjens and Fleer train-loop-tail conceptual model for homopolymer sorption. More polydisperse samples containing larger particles (several hundred nanometers) are less mobile than monodisperse samples containing only small particles (<100nm). The concentration of the injected Fe0 nanoparticle suspensions also impact mobility. The higher deposition rate of the polydisperse samples and lower degree of deposition reversibility is attributed to increased particle aggregation from the magnetic attractive forces between particles which increase with r6. This study emphasizes the important role of aggregation on nanoparticle transport. A systematic study of mobility enhancement by different polyelectrolytes may yield a new semi-empirical approach to predicting the transport of polyelectrolyte or NOM coated nanomaterials in porous media.

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