Microscale Simulation of Nanoparticles Transport in Porous Media for Groundwater Remediation

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Abstract

Nanoscale zerovalent iron (NZVI) is one of the most promising reagent for the remediation of contaminated groundwater. These particles can degrade through redox reactions recalcitrant and carcinogenic compounds such as perchloroethylene and trichloroethylene. NZVI is characterized by a high reactivity and can be injected in the subsurface more easily if compared to the emplacement of granular iron commonly used in permeable reactive barriers (PRBs).
The aim of the study is to simulate the transport of iron nanoparticles and their interaction with the porous media. The capture and deposition of iron particles on the porous media is an important mechanism controlling the mobility of colloids in aquifer systems and the effectiveness of the technology.
A microscale domain (few micron) was reconstructed through SEM images of a sandy aquifer and the flow field was calculated using Navier-Stokes equations over a wide range of flow velocities, but always in laminar conditions. The dynamic of the particles is the center of a pore is governed by drag, gravity and Brownian forces, but close to the sand surface also the electric double layer (EDL) and the Van der Waals forces (VdW) come into play and become prevailing. In order to simulate the trajectories of the NZVI particles a Lagrangian approach was implemented by means of Particle Tracing for Fluid Flow module.
Since EDL and VdW forces are characterized by high gradients close (100 nm) to the grain surfaces, a reduction of the time step of the Lagrangian simulation is required for accurate simulations, but this is also leading to very high computational costs. Since the trajectories of few particles can be calculated on all the domain, a dual region approach implementing different criteria for particles motion (i.e. high time step in the bulk of the fluid, small time step close to the sand grains) would be desired. A further development would be to implement particle particle interactions.