



E-MNM1D: A model for the simulation of shear thinning suspensions of zerovalent iron micro and nanoparticles in porous media

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Colloidal suspensions of engineered nanoparticles have been studied in recent years for waste water and in-situ groundwater remediation. However, the use of zerovalent iron micro- and nanoparticles for groundwater remediation is hindered by colloidal instability, causing aggregation and sedimentation of the particles. The use of viscous shear-thinning fluids based on biopolymers dispersions was shown to significantly increase mobility of iron particles in porous media.

The aim of this work is to develop a numerical model, namely E-MNM1D, able to describe the transport of highly concentrated suspensions of iron particles, in particular during their injection in the subsurface, and in the early stages of migration through the porous matrix. The model is intended to be used as a tool in the development of an efficient injection technology for field-scale applications of nano- and microscale iron suspensions.

The model is based on a numerical solution of a system of coupled partial differential equations simulating the transport of the iron particle in the liquid phase and the interaction with the porous medium. The deposition/release and straining phenomena have been simulated by means of dual site non-equilibrium, reversible sorption sites (Tosco and Sethi 2010). Clogging of the porous medium due to the progressive retention of iron particles is described by a decrease in porosity and permeability. Finally, the shear-thinning properties of the suspensions are included introducing an apparent viscosity, which is function of polymer and suspended iron particle concentrations. Therefore, the transport equations for the concentrations of deposited and suspended colloids, the pressure losses and the constitutive equations for porosity, permeability and viscosity are coupled. The set of equations and boundary conditions are solved for monodimensional geometries using a finite-differences approach. An iterative scheme is used to solve the coupling of the equations.

E-MNM1D can be freely downloaded from www.polito.it/groundwater/software and is provided with an Excel interface for input/output. The work is co-funded by European Union project SQUAREHAB (FP7 - Grant Agreement Nr. 226565).

References

Tosco, T.; Sethi, R. Transport of non-Newtonian suspensions of highly concentrated micro- and nanoscale iron particles in porous media: a modeling approach. *Environmental Science & Technology* 2010.