Modelling field-scale injection and transport of nanoparticles suspensions in 3D geometries

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ABSTRACT

Natural and anthropogenic nanoparticles are widely spread into the environment, and in particular in groundwater, representing a concrete risk for human health. On the other hand, injection into the subsurface of suspensions of microscale and nanoscale zerovalent iron particles (MZVI and NZVI) have been studied in recent years for the remediation of contaminated aquifers. Consequently, understanding and modelling transport and deposition of colloidal particles in saturated porous media is a key aspect in short term (design of a field-scale injection) and long term (spreading in the environment) prediction of particles distribution.

Nanoparticles transport in porous media is usually described by a modified advection-dispersion equation that takes into account the mass exchanges between liquid and solid phase due to physical and physico-chemical interactions. These interaction kinetics, resulting in particles deposition on and release from the solid matrix, are strongly influenced by chemistry, e.g. pH, ionic strength, etc. [3, 4], and velocity [1, 6] of the pore water. However, up to date, modelling of colloids transport in the presence of such complex interaction phenomena has been mainly faced in one-dimensional Cartesian coordinates for the simulation of laboratory column tests [4], or at larger scales in simplified radial domains [5]. A numerical solution to 1D Cartesian and radial colloid transport equations was implemented by the authors in MNMs (www.polito.it/groundwater/software/MNMs.php).

In this work, the modelling tool MNM3D is developed for the simulation of nanoparticles suspensions injection and transport in more complex scenarios. MNM3D, standing for Micro and Nanoparticles transport Model in 3D geometries, is a modified version of the well-known transport model RT3D [2], in which the colloid transport equations and the dependencies of attachment and detachment kinetic coefficients on transients in pore water ionic strength and velocity have been implemented. The approach is validated comparing the simulation results of MNMs and MNM3D run on one-dimensional and 2D (radial symmetry) domains. The tool can be used for multi-dimensional simulations and employed in many practical field-scale applications, including the long-term behavior of engineered nanoparticles released in the environment (eg. from landfills), and the preliminary design of in situ aquifer remediation via injection of reactive nanoparticles injection (thus providing an estimate of operative parameters, such as particles distribution around the injection well, influence radius for a target concentration, number of required injection wells, etc.).

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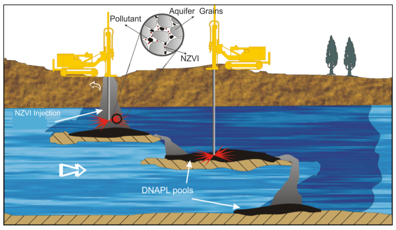
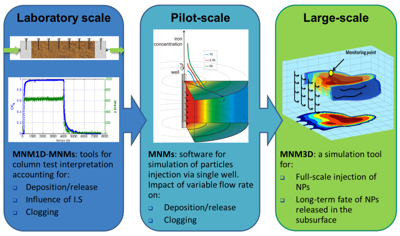
GRAPHICS



Field scale injection of zerovalent iron nanoparticles for remediation of polluted aquifers.

Graphic1



MNM3D development approach: extension of the micro- and nanoparticles transport equations from simplified 1D and radial geometries to complex and more realistic 3D domains.

Graphic2