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Simulating nanoparticle transport in 3D geometries with MNM3D

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The application of NP transport to real cases, such as the design of a field-scale injection or the prediction of the long term fate of nanoparticles (NPs) in the environment, requires the support of mathematical tools to effectively assess the expected NP mobility at the field scale.

In general, micro- and nanoparticle transport in porous media is controlled by particle-particle and particle-porous media interactions, which are in turn affected by flow velocity and pore water chemistry. During the injection, a strong perturbation of the flow field is induced around the well, and the NP transport is mainly controlled by the consequent sharp variation of pore-water velocity. Conversely, when the injection is stopped, the particles are transported solely due to the natural flow, and the influence of groundwater geochemistry (ionic strength, IS, in particular) on the particle behaviour becomes predominant. Pore-water velocity and IS are therefore important parameters influencing particle transport in groundwater, and have to be taken into account by the numerical codes used to simulate NP transport.

Several analytical and numerical tools have been developed in recent years to model the transport of colloidal particles in simplified geometry and boundary conditions. For instance, the numerical tool MNMs was developed by the authors of this work to simulate colloidal transport in 1D Cartesian and radial coordinates. Only few simulation tools are instead available for 3D colloid transport, and none of them implements direct correlations accounting for variations of groundwater IS and flow velocity.

In this work a new modelling tool, MNM3D (Micro and Nanoparticle transport Model in 3D geometries), is proposed for the simulation of injection and transport of nanoparticle suspensions in generic complex scenarios. MNM3D implements a new formulation to account for the simultaneous dependency of the attachment and detachment kinetic coefficients on groundwater IS and velocity. The software was developed in the framework of the FP7 European research project NanoRem and can be used to predict the NP mobility at different stages of a nanoremediation application, both in the planning and design stages (i.e. support the design of the injection plan), and later to predict the long-term particle mobility after injection (i.e. support the monitoring, final fate of the injected particles). In this work MNM3D an integrated experimental-modelling procedure is used to assess and predict the nanoparticle transport in porous media at different spatial and time scales: laboratory tests are performed and interpreted using MNMs to characterize the nanoparticle mobility and derive the constitutive equations describing the suspension behavior in groundwater. MNM3D is then used to predict the NP transport at the field scale. The procedure is here applied to two practical cases: a 3D pilot scale injection of CARBO-IRON® in a large scale flume carried out at the VEGAS facilities in the framework of the NanoRem project; the long term fate of an hypothetical release of nanoparticles into the environment from a landfill is simulated.