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HS8.1.5 - Fate and transport of biocolloids and nanoparticles in soil and groundwater systems

Simulating nanoparticle transport in 3D geometries with MNM3D

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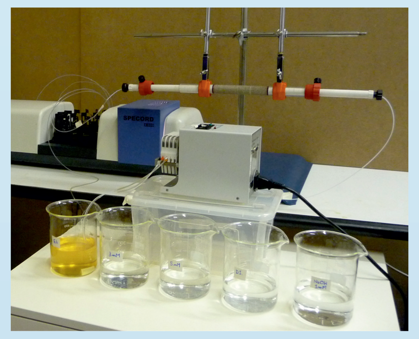
Background and motivation

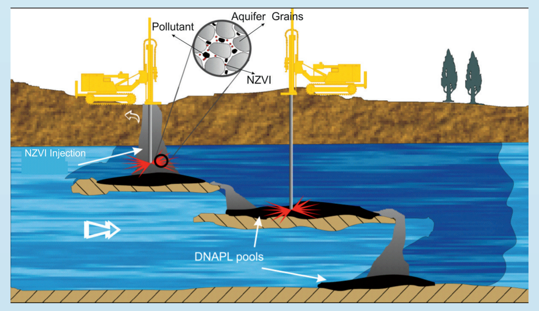
Particle transport and deposition in saturated porous media are important processes occurring in natural and engineered systems:
- Virus, microorganism or contaminant transport in aquifer systems;
- Injection of engineered nanoparticle suspensions (e.g. zero-valent iron nanoparticles) for contaminated aquifer remediation;
- Clogging of depth filters and wells, etc.

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 this work, carried out in the framework of the EU Research Projects NanoRem and Reground, the numerical tool **MNM3D** (Micro- and Nanoparticle transport Model in 3D geometry) is proposed for the simulation of colloid transport in field scale applications. Moreover, an **integrated experimental-modelling procedure** is applied to assess the nanoparticle transport in laboratory-scale conditions and predict the behavior at different spatial and time scales.

Laboratory scale
Modelling 1D experiments to characterize nanoparticle transport



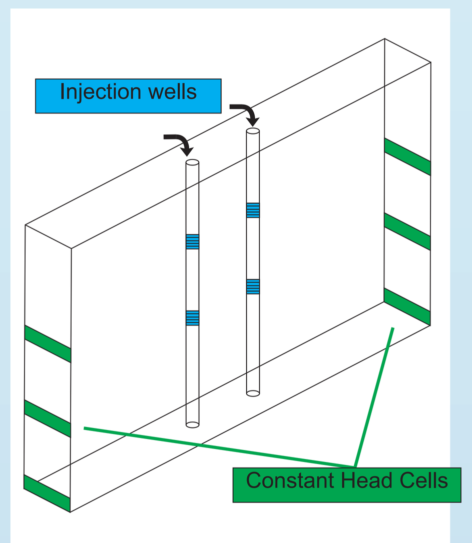
Field scale applications
Simulation of particle injection and transport in complex scenarios, e.g. aquifer reclamation



Injection of CarboIron in a small scale flume

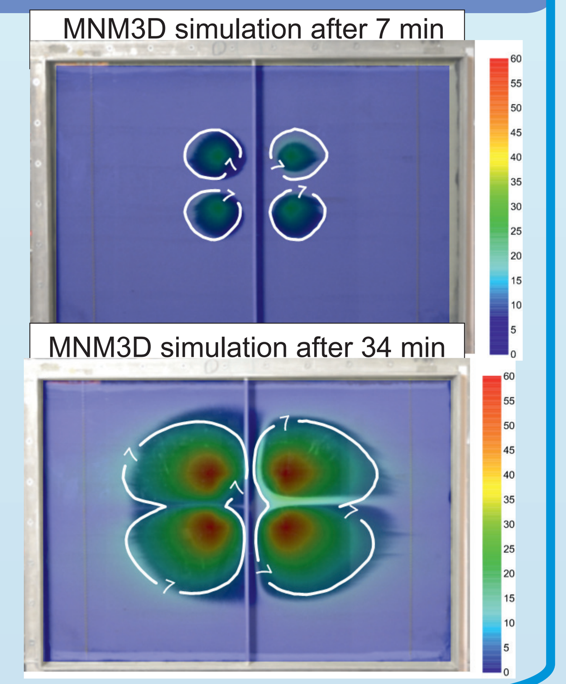
CARBO-IRON® particles (800 nm, 20 g/L) stabilized with CMC (4 g/L) were injected in a 2D confined aquifer (small scale flume SSF), located at the VEGAS facilities in Stuttgart (Germany).
The container was 1 m x 0.7 m x 0.2 m (L x H x W) large, with a glass wall for visual analysis of particle distribution.
The nanoparticle injection was simulated using MNM3D (velocity dependent kinetics) and visually compared to partial experimental results.
Good agreement was found between experimental and modelling data.
Quantitative validation is still necessary.

SSF set-up



LEFT: Experimental setup of the large scale flume.

RIGHT: Spreading area of CARBO-IRON® concentration (front view, courtesy of VEGAS) after 7 (A) and 34 (B) minutes from the start of the particle injection. Visual comparison between experimental (black plume) and simulated (colored) results of nanoparticle transport.
Total concentration of particles is shown (suspended + deposited concentration).



Governing equations

Colloid-porous medium interactions:

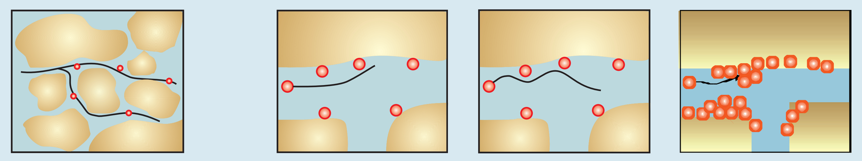
Transport equations for liquid and solid phase:

$$\begin{cases} \frac{\partial(\varepsilon C)}{\partial t} - \sum_k \frac{\partial(\rho_b S_k)}{\partial t} + \frac{\partial(q_i C)}{\partial x_i} - \frac{\partial^2(\varepsilon D_{ij} C)}{\partial x_i^2} - q_s C = 0 \\ \frac{\partial(\rho_b S_1)}{\partial t} = \varepsilon k_{a,1}\left(1 + A S_1^B\right)C - \rho_b k_{d,1} S_1 \\ \frac{\partial(\rho_b S_2)}{\partial t} = \varepsilon k_{a,2} C - \rho_b k_{d,2} S_2 \end{cases}$$

Hydrological processes (advection + dispersion)

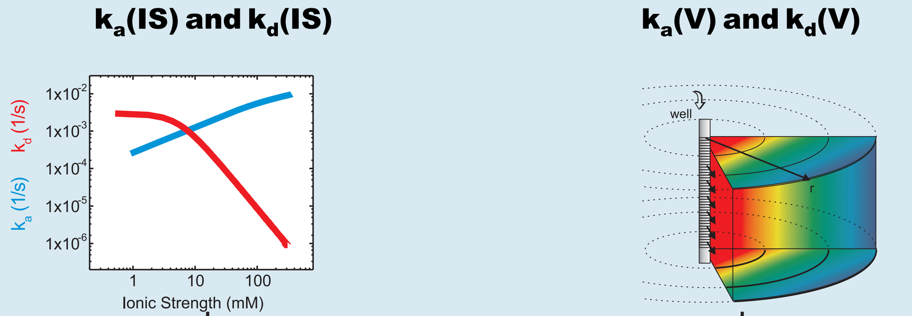
Physico-chemical interactions

linear attachment | **blocking** | **ripening**



Coupled influence of ionic strength and pore water velocity:

In field conditions, the **mobility** of colloidal suspensions is strongly influenced by the groundwater **ionic strength** and **flow velocity**:

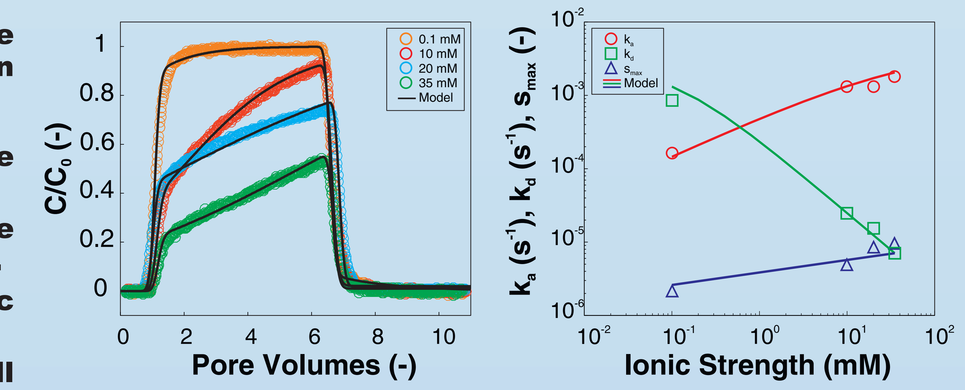


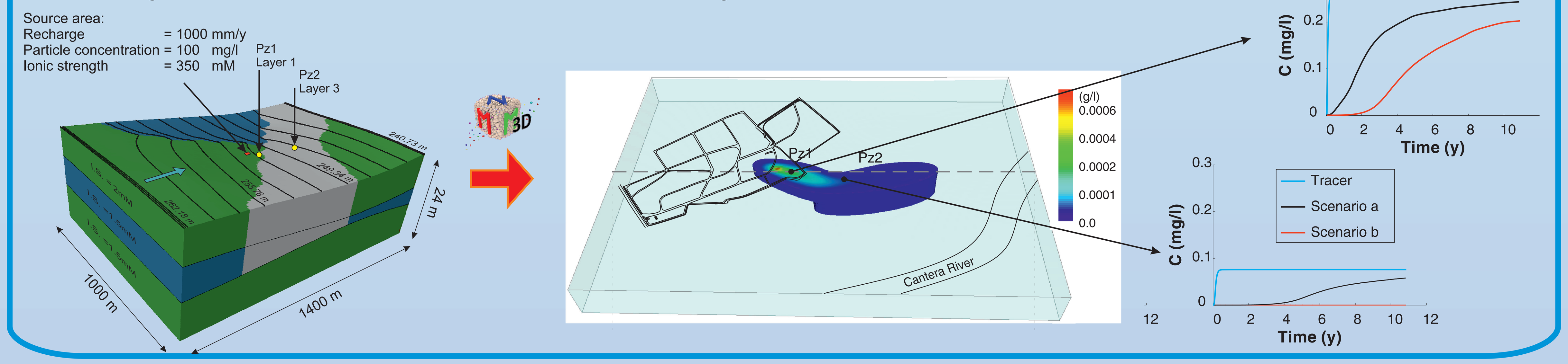
$$k_a(V, c_t) = \frac{3}{2}\frac{(1-\varepsilon)}{\varepsilon d_s}\frac{C'_a}{1+\left(\frac{CDC}{c_t}\right)^{\beta_a}}\eta_0 V \qquad k_d(V, c_t) = \frac{C'_d}{1+\left(\frac{c_t}{CRC}\right)^{\beta_d}}\mu V$$

Prediction of long term fate of graphene oxide NPs with MNM3D

An **integrated experimental-modelling approach** was used to characterize graphene oxide (GO) nanoparticles at the laboratory scale and predict the long term mobility of the NPs in field conditions.

- Column tests of graphene oxides nanoparticles (400 nm, 10 mg/L) transport were carried out at different NaCl concentrations (i.e. DI, 10, 20, 35 mM).
- Experimental BTs were fitted using MNMs to characterize NP transport and derive attachment and detachment coefficients. A reversible blocking kinetics was identified.
- Semi-empirical correlation equations were used to model the effect of variable ionic strength on the graphene oxides NP transport.
- A 3D heterogeneous model was built in Visual Modflow to simulate the hypotetical spill of Graphene oxides NP from a landfill.
- The long term fate of GO was simulated under field conditions using MNM3D.

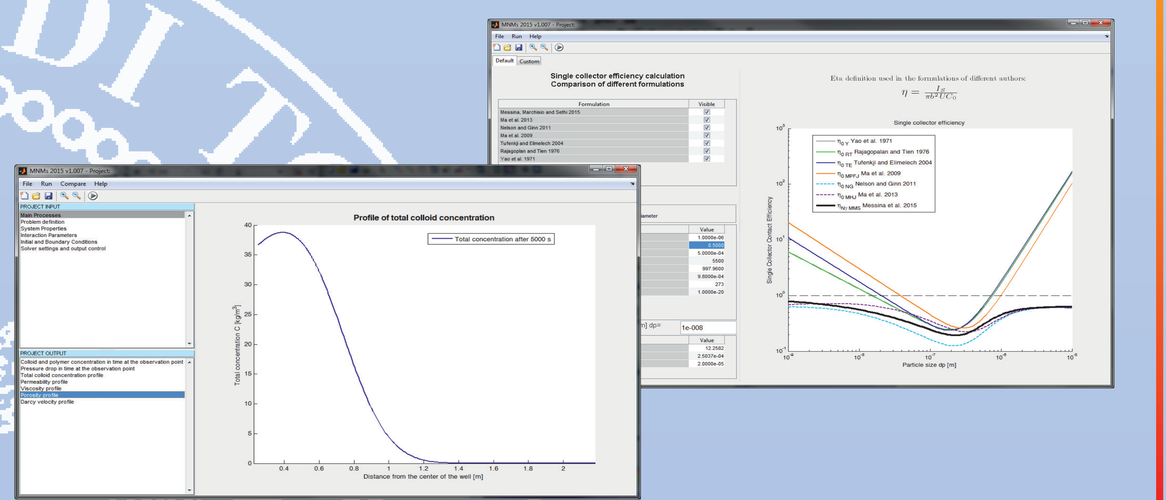




Numerical tools

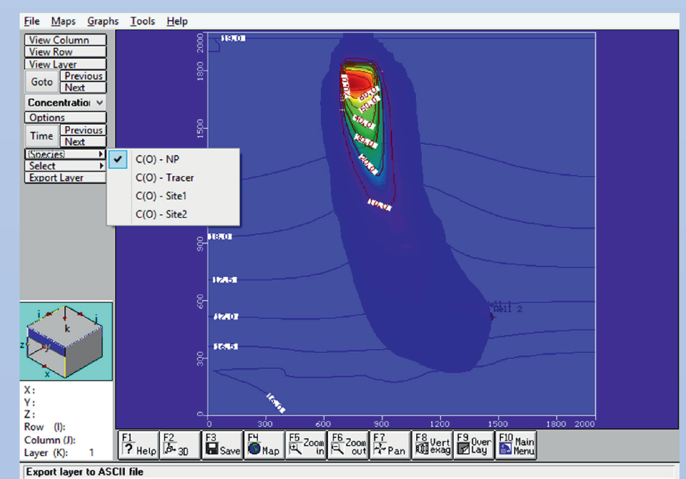
MNMs

MNMs, which stands for **Micro- and Nanoparticle transport, filtration and clogging Model – suite**, is a Matlab-based software developed at Politecnico di Torino for:
- interpretation of column transport tests of solutes and nanoparticles (1D Cartesian geometries);
- simulation of pilot injections through a single well (1D-radial geometry);
- calculation of DLVO interaction profiles and single collector effciency.



MNM3D

MNM3D (**Micro and Nanoparticles transport Model in 3D geometries**) is an RT3D based numerical code developed at Politecnico di Torino for the simulation of the injection and transport of nanoparticle suspensions in generic complex scenarios. MNM3D implements a new formulation of the kinetic coefficients for the simulation of the **simultaneous effects of pore water velocity and ionic strength** transients.
MNM3D can be used to simulate nanoparticle transport within the **Visual Modflow** graphical interface.



Conclusions

The numerical code **MNM3D** was developed for the simulation of nanoparticle transport in **full 3D geometries** under transient conditions of pore water chemistry and velocity. MNM3D was implemented in the **Visual Modflow** classical interface and successfully applied to simulate CarboIron® NP injection in a small scale flume.
An **integrated experimental-modelling approach** was applied to simulate graphene oxides NP transport at different scales using **MNMs** (1D cartesian model) and MNM3D.

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For further information:
http://areeweb.polito.it/ricerca/groundwater/software/MNMs.php