Microscale simulation of nanoparticles transport in porous media for groundwater remediation

Francesca Messina, Matteo Icardi*, Daniele Marchisio**, Rajandrea Sethi**

* Politecnico di Torino – DIATI – C.so Duca degli Abruzzi 24, 10129 - Torino, Italy
** Politecnico di Torino – DISAT – C.so Duca degli Abruzzi 24, 10129 - Torino, Italy

COMSOL CONFERENCE EUROPE 2012

Introduction

Micro and nanoscale zerovalent iron (MZVI - NZVI) is a promising reagent for the remediation of **contaminated groundwater**.
MZVI and NZVI can degrade recalcitrant and carcinogenic compounds.
The aim of this study is to simulate the **transport** of iron nanoparticles and their interaction with the porous media from a **microscale** point of view.
The mechanism of attachment can bring the iron particles to be captured from the grains of porous media, as showed in Fig.1, and, in this way, they can't carry on their remediation activity in groundwater.
The goal of the study is to evaluate the **collector efficiency**, the number of particles captured by the aquifer grains respect to the total number of particles released.

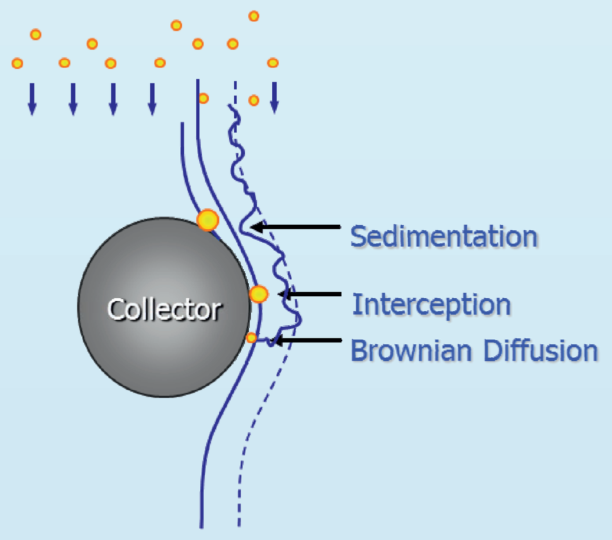

Fig. 1: Mechanisms of particle adhesion to the grain.

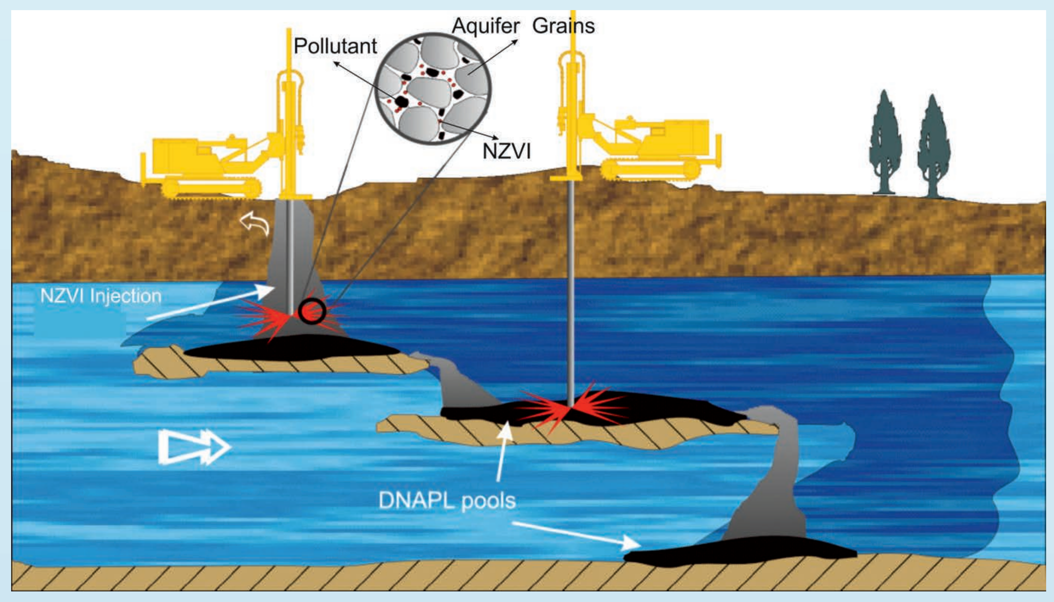

Fig. 2: NZVI injection in the aquifer system.

Methods

A **Lagrangian approach** (Fig.3) has been used, implementing all the forces acting on MZVI and NZVI, whose mathematical expressions are shown in Table 1.
The *COMSOL Multiphysics 4.2a Particle Tracing for Fluid Flow* module has been used.

The particles motion has been studied in two pore-scale configurations: the first is the **Happel model** (Fig.4) where the grain is represented by a circle surrounded by a fluid film that implicitly takes into account the effects of the neighbouring grains. Then a more realistic two-dimensional domain, recreated from a **SEM image** of a real sand sample, has been used (Fig.5 and 6).

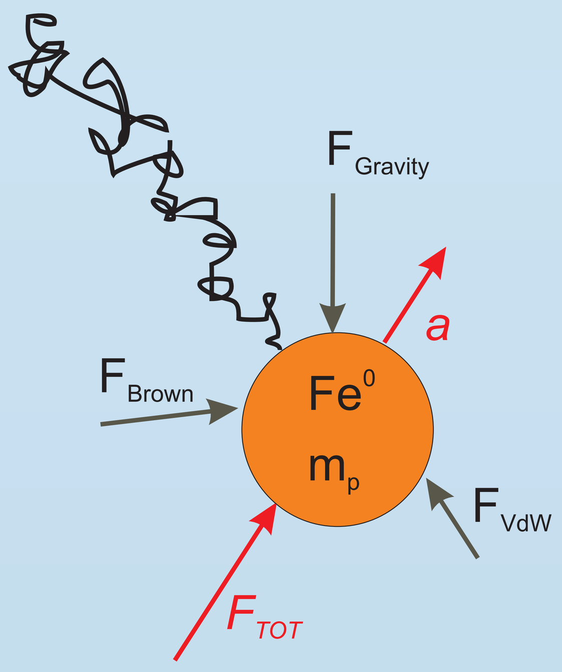

Fig. 3: The total force is the sum of all forces acting on the particle. The particle acceleration is proportional to the total force and it determines the particle trajectory.

Forces	Mathematical expression
Drag force	$\vec{F}_D = 6\pi\mu a_p(\vec{u}-\vec{v})$
Gravity force	$\vec{F}_G = \frac{4}{3}\pi a_p^3(\rho_p - \rho_f)\vec{g}$
Electric double layer force	$\vec{F}_{EDL} = \varepsilon_0\varepsilon_r a_p \frac{(\xi_p^2+\xi_c^2)\kappa e^{-\kappa h}}{2(1-e^{-2\kappa h})}\left[2\frac{\xi_p\xi_c}{(\xi_p^2+\xi_c^2)} - e^{-\kappa h}\right]\vec{n}$
Van der Waals force	$\vec{F}_{VdW} = -\frac{Ha_p}{6h^2}\frac{\lambda(\lambda+28h)}{(\lambda+14h)^2}\vec{n}$
Brownian force	$F_B = R\sqrt{\frac{2\xi kT}{\Delta t}}$

The parameters are: u fluid velocity, v particle velocity, a_p particle radius, ρ_p particle density, ρ_f fluid density, g acceleration of gravity, H Hamaker constant, h particle – collector distance, λ average wavelength of electron oscillation (100 nm), R randomnormal distribution number, k Boltzman's constant, T absolute temperature, ξ friction coefficient (equal to $6\pi\mu a_p$), k Debye - Huckel parameter.

Table 1: The implemented forces.

Results

The results of collector efficiency as a function of the particle radius and the flow field velocity are shown in Table 2.
The flow velocity improves particles transport and the smallest particles are more mobile.
There are some differences with the other studies: the electric double layer effect has been also considered and a Lagrangian approach has been used in place of the more diffused Eulerian approach.

This study is currently being improved in order to simulate a larger number of particles trying to overcome problems due to the time discretization used by the solver that, in the current version of the code, is not adaptive.

Other **future developments** would include the use of more complex geometries and the implementation of particle-particle interactions.

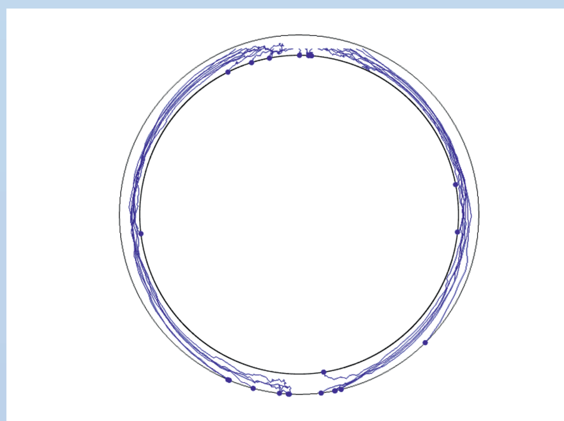

Fig. 4: The particles trajectories in the Happel's geometry.

COLLECTOR EFFICIENCY η [%]

Velocity field [m/s]	MZVI and NZVI particle radius [m]: $a_p = 4\cdot10^{-6}$	$a_p = 4\cdot10^{-7}$	$a_p = 4\cdot10^{-8}$
$U = 10^{-6}$	71	46	59
$U = 10^{-5}$	66	19	19
$U = 10^{-4}$	42	8	10
$U = 10^{-3}$	18	3	1

Table 2: Happel's model results of collector efficiency.

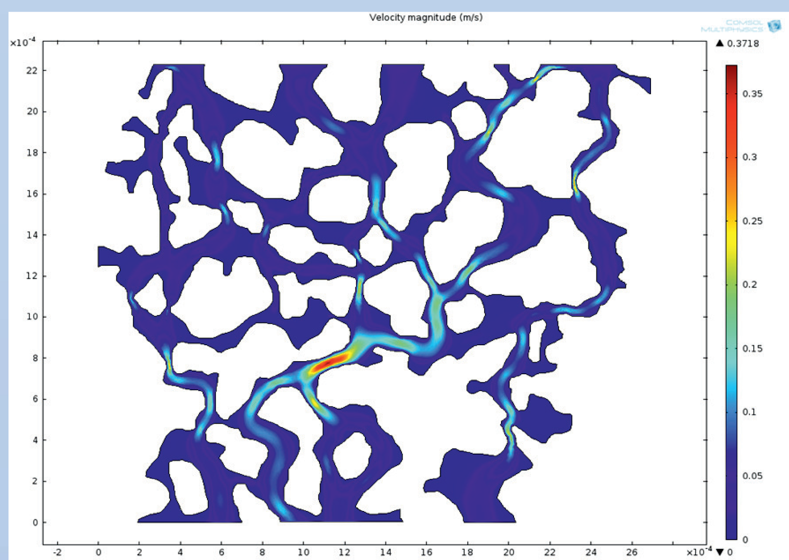

Fig. 5: The flow field in the geometry obtained from the SEM image.

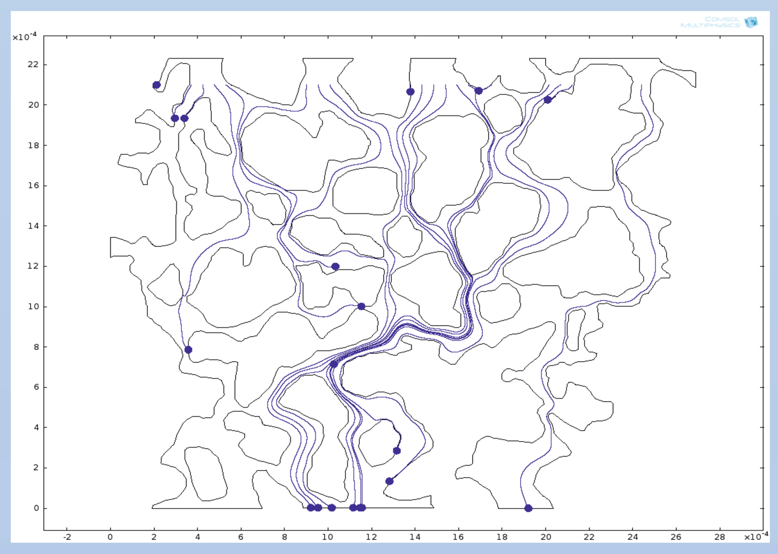

Fig. 6: The particles trajectories in the geometry obtained from the SEM image.

References
[1] Elimelech M., Tufenkji N. - *Correlation equation for predicting single-collector efficiency in physicochemical filtration in saturated porous media* - Environmental Science & Technology,38(2), 529-536
[2] Elimelech M. - *Particle deposition on ideal collectors from dilute flowing suspensions: Mathematical formulation, numerical solution, and simulations* - Sep. Technol., 1994, vol. 4, October
[3] Happel J. – *Viscous Flow in Multiparticle System: Slow Motion of Fluid Relative to Beds of Sherical Particles* – A.I.Ch.E Journal, Vol.4, No.2 p.197
[4] Ma H., Pedel J., Fife P., Johnson W.P. - *Hemispheres-in-Cell Geometry to Predict Colloid Deposition in Porous Media* - Environmental Science & Technology, 2009, 43, 8573-8579
[5] Tosco T., *Modelling the transport of iron- based colloids in saturated porous media*, Tesi di dottorato, Politecnico di Torino, 2010
[6] Tosco T. , Tiraferri A., Sethi R. - *Ionic Strength Dependent Transport of Microparticles in Saturated Porous Media: Modeling Mobilization and Immobilization Phenomena under Transient Chemical Conditions* - Environ. Sci. Technol. 2009, 43, 4425–4431
[7] Tosco T., Sethi R. - *Transport of Non-Newtonian Suspensions of Highly Concentrated Micro- And Nanoscale Iron Particles in Porous Media: A Modeling Approach* - Environ. Sci. Technol. 2010, 44, 9062–9068