NanoRem

Modelling nanoparticle transport in porous media across the scales: from the pore scale to the field-scale injection

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NanoRem is a four year, €14 million research project funded through the European Commission FP7.
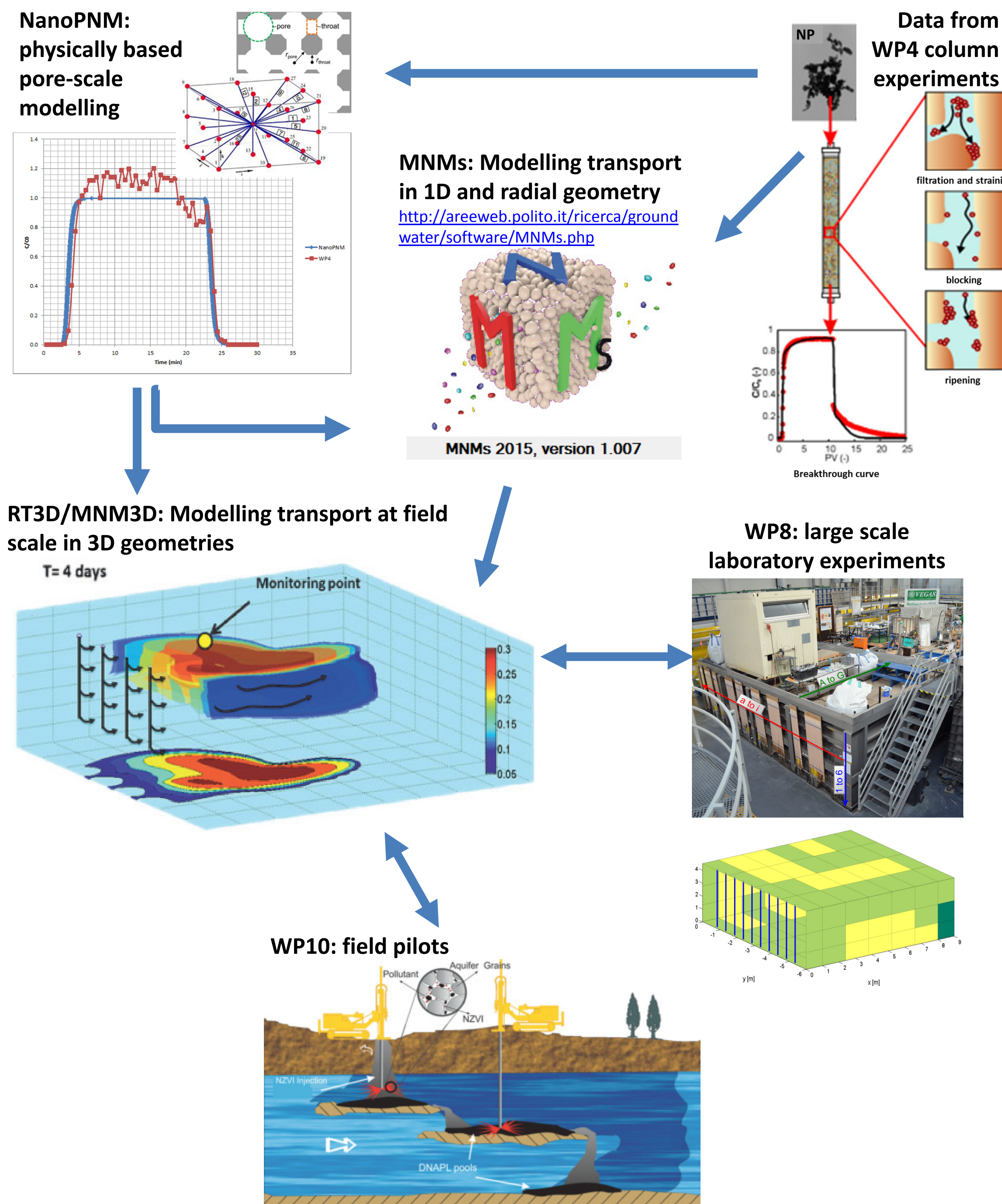
Rationale

The design of a field-scale injection of engineered nanoparticle (NP) suspensions (e.g. zero-valent iron nanoparticles) for remediation of polluted sites requires a reliable estimation of the particle distribution after injection. In addition, regulators will require information on the longer term mobility of the injected particles in case they do not encounter and react with the contaminant.

While numerical models for the simulation of dissolved contaminant transport are widely available, field-scale models for the transport of NPs, with proven predictive ability, are yet developed. This is, in part, due to the lack of understating of fundamental controlling mechanisms for the transport of NPs in the subsurface at the field scale.

Therefore, as part of the EU research project NanoRem, WP7 set out to develop a NP transport simulation module, based on fundamental physics, to be incorporated into the existing reactive transport models like RT3D. The research aim is approached from both ends: understanding NP behaviour at the pore scale and finding up-scaled relationships that are validated using experimental or field data at the macro-scale.

General Approach

NanoPNM: physically based pore-scale modelling

Data from WP4 column experiments

MNMs: Modelling transport in 1D and radial geometry
http://areeweb.polito.it/ricerca/groundwater/software/MNMs.php

MNMs 2015, version 1.007

filtration and straining

blocking

ripening

Breakthrough curve

RT3D/MNM3D: Modelling transport at field scale in 3D geometries

T= 4 days

Monitoring point

WP8: large scale laboratory experiments

WP10: field pilots

Basic Equations

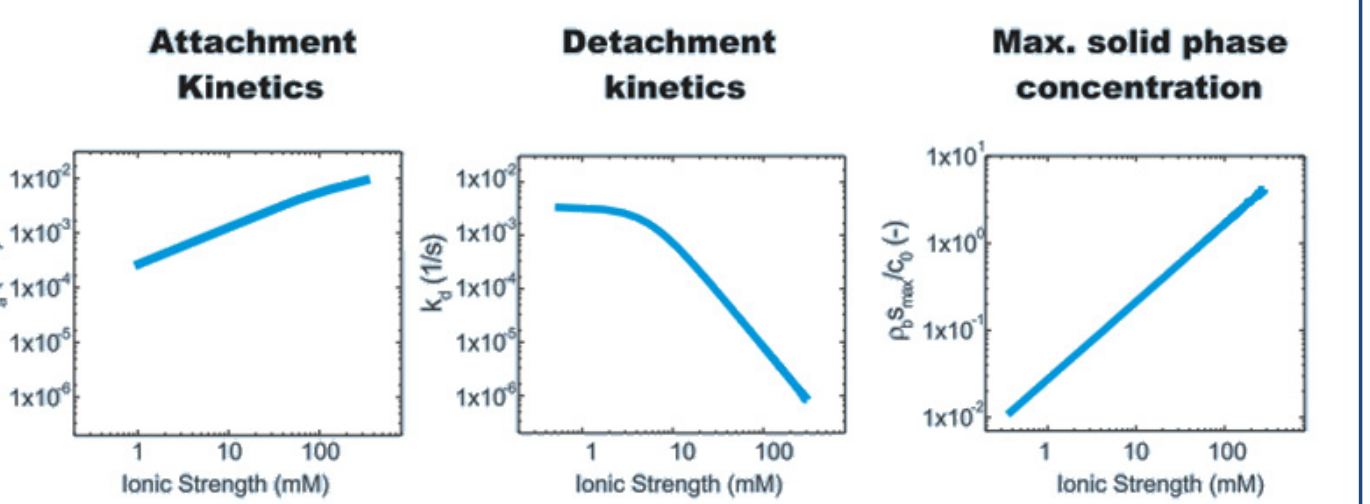**Transport equations for liquid and solid phase:**

$$\frac{\partial (nC)}{\partial t} - \sum_k \frac{\partial (\rho_b S_k)}{\partial t} + \frac{\partial (q_i C)}{\partial x_i} - \frac{\partial^2 (nD_{ij}C)}{\partial x_i^2} - q_s C = 0$$

$$\frac{\partial (\rho_b S_1)}{\partial t} = n k_{a,1}\left(1 + AS_1^B\right)C - \rho_b k_{d,1} S_1$$

$$\frac{\partial (\rho_b S_2)}{\partial t} = n k_{a,2} C - \rho_b k_{d,2} S_2$$

Influence of ionic strength:

Salt concentration is coupled with colloid equations via semi-empirical relationships:

$$\frac{\partial (nc_i)}{\partial t} + \frac{\partial (q_i c_i)}{\partial x_i} - \frac{\partial^2 (nD_{ij} c_i)}{\partial x_i^2} - q_s c_i = 0$$
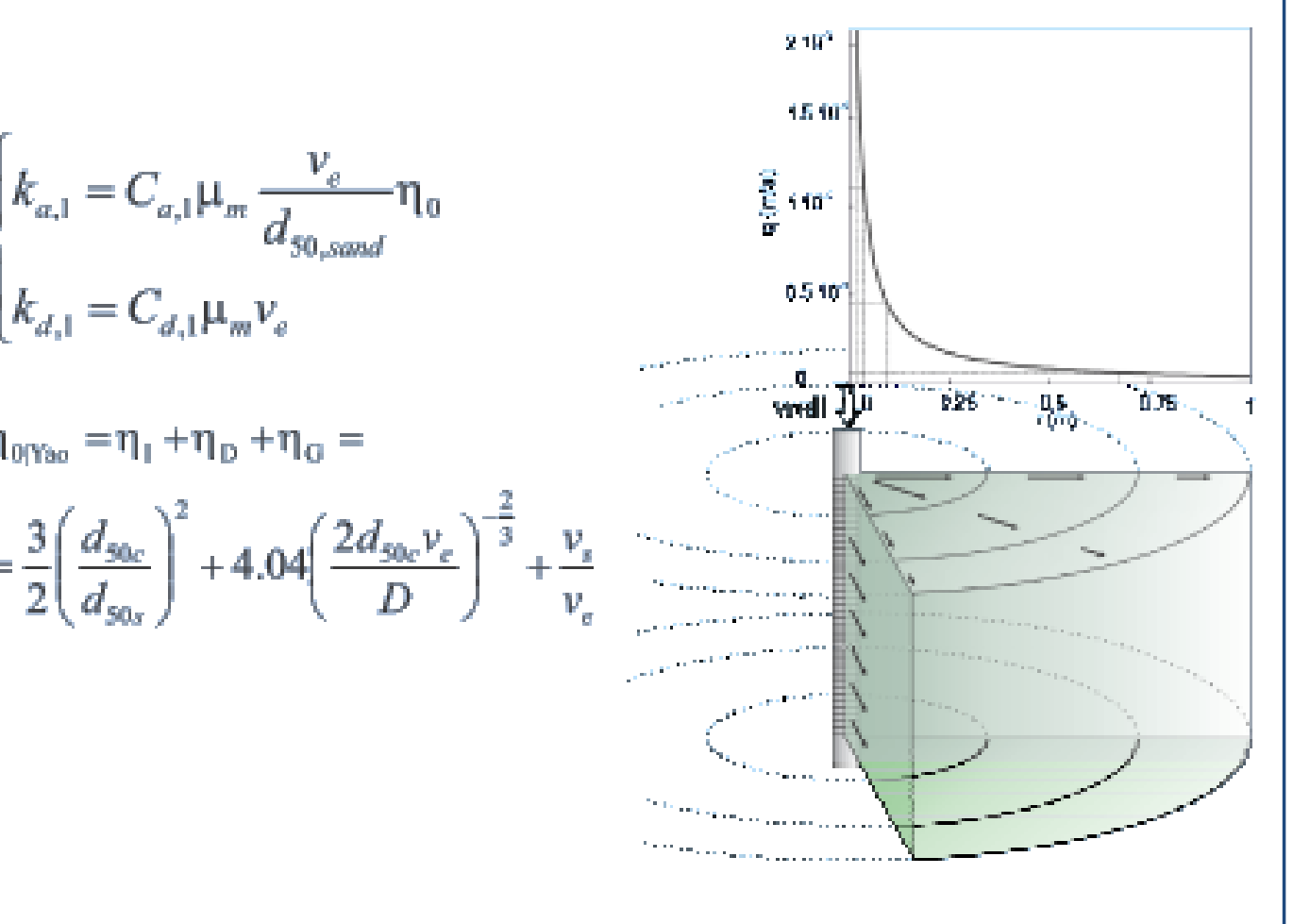
Attachment Kinetics | **Detachment kinetics** | **Max. solid phase concentration**

Ionic Strength (mM)

$$k_{a,i} = \frac{k_{a,0,i}}{1 + \left(\frac{CDC_i}{c_i}\right)^{\beta_{a,i}}} \qquad k_{d,i} = \frac{k_{d,0,i}}{1 + \left(\frac{c_i}{CRC_i}\right)^{\beta_{d,i}}} \qquad s_{\max,i} = \gamma_{d,i} c_i^{\beta_{s,i}}$$
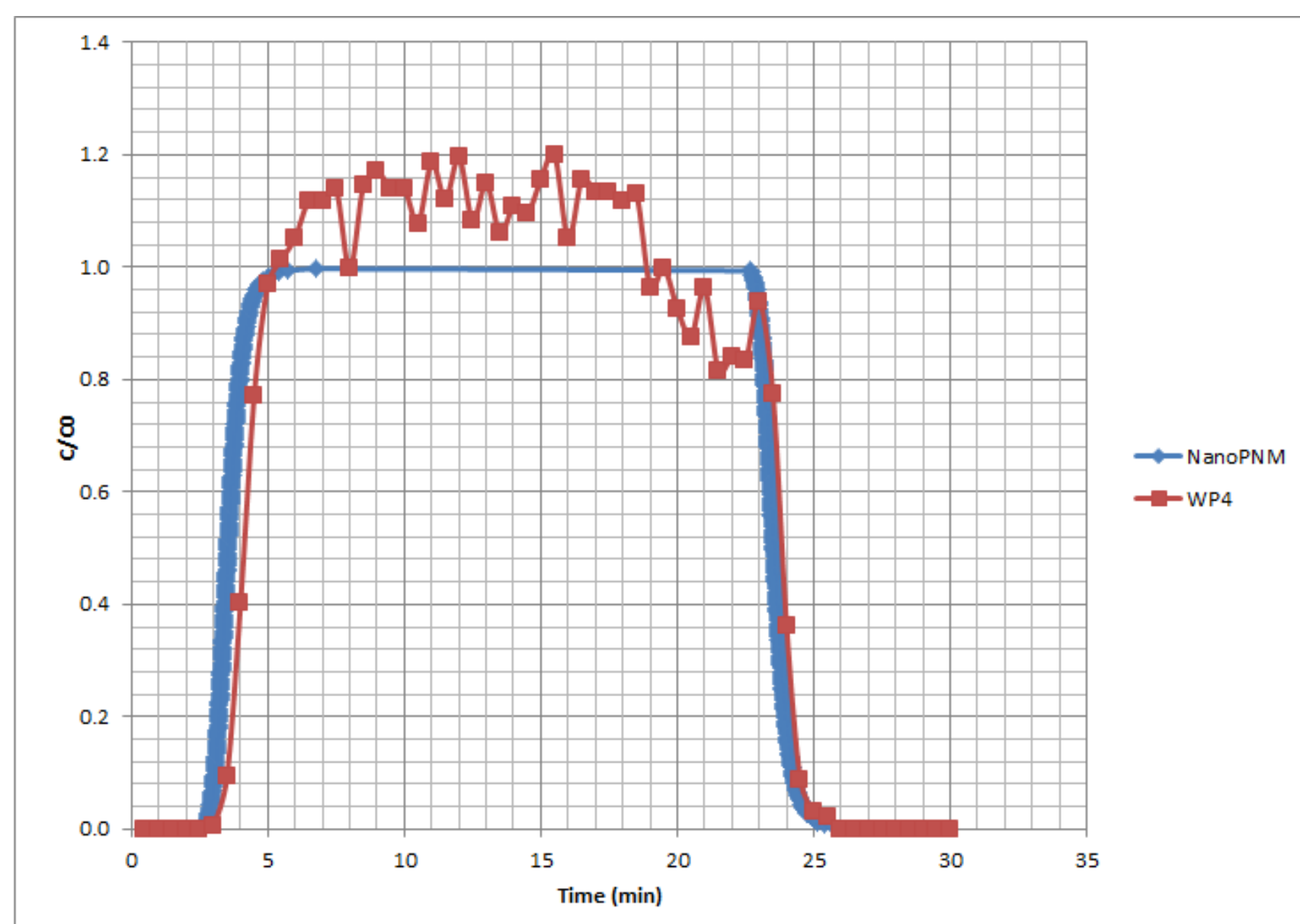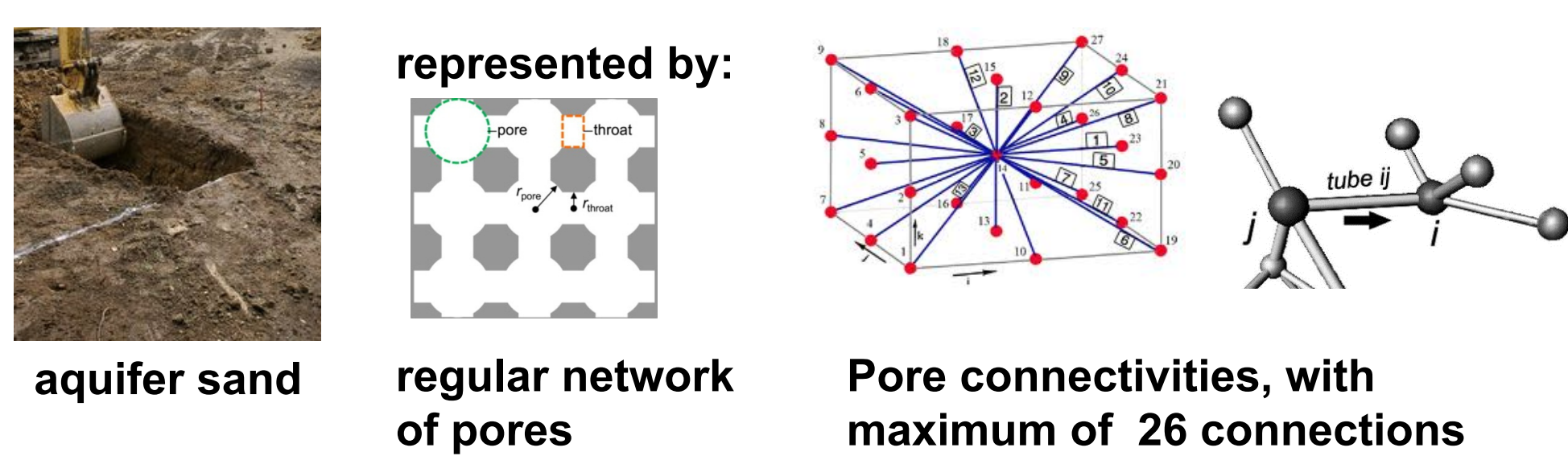
Equations/parameters to be refined based on NanoPNM model experiments

Influence of velocity and flow-rate:

Flow velocity decreases with distance from the injection well. At high flow rates, drag forces increase, reducing retention of particles. Conversely, low flow rates at distances from the well facilitate NP deposition.

$$\begin{cases} k_{a,1} = C_{a,1} \mu_m \frac{v_e}{d_{50,sand}} \eta_0 \\ k_{d,1} = C_{d,1} \mu_m v_e \end{cases}$$

$$\eta_{0,Yao} = \eta_1 + \eta_D + \eta_G =$$

$$= \frac{3}{2}\left(\frac{d_{50c}}{d_{50s}}\right)^2 + 4.04\left(\frac{2d_{50c}v_e}{D}\right)^{-\frac{2}{3}} + \frac{v_s}{v_e}$$

Pore-scale Modelling (NanoPNM)

Using pore-network modelling, PoreFlow, we simulate fluid flow and transport of NPs within a network of interconnected pores. Colloidal processes such as deposition and aggregation are implemented at the scale of individual pores. Averaging over the network domain composed of thousands of pores, we derive macro-scale parameters to be used within macro-scale model.

aquifer sand

represented by:

regular network of pores

Pore connectivities, with maximum of 26 connections

Parameters:
- Lattice distance
- Pore size distribution (mean and variance)
- throat radius: pore radius
- elimination rate (connection number)
- pore scale NP attachment/detachment

Results from a column test using iron oxide NPs, from WP4, were simulated with NanoPNM. There is a good match, however, due to the high flow velocity used in the column experiment, no significant attachment was observed.

Macroscale models for 1D (MNMs) and 3D (MNM3D) geometries
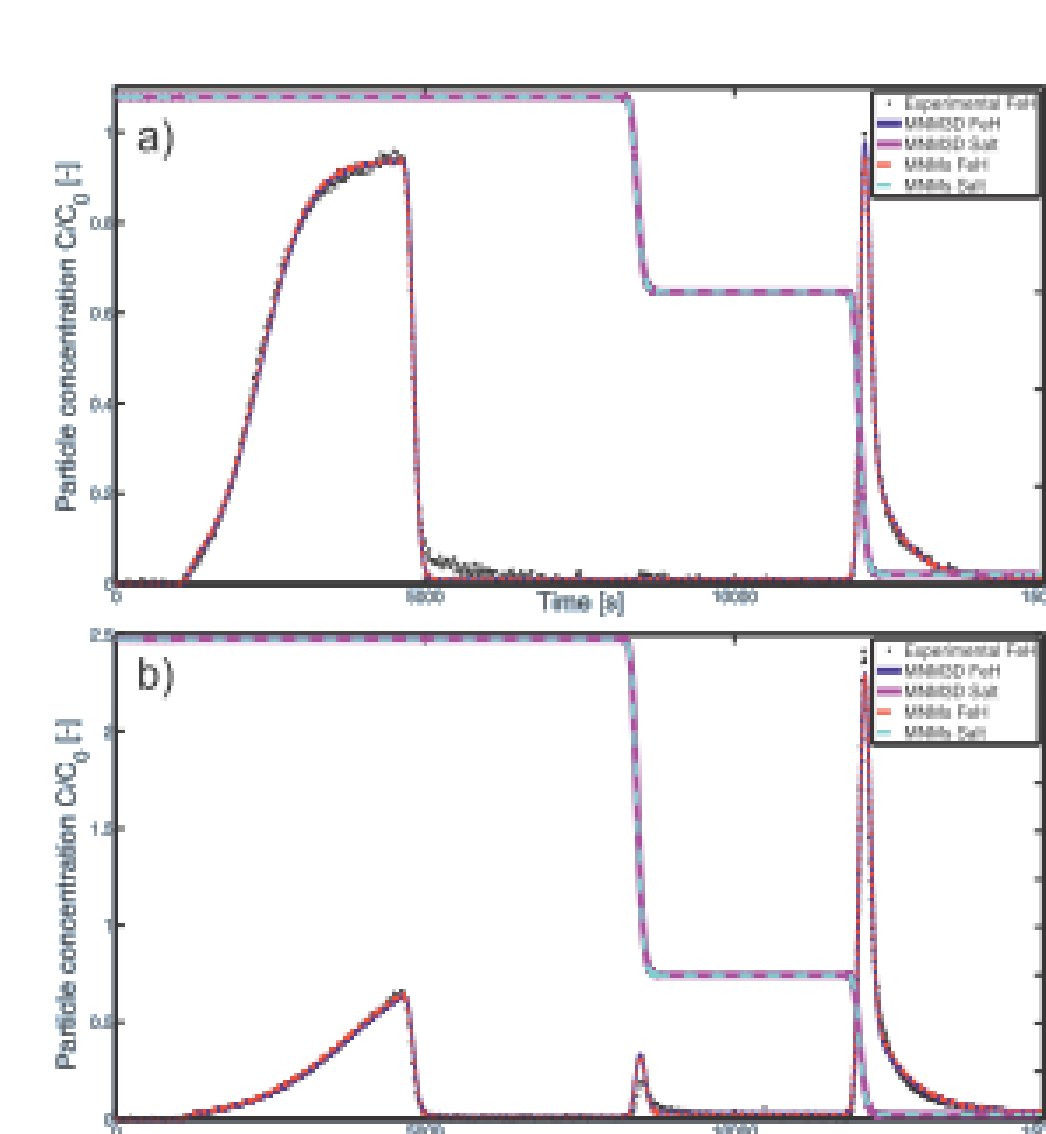
Validation of MNM3D in 1D geometry was performed against both experimental data of a Ferrihydrite microparticle column test and MNMs simulation results (figure on the left; a: 5 mM, b: 10mM).

An application in 3D geometry (figure below) simulated the water flow and the hypothetical NP transport in a large-scale container (LSC) located at the VEGAS facility in Stuttgart University (Germany), where particles will be injected as part of NanoRem WP8. The simulation involved the NP injection through 4 wells and, then, flushing with a lower ionic strength solution (i.e., 50, 30,10 and 1mM).

LSC set-up

Size (L xW x H)	9m x 6m 4.5m
Aquifer type	Unconfined
Soil structure	Blocks with 2 different types of sand (medium sand and coarse sand) "randomly" distributed
Inflow boundary condition	Constant flux: 12 injection wells
Outflow boundary condition	Constant head

Colloid concentration in liquid phase compared with an ideal conservative tracer (gray).
A = End of the injection of the colloidal particles (24h);
B = 6 hours after the beginning of the ionic strength lowering (102h);
C = Ionic strength decrease completed and particles release at an advanced stage (129 h).

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