Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting information (SI)

for the article entitled:

Effect of Deposition, Detachment and Aggregation Processes on Nanoparticle Transport in Porous Media using Monte Carlo Simulations

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SI1. Example of ENPs trajectories.

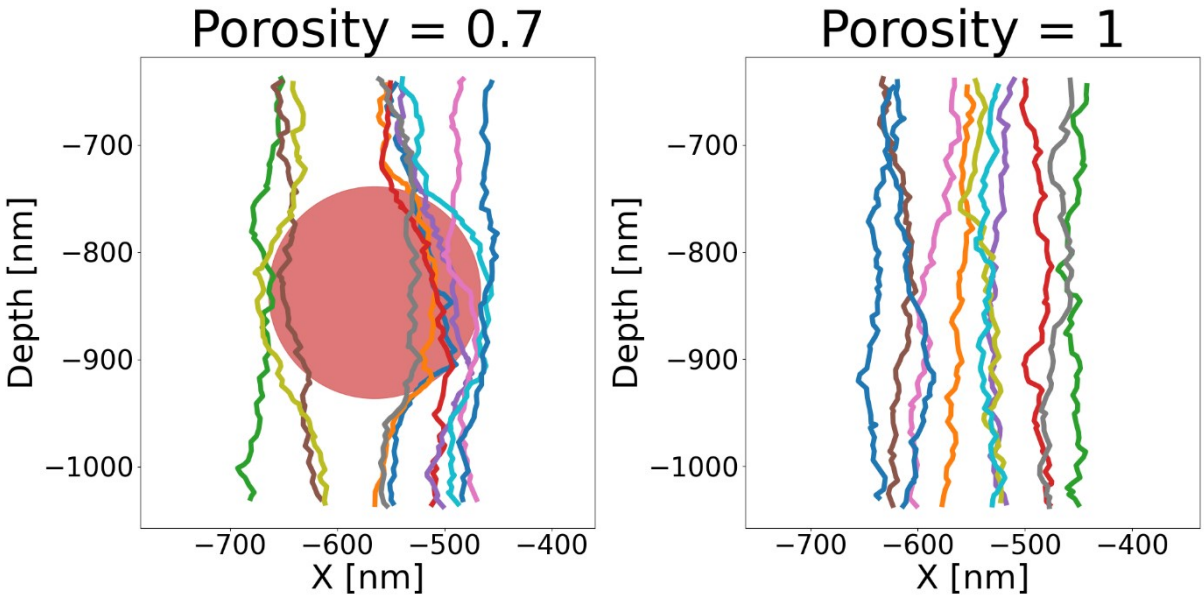

Figure S1. 2D projection of several ENPs trajectories in the presence (left) and in the absence (right) of collectors.

SI2. Changes of effective porosity.

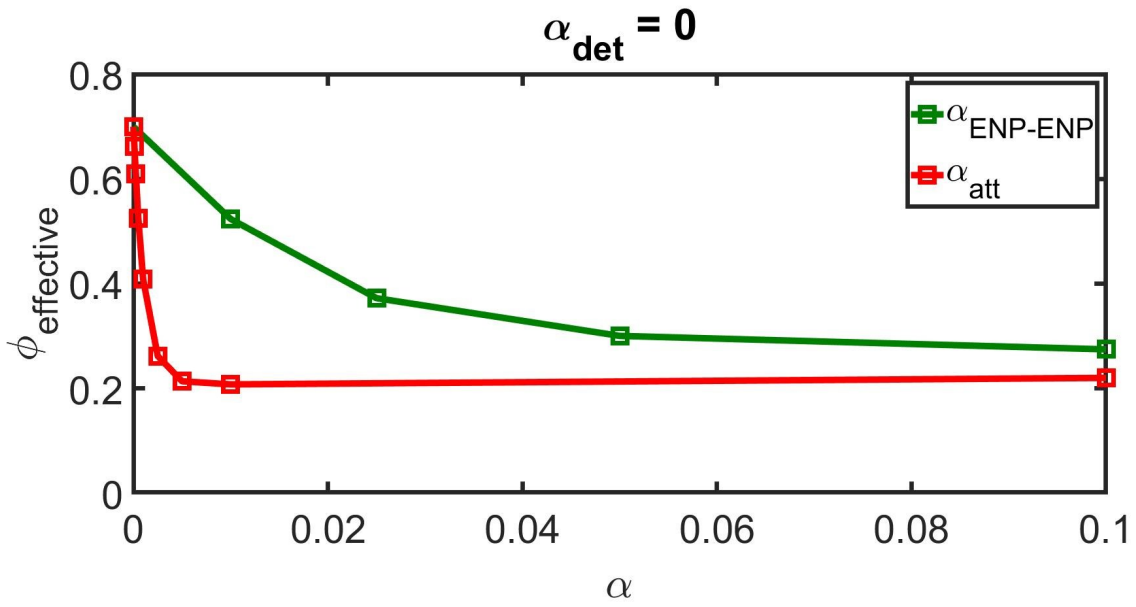

Figure S2. Effective porosity changes of the soil matrix as a function of different homoaggregation efficiencies ($\alpha_{ENP-ENP}$) and different attachment efficiencies (α_{att}). In both cases, effective porosity values decrease and stabilize for α values equal or greater to 0.1.

SI3. Retention profiles generation

During simulation, position and status of each ENP is verified and memorized for each Monte Carlo time. Information about position and status of each ENP memorized for the last MC step is used for the calculation of ENPs retention profiles. To follow ENPs distribution with depth, porous media matrix is first divided into 100 sections, and each section has 40 nm of depth. Then, position of each attached ENP is verified and the number of attached ENPs within the corresponding sections is increased. For example, if an attached ENP is localised between 0 and 40 nm, the number of attached ENPs within this section is increased by 1. Finally, the total number of attached ENPs in each section is plotted as a function of depth.

SI4. Calculation of ENPs that are attached, strained inside and outside of porous media matrix

Information about positions and status of each ENP memorized for the last MC step is also used during calculation of numbers of ENPs that are attached or strained inside/outside of the porous media matrix. A number of ENPs that are outside of the simulation box corresponds mostly to the ENPs that are strained at the top of the porous media matrix. A number of ENPs that are inside of porous media matrix is calculated by subtracting a number of ENPs present outside of the simulation box from a total number of ENPs. A number of ENPs that are strained inside porous media matrix is calculated by subtracting a number of attached ENPs from the number of ENPs present inside of the porous media matrix.