Study of the mobility of zero-valent iron nanoparticles in porous media – Effect of grain size and composition

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This work aims at advancing our understanding of the mobility and entrapment of nanoparticles (NPs) in porous media. The findings of this study are important for remediation of contaminated groundwater using nanoparticles (e.g. zero-valent iron). We focus on identifying the key NP transport mechanisms at pore scale in a non-destructive way using X-ray computed micro-tomography (X-ray micro-CT). In the modelling of particle transport in porous media, several key particle entrapment mechanisms are commonly considered, these are namely ripening, site blocking, straining, attachment, and detachment. These studies use data such as breakthrough curves, particle and grain size distribution as input to calculate the relevance and extent of the above-mentioned mechanisms[1]. In this work, the objective is to use X-ray micro-CT to directly observe the pore-scale mechanisms involved in particle mobility.

We report the outcomes of an experiment that was performed on small columns packed with grains of different size ranges and different compositions (fine sand, coarse sand, carbonate, and a mixed sample of carbonate and sand). The columns were initially saturated with water. A suspension of NP (zero-valent iron) was then injected in the columns, followed by a water flush step that removed the mobile particles. X-ray micro-CT imaging was performed at this stage. Our experimental dataset comprises 3D micro-CT images of these four columns.

The collected images have captured the distribution and characteristics of the trapped NP clusters. To analyse these images, we used the following workflow. The analysis started from filtering the collected images to remove the measurement noise. We then performed segmentation using a range of algorithms including watershed and WEKA segmentation. Subsequently, the segmented pore and NPs phases were quantitatively analysed. The image analysis was performed using Avizo and ImageJ software packages.

The focus of this work is developing a quantitative understanding of the effect of NP entrapment on the properties (e.g. porosity, permeability, and tortuosity) of porous media with different grain structures and compositions. We used the pore network modelling (PNM) module implemented in the Avizo software to extract PNMs from the 3D images of the segmented pore phase before and after the NP injection process.

For the samples under investigation the calculated properties (porosity, permeability, and tortuosity) agree with the range of values reported in the literature for similar pore systems. Our study shows that the permeability reduces by an order of magnitude as a result of this NP injection. Although the calculated tortuosity displays an increase, as expected, the extent of this increase is not significant (less than 10%). The number of pores shows a slight increase while a significant reduction in pore-throat count is observed. The latter can be associated with clogging of pore-throats as a result of NP injection.

This work uses the numerical micro- and nanoparticle transport, filtration, and clogging modelling suite (MNM's 2021) to simulate this 1D column experiment and to specifically study the mechanisms involved in NP mobility at the pore scale. Based on model results, mechanical straining is suggested to be the key mechanism responsible for NP mobility in this study.

References:

1. Hosseini, S. M. & Tosco, T. Transport and retention of high concentrated nano-Fe/Cu particles through highly flow-rated packed sand column. *Water Res.* **47**, 326–338 (2013).