Quantifying the Influence of EDTA on Polymer Nanoparticle Deposition and Retention in an Iron-oxide-coated Sand Column

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SUPPLEMENT

Figure S1: Scanning Electron Microscope (JEOL JSM 6500F Field Emission Scanning Electron Microscope) images of uncoated and Fe-oxide-coated sands. Both sands are well rounded to sub-angular with localised rough surfaces and cracking on individual grains. Sand dimensions between 120µm and 320µm. (A) Uncoated quartz sand (Sigma-Aldrich, Dorset, England) showing dimensions of representative grains. (B) Iron-oxide coated sand showing dimensions of representative grain sizes. (C) Detail of smooth surface on uncoated sand. (D) Detail of smooth surface on iron-oxide-coated sand. (E) Detail of rough surface on uncoated sand. (F) Detail of rough surface on Iron-oxide coated sand. Note the greater abundance of micron to sub-micron-sized particles on coated sands.
Figure S2: VWD optical signals of EDTA measured continuously in column effluent during a single pulse injection of EDTA through uncoated sand. Note that a plateau was developed at an altitude of about 266 (AU), corresponding to the optical signal of EDTA in the source reservoir.
Figure S3\textsuperscript{18}: Model validation based on experimental results of triple pulse nanoparticle injection. Top: nanoparticle BTCs used for model validation with the first pulse for model calibration and the rest pulses for model testing; Middle: model calibration on the first nanoparticle BTC; Bottom: application of calibrated model for predicting transport of nanoparticles in the second and third pulses. A close match between the model predicted and the experimental BTCs confirms the model’s competency for predicting nanoparticle movement in this experimental system.
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| 1    | Calculating theoretical single collector efficiency ($\eta_0$) for favorable deposition using the Filtration Model of Tufenkji and Elimelech | $\eta_0 = \eta_D + \eta_I + \eta_G$ (S1) 
$\eta_D = 2.4A_s^{1/3}N_R^{-0.081}N_{Pe}^{-0.715}N_{vdw}^{0.052}$ (S2) 
$\eta_I = 0.55A_sN_R^{1.55}N_{Pe}^{-0.125}N_{vdw}^{0.125}$ (S3) 
$\eta_G = 0.22N_R^{-0.24}N_{G,11}^{0.053}$ (S4) |
| 2    | Calculating single collector efficiency ($\eta$) based on experimental data using the approach of Yao et al. | $\eta = -\frac{2d_c}{3L(1-f)}ln(\frac{n_e}{n_0})$ (S11) |
| 3    | Calculating collision efficiency ($\alpha$) | $\alpha = \eta/\eta_0$ (S12) |