Electronic Supplementary Material (ESI) for Journal of Environmental Monitoring

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[18]: 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 120 µm and 320 µm. (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.

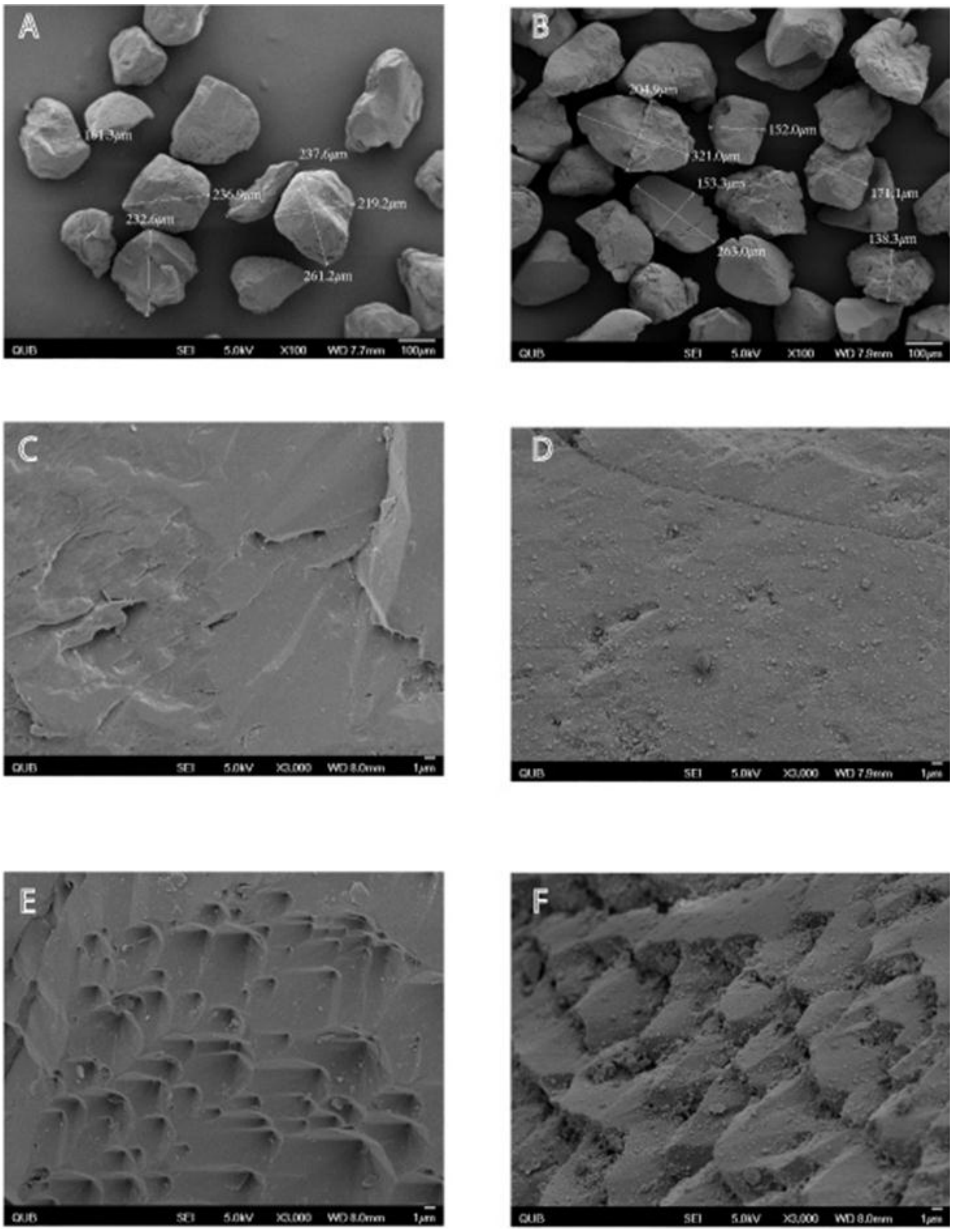

Figure S2: VWD optical signals of EDTA measured continuously in column effluent during a single pulse injection of EDTA through uncoated sand. Note that a plateau was developed at an altitude of about 266 (AU), corresponding to the optical signal of EDTA in the source reservoir.

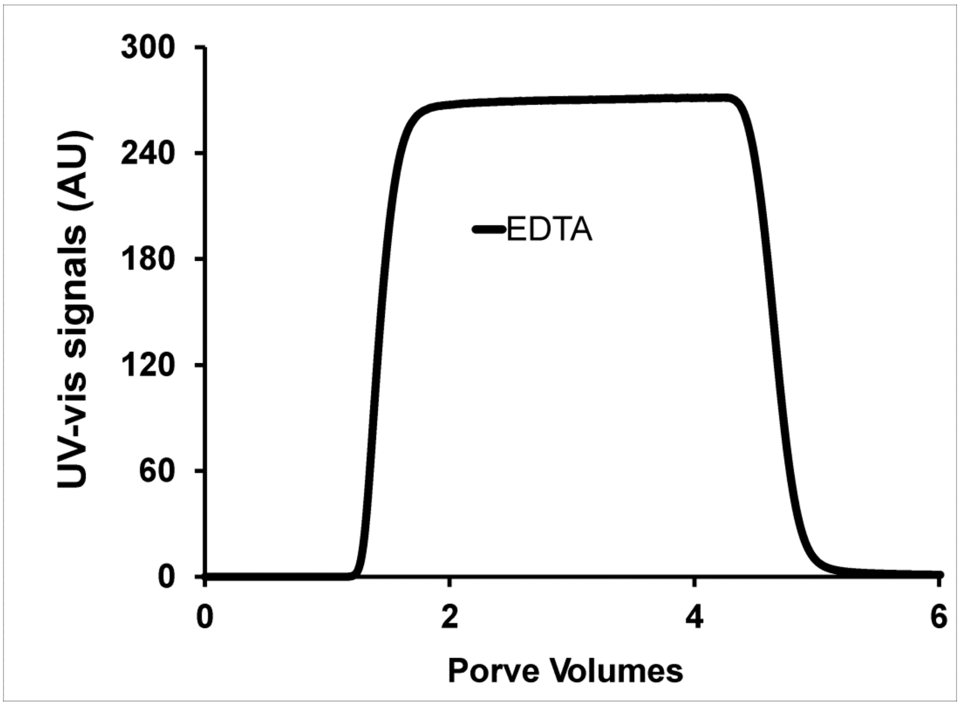

Figure S3[18]: Model validation based on experimental results of triple pulse nanoparticle injection. Top: nanoparticle BTCs used for model validation with the first pulse for model calibration and the rest pulses for model testing; Middle: model calibration on the first nanoparticle BTC; Bottom: application 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.

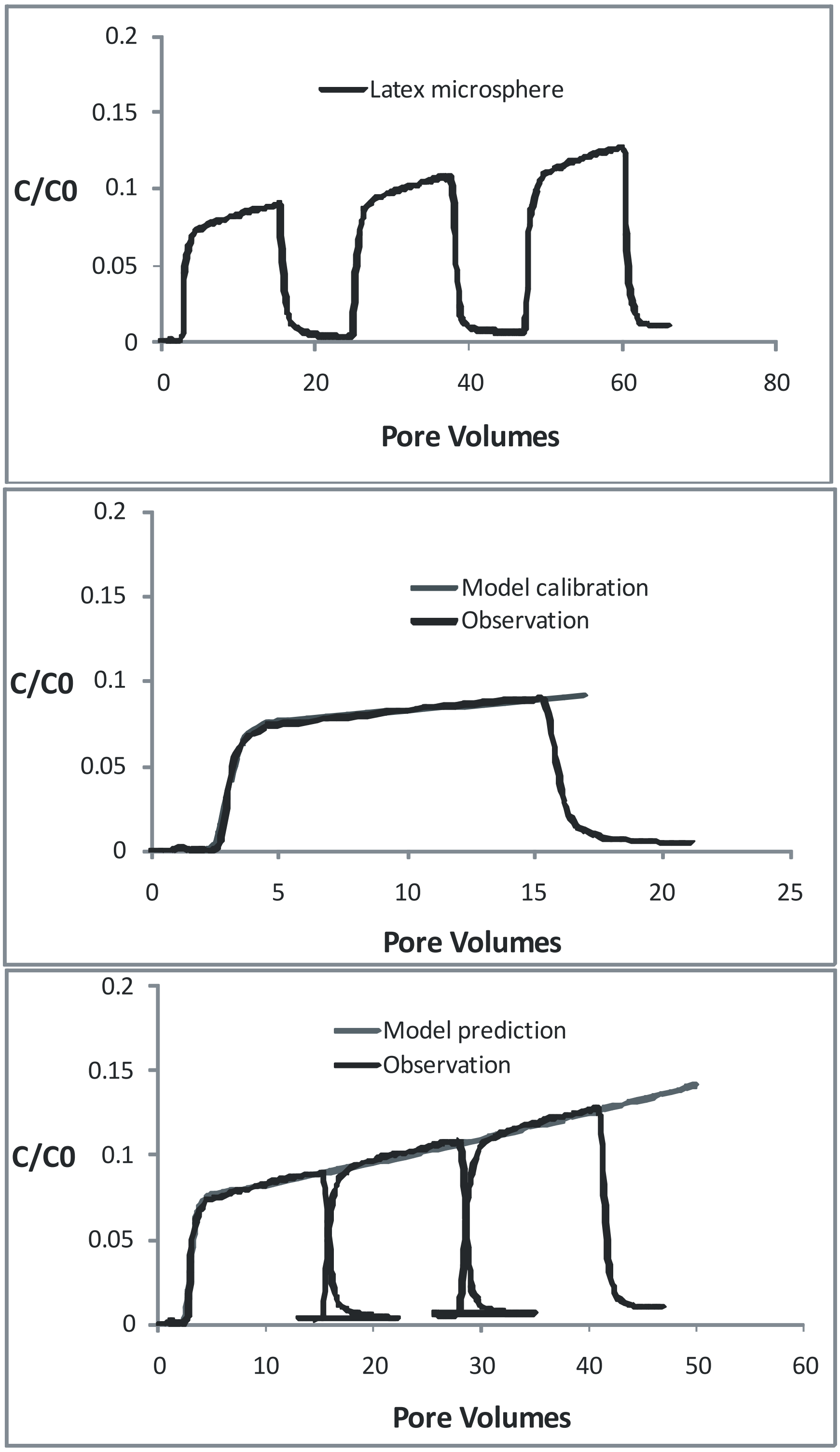

Table S1: Summary of formula and parameter values used in calculation of collision efficiency

Step 1--- Calculating theoretical single collector efficiency (η_0) for favorable deposition using the Filtration Model of Tufenkji and Elimelech[49]

$$\eta_0 = \eta_D + \eta_I + \eta_G \quad \text{(S1)}$$

$$\eta_D = 2.4A_s^{1/3}N_R^{-0.081}N_{Pe}^{-0.715}N_{vdw}^{0.052} \quad \text{(S2)}$$

$$\eta_I = 0.55A_sN_R^{1.55}N_{Pe}^{-0.125}N_{vdw}^{0.125} \quad \text{(S3)}$$

$$\eta_G = 0.22N_R^{-0.24}N_G^{1.11}N_{vdw}^{0.053} \quad \text{(S4)}$$

Where

$$N_R = d_p/d_c \quad \text{(S5)}$$

$$N_{Pe} = (Ud_c)/D_\infty \quad \text{(S6)}$$

$$N_{vdw} = A/kT \quad \text{(S7)}$$

$$N_{gr} = \frac{4}{3}\frac{\pi a_p^4(\rho_p - \rho_f)g}{kT} \quad \text{(S8)}$$

$$N_A = A/(12\pi\mu a_p^2 U) \quad \text{(S9)}$$

$$N_G = \frac{2}{9}\frac{a_p^2(\rho_p - \rho_f)g}{\mu U} \quad \text{(S10)}$$

Model parameters: particle diameter (dp=200nm), collector diameter (dc=0.125mm), fluid approach velocity (U=7.2m/day), Hamaker constant (A=1.98×10^{-21}J), fluid absolute temperature (T=298K), porosity (f=0.39).

Step 2--- Calculating single collector efficiency (η) based on experimental data using the approach of Yao et al.[48]

$$\eta = -\frac{2d_c}{3L(1-f)}\ln(n_e/n_0) \quad \text{(S11)}$$

Model parameters: column length (L=0.03m), relative effluent concentration shown by the inflection point on experimental BTC ($\frac{n_e}{n_0} = 0.06$).

Step 3--- Calculating collision efficiency[49] (α)

$$\alpha = \eta/\eta_0 \quad \text{(S12)}$$