In Situ Measurement and Simulation of Nano-Magnetite Mobility in Porous Media Subject to Transient Salinity

Supporting Information

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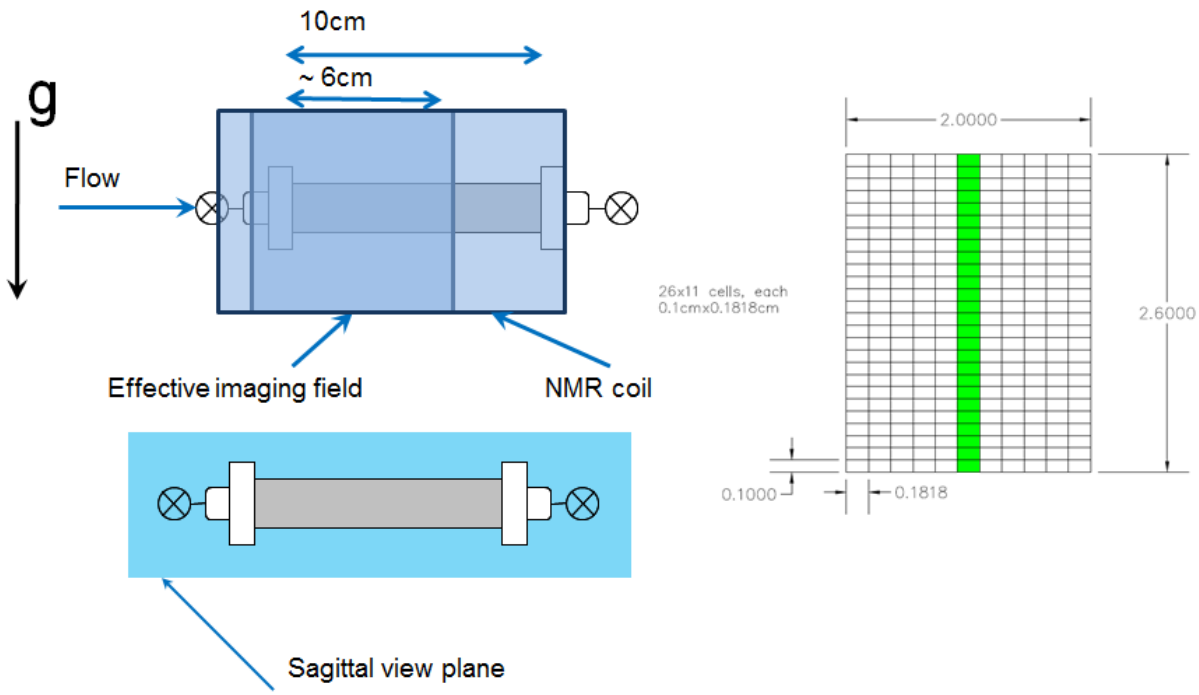

Figure S1. Column setup in the MRI apparatus and model discretization domain. The green column in the discretization domain represents the plane from which the sagittal images in Figure 4 are taken.

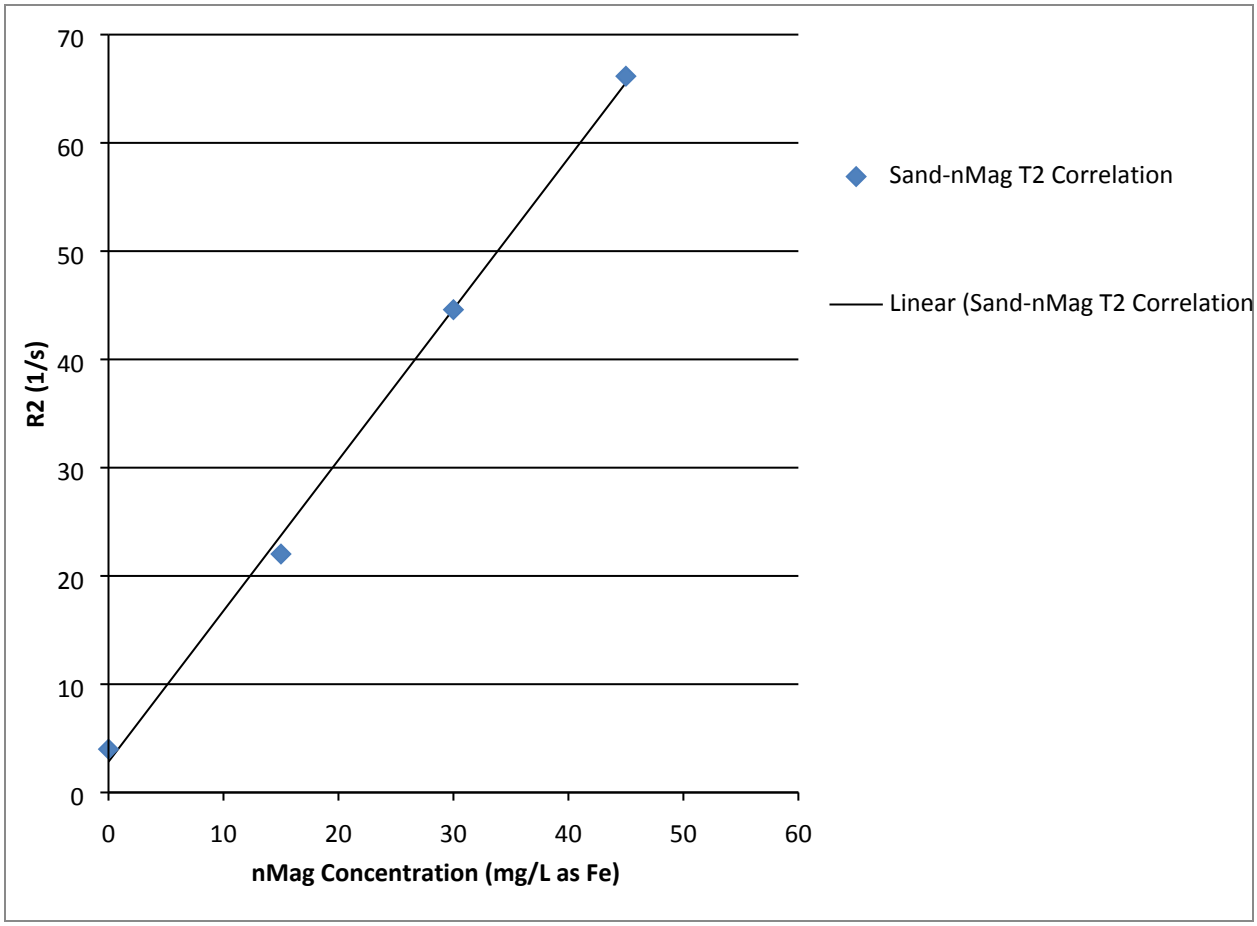

Figure S2. Relaxation rate ($R_2 = 1/T_2$) calibration with nMag concentration measured in 40-50 Mesh Ottawa sand under API brine conditions (80 g/L NaCl, 20 g/L $CaCl_2$). The relaxivity of the nMag particles is 1.39 $(s\ mg/L)^{-1}$ and can depend on the exact particle synthesis and preparation as well as aggregation state[1], The intercept of 2.83 s^{-1} corresponds to a 352ms T_2, consistent with the expected range of possible T_2 values for a clastic material.

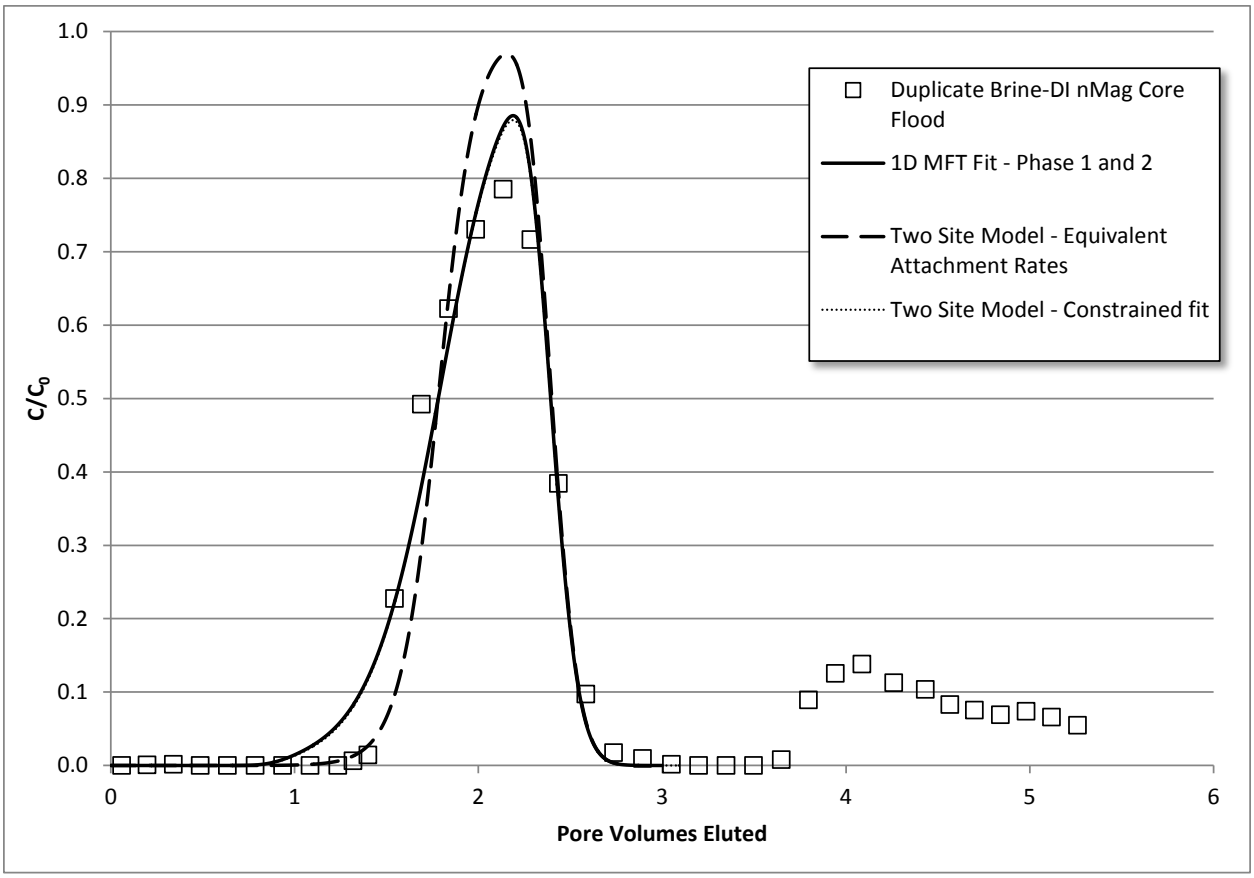

Figure S3. Sensitivity of the two-site model implemented in one dimension for phases 1 and 2 of the experiment. The solid line indicates the one-site model fit, which corresponds to the model result shown in Figure 1 of the manuscript. The dashed line represents two-site attachment model prediction using the attachment parameters from the one site model (Figure 1). The dotted line indicates the two site model fit to the experimental data with equivalent attachment parameters for each deposition site, and a retention capacity for non-releasable sites equivalent to the value fitted in Figure 1 ($S_{max,r} = f_r * S_{max} = 2.16$ ug/g). The fitted parameters for this result ($k_{att,r} = k_{att,nr} = 4.4 \times 10^{-2}$ min^{-1}; $S_{max,nr} = 3.29$ ug/g) resulted in parameters which were not substantially different from those fitted by the one site model ($f_r = 0.39$, $S_{max} = 5.46$ ug/g). This suggests that the one site model fitted to the breakthrough curve provided a reasonably accurate estimation of the total retention capacity of the system, an inherent assumption of the approach taken to estimate these

parameters. The best fit attachment rates for each site of the two site model (dotted line) were half the value of the value fitted by the one site model (see Table 1), an expected result because it is consistent with the fact that there are two sites which are superposed to create the total deposition profile. Based on these results, it was concluded that the one-site model provided an accurate representation of the two-site model for the breakthrough phase of the experiment.

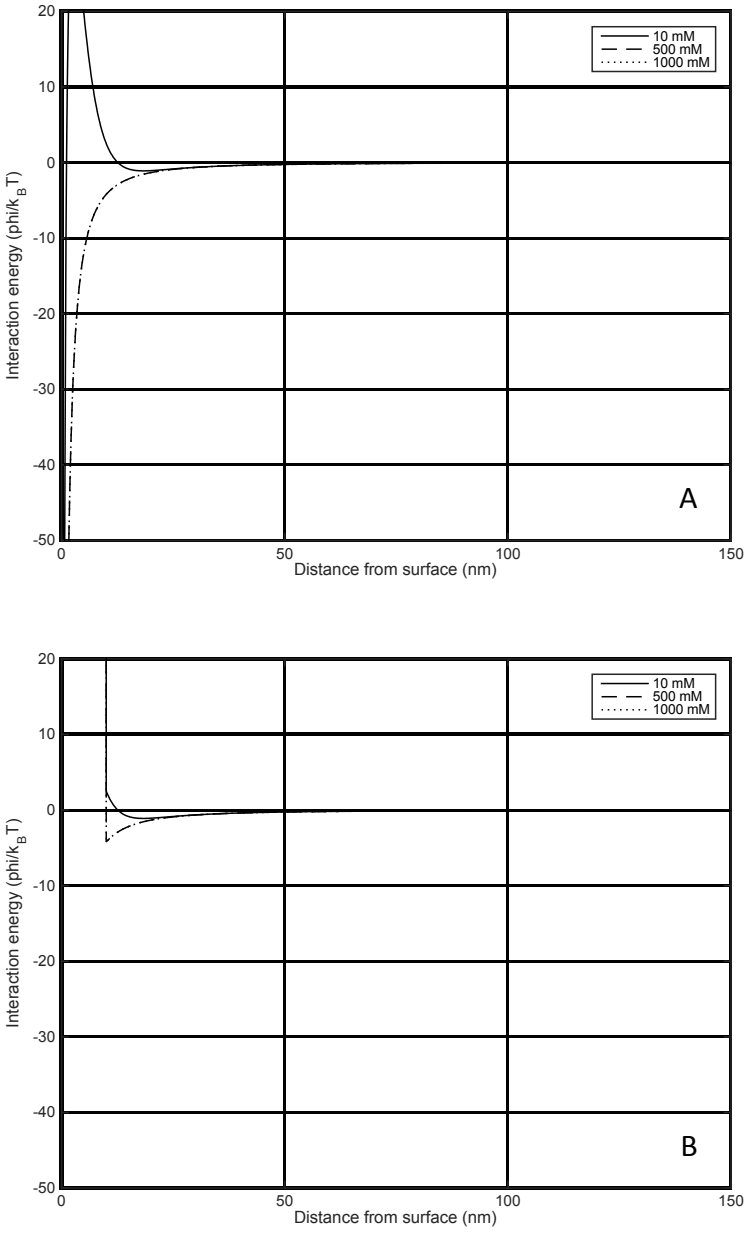

Figure S4. Calculated traditional (A) and extended (B) DLVO interaction energy profiles for three representative ionic strength values (10 mM ≈ 1 g/L API Brine; 500 mM ≈ 48 g/L API Brine; 1000 mM ≈ 96 g/L API Brine). Traditional DLVO represents the superposition of van der Waals interactions and electrostatic interactions, while extended DLVO accounts van der Waals, electrostatic, and steric interaction effects (for review and equations, see Petosa et al.[2]). For these

calculations, the Hamaker constant for nMag-PAMPS particles were estimated based on Hu et al.,[3] zeta potentials for nMag-PAMPS were estimated using electrophoretic mobility measurements by Bagaria et al.,[4] and surface potentials of Ottawa Sand were estimated based on Wang et al.[5]

References

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