Electronic Supporting Information for:

Synthesis and laboratory testing of novel calcium-phosphonate reverse micelle nanofluid for oilfield mineral scale control

Ping Zhang [a] *, Dong Shen [a, c], Amy T. Kan [a] and Mason B. Tomson [a, b] *

[a] Department of Civil and Environmental Engineering,

Rice University, Houston, Texas

[b] Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment,

Rice University, Houston, Texas

[c] Presently with Baker Hughes Inc., Houston, Texas

Manuscript prepared for *RSC Advances*

* To whom correspondence should be addressed: ping.zhang@alumni.rice.eduand mtomson@rice.edu

1. Characterization of porous medium via tracer breakthrough test:

A tracer (tritiated water) test was carried out to measure the PV and the hydrodynamic dispersion coefficient (D) of the packed column. According to the breakthrough curves of the tracer in each medium, the D values for each medium can be obtained by fitting the one-dimensional advection-dispersion equation (Eq. ESI-1) to the acquired data using CXTFIT code,[1] by setting the retardation factor (R) to one:

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \quad \text{(ESI-1)}$$

where C (mg L^{-1}) is the effluent nanomaterials concentration at a certain time; t (min) denotes the time. X is the distance of transport. D value is calculated to be 0.065 $cm^2\ min^{-1}$.

Table ESI-1 Properties of the calcite medium and parameters from the tracer tests

Formation medium	**Particle size Range (μm)**	**Particle density ρ_p (g cm^{-3})**	**Bulk density ρ_b (g cm^{-3})**	**Porosity, ε**	**Pore velocity, v (cm min^{-1})**	**Dispersion coefficient, D ($cm^2\ min^{-1}$)**
Calcite	106-180	2.71	1.54	0.43	2.85	0.065

D value ($cm^2\ min^{-1}$) can be calculated as:

$$D = \alpha_d \times v \quad \text{(Eq. ESI-2)}$$

where α_d (cm) is the dispersivity and v (cm min^{-1}) is the linear pore velocity. Based on Eq. ESI-2, α_d for calcite medium at 2.85 cm min^{-1} pore velocity is calculated to be 0.0228 cm. α_d is a characteristic property of a formation media.[2] Thus, the dispersivity of calcite should be maintained the same at different pore velocities. The D value for the other flow velocity evaluated (2.99 cm min^{-1}) can be easily calculated as 2.99 * 0.0288 = 0.068 $cm^2\ min^{-1}$.

2. Classical colloidal filtration theory (CFT):

The deposition due to Brownian diffusion, interception and sedimentation can be lumped into the η_0 value:

$$\eta_0 = \eta_D + \eta_I + \eta_G \qquad \text{(ESI-3)}$$

where η_D, η_I and η_G are the single collector efficiency components as a results of diffusion, interception and sedimentation, respectively. Following the strategy of Tufenkji and Elimelech,[3] these three components can be calculated as a function of several dimensionless groups as follows:

$$\eta_D = 2.4A_s^{1/3}N_R^{-0.081}N_{pe}^{-0.715}N_{vdW}^{-0.052} \qquad \text{(ESI-4)}$$

where A_s is the porosity-dependent parameter of Happel's model, N_R is the aspect ratio, N_{Pe} is the Peclet number, and N_{vdW} is the van der Waals number. A_s is the porosity-dependent parameter of Happel's model and is defined as

$$A_s = \frac{2(1-\gamma^5)}{2-\gamma+3\gamma^5-2\gamma^6} \qquad \text{(ESI-5)}$$

where $\gamma = (1-\varepsilon)^{1/3}$, ε is the porosity of the porous medium. N_R is the ratio of particle diameter (d_p) to spherical collector diameter (d_c) (i.e. $N_R = \frac{d_p}{d_c}$ and d_p=500 nm, d_c=150 μm).

$$N_{Pe} = \frac{vd_c}{D_\infty} \qquad \text{(ESI-6)}$$

where v (m s^{-1}) is the pore velocity, D_∞ (m^2 s^{-1}) is the diffusion coefficient in an infinite medium, which, according to Stocks-Einstein relation, is defined as

$$D_\infty = \frac{kT}{3\pi\mu d_p} \qquad \text{(ESI-7)}$$

where k is the Boltzmann constant (1.38×10^{-23} J K^{-1}); T (K) is the absolute temperature; μ (kg m^{-1} s^{-1}) is the absolute viscosity of the fluid (water). The van der Waals number N_{vdW} is defined as

$$N_{vdW} = \frac{A}{kT} \qquad \text{(ESI-8)}$$

where A is the Hamaker constant (assumed to be 10^{-20} J). Moreover,

$$\eta_I = 0.55A_sN_R^{1.55}N_{pe}^{-0.125}N_{vdW}^{0.125} \qquad \text{(ESI-9)}$$

$$\eta_G = 0.475 N_R^{-1.35} N_{pe}^{-1.11} N_{vdW}^{0.053} N_{gr}^{1.11} \qquad \text{(ESI-10)}$$

where N_{gr} is the gravitational force number, defined as

$$N_{gr} = \frac{d_p^4(\rho_p - \rho_f)g}{3kT} \qquad \text{(ESI-11)}$$

where ρ_p is the density of the nanoparticles; ρ_f is the density of fluid and g is the gravitational acceleration, 9.81 m s^{-2}.

References:

1. Parker, J. C.; van Genuchten, M. T., Determining Transport Parameters from Labotoary and Field Tracer Experiments. Blacksburg, VA, 1984; Vol. Bulletin 84-3.
2. R. J. Charbeneau, Groundwater Hydraulics And Pollutant Transport, 1st edn, Waveland Press, Long Grove, IL, 2006.
3. N. Tufenkji, M. Elimelech, Correlation Equation for Predicting Single-Collector Efficiency in Physicochemical Filtration in Saturated Porous Media. Environmental Science & Technology 2004, 38, 529-536.