Supporting Information for: Enhanced transport of novel crystalline calcium–phosphonate scale inhibitor nanomaterials and their long term flow back performance in laboratory squeeze simulation tests

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Submitted to *RSC Advances*

Number of pages: 7

Number of figures: 2

Number of tables: 2

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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 (Fig. SI-1), the D values for each medium can be obtained by fitting the one-dimensional advection-dispersion equation (1-D ADE) (Eq. SI-1) to the acquired data using CXTFIT code[1], by setting the retardation factor (R) to one:

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

where C (mg L^{-1}) is the effluent nanomaterials concentration at a certain time; t (min) denotes the time.

Table SI-1 Properties of the porous media and parameters from the tracer tests

Porous medium	Particle size (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})	r^2
Calcite	106-180	2.71	1.39	0.449±0.006	3.406±0.0499	0.0897±0.066	0.994
Louise sandstone	106-180	2.52	1.48	0.453±0.005	3.442±0.0434	0.0690±0.0762	0.999

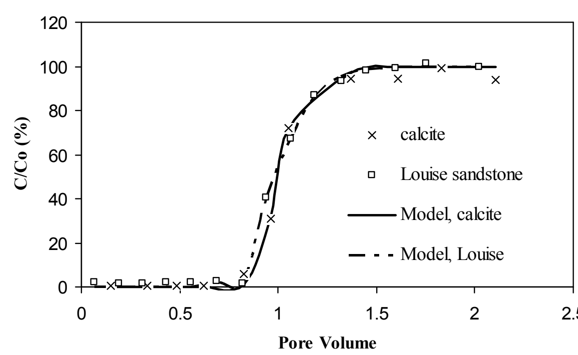

Figure SI-1 Tracer breakthrough tests in calcite and Louise sandstone media. This figure is adopted from a previous study[2].

2. Describing nanomaterials transport by ADE and filtration theory:

The transport of Si-Ca-DTPMP nanomaterials through the formation porous medium can be described by the ADE with an additional term representing the first-order removal[3-5]:

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - J_d C \qquad \text{(SI-2)}$$

where J_d (min^{-1}) is the first-order removal rate coefficient and can be calculated as[6, 7]:

$$J_d = -\frac{v}{L}\ln(C_e / C_o) \qquad \text{(SI-3)}$$

where L (cm) is the length of the porous medium; C_e (mg L^{-1}) is the steady-state effluent concentration of the nanomaterials; and C_o (mg L^{-1}) is the influent particle concentration. The solution of Eq. S-2 follows the effort of Parker and van Genuchten[1], where both the first-order removal and zero-order production in the solid phase were considered.

The solution for a clean bed filtration model can be obtained simply by forcing the zero-order production coefficient to be zero in the analytical solution, which is in the following manner:

$$C(x,t)=\frac{1}{2}\exp[\frac{(v-w)x}{2D}]erfc[\frac{Rx-wt}{2(DRt)^{0.5}}]+\frac{1}{2}\exp[\frac{(v+w)x}{D}]erfc[\frac{Rx+wt}{2(DRt)^{0.5}}] \quad \text{(SI-4)}$$

$$and \quad w=(v^2+4J_dD)^{0.5}$$

The retardation factor R in Eq. SI-2 accounts for the retardation effect arising from the sorption of nanomaterials to the porous medium. Since the R value is characteristic of the sorptive behavior of the nanomaterials to the medium surfaces, it should be independent of the pore flow velocity.

From the perspective of filtration theory, the removal of colloidal particles by the porous medium can be characterized by the removal efficiency (η_0) term, which summarizes the removal resulted from diffusion, interception and sedimentation[8]. Following the calculation of the η_0 value, the attachment efficiency (α) can be obtained via:

$$\alpha=-\frac{2\mathrm{d_c}}{3(1-\varepsilon)\mathrm{L}\eta_0}\ln(\frac{\mathrm{C}}{\mathrm{C_0}}) \qquad \text{(SI-5)}$$

where ε denotes the porosity of the medium; d_c represents the diameter of the medium particle and L is the length of the porous medium bed.

3. Brine composition and field conditions for Scalesoftpitzer calculation:

$$SI = \log_{10} \frac{(Ca^{2+})(CO_3^{2-})}{K_{sp}(T,P)} \quad \text{(SI-6 for calcite scale)}$$

$$SI = \log_{10} \frac{(Ba^{2+})(SO_4^{-})}{K_{sp}(T,P)} \quad \text{(SI-7 for barite scale)}$$

Table SI-2 Brine composition used for Scalesoftpitzer software calculation.

Parameters	Units	Input
Na^{+}	(mg/l)	**19,872.00**
K^{+}	(mg/l)	**500.00**
Mg^{2+}	(mg/l)	**54.00**
Ca^{2+}	(mg/l)	**6,500.00**
Sr^{2+}	(mg/l)	**700.00**
Ba^{2+}	(mg/l)	**550.00**
Fe^{2+}	(mg/l)	**12.00**
Zn^{2+}	(mg/l)	**10.00**
Pb^{2+}	(mg/l)	**1.00**
Cl^{-}	(mg/l)	**43,000.00**
SO_4^{2-}	(mg/l)	**5.00**
F^{-}	(mg/l)	**1.00**
Br^{-}	(mg/l)	**10.00**
SiO_2	(mg/l) SiO_2	**10.00**
Alkalinity	(mg/l)	**281.00**
TDS (Measured)	(mg/l)	**70,000.00**
CO_2 Gas Analysis	(%)	**1.04**
H_2S Gas Analysis	(%)	**0.0283**
Total H_2S_{aq}	(mgH_2S/l)	**4.32**
pH, measured (STP)	pH	**7.16**
Initial T	(F)	**340.0**
Final T	(F)	**77.0**
Initial P	(psia)	**7,000.0**
Final P	(psia)	**14.7**

4. XRD characterization of both amorphous and crystalline Si-Ca-DTPMP

The crystallinity of the developed Si-Ca-DTPMP solids after diafiltration treatment can be provided by the XRD spectra[2] (Fig. SI-2).

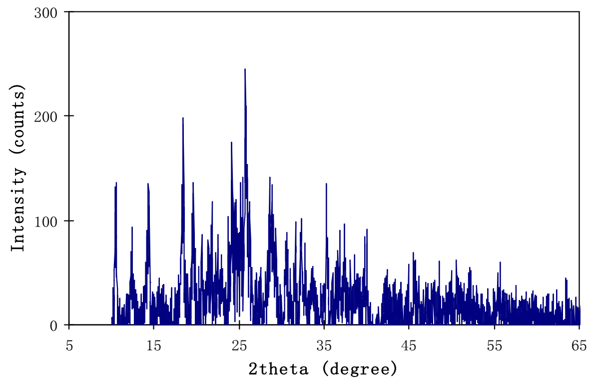

Figure SI-2. XRD profiles of crystalline phase Si-Ca-DTPMP solid after diafiltration treatment (Adopted from a previous study[2])

References:

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