TRANSPORT OF FULLERENE NANOPARTICLES IN SATURATED POROUS MEDIA



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Introduction

- Studies with C₆₀ and its derivatives have shown that fullerenes can form charged aggregates in aqueous media that result in stable aqueous fullerene suspensions.
- The interaction of aqueous C₆₀ aggregates (aqu/C₆₀) with environmental surfaces is incompletely understood.
- As a result, modeling the transport of *aqu/C*₆₀ through porous media (soils, sediments) is problematic.
- The utility of existing particle transport models adequately describe aqu/C₆₀ transport in watersaturated porous media needs to be evaluated
- Although the formation of aqu/C₆₀ is pH and ionic strength dependent, the suspensions are highly negatively charged under a wide range of solution conditions.

Methods and Materials

- The 125 μm to 250 μm size fraction of lota sand was DDI-washed and wet-packed in an Omnifit column (100 mm x 25 mm ID).
- Aqu/C_{60} suspensions were continuously stirred in various buffers for > 111 days. The buffers were either acetate (pH = 4.00 ± 0.01), HEPES (pH = 7.01 ± 0.04), or Tris (pH = 10.03 ± 0.06). Ionic strength was 0.010 M.
- The hydrodynamic diameters and zeta (ζ) potentials of the *aqu*/C₆₀ suspensions were analyzed by dynamic light scattering.
- The pH titrations were performed using an autotitrator in conjunction with real time monitoring of size and ζ-potential changes.
- The streaming potentials of lota sand in various buffers were measured using a SurPass electrokinetic analyzer.









Figure 1. Measured and simulated aqu/C_{60} breakthrough curves under different pH in saturated quartz sand columns. A typital tracer breakthrough curve is included as a reference.





Figure 3. Simulated breakthrough curves show the effects of $\rm K_{att}$ and $\rm S_{max.}$



Conclusions

- Solution chemistry affects the transport of aqu/C₆₀ aggregates in porous media.
- The aqu/C₆₀ aggregates have highly negatively charged surfaces.



Results

- Aqu/C₆₀ aggregates were more mobile at higher pH (Figure 1).
- The aqu/C₆₀ attachment efficiencies (α) generated under different pHs are significantly

Figure 5. DLVO interaction energy profiles as a function of pH for aqu/C_{60} . The secondary minimums under different pH shown in the insert.



Figure 6. $\,\zeta$ potential and Z-average diameter of unfiltered aqu/C_{60} in pH 10 titrated as a function of pH.

- different (Figure 2).
- α controls the frontal region of the curves while maximum sorbed concentration (S_{max}) controls the height of the curves (Figure 3).
- Initial concentrations of *aqu*/C₆₀ greatly influence the shapes of breakthrough curves (Figure 4).
- The *aqu*C₆₀ suspensions formed were pH sensitive (Figure 5 and 6).
- The aggregates in aqueous systems were highly negatively charged (Figure 6).
- Both linear and non-linear models can describe the breakthrough curves of *aqu*/C₆₀ at pH 10.
- Details of the breakthrough curves of aqu/C₆₀ in pH 4 are not well modeled by the nonlinear model, even when covered sites are included.

- Aqu/C₆₀ is highly mobile as pH increases.
- The existing non-linear model with no covered area included may not accurately describe the aqu/C_{60} transport under acidic conditions (highly retained).

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Disclaimers

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