1. BACKGROUND

- Compared with single-component nanomaterials (NMs), the “new-horizon” nanohybrids (NHs) are multifaceted in various applications due to enhanced properties, optimized multifunctionalities, and maximized performances.
- Owing to the excellent physicochemical (electronic, thermal, mechanical, optical, photocatalytic) and biological (antimicrobial) properties, reduced graphene oxide (RGO)-metal oxide NHs are widely used in many applications like drug delivery, supercapacitors, solar cells, and environmental remediation.
- However, little is known about the fate and transport of the “new-horizon” multifunctional RGO-metal oxide NHs in the subsurface.
- Numerical modeling can describe the transport and retention of colloids via inverse simulation, but also has the ability to forecast possible outcomes of colloids via forward simulation.

This work is to simulate and then predict the transport and retention of RGO-metal oxide NHs in water-saturated porous media.

2. MATERIALS AND METHODS

- Cleaned quartz sands (360-µm mean size) were used to pack 1.7-cm i.d. × 10-cm long glass chromatography columns for transport experiments.
- Experimental conditions: 1-100 mM NaCl, 0.5-10 mM CaCl2, 0-10 mg C/L Suwannee River humic acid (SRHA), 0.64 cm/min flow velocity, and pH 7.0.
- Six transport models based on 1D convection-dispersion equation (CDE):

\[
\frac{dC}{dt} = \frac{d}{dx} \left( D \frac{dC}{dx} \right) - u C
\]

\[
C(t) = \frac{1}{\sqrt{4 \pi D t}} \int_{-\infty}^{\infty} e^{-\frac{(x-u t)^2}{4 D t}} d\xi
\]

\[
C(x, t) = \frac{1}{\sqrt{4 \pi D t}} \int_{-\infty}^{\infty} e^{-\frac{(x-u t)^2}{4 D t}} d\xi
\]

where:

- \( D \) is the diffusion coefficient (m^2/s)
- \( u \) is the mean flow velocity (cm/s)
- \( t \) is the time (s)
- \( x \) is the horizontal distance (cm)

3. RESULTS AND DISCUSSION

3.1. Inverse Simulation (Obtaining the Best Model)

- Transport capacity order: RGO-Fe3O4 > RGO-TiO2 > RGO-ZnO.
- Six particle transport models were used to simulate breakthrough curves and retention profiles of NHs concurrently.
- Model 4 (M4) performed the best simulation with the highest R^2 and lowest AIC and BIC (Akaike and Bayesian Information Criterion) values.

3.2. Direct Simulation (Predicting NHs Retention)

- Based upon the observed breakthrough curves and retention profiles (Figs. 2-3), M4 provided the most reliable simulation outcomes.

3.2.1. Direct Simulation (Predicting NHs Retention Using M4) (M4-fitted \( S_{\text{max}} \) and \( k_b \) as initial parameters in direct simulation)

- Predicted retention for NHs varied significantly (log-scale y-axis).

4. CONCLUSIONS

- Like the transport behaviors of single-component NMs, blocking breakthrough curves and hyper-exponential retention profiles frequently occurred for NHs.
- M4 that considers time- and depth-dependent retention kinetics (one-site model) captured the transport and retention of NHs.
- More complicated models (two-site model) do not perform better than simpler models due to over-parameterization.
- M4 can predict possible outcomes of NHs using M4-fitted parameters \( S_{\text{max}} \) and \( k_b \) via forward simulation.
- At similar solution chemistries, RGO-metal oxide NHs’ mobility was lower than RGO due likely to the larger size of the NHs (~μm).