Theme 1. Exposure: Transport and Transformations
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Reason for research
The fate and transport of manufactured nanoparticles (NPs) released into the environment is of great interest due to their increasing use in consumer products and their potential risks to the environment and human health. Most NPs are manufactured with a surface coating such as polymers or polyelectrolytes to provide specific functionality. Nanoparticles can also acquire a natural coating once released into the environment due to adsorption of natural organic matter (NOM) including humic and fulvic acids. Several recent studies indicate the need for mechanistic understanding of the effect of adsorbed engineered and natural macromolecules on nanoparticle transport (i.e. attachment efficiency, $\alpha$) in porous media. It is unsure if existing empirical models capable of predicting $\alpha$ of electrostatically stabilized (bare) particles can predict $\alpha$ of NPs coated with organic macromolecules.

Hypothesis
1) Existing empirical models capable of predicting $\alpha$ of bare particles cannot predict the $\alpha$ of NPs coated with organic macromolecules because they do not account for forces originated by adsorbed macromolecule layer.
2) Adding a dimensionless parameter ($N_{LEK}$) which includes adsorbed macromolecule layer properties representing steric repulsions and the decreased friction force afforded by adsorbed NOM or polyelectrolytes in the correlation significantly improves the correlation.

Approach and Results
Deposition data for a variety of nanoparticles with different types of organic coatings, including natural organic matter (NOM)-coated latex and hematite NPs, and poly(styrenesulfonate)-, carboxymethylcellulose-, and polyaspartate-coated hematite and titanium dioxide NPs (80 data points), was used to develop an empirical correlation between measureable NP properties and their deposition under a variety of electrolyte conditions and flow velocities. Adsorbed macromolecule layer thickness was quantified using Ohshima soft particle analysis. Buckingham-Pi theory was used to develop a dimensionless parameter ($N_{LEK}$) representing steric repulsions and the decreased friction force afforded by adsorbed NOM or polyelectrolytes. Existing correlations (developed for bare particles) were unable to predict the $\alpha$ of NPs coated with organic macromolecules (Figure A) while the new correlation with the inclusion of $N_{LEK}$ can (Figure B).

Implications
This establishes the importance of including the adsorbed NOM- and polymer-coated layer properties for predicting the attachment efficiency of NPs in the environment. The form of $N_{\text{LEK}}$ suggests that limiting unintended transport and exposure to NPs could be achieved by using coatings with the smallest adsorbed mass and polymer density, shortest extended layer thickness, and largest molecular weight that would still afford the desired functionality of the coating.