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Goals

- The goal of this semester is to focus on the nanoparticle transport modeling using two kinetic site model. The model focuses on the attachment of nanoparticles using two different sites of collector sand grains and also includes a blocking function.
- Nanoparticle-nanoparticle and nanoparticle-sand interactions are also calculated according to DLVO theory. These calculations are based on surface charge measurement of nanoparticle and sand grains. These results will help to understand the chemical interactions going inside the sand column.
- Sensitivity analyses with nanoparticle transport parameters are also aimed to perform.

Brief Description

The research includes both experimental and computational approach. Experiments are conducted using glass column packed with sand. Suspended nanoparticles are injected with a syringe injection pump at a constant flow rate and effluents are collected using a fraction collector. The concentration of effluents is measured. The size of influent and effluent nanoparticle is also measured. Breakthrough curves are prepared as a function of pore volume passing through the sand column. The experiments are performed under varying factors such as ionic strength, flow rate, nanoparticle concentration, pH etc.
A one dimensional transport model is used to fit the experimental breakthrough curves with two removal rate constants for fast and slow attachments where fast attachment is subject to a site blocking term and the slow attachment is not.

The breakthrough curves for 150 mg/L aluminum oxide nanoparticles in DI water, 1 mM NaCl, 10mM NaCl and 100 mM NaCl background were fitted using Hydrus. Two kinetic site model was used for the purpose. The model was used in the following ways:

Model M1: Only k_1 (attachment coefficient 1) was fitted

Model M2: k_1 (attachment coefficient 1) and $Smax_1$ (maximum solid phase particle concentration) were fitted

Model M3: k_1 (attachment coefficient 1), k_2 (attachment coefficient 2) and $Smax_1$ (maximum solid phase particle concentration) were fitted

The tracer data were fitted using advective dispersive equation (ADE) and the column porosity and dispersivity were obtained by minimizing the square of the difference between experimentally and simulated breakthrough curves.

Highlights of achievements this semester

- Aluminum oxide nanoparticle and sand zeta potential (measurement of surface charges) were measured using zeta potential analyzer.
- Calculations were done for interaction energy between aluminum oxide nanoparticles and nanoparticle and sand (quartz). Graphs were plotted and interactions were explained according to DLVO theory.
- Aluminum oxide nanoparticle breakthrough curves were fitted using two kinetic site model. Attachment coefficients for two sites and a blocking function were used to best fit the curves. These parameters were fitted using inverse optimization. Hydrus 1D software was used for the purpose.

Representative Figures/Diagrams/Videos that highlight your research methodology and results

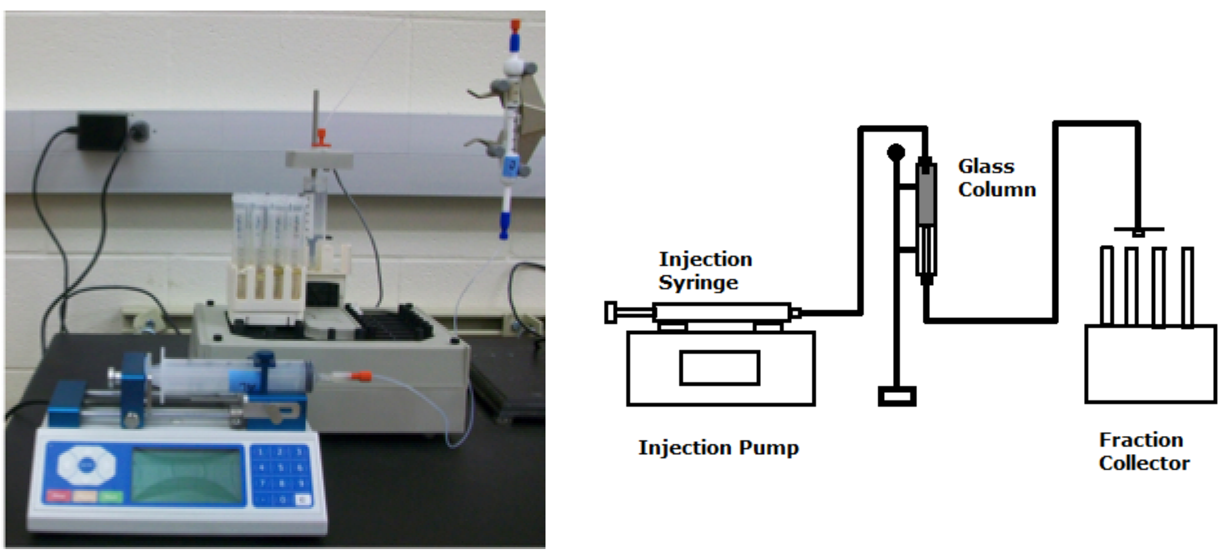

Figure 1: Experimental Setup

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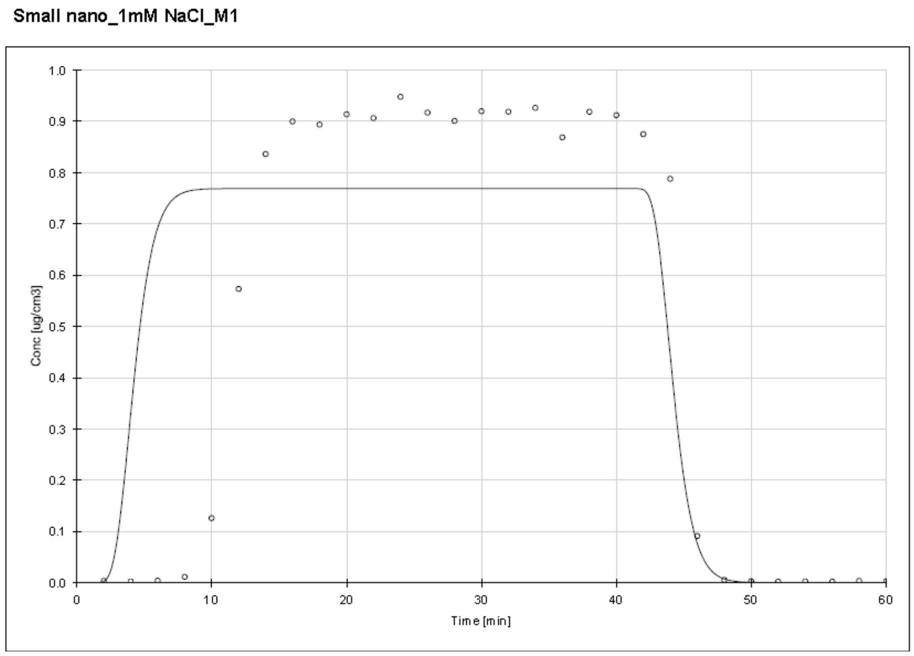

Figure 2: Experimental breakthrough curve fitted with two kinetic site model for model condition M1

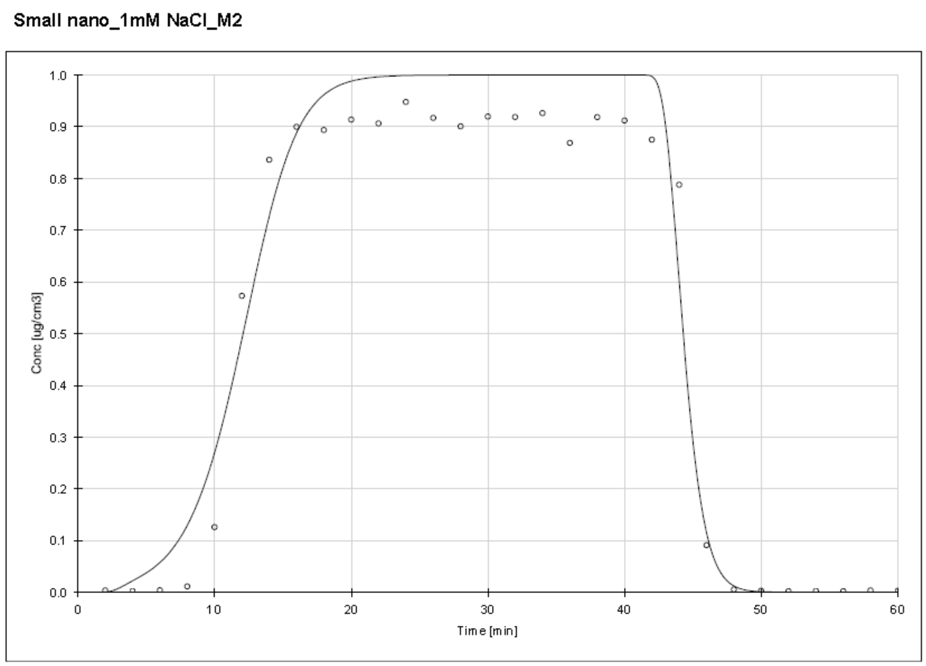

Figure 3: Experimental breakthrough curve fitted with two kinetic site model for model condition M2

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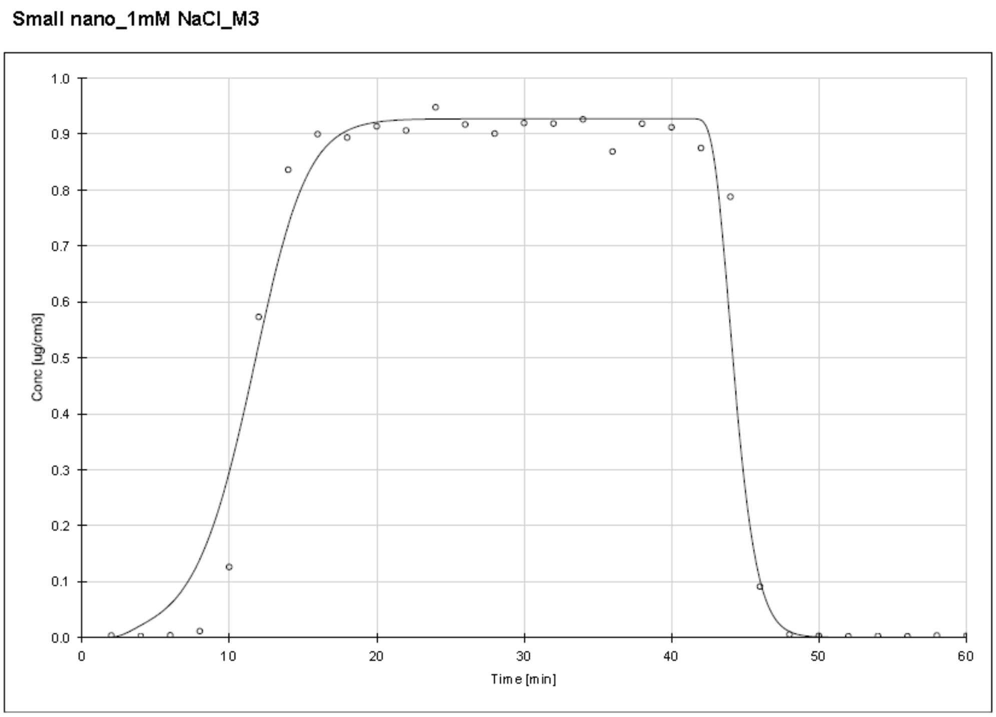

Figure 4: Experimental breakthrough curve fitted with two kinetic site model for model condition M3

Comment: M1 model was least fitted and M3 model was best fitted for all conditions.