Stability of engineered nanoparticles under various environmental conditions: Measurements and modeling

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To better understand and predict the environmental fate of engineered nanoparticles (ENPs) and their biological effects, characterization of their aqueous stability (e.g., aggregation and ion release) is important. In this study, we investigated and developed models to describe aqueous behaviors of serval selected ENPs. The ENPs include CeO_2, Ag, and quantum dots (QDs), which have broad commercial applications and toxicological relevance. The primary physicochemical properties of ENPs (i.e., morphology, size distribution and surface potential) were characterized by transmission electron microscopy (TEM), atomic force microscopy (AFM), dynamic light scattering (DLS), and zeta potential instrument. The aqueous stability was evaluated by studying the aggregation kinetics under different levels of salt, natural organic matter (NOM) and temperature by time resolved-dynamic light scattering (TR-DLS). Extended Derjaguin–Landau–Verwey–Overbeek (EDLVO) theory and the attachment efficiency (or inverse stability ratio) were both used to interpret the aggregation mechnisms. Moreover, we developed models by combining EDLVO with Arrhenius equation or von Smoluchowski's population balance equation to describe aggregation kinetics of ENPs. Particularly, the model derived from EDLVO and Arrhenius equation was also used to simulate the Ag^+ release kinetics and the influences of particle size, concentration, dissolved oxygen, and other environmental factors (e.g., temperature) on ion release kinetics. Finally, we investigated the oxidative dissolution of QDs under irradiation of ultravoliet (UV) light at 254 nm.. The effects of irradiation intensity, dissolved oxygen (DO), temperature, and surface coating on the dissolution kinetics of QDs were systematically investigated. Our results showed that the possible mechanism of the oxidative dissolution of QDs involved the formation of reactive oxidative species (ROS) on the surface of QDs under UV irradiation, and ROS may further oxidize the core-shell compositions of QDs and subsequently release the metal ions (Cd^{2+}, Se^{2+}, and Zn^{2+}). The knowledge gained from this study proivdes insight information about aqueous stability of ENPs, which lays out groundwork toward a better understanding of environmental impacts of ENPs.

Quantification non-linear flow and transport in fractures based on boundary layer theory and MIM

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Solute transport in fractures or fractured media becomes a big issue in CO_2 geological sequestration, groundwater reservoir finding, oil exploiting, nuclear waste disposal and many other fields[1-4]. More and more attentions were drawn on solute transport in single rough fracture. Among which, Fickian Law is believed to be the "right" form of governing law, however, extensive evidences such as "early arrival" and "the long tail" show non-Fickian transport [5-6].

The roughness of the fracture and the non-linear flow were considered to be two important reasons for non-Fickian transport [7]. Application of boundary layer theory in describing the flow condition in fracture seems to be a choice in non-Fickian explanation by Qian *et al*. [8]. A viscous boundary layer existed near fracture wall and the flow velocity changed rapidly. A low velocity zone (or zero velocity in cavities caused by roughness) and a fast velocity zone exist based on boundary layer theory. As a simplification of the boundary layer dispersion problem in single rough fracture, the mobile-immobile (MIM) model may be applicable. MIM approah assign a mobile domain and a immobile domain for the transport. The mobile domain was used to approximate the region near the symmetry of the fracture and the immobile domain used in low velocity zone.

By fitting the experimental data of solute breakthrough curve (BTC) through a single rough fracture using MIM we found that MIM did an excellent work. The early arrival of peak value can be explained by the dispersion in fast velocity zone and the long tailing phenomenon can be explained by the delayed transport in low or zero velocity zone. Further work can be carried out on finding the relationship between the thickness of boundary layer and mobile water fraction coefficient in MIM.

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