



Interaction between carboxyl-functionalized carbon black nanoparticles and porous media

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Carbon nanomaterials, such as carbon nanotubes, fullerene, and graphene, have received considerable attention due to their unique physical and chemical characteristics, leading to mass production and widespread application in industrial, commercial, and environmental fields. During their life cycle from production to disposal, however, carbon nanomaterials are inevitably released into water and soil environments, which have resulted in concern about their health and environmental impacts. Carbon black is a nano-sized amorphous carbon powder that typically contains 90–99% elemental carbon. It can be produced from incomplete combustion of hydrocarbons in petroleum and coal. Carbon black is widely used in chemical and industrial products or applications such as ink pigments, coating plastics, the rubber industry, and composite reinforcements. Even though carbon black is strongly hydrophobic and tends to aggregate in water, it can be dispersed in aqueous media through surface functionalization or surfactant use. The aim of this study was therefore to investigate the transport behavior of carboxyl-functionalized carbon black nanoparticles (CBNPs) in porous media. Column experiments were performed for potassium chloride (KCl), a conservative tracer, and CBNPs under saturated flow conditions. Column experiments were conducted in duplicate using quartz sand, iron oxide-coated sand (IOCS), and aluminum oxide-coated sand (AOCS) to examine the effect of metal (Fe, Al) oxide presence on the transport of CBNPs. Breakthrough curves (BTCs) of CBNPs and chloride were obtained by monitoring effluent, and then mass recovery was quantified from these curves. Additionally, interaction energy profiles for CBNP-porous media were calculated using DLVO theory for sphere-plate geometry. The BTCs of chloride had relative peak concentrations ranging from 0.895 to 0.990. Transport parameters (pore-water velocity v , hydrodynamic dispersion coefficient D) obtained by the model fit from the tracer BTCs were 0.274 ± 0.007 cm min⁻¹ and 0.102 ± 0.025 cm² min⁻¹, respectively. Mass recoveries of chloride were in the range of 94.7 to 101.9%, indicating that chloride behaved as a conservative tracer and that the column experiments were successful. The BTCs of CBNPs had different relative peak concentrations depending on the porous media used in the experiments. In quartz sand, the relative peak concentration was 0.768 ± 0.005 . The mass recovery of CBNPs in quartz sand was $83.1 \pm 2.7\%$, whereas no breakthrough of CBNPs (mass recovery = 0 %) was observed in IOCS or AOCS at the same flow rate, indicating that all CBNPs were retained in the IOCS and AOCS columns under the experimental conditions. These results indicate that metal (Fe, Al) oxides can play a significant role in the attachment of CBNPs to porous media. For the given solution conditions, both CBNPs and quartz sand were negatively charged with zeta potentials of -31.8 ± 0.1 and -39.0 ± 0.6 mV, respectively. Therefore, the electrostatic interactions between CBNPs and quartz sand were repulsive. Meanwhile, both IOCS and ACOS were positively charged with zeta potentials of 10.1 ± 1.3 and 39.9 ± 1.9 mV, respectively, such that the interaction between CBNPs and metal oxide-coated sands was electrostatically attractive, resulting in enhancement of CBNP attachment to the coated sands. Interaction energy profiles for CBNP-porous media were calculated using DLVO theory for sphere-plate geometry. Interaction energy profiles demonstrated that the interaction energy for CBNP-quartz sand was repulsive with a primary maximum (energy barrier) of 63.2 KBT, whereas the interaction energies for CBNP-IOCS and CBNP-AOCS were attractive with no energy barriers.

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