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Assessing the Environmental Fate of Graphene Oxide Nanoparticles and Their Reaction Products in Surface Waters Using the Water Quality Analysis Simulation Program (WASP8)

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Assessing the Environmental Fate of Graphene Oxide Nanoparticles and Their Reaction Products in Surface Waters Using the Water Quality Analysis Simulation Program 8 (WASP8)

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Abstract: The risk assessment of engineered nanomaterials in the environment significantly relies on mathematical models. The Water Quality Analysis Simulation Program (WASP) is one of the most widely used water quality models throughout the world, and has recently been updated (WASP8) to include numerical algorithms for simulating the fate and transport of engineered nanomaterials in surface waters. Sunlight exposure induces the phototransformation of graphene oxide (GO) nanoparticles in surface waters, resulting in products that include photoreduced GO (rGO) and polycyclic aromatic hydrocarbons (PAHs). In this study, we assume that GO releases into a river at a constant loading for 20 years, and investigate the fate and transport of GO and its major phototransformation products, rGO and PAHs. Simulation results indicate that GO dominates the GO-derived species, and accounts for 99% of the mass throughout the whole river of interest; rGO species, including free rGO and rGO aggregated to suspended solids (rGO-SS), accounts for only 1%. GO and rGO are present in the water column due to their physicochemical properties. Approximately 1% of rGO aggregates with suspended solids and is removed from the water column. Three major PAHs products are detected during GO phototransformation. The highest concentration of these three PAHs in the water column is found at 0.025 ng/L throughout the river. In the sediment, these three PAHs gradually accumulate and the highest total concentration is 1.64 ng/kg. After GO stops loading in the river, rGO-SS and PAHs can be present in the water column for more than 60 years due to sediment resuspension and pore water exchange processes. The removal of rGO-SS and PAHs from the sediment can take more than 80 years.

Keywords: engineered nanomaterials; graphene oxide; modeling; water quality analysis simulation program