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ABSTRACT

The fate and behavior of engineered nanoparticles (NPs) released in aquatic environments will be influenced by the water chemistry, as well as the pesticide load due to the potential for NP interaction with anthropogenic organic molecules (AOMs). As such, surface charge and aggregation of pure hydrophilic 100 % rutile and pure hydrophilic 100 % anatase titanium dioxide nanoparticles (TiO_2 NPs, 5−30 nm)were evaluated in a modeled water solutionin the presence of three common AOMs,glyphosate, aminomethylphosphonic acid (AMPA), and 2.4-D. Thesurfacecharge and size distribution were assessed over time as a function of various factors including surface chemistry of the NPs andAOMs, presence of mono- and bi-valent cations, pH, and ionic strength of the aqueous solution.Thepresence of AOMs(5µg/L) affectedTiO_2 NP(5 mg/L) homoaggregationin solutions (IS=10^{-3}M - 10^{-2}M)

with pH values below the NP point of zero charge (PZC) for the anatase NPs (pH=6.5)and with pH values above the NP PZC for the rutile NPs (pH=4.5). No changes in NP aggregationwere observed in very low(IS=10^{-4}M) or very high(IS= 10^{-1}M) ionic strength solutions. Passing through the PZCresulted inirreversibleaggregation of the NPs,even in the presence of AOMs.The presence of the pesticides also caused a significant modification of the NP surface charge (zeta potential) over a large range of salt concentrations (IS=10^{-4}M - 10^{-1}M). Compared to mono-valent cations, bi-valent cations (Ca^{2+}) favored NP aggregation and an increase in zeta potential. Finally, these results demonstrated that,among the studiedAOMs,glyphosate (with 4pKa-s from 0.8 to 11)affects NP aggregation/stabilization in a widerrange of physicochemical conditions.Overall, these results will aid in the evaluation of potential environmental risks posed by engineered NPs in the aquatic environments exposed to pesticide load.