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Fate of TiO₂ nanoparticles in the aquatic environment in the presence of anthropogenic compounds

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ABSTRACT

The increasing production and use of nanoparticles (NP) in consumer products inevitably lead to ENP emissions into the environment. The physicochemical properties of NP depend on various parameters (e.g. pH, cations, IS). In natural waters, the stability of NP can vary as a function of a sum of these parameters and occurs by one of the numerous scenarios. In particular, the presence of anthropogenic organic molecules (AOM) can change the NP fate. Also, the presence of NP may affect the organic pollutants (fate and toxicity). The main objective of the work was to study the aggregation of TiO₂ NP (pure hydrophilic 100 % rutile and pure hydrophilic 100 % anatase, 5–30 nm) in the presence of the most frequently occur and representative pesticides (glyphosate, AMPA, 2.4D) in natural waters considering lab experiments under relevant aqueous conditions (pH, ionic strength, presence and

concentrations of mono- and bivalent cations). The presence of pesticides affected TiO_2 NP homoaggregation in solutions ($\text{IS}=10^{-3}\text{M} - 10^{-2}\text{M}$) 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 NP (pH=4.5). No changes in NP aggregation were observed in very low ($\text{IS}=10^{-4}\text{M}$) or very high ($\text{IS}=10^{-1}\text{M}$) ionic strength solutions. The presence of the pesticides caused a significant modification of the NP surface charge (zeta potential) over a large range of salt concentrations ($\text{IS}=10^{-4}\text{M} - 10^{-1}\text{M}$). Compared to mono-valent cations (Na^+), bi-valent cations (Ca^{2+}) favor an increase in zeta potential of NP (anatase and rutile) at pH 8. There is no significant difference between at pH 5. Finally, these results demonstrated that, among the studied AOMs, glyphosate (with 4 pKa-s from 0.8 to 11) affects NP aggregation/stabilization in a wide range of physicochemical conditions. Overall, these results will aid in the evaluation of potential environmental risks posed by engineered NP in the aquatic environments exposed to pesticide load.