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Measuring and predicting the ζ-potential of anthropogenic TiO_2-nanoparticles in surface waters

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The increasing use of TiO_2-nanoparticles in commercial products such as sunscreen, paint, and food results in an increasing presence of these anthropogenic particles in surface waters due to direct (e.g. recreational activities) or indirect (e.g. urban runoff) release. Predicting the fate of those emerging pollutants requires modeling their interactions with natural colloids and surfaces, which depends strongly on the particles' ζ-potential. Since this parameter depends on the water composition (pH, ions concentrations, dissolved organic matter, etc.), a systematic investigation under controlled conditions would be extremely time and cost intensive and it is unclear if these results could be extrapolated to environmental conditions.

In this context, we proposed a novel approach for determining and predicting the ζ-potential of nanoparticles in surface water based on the water composition and environmental parameters. For that, the dialysis bag method was applied to expose five different types of TiO_2-nanoparticles representing the most common TiO_2-particles in commercial products *in situ* to a set of representative surface waters. We then determined the ζ-potential of these environmentally coated particles in the surface waters. These values ranged from -58 to 13 mV and were used together with detailed data on the water composition to train models for predicting the ζ-potential from the water composition. With an average root mean square error of 3.6 mV for the 50 generated models, the XGBoost models outperformed random forest and various linear models. The importance of explaining parameters for prediction was evaluated and discussed in detail. Furthermore, we characterized the surface coating of a selection of samples using XPS and TG-QMS. Using these techniques, we could confirm the presence of an organic coating and explore the connections between ζ-potential values and environmental coating. As expected from batch experiments studies, the concentration of divalent cations is the most important factor for predicting ζ-potential in surface water. However, pH and dissolved organic matter content do not play a major role, whereas the quality of dissolved organic matter has a significant effect. This study demonstrates the potential of our in-situ exposure method combined with multivariate analysis to explore the fate of nanoparticles in aquatic environments.