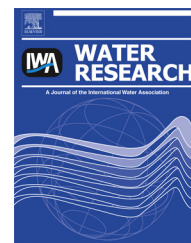


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Geographically distributed classification of surface water chemical parameters influencing fate and behavior of nanoparticles and colloid facilitated contaminant transport

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ABSTRACT

The current production and use of nanomaterials in consumer products have increased the concern about the possibility that these enter the rivers during their entire life cycle. Further, many aquatic contaminants undergo partitioning to the ubiquitous aquatic colloids. Here is presented the development of a set of European water types for environmental risk assessment of chemicals transported as nanovectors as is the case of environmental fate of manufactured nanoparticles and colloid-bound contaminants.

A compilation of river quality geochemical data with information about multi-element composition for near 800 rivers in Europe was used to perform a principal component analysis (PCA) and define 6 contrasting water classes. With the aid of geographical information system algorithms, it was possible to analyse how the different sampling locations were predominantly represented within each European water framework directive drainage basin. These water classes and their associated Debye–Hückel parameter are determining factors to evaluate the large scale fate and behaviour of nanomaterials and other colloid-transported pollutants in the European aquatic environment.

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1. Introduction

Colloidal particles are today known to be effective sorbents for both, metals and organic contaminants and thus influence their fate and transport in aquatic environments (Hassellöv and von der Kammer, 2008; Hofmann and von der Kammer, 2009; McCarthy and Zachara, 1989; Plathe et al., 2010). In addition to conventional chemicals, a new group of colloidal contaminants – engineered nanoparticles (ENP) – is an emerging environmental concern (Colvin, 2003; Handy et al., 2008; Maynard et al., 2011) owing to the potential

environmental hazard of the uniqueness of their properties and the possibility that their incorporation into consumer products will inevitably lead to environmental releases (Arvidsson et al., 2011; Gottschalk and Nowack, 2011; Hendren et al., 2011).

In order to predict the environmental concentration there is a need to assess the fate and behaviour of colloidal particles and ENP released from products in any stage of their life cycle (Westerhoff and Nowack, 2013). The possible entry ways to the aquatic environment for these particulate materials are waste water treatment plants effluents (Gottschalk and

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Nowack, 2011) or direct disposal depending on local sanitation coverage, stormwater runoff, and other indirect ways (e.g. leaching from landfills or airborne deposition). Since rivers are not only important as drinking water supply but are also essential components of watersheds and these in turn are essential units to measure ecosystem's health (Cardinale et al., 2012), understanding the fate and behaviour of nanoparticles and contaminant-colloid assemblies (NP&C) in river waters will aid to the development of integrated and physically-based environmental risk analysis of contemporary contaminants.

von der Kammer et al. (2010) identified two different approaches to assess the behaviour of ENP in natural waters: mechanistic studies performed in water with only one or two chemical components such as single electrolytes or natural organic matter (NOM), and studies with complex media like natural waters. While the first approach is aiming to identify factors that control processes and gain quantitative data, the latter approach tries to gain highly relevant information about the behaviour of particles under natural relevant conditions. While the experiments with natural waters give a more realistic approach, they are also prone to be affected by seasonal and local variations increasing the complexity and the amount of unknown parameters which ultimately leads to a lower degree of understanding of the underlying environmental processes (Bhavsar et al., 2004). Studies performed under simplified conditions are reproducible and valuable to investigate single processes, but are only valid for the limited set of hydro-chemical conditions and due to complex electrolyte, solute and NP interactions these do not allow for mimicking environmental conditions (von der Kammer et al., 2010). For emerging contaminants, like ENP, the situation is more complex owing to the non-stationary behaviour, the intrinsic heterogeneity of physico-chemical parameters (Hassellöv and Kaegi, 2009) and the likelihood of being transformed in the environment (Lowry et al., 2012; Nowack et al., 2012). For this reason, fate and transport models need to be underpinned by standardized test systems under conditions covering the relevant parameter-space.

The objective of this work is to merge the relevance of experiments in natural waters and the controllable factors of simplified mechanistic studies to create a European water classification with large-scale hydro chemical classes and to evaluate in a very simplified way the effects of the physico-chemical properties of the water on the ultimate fate of NP&C across the continent.

2. Theory on colloidal stability

There are many different ways in which NP&C can be influenced by the surrounding physico-chemical properties of the water body (Lowry and Casman, 2009; Lowry et al., 2012; Nowack et al., 2012); NP&C can undergo aggregation, dissolution, redox reactions, photo-transformations, among others and these transformation processes will be dependent on the nanoparticle intrinsic properties (material, size, shape, surface coating, etc.), the abundance of both the contaminant particles and other interacting particles, the water chemistry of the surrounding medium including electrolyte ions and

organic molecules, as well as the hydrodynamic conditions of the water body. To evaluate the effects that the ambient dissolved ions would have on nanoparticles and colloids, the effects on destabilization (likeliness to aggregate) can be evaluated theoretically in a simple way for a generic case by calculating the Debye length ($1/\kappa$), also called the inverse Debye–Hückel parameter (κ) (Elimelech et al., 1995). The Debye length is common to most mathematical solutions of the Poisson–Boltzmann (P–B) equation which resolve the electrical potential as a function of the distance away from a charged surface immersed in an electrolyte solution which is modelled as a diffuse double-layer (Ohshima, 2010; Petosa et al., 2010). It has the form:

$$\frac{1}{\kappa} = \sqrt{\frac{\epsilon \cdot \epsilon_0 \cdot k_B \cdot T}{\sum_i (n_i)_0 \cdot z_i^2 \cdot e_0^2}} \quad (1)$$

Where $(n_i)_0$ is the concentration of the i th ion in the bulk phase and z_i is its valence, e_0 is the elementary charge (1.602×10^{-19} C), ϵ is the dielectrically constant for the medium, ϵ_0 is the permittivity for vacuum (8.85×10^{-12} C² J⁻¹ m⁻¹), k_B is Boltzmann's constant (1.38×10^{-23} m² kg s⁻² K⁻¹) and T is the temperature in K. The term $\sum_i I(n_i)_0 \cdot z_i^2$ corresponds to the ionic strength scaled by $(N_A/2)$ where N_A is the Avogadro number.

The theoretical solutions for the linearized P–B equation for the electrical double layer potential usually express the repulsive interaction potential between two spheres using values such as $\kappa \cdot H$ or $\kappa \cdot a_i$, where H is the distance between the charged surfaces and a_i is the radius of the sphere i , (Ohshima, 2010; Petosa et al., 2010). The potential decays as the value of $\kappa \cdot H$ increases and, for this reason, the Debye length is often referred to as a measure of the thickness of the diffuse layer (Elimelech et al., 1995). For NP&C with other shapes than spherical (e.g. nanotubes) the interaction potential between charged surfaces can be modelled using similar approaches as those for simpler geometrical shapes (i.e. planar or spherical) which are also functions of the Debye–Hückel parameter and are usually valid as long as the assumptions for P–B approximation are sufficient (Ohshima, 2010). The overall effect of the shape in the electrostatic stability must take into account the effects that anisotropy could have on the attractive and repulsive forces (Schwyzer et al., 2012).

The decay of the electrical potential, even though simplified here, is also similar for more complex systems where electrostatic interactions dominate and therefore the calculation of Debye length can be used as a preliminary indicator for the stability of NP&C in natural waters. Some caution must be taken in cases where the concentrations of multivalent ions are high (ion–ion correlations that are neglected by P–B approximation can induce charge reversal or attractions between oppositely charged surfaces (Labbez et al., 2009)), there are ion-specific interactions with the surface (both cases when the P–B equation conditions are no longer valid) or there are other non-DLVO forces acting on the surfaces (highly steric stabilization or hydration effects). However, the knowledge of the water chemistry and, therefore, the Debye length could serve as a good first approximation to evaluate the trends of destabilization of particles from the effects of surrounding water chemistry.

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