

NanoFASE Deliverable D9.1

Comparative physiology study to parametrize in vitro and in silico models for the evaluation of the bioaccumulation potential in (in)vertebrates

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Research Report Summary

The use of engineered nanoparticles (NPs) is rapidly increasing in a wide variety of industrial sectors. As a result engineered NPs may be found in all environmental compartments. The NPs may not remain in pristine form, and transformation of engineered NPs is a process determined by the physicochemical properties of the NPs and by their interactions with the environment. Influencing factors on NP fate and behaviour can be divided into physical processes (including aggregation and adsorption to materials like organic and particulate matter in the environment), chemical processes (including oxidation/reduction reactions, complexation, and dissolution), and biological processes (biologically mediated NP transformations, and absorption of macromolecules onto the NP surface).

Transformation of NPs in the environment can at least partly be understood by extrapolations from the Derjaguin Landau Verwey Overbeek (DLVO) theory describing colloidal systems. This theory combines the effects of van der Waals attraction forces with the electrostatic repulsion, due to the double layer of counterions formed around charged particle surfaces. Environmental conditions like changes in pH, ionic strength, the presence of divalent ions, and the type/concentration of organic matter play a crucial role in NP transformation. pH variations change the surface charge of NPs to become either more positively or negatively charged, depending on their isoelectric point, inducing particle repulsion and thus better dispersion. Ionic strength either increases or decreases the double layer thickness around the particles, inducing dispersion or aggregation of the particles,



respectively. Furthermore, changes in pH and ionic strength also affect chemical processes like dissolution of metallic NPs. The effects of pH, ionic strength, electrolyte composition and presence of organic matter can also be considered in the context of bioavailability of engineered NPs in the gut of organisms, and the consequences for bioaccumulation potential. To enable environmental protection, the potential uptake of NPs (and subsequent potential adverse effect) of NPs can be tested in a wide range of test organisms. Several exposure scenarios are possible, and the species of organism affected, will depend on their habitat choice. Ingestion of NPs (while feeding) is considered an important exposure route, although, other routes like dermal uptake may be important for some species. After oral uptake, gut conditions and digestive processes (including gut motility, secretion of digestive juices, digestion, and absorption) may affect transformation and the fate of NPs and thus determine the so-called bioaccessible fraction. To assess the potential effects of gut conditions on the uptake kinetics of nanomaterials, a comparative literature study of the digestive physiology of the most frequently used species in regulatory toxicology is performed to identify the dynamic ranges of pH, ionic strength, and other factors known to affect the physicochemical properties of NPs. This information is crucial for parametrization of *in vitro* or *in silico* models that may be deployed to predict the bioaccessible fraction and the bioavailability and bioaccumulation potential of NPs.

The objectives of deliverable 9.1 are; i) to derive the dynamic ranges of parameters that play a role in accumulation efficiency, uptake, and translocation of NPs in the gut across a range of (eco)toxicological species, and ii) to identify critical parameters for prediction of the bioavailability and bioaccumulation potential of NPs and how to apply them to improve *in vitro* and *in silico* testing procedures. First, a set of parameters in the gastrointestinal environment was selected based on expert opinion. Subsequently, data on these parameters was derived by a comparative literature study on animal species physiology, taking key aspects of the anatomy of each model species into account. For all species, the anatomy and luminal chemistry depends on their feeding traits (*e.g.* herbivores *versus* carnivores), amongst many other factors. However, for simplicity and standardisation, the focus here is especially on the acid digestion of carnivorous animals, which is likely of major importance when studying nanomaterials. Fourteen model species were selected representing vertebrate and invertebrate species used in environmental and human toxicology.

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