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A modelling framework for the transport, transformation and biouptake of manufactured nanoparticles in the aquatic environment

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The development of innovative new chemical products is a key aspect of the modern economy, yet society demands that such development is environmentally sustainable. Developing knowledge of how new classes of chemicals behave following release to the environment is key to understanding the hazards that will potentially result. Nanoparticles are a key example of a class of chemicals that have undergone a significant expansion in production and use in recent years and so there is a need to develop tools to predict their potential hazard following their deliberate or incidental release to the environment. Generalising the understanding of the environmental behaviour of manufactured nanoparticles in general is challenging, as they are chemically and physically diverse (e.g. metals, metal oxides, carbon nanotubes, cellulose, quantum dots). Furthermore, nanoparticles may be manufactured with capping agents to modify their desired behaviour in industrial applications; such agents may also influence their environmental behaviour. Also, nanoparticles may become significantly modified from their as-manufactured forms both prior to and after the point of environmental release.

Tools for predicting nanoparticle behaviour and hazard need to be able to consider a wide range of release scenarios and aspects of nanoparticle behaviour in the environment (e.g. dissolution, transformation of capping agents, agglomeration and aggregation behaviour), where such behaviours are not shared by all types of nanoparticle. This implies the need for flexible, futureproofed tools capable of being updated to take new understanding of behavioural processes into account as such knowledge emerges.

This presentation will introduce the NanoFASE model system, a multimedia modelling framework for the transport, transformation and biouptake of manufactured nanoparticles. The complete system will comprise atmospheric, terrestrial and aquatic compartments to allow holistic simulation of nanoparticles; this presentation will focus on the aquatic compartment but will demonstrate the linkages with the other compartments. The system is intended for application at scales up to a large European river catchment at a resolution suitable for assessing spatially-resolved fate and biouptake. The model will be built around a transport framework which will deal with the bulk movement of water, sediments and nanoparticles through the system. Transformation processes such as dissolution, capping agent transformation, sorption of environmental molecules to particle surfaces, heteroaggregation with sediments, will be dealt with within 'reactors' with each grid cell. The reactor concept is intended to provide a separation between transport and transformation process, to allow alternative formulations of transformation processes for different classes of nanoparticles, and to allow new and updated formulations to be readily incorporated. Using this structure we aim to develop a flexible system capable of simulating the environmental transformation and fate of diverse nanoparticle classes under varying release scenarios. We will show conceptual model structures for release scenarios most relevant to the aquatic environment.