Abstract
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A Multimedia Model For Nanoparticle Fate And Biotic Update In The Environment

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Predicting the behaviour of manufactured nanomaterials (MNMs) following release into the environment is key to assessing their ultimate fate and potential risks. Developing models of MNM transfer through environmental compartments following release is therefore an essential component of assessing their environmental sustainability.
MNMs present a specific challenge to models due to their chemical and physical diversity, for example metals, metal oxides, carbon nanotubes, quantum dots. Furthermore, MNMs are frequently manufactured with capping agents or other types of coatings, or may be enclosed within product matrices (for example, antifouling paints containing zinc or copper-based MNMs). Such modifications increase the physicochemical complexity of the particles and may further modify their environmental behaviour. Additionally, MNMs may transform prior to environmental release (for example, in sewage treatment works) or following environmental release (for example, by dissolution or heteroaggregation). Environmental models of MNMs thus require the capability to simulate a wide range of physicochemical forms and behaviours, within a single framework. Such a framework ideally needs to be readily updatable, to permit simulation of MNMs not yet in commercial use.

The NanoFASE Horizon2020 project (2015-2019) aims to tackle the particular issues of multimedia nanoparticle modelling by developing a spatially-explicit, gridded dynamic model of nanoparticle transport, transformation and biouptake (the NanoFASE model) using object-oriented programming (OOP) concepts. The OOP approach allows for the system to be considered as a linked set of 'objects' representing entities such as a layer of soil or sediment, a population of organisms, or a population of nanoparticles. The complete model system will comprise terrestrial and aquatic compartments, with a link to atmospheric deposition modelling, to allow holistic simulation of nanoparticle fate and biouptake. It is intended for application at scales up to that of a large European river catchment.

The model will be divided into 'transport' and 'transformation' components. The transport component will handle the bulk movement of MNMs, for example in river flow, settling sediments, soil porewater and surface soil erosion to waters. The transformation component will handle key MNM transformations and reactions within environmental compartments, such as heteroaggregation and adsorption of environmental species such as dissolved organic matter. MNMs will be categorised by 'type', where all MNMs within a single 'type' will share common algorithms for transformations within each environmental compartment. The number and nature of the types simulated will be readily extensible, thus allowing for the efficient addition of new nanoparticle types to the model.