



NanoFATE Deliverable 2.1

Issues for consideration during development and refinement of fate models

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Research report - Summary

Fate evaluations form a central part of the exposure assessment of chemicals in the environment and are often implemented by means of multi-media models, such as e.g. the SimpleBox model of EUSES for industrial chemicals or the pesticide fate models from the FOCUS suite. These models, however, depend to a great deal on mass-balances and steady-state equilibrium assumptions that are violated by the fundamental behaviour of nanoparticles. As colloids, nanoparticles are never in thermodynamic equilibrium, but continuously collide, attach and detach to/from themselves and surrounding materials (e.g. natural organic matter). The net effect of these processes inevitably leads to agglomeration over time and nanoparticle dispersions hence cannot be treated as a static system. Instead their rates of changes due to agglomeration and sedimentation need to be described and modelled. Additional fate processes, such as surface modifications due to interactions with other colloidal or solved matter in aqueous systems, dissolution processes and redox transformations might also impact the fate of nanoparticles in environmental matrices. These specific properties need principal consideration during the development, adaptation and validation of environmental fate models for nanoparticles.

Next steps within the NanoFATE project

NanoFATE will explore needs, possibilities and consequences of accounting for the specific properties of nanoparticles in GIS-aware models for river-basin modelling. As well, STP-models and fate models in the context of EUSES will be applied within NanoFATE. As a first step, sensitivity analyses will be performed and a set of worst case assumptions will provide the range of possible estimates of environmental concentrations of zinc-oxide, silver and cerium-oxide particles in soil and receiving waters. A subsequent comparison to ecotoxicological data (hazard assessment) will identify the need for further refinements. Should the first, rough fate and exposure estimates indicate a potential reason for concern, the models need to be further adapted to the specific properties of nanoparticles. Should even rough, highly conservative exposure and fate estimates indicate no reason for environmental concern, the need for advanced fate models might not be substantial. Experimental model-systems will provide validated data on the fate of nanoparticles in STPs.

This report is to be published as a refereed journal paper.