The world's first model for engineered nanoparticles in surface waters

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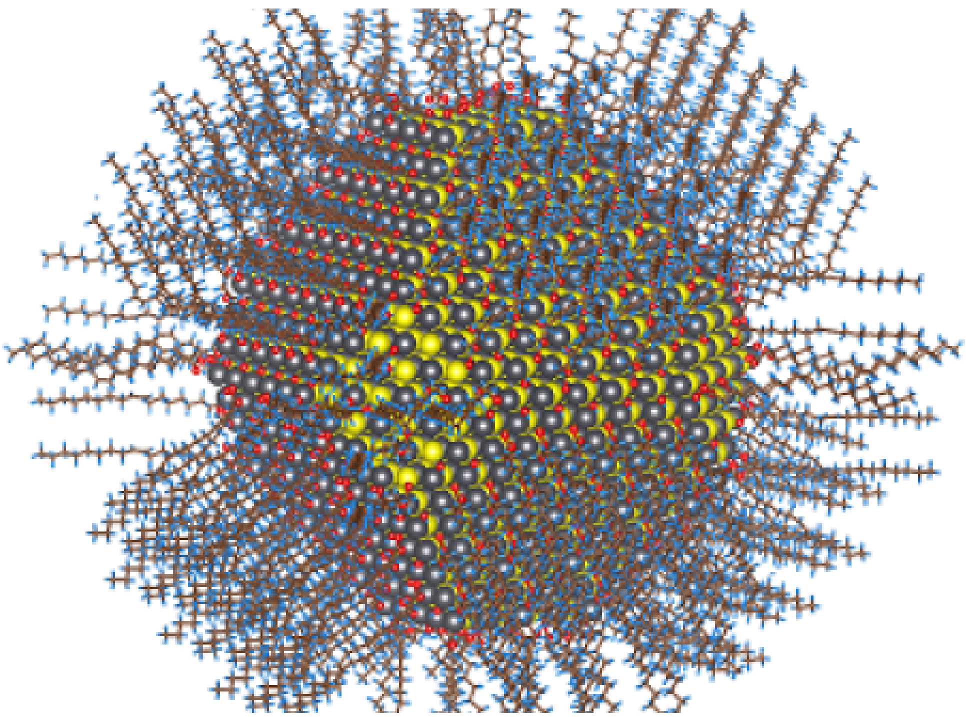

Researchers of Wageningen University provide the world's first spatiotemporally explicit model that simulates the behaviour and fate of engineered nanoparticles (ENPs) in surface waters. Wageningen researcher Bart Koelmans: "This is important in order to assure safe nanotechnology. We do need to have an assessment of the risks of ENPs to man and the environment."

Nanotechnology is developing fast, with the fast growing emission of less than 100 nm engineered nanoparticles as a consequence. ENPs are hard to measure in the environment so that exposure assessments have to rely on modelling. Previous models could only predict average background concentrations on a continental or national scale.

NanoDUFLOW

The new NanoDUFLOW model however, developed by Joris Quik, Jeroen de Klein and Bart Koelmans and recently described in Water Research magazine, is capable of simulating the concentrations of ENPs, and their homo- and heteroaggregates in space and time, for any hydrological flow regime of a river. Under the hood of NanoDUFLOW is an 'engine' that calculates all relevant interactions among 35 types of particles including the ENPs, and that decides upon aggregation, settling or prolonged flow in the river. The rate of these interactions depends on the flow conditions in the river, which are calculated in the hydrology module of NanoDUFLOW. This module can be set to match the channel structure of any catchment as defined by the user, allowing for a great flexibility.

Development of the model

Development of the model took a long and winding road. ENPs are emerging chemicals with unique properties, which implies that some new process descriptions needed to be developed. One of the main parameters in this new type of models is the attachment efficiency. The attachment efficiency is the chance that two particles stay together when they collide, a chance that depends on the nature of the colliding particles and the chemistry of the water. A smart calculation method needed to be developed that enabled the estimation of the attachment efficiency from laboratory experiments with ENPs and natural particles and waters collected in the field.

Using NanoDUFLOW for the risk assessment of nanomaterials

In order to assure safe nanotechnology, society calls for an assessment of the risks of ENPs to man and the environment. A risk assessment for ENPs requires an assessment of ENP exposure, and of the effects caused by ENPs, which then can be compared in a risk characterisation. Whereas previous screening-level models still may be first choice for lower tiers in the risk assessment, NanoDUFLOW is believed to be useful for higher tiers of the risk assessment, where site specific risks need to be addressed. Simulations with NanoDUFLOW showed the occurrence of clear ENP contamination 'hot spots' in the water column and in sediments. Furthermore, NanoDUFLOW was capable of simulating the speciation of ENPs over different size fractions. This speciation defines the ecotoxicologically relevant fractions of ENPs, for a variety of species traits. Also in this respect NanoDUFLOW will add to refining the risk assessment for ENPs.

Provided by Wageningen University

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