WATER RESEARCH COMMISSION

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The WRC operates in terms of the Water Research Act (Act 34 of 1971) and its mandate is to support water research and development as well as the building of a sustainable water research capacity in South Africa.

TECHNICAL BRIEF

Nanotechnology

Determining the toxicity of engineered nanomaterials

A completed Water Research Commission (WRC) study modelled the fate, behaviour and toxicity of engineered nanomaterials in aquatic systems.

Background

Growth in the production and use of engineered nanomaterials (ENMs) has raised concerns with regard to their potential impact on the environment, and aquatic media in particular. These materials mostly consist of metal nanoparticles and their oxides, which could be released in large quantities into aquatic environments.

At present, assessment of the risk posed by these pollutants is stymied by the severe lack of information on the effects of nanoparticles on the environment, since they have differently from their bulk material counterparts.

It is therefore imperative that the potential risks that may be associated with ENMs are identified as soon as possible during the early stages of nanotechnology development. Therefore, this WRC project was initiative to investigate the potential impact of ENMs on aquatic invertebrates using both experimental approaches (bioassays) and modelling methods.

Methodology

The development of the toxicological database of ENMs was accomplished through the sourcing and acquisition of scientific reports (mostly peer reviewed articles) detailing experimental work related to the behaviour and effect of ENMs in aquatic media. Although this methodology is applicable to ENMs in general, the project scope was limited to titanium nanoparticles ($nTiO_2$), since they are among the ENMs with the most widely reported exposure and toxicity data in aquatic systems.

The data described in each of these reports were collected in an Excel database. This consisted for qualitative and quantitative variables annotated by comments on the sources or quality of the data.

Neural network models

The data was used to develop multilayer perceptron neural networks to predict the behaviour and toxicity of $nTiO_2$ in aquatic media. This behaviour of the nanoparticles in water was represented by two response variable and hence two neural network models, as different sets of predictor variables were used to predict each response, namely a) their ability to adsorb organic substances in their environment and b) aggregation of the particulates in aqueous media.

In contrast, the effect of the particles on the environment were represented by six response variables (and hence six neural network models). These were the effect of the particles on the a) immobilisation of ***Daphnia magna***; b) mortality of ***D. magna***; c) growth rate of ***D. magna***; d) growth rate of algae; e) reproduction in ***D.magna*** and f) biomass of algae.

Results of the study

With the exception of the algae biomass (as an effect on the environment) model, the models could explain the variation in the response variables satisfactorily (with coefficients of determination or R^2 ranging from approximately 74 to 93% on test and validation data).

The algae biomass model could not explain more than approximately 43% of the variation of the response variable based on test and validation data. Therefore, the results from this model should be treated with caution.

Although the variables identified as significant predictors of the response variables could also have been derived from first principles, the models provided a quantitative assessment of the variables that could not be acquired in any other way.

Conclusions

With the neural network models, data from different sources could be combined to generalise the behaviour and toxicity of $nTiO_2$ using reported scientific data. This facilitated the identification of complex relationships involving many variables that would otherwise not have been possible with deterministic models. This knowledge extraction and feasible inductive learning from the published data could be used to direct future research and early regulation of nanomaterials in the environment.

In principle, the models could be applied to pilot-scale or full-scale scenarios, e.g. water bodies, to predict response patterns without requiring extensive analytical work. Output from the regression models derived from laboratory data provides generic first-tier risk assessment.

The natural environment comprises multiple associations or organisms and conditions that might contribute to a) effects to organisms that are not related to nanomaterials and b) enhanced or antagonised effects that are different from those observed in pure cultures.

Laboratory studies simulate aquatic systems where natural associations are simplified. The models were built on this simplification by incorporating predictor variables drawn from characteristics of nanomaterial, environmental conditions and organism factors to forecast exposure mechanisms.

Finally, the neural network models could be integrated as management tools to predict the dynamics of $nTiO_2$ after release into aquatic systems and interrogation of the models could be used to explain the effects of the $nTiO_2$ on the environment. For example, adsorption and aggregation processes may have both negative and positive impacts on aquatic systems.

An understanding of the aftermath e.g. enhanced flocculation and removal, deposition, accumulation etc. may influence mitigation planning. The model is flexible and can be improved by adapting it to new data to generalise risk-based outcomes in diverse aquatic systems, as ad when new data are obtained.

Further reading:
To order the report, ***Modelling the fate, behaviour and toxicity of engineered nanomaterials in aquatic systems*** *(***Report No. 2107/1/14***)* contact Publications at Tel: (012) 330-0340, Email: orders@wrc.org.za or Visit: www.wrc.org.za to download a free copy.