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ABSTRACTS

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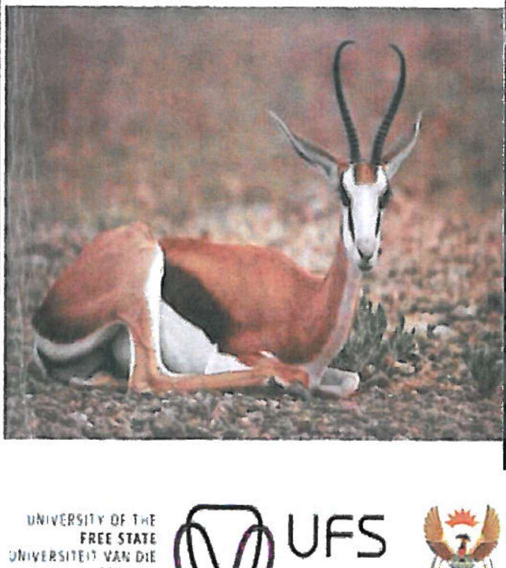

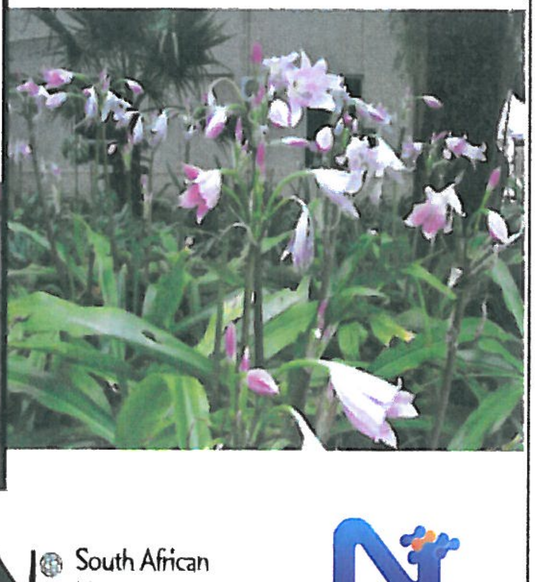

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Application of Modeling Tools for Risk Assessment of Engineered Nanomaterials in Aquatic Systems

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1. Introduction

Globally, engineered nanomaterials (ENMs) are increasingly being used in nanoproducts [1–3] to improve their performance. The multi-stage lifecycle of ENMs increases their potential risk profiles to different environmental systems, for example, due to release of nanowastes [1]. Both the physicochemical properties of ENMs (e.g. size, shape, zeta potential, etc) and abiotic factors (e.g. pH, ionic strength, natural organic matter, etc) influence their; exposure, fate, transport, and effects in aquatic systems [4]. Until now, there is limited scientific data on the exposure, fate, transportation, and effects of ENMs in the aquatic systems. Therefore, use of modeling tools are an attractive approach for estimating the potential ENMs risks [2, 5], and provides a rigorous alternative approach to elucidate linkages of their physicochemical properties, abiotic factors, and the observed biological effects.

To date, several modeling techniques have been exploited in estimating the potential environmental exposure risks of ENMs under different environmental conditions. These models include; material flow analysis (MFA), particle flow analysis (PFA), stochastic, dose-response, and quantitative structure-activity relationship (QSAR). Results from each model type are limited in estimating the ENMs risks in the aquatic systems. Perhaps the limitations are linked to their fundamental design which did not take into account data complexity as a result of interactions between physicochemical properties of ENMs and abiotic factors that underpins the observed exposure and effects. Here, we illustrate the strengths and the weaknesses of each model, and provide a conceptual framework on how the models can be integrated to derive more useful risk estimation data of ENMs in the aquatic systems. The strengths and weakness of each model are summarized in Table 1.

2. Proposed conceptual framework

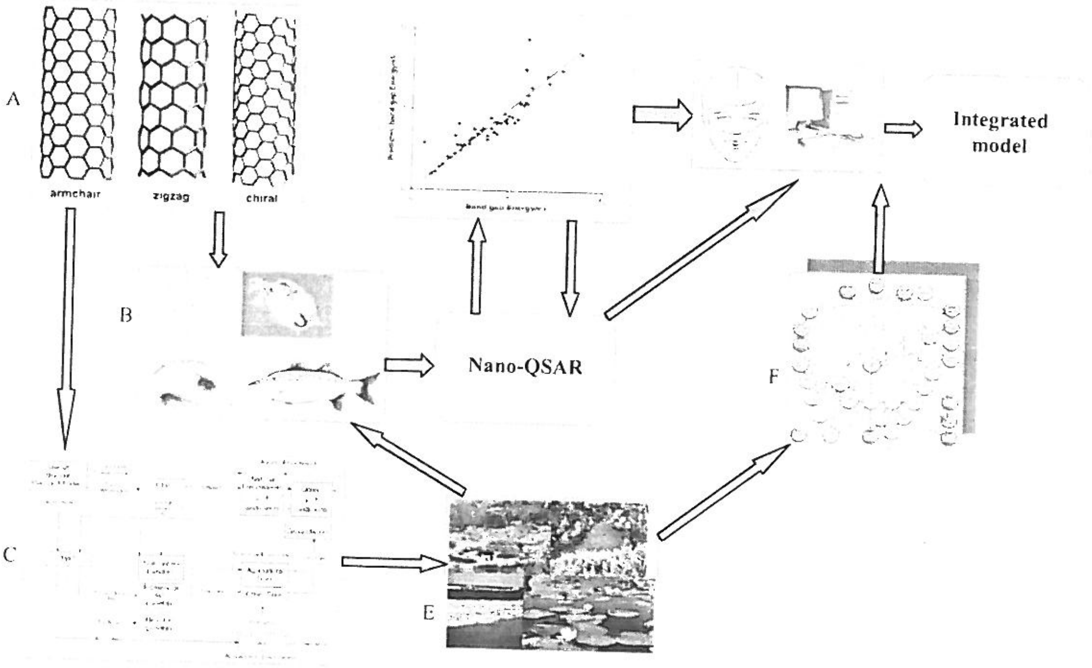

Fig. 1: Conceptual framework on integrated modeling; A, physicochemical & structural properties of ENMs; B, *in vitro* & *in vivo* toxicity data; C, ENMs emission (material flow); E, fate and transport in aquatic ecosystems; D, data mining and regression models; F, Bayesian networks; and G, expert systems & reasoning.

A holistic and integrated modeling approach of forecasting ENMs environmental risks is proposed to establish the best predictive model through a combination of models previously used in forecasting ENMs risks in aquatic systems. The proposed methodology offers the possibility of exploring and developing more resilient and robust predictive models that account for the unique aspects of the most used ENMs with elevated likelihood of release into the environment. The integrated modeling approach would see estimate the fate, transport, exposure to receptor cells or organisms, and toxicity of ENMs. Accessible data and knowledge will be integrated systematically, for example, one model output may be used as input variables to another model as means of developing higher level models.

Table 1: The strength and weakness of modeling techniques for estimating ENMs toxicity in the environment.

Model	Strengths	Weaknesses
Material flow analysis (MFA)	• Forecast likely production, emission, exposure, risks, and concentration of ENMs in environment • Provide good measure of life-cycle mass balances	• Regional specific and cannot be replicated • ENMs toxicity to ecological systems not considered • Physicochemical properties of ENMs not considered
Probabilistic material flow analysis (PMFA)	• An improvement to MFA models • Considers stochastic temporal and spatial data e.g. for river systems and emission uncertainties in environmental compartments.	• Exclude uncertainties from abiotic and biotic parameters that forecast colloid sedimentation risks to aquatic organisms • Regional specific and cannot be replicated • ENMs toxicity to ecological systems not considered • Physicochemical properties of ENMs not considered
Particle flow analysis (PFA)	• Forecast the potential sources of ENMs emissions to the environment • Introduces the concept of using the particle number as the unit of measuring the ENMs effects to receptor organisms	• Do not quantify expected emission pathways • Are not practical in quantifying emissions of non-particle, non-spherical, bulk & coated ENMs • Regional specific and cannot be replicated • ENMs toxicity to ecological systems not considered • Physicochemical properties of ENMs not considered
Stochastic modeling	• Predicts colloidal behaviour of ENMs in fluid media under different media conditions • Reveal settling properties due to the effects of surface properties of ENMs	• Limited in predicting risks of ENMs suspensions or colloids in terrestrial or aquatic organisms due to settling • Unrealistic as assumes purified water in box simulations • Ideal agglomeration and colloid computations for a typical water flow process in an aquatic system
Dose-response modeling	• Forecast toxicity effects of ENMs to cells, biological, and ecological organisms • Insightful on ENMs risks that support development of a regulatory framework • Data generated used in developing other models including MFA and QSAR	• Inconsistency and uncertainty in parameterization and naming due lack unified framework • Use no observed effect concentration (NOEC), a parameter associated with statistical limitations Physicochemical properties of ENMs not considered
Quantitative structure activity modeling (QSAR)	• Insightful on computational modeling where suitable descriptors are used to predict toxicity of ENMs to biological organisms • Significantly support development of protocols for testing of toxic ENMs	• Lack of knowledge of ENMs properties, and use of limited descriptors inhibits development of suitable models • Lack of reference standards to guide model development • Unique properties of ENMs render classical QSAR models unlikely to predict toxic effects using *in vitro* results

3. References

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