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Freshwater ecotoxicity characterisation factor for metal oxide nanoparticles: A case study on titanium dioxide nanoparticle

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HIGHLIGHTS

- The present study proposes a method to calculate the freshwater ecotoxicity CF for nano-TiO2;
- We applied the recent USEtox model, and Nano-specific descriptors have been considered.
- An adjusted model has been developed which accounts nano-specific description to estimate the FF of n-TiO2 in freshwater
- On our knowledge our study is the first which combine the nano-specific fate process within the USEtox framework.
- The CF may be used in LCA study allowing the calculation of freshwater ecotoxicity impact of ENP until now scarcely assessed

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ABSTRACT

The Life Cycle Assessment (LCA) methodology is widely applied in several industrial sectors to evaluate the environmental performance of processes, products and services. Recently, several reports and studies have emphasized the importance of LCA in the field of engineered nanomaterials. However, to date only a few LCA studies on nanotechnology have been carried out, and fewer still have assessed aspects relating to ecotoxicity. This is mainly due to the lack of knowledge in relation on human and environmental exposure and effect of engineered nanoparticles (ENPs). This bottleneck is continued when performing Life Cycle Impact Assessment, where characterization models and consequently characterization factors (CFs) for ENPs are missing. This paper aims to provide the freshwater ecotoxicity CF for titanium dioxide nanoparticles (nano-TiO_2). The USEtox™ model has been selected as a characterisation model. An adjusted multimedia fate model has been developed which accounts for nano-specific fate process descriptors (i.e. sedimentation, aggregation with suspended particle matter, etc.) to estimate the fate of nano-TiO_2 in freshwater. A literature survey of toxicity tests performed on freshwater organism representative of multiple trophic levels was conducted, including algae, crustaceans and fish in order to collect relevant EC_{50} values. Then, the toxic effect of nano-TiO_2 was computed on the basis of the HC_{50} value. Thus, following the principle of USEtox™ model and accounting for nano-specific descriptors a CF for the toxic impact of freshwater ecotoxicity of 0.28 PAF day m^3 kg^{-1} is proposed.

1. Introduction

The advent of nanotechnology is considered as one the greatest innovations since the beginning of industrial engineering (Som et al., 2010). Nanotechnology is used in a rapidly increasing number of products available to industries and private consumers: electronics, cosmetic, nutrition, medical drug designing and other. The term engineered nanoparticles (ENPs) refers to a subset of nanomaterial which is a material with at least one external dimension in the size range from 1 to 100 nm (ISO, 2008).

The increasing use of ENPs in consumer and industrial products has also increased the concerns on their adverse effect on human health and ecosystems (Alvarez et al., 2009; Klaine et al., 2012). Therefore considerable effort has been made to assess the impacts of ENPs to humans and the environment. Among the several tools available, the European Commission encouraged life cycle-based methods to assess the sustainability of nanotechnology (UNEP, 2011). Life Cycle Assessment (LCA) is regulated by the international standards ISO 14040 series (ISO, 2006 a, b).

Abbreviations: EC_{50}, The chemical concentration that is expected to have one or more specified effects in 50% of a group of organisms; HC_{50}, Hazardous Concentration for 50% of the species.

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LCA has been proposed and adopted as essential tool to analyse, evaluate, understand and manage the environmental and health effects of the ENMs (Hischier, 2014). Despite all, the LCA studies often do not cover the complete life cycle of ENMs (Hischier and Walser, 2012; Gavankar et al., 2012; Miseljic and Olsen, 2014). Hence, most of the studies are cradle-to-gate and the environmental impacts primarily reflect the energy and material flows for the extraction of raw materials and manufacturing phases, whereas the environmental impacts related to the release of ENPs into the environment are rarely assessed. This is due to gaps in knowledge concerning both the release of ENPs (Life Cycle Inventory) and their potential effects on the environment and humans (Life Cycle Impact Assessment). The latter of these is expressed by the so-called eco/toxic characterisation factors (CFs) describing and quantifying the cause–effect chain of an emission of a substance to the environment. The development of freshwater-ecotoxicity CFs for ENPs is still in its infancy due to the scarce knowledge of the exposure and effects to aquatic organisms. More fate and transport models (F&T) to assess the concentration of ENPs in the environmental media are yet to emerge (Liu and Cohen, 2014; Gottschalk et al., 2010, 2013). It is evident that the lack of ecotoxicity CF of ENPs impedes the evaluation of ecotoxicological impacts caused by their emissions into the environment. So far, only two studies have calculated the freshwater- and seawater-ecotoxicity CF of ENPs: Eckelman et al., 2012 and Walser et al., 2011 calculated the CF for carbon nanotubes (CNT) and silver nanoparticles, respectively.

Many metal containing materials, particularly metal oxides, belong to the class of ENPs: zinc oxide (ZnO),titanium dioxide (TiO_2), cerium dioxide (CeO_2), chromium dioxide (CrO_2), molybdenum trioxide (MoO_3), bismuth trioxide (Bi_2O_3) and binary oxides such as, lithium Cobalt dioxide ($LiCoO_2$), indium tinoxide (InSnO) (Bhatt and Tripathi, 2011).

The estimated worldwide production of nano-TiO_2 is 3000 t/year for 2010 (Piccinno et al., 2012). The environmental nano-TiO_2 realise into aquatic system can occur through wastewater treatment plant effluents, form exterior facades or accidents during transport (Gottschalk et al., 2010).

This study proposes a method for calculating the freshwater-ecotoxicity characterization factors of metal oxide ENPs. In particular, nano-TiO_2 ENPs have been chosen as representative substance based on their extensive application, the availability of data regarding their ecotoxicological effect and on their environmental behaviour. Based on the USEtox™ model and on the multimedia fate models for organic chemicals, this paper develops an adjusted model which includes nano-specific descriptions to estimate the fate of nano-TiO_2 in freshwater and thereby calculates a CF for freshwater ecotoxicity.

2. Materials and methods

2.1. Characterization model

Several characterization models are available for the ecotoxicity impact category and often the final results vary substantially among the models. It must be noted that the quantification of the ecotoxicity impacts is one of the most debatable items in LCA (Hischier and Walser, 2012). The variability in model outcomes has been reduced thanks to the USEtox™ model, recently developed by an international collaboration of leading LCIA specialists (Rosenbaum et al., 2008). The USEtox™ provides CFs for organic and inorganic substances for both human toxicity and aquatic freshwater ecotoxicity. However, it does not yet consider marine ecosystems or sediments (where sedimentation is considered a removal process). The International reference for Life Cycle Data System (ILCD) Handbook (JRC-IES, 2011) recommends using USEtox™ to model impacts related to ecotoxicity and human toxicity. Thus, in this study, the USEtox™ model has been selected as characterisation model and its framework has been applied to calculate the CF for nano-TiO_2.

Since it was developed for organic chemicals, the application of the USEtox™ to model ENPs has some inherent difficulties. And also, a new approach based on the colloidal science is required. As will be explained in Section 2.5.2 ENPs show different environmental behaviours (and thus descriptors), relative to their bulk phases and other chemicals. Therefore, environmental fate modelling has to be adapted to ENP's specific fate processes and to the physicochemical properties governing them.

2.2. Characterization factor calculation

The USEtox™ model estimates the CF of a substance for the impact category of freshwater ecotoxicity, as:

$$CF = EF \cdot FF \cdot XF \qquad (1)$$

where EF (PAF m^3 kg^{-1}) is the effect factor that represents the ecotoxicity of the substance and it is expressed in term Potentially Affected Fraction of species-PAF, FF (day) is the fate factor and expresses the residence time of a substance in a particular environmental compartment (such as freshwater) and XF [dimensionless] is the exposure factor. The development of each factor for nano-TiO_2 is discussed below. The CF for nano-TiO_2 was then calculated, with units describing the temporal and volumetrically integrated potentially affected fraction of aquatic organisms per unit mass of released nano-TiO_2 (PAF m^3 day kg^{-1}).

2.3. The effect factor calculation

USEtox™ adopts a PAF (Potentially Affected Fraction of species) based approach to calculate the EF for aquatic ecotoxicity of a substance (Larsen and Hauschild (2007a, 2007b); Rosenbaum et al., 2008). The PAF is the fraction of species exposed to a concentration above their EC_{50} (Klepper et al., 1998). The EF is defined as:

$$EF = \frac{0.5}{HC50_{EC50}} \qquad (2)$$

where, $HC50_{EC50}$ represents the concentration at which 50% of species is exposed above their chronic EC_{50} and 0.5 is the working point (PAF = 0.5) on the PAF curve. At least three EC_{50} values from three different phyla are required to reflect the variability of the physiology and to ensure a minimum diversity of biological responses (Henderson et al., 2011). USEtox™ suggests to calculate the $HC50_{EC50}$ as the geometric mean of the available single species EC_{50} for organisms representative of three trophic levels: algae, crustaceans and fish. In this study, the EF of nano-TiO_2 was estimated from toxicity values reported in previous studies on freshwater organism representative of the three trophic levels recommended by the USEtox™ model (algae, crustaceans and fish).

As highlighted by the literature, the toxicity of nano-TiO_2 is influenced by: i) type of nano-TiO_2: crystalline structure, nominal size, content of impurities (Crane et al., 2008; Navarro et al., 2008; Ji et al., 2010; Seitz et al., 2013, 2014); ii) procedure followed to conduct the toxicity test, i.e. suspension preparation method with use of solvent, sonication, filtration, (Clement et al., 2013; Aruoja et al., 2009; Handy et al., 2008,); and iii) mode of exposure to organism i.e. the time of exposure, UV exposure (Zhu et al., 2010; Dabrunz et al., 2011; Seitz et al., 2013; Ma et al., 2012). In order to increase the reliability of the estimated EF criteria have been applied to select the toxic value involved into the EF calculation. The toxic values applied are reported in Tables S.1–S.3. The criteria are listed below and aim account for the main sources of variability.

i) Chemical tested concerning crystalline structure, anatase form seems more toxic than rutile. Thus, toxicity tests performed with nano-TiO_2 composed mainly of anatase are preferred to those