

How suitable is LCA for nanotechnology assessment? Overview of current methodological pitfalls and potential solutions: 65th LCA Discussion Forum, Swiss Federal Institute of Technology, Zürich, May 24, 2017

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1 Foreword

The 65th Life Cycle Assessment Discussion Forum was held on May 24, 2017, to discuss the state of research and application with regard to nanotechnology. This conference report presents the highlights of the forum. While all presenters agreed on the relevance of the life cycle assessment (LCA) and risk assessment (RA) methods to offer valuable environmental sustainability assessment of manufactured nanomaterials (MNMs), a recurring theme during the forum was the continued lack of environmental data on the manufacturing, release and impacts of such MNMs. Different strategies and research pathways were proposed to tackle this dearth of representative data. The first session provided an overview of the current state-of-the-art in environmental assessment of MNMs from the perspective of regulation, industry and research. The main concern for all these stakeholders is to offer representative environmental assessment and avoid risks in a sector that is rapidly developing. System modellers then proposed, in the second session, different strategies to consider the current lack of knowledge (e.g. uncertainty and potential evolution) in representation of MNMs production pathways. Prospective modelling, global sensitivity analysis and dynamic probabilistic methods were all shown to be relevant tools to deal with the scarce information. Presenters from the third session subsequently discussed the requirements of evaluating potential impacts (i.e. toxicity) of MNMs if they

are released into the environment. Techniques for the characterisation of their effects were introduced, but the consideration of nano-specificities and a clear focus on a limited amount of MNMs were identified as major research challenges that still need attention. The final session then offered a review of how the RA method can be used to complement LCA studies and quantify adverse environmental and human health effects due to exposure at specific sites.

All presentations from the 65th discussion forum are available for download (www.lcaforum.ch), and the video recordings can be watched online (<http://www.video.ethz.ch/events/lca/2017/spring/65th.html>).

2 Introduction

Almost half a century after Richard P. Feynman's famous declaration, "there is plenty of space at the bottom" (Feynman 1960), nanotechnology is now considered by the European Commission as being one of the six key enabling technologies for the twenty-first century. Today, manufactured nanomaterials (MNMs) are being used in an ever increasing number of consumer products, which raises concerns about their potential environmental and human health impacts. To alleviate these concerns, there is a need to assess the potential impacts of MNMs during their life cycles and when they are released into the environment (Liu et al. 2015).

Life cycle assessment (LCA), defined in the ISO standards, is recognised as being fully suitable for the assessment of nanomaterials and nano-enabled products, despite notable shortcomings in the availability of specific inventory data and impact assessment models (Ettrup et al. 2017, Klöpffer et al. 2007, Pini et al. 2016). Various actors have been working extensively on overcoming these shortcomings (see e.g.

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Hischier et al. 2017; van Harmelen et al. 2016; Walser et al. 2017) to ensure that traditional, as well as nano-specific environmental issues, could be assessed within one, unified, comprehensive and consistent LCA framework. Notably, the OECD published, in 2015, a guidance manual about the smart exchange of data between risk assessment (RA) and LCA studies specifically for nano-enabled application studies (OECD 2015).

The 65th Swiss LCA Discussion Forum, a one-day event that fosters exchanges between industry, consultancies and academia, aimed to provide an overview of the key challenges that LCA practitioners and data providers are still facing when they undertake LCA studies of nanotechnology, as well as possible solutions. The discussion during that day can be split into four distinct parts. The first part provided a general overview of the current context, looking at the issues from different perspectives. Different strategies for undertaking prospective modelling of novel MNMs and nanotechnology were discussed during the second part. As a third part, the afternoon session focused on why and how existing impact assessment (LCIA) methods should be modified to be appropriate for the assessment of nanoparticles/nanomaterials. Last but not least, the final part explored the benefits of combining LCA and RA approaches for MNM environmental assessment.

3 General overview of current development

There is a growing need for robust and objective information on the environmental, human and safety (EHS) aspects of MNMs. Regulatory and industrial stakeholders rely on scientists to develop and use assessment methods, such as RA and LCA, to provide such information. The first session of the day offered an overview of the current status and related key challenges in view of the use and release of MNMs from the perspectives of regulation, industry and academia.

Roland Hischier (group leader, Empa, Switzerland) presented as introduction into the day a critical review of LCA studies on MNMs, focusing on developments since his 2012 publication (Hischier and Walser 2012). Although many studies have been published in recent years, most of the key issues originally identified in 2012 still remain unresolved, namely (i) inadequate functional unit definition, (ii) insufficient coverage of environmental emissions of MNMs in LCI datasets, (iii) no consensus on the modelling of nano-releases and (iv) lack of characterisation factors for MNM releases (particularly for toxicity-related impact categories). The consequences of these issues on the variability and uncertainty of LCA results were investigated with the example of nano-titanium dioxide use in facade coatings (Hischier et al. 2017). Adequate and comprehensive consideration of MNM functionality during goal and scope definition was found to be the principal cause of variability in LCA results.

Tobias Walser (Vereala GmbH, Zurich, Switzerland) continued the session with a presentation on the relevance of LCA and RA for MNM policymaking. The need for clear rules on the identification and grouping of MNMs was highlighted, particularly given the wide variety of MNMs being used and developed. These would ensure that nanomaterial RA is conducted in a manner that is appropriate for the purpose of regulatory decision support. Walser then presented a classification method, based on core and coating composition, size distribution and shape (Walser and Studer 2015). Furthermore, he suggested that LCA studies, complemented by RA, were providing added value which is a conclusion that was also made during the final session of the day (Walser et al. 2017).

Providing an industrial perspective, Karl Höhener (business owner at TEMAS, Switzerland) presented the NANoREG Safe-by-Design (SbD) concept, in which safety information on MNMs and nanoproducts is integrated into the innovation process of product development (Gottardo et al. 2017). The SbD concept is based on the precautionary principle and can help reduce the need for downstream risk management, thus benefitting both industry and regulatory authorities.

4 System modelling and environmental releases

The current dearth of experimental data in the field of nanotechnology makes LCA models of MNMs challenging for two principal reasons. Firstly, practitioners are tasked with characterising and modelling MNMs/nanoproducts and processes that remain under development. Secondly, data on MNM flows and concentrations into different environment compartments are currently lacking. Implications of this data void in LCA studies of MNMs were discussed in the second part of this Forum.

Marco Villares (consultant/researcher, Netherlands) presented a framework for undertaking prospective LCA while technological development is ongoing (Villares 2015; Villares et al. 2016). This framework is based on the use of lab-scale data and scenario analysis to model future commercial-scale production. Villares emphasised the importance of sound assumptions on process efficiency changes when upscaling lab-scale data to the commercial scale. Such prospective, LCA studies enable the identification of environmental hotspots along MNM life cycle, which can then be addressed early in the product innovation process. In conclusion, Villares asserted the need for testing of the framework on new case studies.

Isabelle Blanc (professor, MINES ParisTech, France) provided an overview of stochastic methods, global sensitivity analysis (GSA), which can be used by LCA practitioners to identify those model inputs that most greatly contribute to

uncertainties in outputs. To demonstrate their usefulness, GSA methods were applied in two case studies of emerging technologies: enhanced geothermal systems and graphene production. Independent input variables were identified and defined as probabilistic distributions for both examples. To cope with very uncertain definition of input data for emerging technologies, Blanc then explained how the Sobol's indices can be used to quantitatively evaluate the effects of various distribution definitions for each input variable and their ranking on the model's output uncertainties (Lacirignola et al. 2017). Finally, Blanc suggested that results from such analyses could help in the design of simplified LCA models that focus on key variables and environmental hotspots of specific systems that are the sources of main environmental uncertainties (Padey et al. 2013).

Fadri Gottschalk (researcher, ETSS AG, Switzerland) discussed the application of dynamic and probabilistic modelling for the releases of MNMs along their life cycles (Walser & Gottschalk 2014). Gottschalk highlighted the challenge of fulfilling large data requirements for such modelling (i.e. production, import and export volumes of each MNM and the destinations of releases into the environment). He then suggested that a lack of data availability in release models should be tackled with probabilistic distributions to account for uncertainties in the model inputs. Preliminary findings from an ongoing project on nano-CeO₂ demonstrated that dynamic modelling is possible, despite limited data availability. Nevertheless, Gottschalk stated that further efforts are required to quantify uncertainties in MNM release models and that more information on MNM production volumes, product integration and end of life management are urgently required.

Finally, a short presentation on models of MNM flows was given by Véronique Adam (postdoc, Empa, Switzerland), who discussed the benefits and drawbacks of two different probabilistic methods to describe the MNM releases into the environment: probabilistic material flow analysis (MFA) and Bayesian networks. With probabilistic MFA, the uncertainty on the input values can be defined based on their quality (Laner et al. 2015) or through triangular probability distributions. With Bayesian networks, the parameters and their interrelationships are defined within conditional probability tables. The two methods are powerful and flexible tools for assessing MNM flows. They can be applied at the local or global scales, and can include temporal dynamics. Overall, probabilistic MFA is seen as useful but sometimes oversimplified whilst Bayesian networks can be more informative but more complex to implement.

5 Impact assessment methods for nanomaterials

The third session covered the environmental impact assessment of MNMs. A general overview of the fate, effect and

exposure modelling of MNMs was provided, and recent advances of LCIA methods were discussed.

The session was opened by Savvina Chortarea (postdoc, Empa, Switzerland) with a presentation on the limitations and knowledge gaps of toxic effect assessment for MNMs. Chortarea provided an overview of recent research into the mechanisms of toxicity, modes of action and toxic effects. She then described different approaches used to conduct nano-safety assessments, based on the oxidative stress paradigm, the fibre paradigm, or on analysis of lung fibrotic responses. Lastly, main challenges in nano-safety assessment were presented, namely (i) insufficient physicochemical characterisation of MNMs, (ii) lack of reference materials and standardised toxicity testing protocol, (iii) unrealistic exposure levels of tests and (iv) interference with biological arrays (i.e. quenching and adsorption).

Olivier Jolliet (professor, University of Michigan, USA) then presented recent advances in integrating fate and toxicity assessment of MNMs in LCIA methods. The USEtox model has been applied by several authors to develop characterisation factors (CFs) for the toxic impact categories of human toxicity and freshwater ecotoxicity (Deng et al. 2017; Ettrup et al. 2017; Salieri et al. 2015), but several adaptations have been required to account for nano-specificities (*ibid*). An ongoing project that combines the USEtox model with the nano-specific fate model, SimpleBox4nano (SB4N), was described. The presented approach is consistent with the USEtox framework but it (i) reduces the number of environment compartments (by merging the water and rain compartments) and (ii) defines, for each compartment, the sum of three MNM species (free, attached and agglomerated). The presentation then focused on human exposure and toxic effect assessment. An overview of physiologically based pharmacokinetic (PBPK) models, which have been applied to describe and predict the uptake and disposition of substances in the body, was also presented. In particular, Jolliet described a modified version of a nano-PBPK model developed by Li et al. (2014), for non-degradable MNMs. The model has been used to accurately describe the biokinetic profile of investigated MNMs, leading to several advances in the RA of MNMs (Carlander et al. 2016). Additionally, a recent approach (Laurent et al. 2017) to calculate the NOAEL (no observed adverse effect level) for nano-TiO₂ as function of their primary size was presented and discussed.

Finally, a short presentation was made by Nicole Sani-Kast (PhD student, ETH Zürich, Switzerland) on her review of 260 experimental papers looking at the influence of dissolved organic matter on the fate and properties of MNMs in aquatic environments. The results have revealed a decrease in the number of newly studied materials over the last 25 years, which is driven by an increasing focus on several frequently investigated materials (Sani-Kast et al. 2017).

6 Combining LCA and RA for nanotechnology

Unlike LCA, which remains in the formative stages of applications in the field of MNMs, RA has been applied extensively to evaluate a wide range of MNMs (Grieger et al. 2012b; Savolainen et al. 2010). RA is used to quantify the probability of adverse environmental and human health effects due to exposure to an agent. Risk is then calculated as a function of the hazardousness of the agent and its exposure to human or environmental receptors. Whilst LCA and RA have different aims, their complimentary use to evaluate MNMs has been advocated by many authors in recent decades (Breedveld 2013; Grieger et al. 2012a; Walker et al. 2015). In particular, given the current problems in LCA of MNMs concerning the availability of data on MNM releases and ecotoxicity, the use of combined RA-LCA (Barberio et al. 2014) may provide an opportunity to overcome such deficiencies. During the final part of the forum, different perspectives on the combination of LCA and RA to evaluate MNMs were presented.

Elorri Igos (R&T associate, LIST, Luxembourg) presented an overview of the RA framework and compared it with its LCA counterpart. She introduced how LCA and RA can be combined to better support decision making in nanotechnology, focusing on two possible approaches: (i) use of RA to better inform the toxicity-related impact assessment of MNMs, and (ii) application of life cycle thinking in RA. Regarding the former, Elorri noted how the outputs of RA studies have been used for decades in the development of toxicity-related characterisation factors for LCIA methods. Furthermore, she described how RA can complement LCIA results by providing more detailed information on the potential impacts of released MNMs, helping to overcome data gaps in this area (see Section 5). The latter case (i.e. approach (ii) above) involves the implementation of RA along the entire product life cycle to enhance the scope of the RA study (Grieger et al. 2012a; Walser et al. 2014). Recent examples from the literature (Hellweg et al. 2009; Scanlon et al. 2015; Sleswijk 2011) where RA has been used to enhance the impact assessment of LCA studies were discussed. Finally, key challenges for the application of combined LCA-RA for nanotechnology were presented, including: the difficulty of defining realistic use and disposal scenarios for MNMs and nanoproducts, the lack of standardisation stressing the need for a common framework to combine RA and LCA (Barberio et al. 2014) and the lack of high quality and published toxicological data for MNMs.

Peter Weyell (PhD student, Jena University, Germany) introduced, in a short presentation, a case study where the SbD development framework (i.e. combination of RA and LCA methods) was used to assess the EHS risks of a core-shell iron-oxide MNM. This work showed that the LCA method is applicable even in the early development stage, but that remains difficult to consider the direct impacts of the MNM

due to a lack of available characterisation factors. Still, the RA method indicated that all MNM formulations were appropriate for medical applications.

And finally, Socorro Vázquez-Campos (group leader, LEITAT Technological Center, Spain) provided an overview of GUIDEnano, a recently developed RA tool for MNMs that applies life cycle thinking principles to RA. With this approach, the tool enables the assessment of risks from multiple agents from different sources and at different locations within each stage of the MNM life cycle. The model, developed for use by industry, includes integrated fate, exposure and hazard assessment capacities and supports the quantitative evaluation of risks for workers, consumers and the environment associated with the use of nanotechnology. Unlike the majority of existing RA tools (life cycle-based or otherwise), GUIDEnano includes all RA stages, including risk management options and is based on an iterative data entry procedure that helps users to refine input parameter values when new data are available, thereby improving the quality of model outputs. In the presentation, a demonstration of the tool was provided, highlighting its key features and outputs.

7 Conclusions

The various presentations given during this Discussion Forum reaffirm the conclusions of the workshop on “Nanotechnology and Life Cycle Assessment” that took place in Washington, D.C., in 2007. The LCA framework is still seen as suitable to assess the potential environmental impacts of MNMs but there remain significant challenges in its implementation, principally due to a lack of available information. Here, the presentations outlined different strategies that have been used in an attempt to deal with this dearth of information. For instance, scenario modelling, GSA methods and dynamic probabilistic MFA can be used to model MNM production systems, even if most experts still have low amounts of information on flows of MNMs that are released into the environment during the phases of production, use and end-of-life.

During this Discussion Forum, several contributions discussed how the results of RA studies may be a useful source of information to support LCA of MNMs, particularly in supporting the development of LCIA methods (e.g. as a basis for creating new characterisation factors for MNMs). Nevertheless, concerns about the current state of knowledge in the environmental assessment of MNMs remain. In particular, whilst LCIA methods (e.g. USEtox) have been adapted to consider the specificities of MNMs, a broader range of representative characterisation factors are still urgently required for different types and shapes of MNM to support LCA practitioners. In practice, however, studies remain focused on a few MNM types and many groups of MNMs remain undefined.

Based on this discussion, we conclude that there is a need for regulators to support the creation of more research projects that focus on models of MNM environmental and health effects, and the integration of this information into the field of LCA. Regarding industrial stakeholders, they would likely profit from the sharing of their production data, even during the design phase, as this would increase their capacity to minimise the environmental impacts of their production processes and products.

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