Università
Ca'Foscari
Venezia

Scuola Dottorale di Ateneo
Graduate School

Dottorato di ricerca
in Scienze Ambientali
Ciclo29°
Anno di discussione 2016

Development and Testing of a Framework for Sustainable Nanotechnology

SETTORE SCIENTIFICO DISCIPLINARE DI AFFERENZA: CHIM/12
Tesi di Dottorato di Vrishali Subramanian, Matricola 956104

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SCIENTIFIC OUTPUT

Publications

Published papers

Oksel, C., Subramanian, V., Semenzin, E., Ma ,C.Y., Hristozov ,D., Wang, X., Hunt, N., Costa , A., Fransman ,W., Marcomini ,A. and Wilkins, T. (2016) Evaluation of existing control measures in reducing health and safety risks of engineered nanomaterials. Environmental Science: Nano, 3: 869-882.

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Papers in preparation

Subramanian, V., Semenzin, E. , Zabeo, A., Pizzol, L., Wouter, F., Wilkins, T., Hristozov, D. and Marcomini, A. Controlling The Human Health and Ecological Risks Of Nano-Enabled Products Through The Life Cycle: The Case Of Nano Copper Oxide Paint and Nano Organic Pigment Colourant in Plastic Bumper. In preparation (a).

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Dissemination in Conferences

Oral presentations

Subramanian, V., Semenzin, E. , Zabeo, A., Sailing, P., Ligthart, T., Van Harmelen, T, Malsch, I, Hristozov, D. and Marcomini, A. A methodology for social impact assessment of nano-enabled products. Society of Environmental Toxicology and Chemistry Europe Meeting 2016, Nantes (France)-

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SUMMARY

Nanotechnology is one of the Key Enabling Technologies identified in the European Union (EU) 2020 Strategy, which is expected to enhance economic growth and industrial competitiveness (COM(2009)512, COM(2012)341). While there is not precise information on market penetration of engineered nanomaterials (ENM), consumer nano-enabled product inventories have been registering an increasing number of nano-enabled products over past years (Nanodatabase, 2015; Project on Emerging Nanotechnologies Product Inventory, 2015). While the global nanotechnology value chain is expected to reach $4.4 trillion by 2018 (Lux Research, 2014), large uncertainties persist about the Environmental Health and Safety (EHS) risks of ENM. Moreover, there is a significant time lag between nano-EHS data availability and its use by regulatory agencies to perform risk assessment (RA) and risk management (RM). These challenges, together with ambiguous perceptions of risks, economic viability and social impacts may potentially impede the full realization of the value of nanotechnology Research and Development.

Sustainable nanotechnology is widely mentioned as a means to guide incremental nanotechnology development amidst significant knowledge and data gaps, but it has not been clearly defined. Sustainability is a typical case of a decision problem including multiple trade-offs and conflicting stakeholder needs, and a decision analytic approach is appropriate to address it. A decision analytical approach combines top-down approach of defining stakeholder needs with bottom-up tools (Linkov et al., 2014). This PhD thesis defines sustainable nanotechnology as a decision problem, and proposes a sustainable nanotechnology conceptual decision framework (named SUNDS) and methodology that can support needs of industries, regulators and insurance companies in the nanotechnology sector.

As there is wide agreement that RA and lifecycle assessment (LCA) should be integrated to support nanotechnology decisions (Fadel et al., 2014; Linkov et al. 2014; Greiger et al., 2012b), these form the key tools utilized in the proposed methodology. Existing RA, LCA and decision analysis (DA) tools for nanotechnology are reviewed and their relevance to sustainable nanotechnology is assessed. As there are very few tools on assessing economic and social aspects of nano-enabled products, a systematic literature review is not performed. However, given the increasing interest in addressing all dimensions of sustainability, economic and social counterparts of LCA are also incorporated in the framework.

SUNDS conceptual decision framework is a two-tiered framework designed to address differing data availability and expertise of stakeholders to handle analytical complexity.

SUNDS Tier 1 comprises LICARA NanoSCAN, a screening-level tool developed within the EU FP7 LICARA project that assists SMEs in checking supplier risks, competing products, market opportunities or making an internal risk and benefit analysis (van Harmelen et al., 2016). SUNDS Tier 2 comprises more advanced tools to support sustainable nanotechnology developed in the aegis of EU FP7 SUN project, and includes two methodologies: a) Risk Control (RC) methodology which ranks the most cost-effective RM measures to reduce unacceptable ecological and human health risks to below acceptability thresholds, and b) Socioeconomic Assessment (SEA) methodology which highlights sustainability hotspots in environmental, social and economic pillars. In order to align the two tiers, I spent a month at TNO (The Netherlands) in December 2014 collaborating with Toon van Harmelen and Tom Ligthart, the developers of LICARA NanoSCAN tool.

SUNDS tiers are tested to two case studies of real industrial products: nano-copper oxide based biocidal paint for wood treatment and two pigments (nano-sized red organic pigment (diketopyrrolopyrrole) and nano-sized black pigment (carbon black)) for colouring an automotive plastic part. The analysis shows that the biocidal paint, while an innovative product, is not promising for further development due to high risks and low benefits. On the other hand, bumpers with nano-organic and nano-carbon black fit into the profile of a conventional product with low risks and high economic benefits. The application to case studies yielded important insights on trade-offs between innovation, (eco)toxicological risks, environmental impacts and socioeconomic impacts that was not possible by these analyses individually. Further, application to real case studies allowed to identify current limitations of the research and possible future developments.

SOMMARIO

Le nanotecnologie sono una delle cosiddette “tecnologie abilitanti” (Key Enabling Technologies) identificate dalla Strategia 2020 dell’Unione Europea (UE) che dovrebbe contribuire ad aumentare la crescita economica e la competitività industriale (COM(2009)512, COM(2012)341). Anche se non sono attualmente disponibili informazioni precise sulla penetrazione del mercato dei nanomateriali ingegnerizzati (ENM), negli ultimi anni è stato registrato un crescente numero di prodotti a base nanotecnologica disponibili per i consumatori (Nanodatabase, 2015; Project on Emerging Nanotechnologies Product Inventory, 2015). Inoltre, se da un lato si prevede che la catena globale di valore per le nanotecnologie possa raggiungere i 4.4 trilioni di dollari entro il 2018 (Lux Research, 2014), dall’altro permangono importanti incertezze sui rischi da ENM per la salute e la sicurezza ambientali. In aggiunta, si riscontra un significativo ritardo temporale tra la disponibilità dei dati per la salute e sicurezza ambientale dei ENM e il loro uso da parte di agenzie di regolamentazione al fine di procedere con l’analisi e la gestione del rischi. Queste difficoltà, in aggiunta ad un’ambigua percezione dei rischi, alla fattibilità economica e agli impatti sociali, potrebbero potenzialmente impedire la completa realizzazione del valore della ricerca e dello sviluppo nel settore nanotecnologico.

Il concetto di nanotecnologia sostenibile, sebbene sia citato ampiamente come un modo per guidare lo sviluppo incrementale delle nanotecnologie in un contesto di significative lacune sia di dati che di conoscenza, non è stato ancora chiaramente definito. La sostenibilità è un tipico caso di problema decisionale che include molteplici compromessi e bisogni conflittuali di diversi portatori di interesse, e per risolverlo l’analisi decisionale risulta essere l’approccio più adeguato. L’analisi decisionale infatti combina approcci top-down per la definizione dei bisogni dei portatori di interesse con strumenti di tipo bottom-up (Linkov et al., 2014).

Questa tesi di dottorato definisce il concetto di nanotecnologia sostenibile come un problema decisionale, e propone un framework decisionale concettuale per una nanotecnologia sostenibile (chiamato SUNDS) ed una metodologia che lo implementa, capaci di rispondere ai bisogni delle industrie, dei legislatori e delle compagnie assicurative operanti nel settore nanotecnologico.

Poichè è ampiamente accettato che l’integrazione di analisi di rischio (AR) e analisi del ciclo di vita (LCA) supporterebbe adeguatamente le decisioni relative alle nanotecnologie (Fadel et al., 2014; Linkov et al. 2014; Greiger et al., 2012b), sono proprio questi gli strumeti chiave utilizzati nella metodologia proposta. E’ stata condotta una review degli strumenti di AR, LCA e analisi decisionale esistenti per le nanotecnologie ed è stata valutata la loro

rilevanza rispetto al concetto di nanotecnologia sostenibile. Poichè esistono pochi strumenti per la valutazione economica e sociale dei prodotti nanotecnologici, per questi non è stata condotta una review sistematica della letteratura. Tuttavia, visto il crescente interesse a coprire tutte le dimensioni della sostenibilità, sono state incluse nel framework anche le declinazioni economiche e sociali del LCA.

Il framework concettuale SUNDS è a due livelli, progettato per affrontare diverse disponibilità di dati e competenze dei portatori di interesse nella gestione di analisi complesse. Il Livello 1 consiste in LICARA NanoSCAN, uno strumento di screening sviluppato nell'ambito del progetto 7PQ LICARA che assiste le piccole medie imprese nel controllare il rischio fornitori, i prodotti concorrenti, le opportunità di mercato o nel condurre un'analisi rischi-benefici interna (van Harmelen et al., 2016). Il livello 2 di SUNDS consiste in strumenti più avanzati a supporto della nanotecnologia sostenibile, sviluppati nell'ambito del progetto europeo 7PQ SUN, e include due metodologie: a) la metodologia Risk Control (RC) che prioritizza le misure gestionali per la riduzione dei rischi ecologici e per la salute umana al di sotto delle soglie di accettabilità, sulla base di criteri di maggior efficienza e minor costo, e b) la metodologia Socioeconomic Assessment (SEA) che mette in evidenza gli eventuali hotspot di sostenibilità nei pilastri ambientale, sociale ed economico. Al fine di allineare i due livelli, ho trascorso un mese presso TNO (Olanda), nel Dicembre 2014, collaborando con Toon van Harmelen e Tom Ligthart, gli sviluppatori dello strumento LICARA NanoSCAN.

I livelli di SUNDS sono stati testati su due casi studio relativi a due prodotti industriali reali: una vernice biocida per il trattamento del legno a base di nano-ossido di rame e due pigmenti (nano-pigmento organico rosso (diketopyrrolopyrrole) e nano-pigmento nero (carbon black)) per la colorazione di un paraurti in plastica di un'automobile. L'analisi ha mostrato che la vernice biocida, sebbene sia un prodotto innovativo, non sia promettente per un suo ulteriore sviluppo a causa degli elevati rischi e dei bassi benefici presentati. Diversamente, il paraurti colorato con il nano pigmento rosso o nero ricade nel profilo di un prodotto convenzionale, caratterizzato da bassi rischi e alti benefici economici. L'applicazione ai casi studio ha fornito interessanti spunti sui compromessi tra innovazione, rischi (eco)tossicologici, impatti ambientali e impatti socio-economici che non sarebbe stato possibile individuare tramite l'analisi individuale di ciscuno di questi aspetti. Inoltre, l'applicazione a casi di studio reali ha permesso di identificare le limitazioni di questa ricerca e i possibili sviluppi futuri.

CONTENTS

Part A- Theoretical Background

Part B-Methodological part

Part C- Case study application

CHAPTER 1: Introduction

1.1 Problem formulation and Specific Objectives

The development of safe nano-enabled products is considered an important aspect of its overall sustainability (Dhingra et al., 2010; Mulvihill et al., 2011; Schulte et al., 2013b). However, even as the global value chain of nanotechnology is estimated to reach $4.4 trillion by 2018 (Lux Research 2014), nanosafety research has not yet been translated into practical guidelines that can support nanomanufacturing (Linkov et al., 2009; Linkov et al., 2011). The application of Risk Assessment (RA) and Life Cycle Assessment (LCA) to nano-enabled products is hampered by significant uncertainty with respect to physicochemical properties, environmental fate and transport, environmental impacts, ecological and human exposure and (eco)toxicity through the product lifecycle (Hristozov et al., 2016; Hischier and Walsher, 2012). Nanosafety knowledge gaps have led to technological and institutional lock-in effects, over-balancing regulations and low consumer confidence (Hristozov et al., 2016).

This problem is being partly addressed by understanding stakeholder perspectives and needs with respect to sustainable nanotechnology: industry (Engelman et al., 2012; Conti et al., 2008), regulators (Malloy et al., 2011) and insurance sector (Baublyte et al., 2014; Mullins et al., 2013; Blaustein et al., 2010). The National Nanotechnology Initiative (NNI) conducted a workshop in 2013 that considered nanotechnology stakeholder needs with respect to communication resources, data resources, standards and guidance resources and decision tools (NNI Report, 2015; Fadel et al., 2014). The 2015 and 2016 EU-US Communities of Research (COR) Workshop organized a “Nano Scrimmage” activity to simulate setting occupational, consumer and environmental exposure standards for nanomaterials to analyze the informational and communication bottlenecks in this process (COR, 2016; COR, 2015). These activities reiterate various ways in which the re-alignment of stakeholder values, risk and impact analysis methods and management strategies can release the “stuck gears” and facilitate sustainable nanotechnology.

Decision analysis has been proposed as a way to support sustainable nanotechnology by integrating bottom-up tools like RA and LCA within a decision analytic framework determined by stakeholder needs (Fadel et al., 2014; Linkov et al., 2014). The Triple Bottom Line (TBL) framing of sustainability comprising of environmental, economic and societal pillars has been illustrated in the context of sustainable nanotechnology (Subramanian et al., 2014). A sustainable nanotechnology framework can assist industry, regulators and insurance sector users to evaluate the environmental, economic and social impacts of nano-enabled products, particularly the trade-offs therein, and facilitate safe development of nanotechnology.

This PhD thesis has been carried out under the aegis of the EU FP7 Sustainable Nanotechnologies (SUN) project (http://www.sun-fp7.eu/), which aims to build a repertoire of tools to address various elements of the sustainability of nanotechnologies, including ecological and human health RA, LCA, lifecycle costing (LCC) and social impact assessment. In order to address real world sustainability needs, what is needed is an integration of suitable tools with consideration to analytical structure, stakeholder needs and relevant policy frameworks.

The specific goal of this PhD thesis was to develop and test a framework for sustainable nanotechnology, according to the following specific objectives:

1. Review the needs of stakeholders in addressing the complex risks associated with nano-enabled products through the lifecycle, including industry, regulators and the insurance sector a) in the literature and b) through a user elicitation process;
2. Develop a) a conceptual decision framework for sustainable nanotechnology based on TBL and stakeholders' needs and b) a methodology implementing such a framework;
3. Apply the methodology to commercially available nano-enabled products to assess their sustainability.

1.2 Outline of the thesis

This PhD thesis is split into the following three sections: (a) Theoretical background (Chapter 2 and 3), (b) Methodological development (Chapter 4-7) and (c) Application to case study (Chapter 8). Chapter 9 concludes the thesis by summarising key insights from this research and future directions for research.

Chapter 2 presents the theoretical background and current regulatory perspective on sustainable nanotechnology. The concept of sustainable nanotechnology is defined in the context of emerging literature as well as the by adopting broader ideas of product sustainability. The theoretical background of the following methods relevant to sustainable nanotechnology are elaborated: ecological and human health RA, LCA (including life cycle costing (LCC) and social life cycle assessment (sLCA)), and decision analysis. As the developments in risk regulation have an impact on the sustainability of nanotechnologies, the regulatory frameworks are reviewed with a focus on the issues concerning nanomaterials. As it has the most influence on this thesis, EU Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) regulation (EU Regulation 1907/2006) is explored in some depth.

Chapter 3 presents a literature review of three relevant methods viz. RA, LCA and DA, and their contribution to the operationalization of sustainable nanotechnology described in Chapter 2.

Chapter 4 presents the two tiered SUNDS conceptual decision framework. The first tier comprises of a semi-quantitative tool that supports product development decisions for nano-enabled products by considering their benefits and risk in situations where expertise and precise data are not available. The higher tier has two methodological foci: a) control of risks through the lifecycle using cost effective risk management measures (termed risk control methodology), and b) assessment of the sustainability profile of nano-enabled products through the life cycle (termed socioeconomic assessment methodology). The findings from stakeholder elicitation that led to the development of the proposed framework are described.

Chapter 5 presents the methodology for risk control (RC) implemented within Tier 1 of the SUNDS framework. The aggregation and classification of human health and ecological risks along the life cycle of the nano-enabled product is first explained. RC methodology guides the selection of appropriate Technological Alternatives and Risk Management Measures (TARMM) to reduce unacceptable human health and ecological risks to below safe thresholds.

Chapter 6 presents the methodology for socioeconomic assessment (SEA) to be implemented within Tier 1 of the SUNDS framework. In addition to aggregation and classification steps for ecological and human health RA described in Chapter 5, SEA methodology also does this for LCA, economic assessment and social impact assessment. A sustainability portfolio is thus created for the nano-enabled product at the global and individual lifecycle stage level.

Chapter 7 presents the social impact assessment methodology developed using social lifecycle assessment (sLCA) and multicriteria decision analysis (MCDA).

Chapter 8 presents the two case studies to which the methodology developed in this research is applied viz. nano-copper oxide based biocidal paint for wood treatment and two nano-sized pigments (red and black) for colouring an automotive plastic part. The results from the application of Tier 1 and 2 are discussed and compared.

Chapter 9 summarizes the key insights from this research and directions for future development.

Section A: Background

CHAPTER 2: Conceptual and Methodological Foundation for Sustainable Nanotechnology

The enhanced properties of engineered nanomaterials (ENMs) are suited to applications in information technology, energy production, environmental protection, biomedical applications, food and agriculture (Koehler and Som, 2008). While there is not precise information on market penetration of nano-enabled products, consumer nano-enabled product inventories have been registering an increasing of entries over past years (Nanodatabase, 2015; Project on Emerging Nanotechnologies Product Inventory, 2015). Lux Research (2014) estimates that the global nanotechnology value chain is expected to reach $4.4 trillion by 2018. ENMs with complex functionality are in Research and Development stage and present significant uncertainties for regulation (Kuzma and Roberts, 2016; Maynard, 2016; International Risk Governance Council, 2012; Subramanian et al., 2010). This rapid developmental trajectory emphasizes the need for adaptive processes and tools to manage the potential risks and impacts of ENM and develop more sustainable nano-enabled products.

This chapter briefly introduces key concepts and approaches relevant for the assessment of nanotechnologies in the context of sustainability and risk management which will be utilised in the remainder of the thesis. First, Sustainable Nanotechnology is defined (Section 2.1), and then methodologies that can be used to address its elements are described. Ecological and human health RA (Section 2.2) and LCA (Section 2.3) have been deemed as relevant tools to support sustainable product design (Powers et al., 2012; Shatkin, 2012; Linkov and Seager, 2011). Given the increasing interest in assessing the sustainability of nano-enabled products, economic and social counterparts of LCA are also described in Section 2.3. Decision analysis (DA) (Section 2.4) can be used to integrate these tools in a way that addresses concerns of various stakeholders. Finally, as the development of safe nano-enabled products is pinpointed as a key element in the overall sustainability of nanotechnology (Dhingra et al., 2010; Mulvihill et al., 2011; Schulte et al., 2013b), the nanosafety regulatory context is elaborated (Section 2.5).

2.1 Defining Sustainable Nanotechnology

Sustainable nanotechnology is being touted as a holistic and pragmatic concept that can guide incremental nanotechnology development amidst significant data gaps and uncertainty. A Google Scholar search shows that the number of documents using the term was ~106 annually in 2009—2011, 258 in 2012, and reaching over 819 as of 26 September 2016.

Although there is increasing interest in the topic, there is little consensus on how sustainable nanotechnology should be defined and measured.

The most widely cited definition of sustainable development was first proposed by Gro Brutland at the World Commission on Environment and Development (WCED) as “development that meets the needs of the present without compromising the ability of future generations to meet their own needs’’ (Brutland, 1985). WCED was first convened by the UN in 1983 to address solutions to environment and development issues, followed with another conference in 1992 in which a number of developmental and environmental objectives were identified. Also in the WCED 1992 meeting, the “Rio Declaration on Environment and Development” detailing 21 principles of sustainability was signed (Wirth, 1995). In 2001, UN’s Commission on Sustainable Development (CSD) developed a core set of 58 national-level indicators covering the environmental, economic and social dimensions of sustainability, and updated this list in 2006 (United Nations, 2007). However, there is still a need to define sustainability in the context of the production and use of ENMs. In 1994, John Elkington coined the term Triple Bottom Line (TBL) as a form of accountability that envisions the environment, society, and economy as three pillars of sustainability (Elkington, 2008). TBL requires consideration of each pillar and the interactions between them, and can, in principle, systematically ‘trickle down’ to technology design details (Linkov, 2014).

There has also been an interest in linking the idea of sustainability to governance in the US and EU. In the US, government agencies have been explicitly mandating incorporation of sustainability principles in the areas of procurement, chemical management, electronics stewardship, Environmental Management Systems, energy, greenhouse gases, high performance buildings, National Environmental Policy Act, natural resources, pollution prevention and transportation. Executive Order (E0) 13423 "Strengthening Federal Environmental, Energy, and Transportation Management" was signed in 2007, followed by EO 13514 “Federal Leadership in Environmental, Energy, and Economic Performance” in 2009. These EOs have been translated in terms of agency missions of the Department Of Defense (DoD, 2010) and Environmental Protection Agency (National Research Council, 2011). The European Commission (EC) views industrial sustainability as a multipronged problem that needs to be addressed by building coherence between environmental, climate, energy and industrial policies, as well as a driver of innovation and competitiveness of the EU industry (https://ec.europa.eu/growth/industry/sustainability_en). Table 2.1 lists some recent instruments (e.g. directives, certification labels) that have been developed in the EU to operationalize and benchmark sustainability aspects in a product context.

Table 2.1: Instruments to benchmark Industrial Sustainability

Instrument	Description	Reference Regulation
Eco design and Energy Labelling	Directive that sets out minimum requirements for energy related products	Directive 2009/125/EC (Establishing a framework for the setting of ecodesign requirements for energy-related products), Directive 2010/30/EU (Indication by labelling and standard product information of the consumption of energy and other resources by energy-related products)
Ecolabel	Label to certify products and services that have a reduced environmental impact throughout their life cycle	Regulation (EC) No 66/2010 (EU Ecolabel)
Green Public Procurement	Public procurement process whereby public authorities procure goods, services and works with a reduced environmental impact throughout their life cycle	{SEC(2008) 2124} {SEC(2008) 2125} {SEC(2008) 2126} Public procurement for a better environment
Product Environmental Footprint	Harmonised methodology for the calculation of the environmental footprint of products	SEC(2008) 2110}{SEC(2008) 2111} Sustainable Consumption and Production and Sustainable Industrial Policy Action Plan
Organisational Environmental Footprint	Harmonised methodology for the calculation of the environmental footprint of organizations	SEC(2008) 2110}{SEC(2008) 2111} Sustainable Consumption and Production and Sustainable Industrial Policy Action Plan

Conceptualizing sustainable nanotechnology within the TBL framework can be utilized to help solving nanotechnology problems that have many variables and which call for detailed analysis. In this approach, TBL pillars form the first level of the decision tree, which is further divided into subsequent levels of criteria until the problem is articulated in sufficient breadth and detail. The operationalization of sustainable nanotechnology into a decision model comprises of (a) metrics associated with sustainable nanotechnology and (b) weights associated with nanotechnology stakeholder preferences at each branch of the decision tree. Implementing sustainable nanotechnology as a decision model can provide a comprehensive monitoring framework, including conceptual framework, indicators, and stakeholder values. A variety of decision analysis (DA) techniques like Analytic Hierarchy Process, Bayesian Network, Nominal gap theory, Multi Attribute Value Theory, etc. exist. This thesis hypothesizes that techniques under the umbrella of Multi Criteria Decision Analysis (MCDA) could be most suitable to implement a sustainable nanotechnology decision model.

In a first attempt to conceptualize sustainable nanotechnology in terms of the TBL approach, a project course was developed at Ca' Foscari University of Venice (Italy) in the Fall of 2013[1]. Twenty students were tasked with conducting a literature search on sustainable nanotechnology definitions and operationalizing the TBL approach for evaluating sustainable nanotechnology. Six student groups reviewed government agency documents, peer-reviewed and gray literature, as well as websites of major ENM manufacturers and consumer groups. Though the volume of literature containing an association between sustainability and nanotechnology was significant, the search yielded no concise definitions for sustainable nanotechnology. As a starting point to conceptualize sustainable nanotechnology as a decision problem, the class adopted a TBL definition of sustainability recommended by the Institute of Chemical Engineers (ICE) (ICE Report, 2003). Supplementing the ICE definition with nano-specific criteria from their literature review, the class developed a conceptual model of sustainable nanotechnology (Fig. 2.1). The environmental pillar includes impacts on environment and human health, waste and resources. The economic pillar includes impacts on investment, cost, material efficiency and technological risk. The societal pillar contains impacts on workplace, key stakeholders and society.

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[1] I served as teaching assistant for this course. Detailed results of the activity are reported in Subramanian et al. (2014).

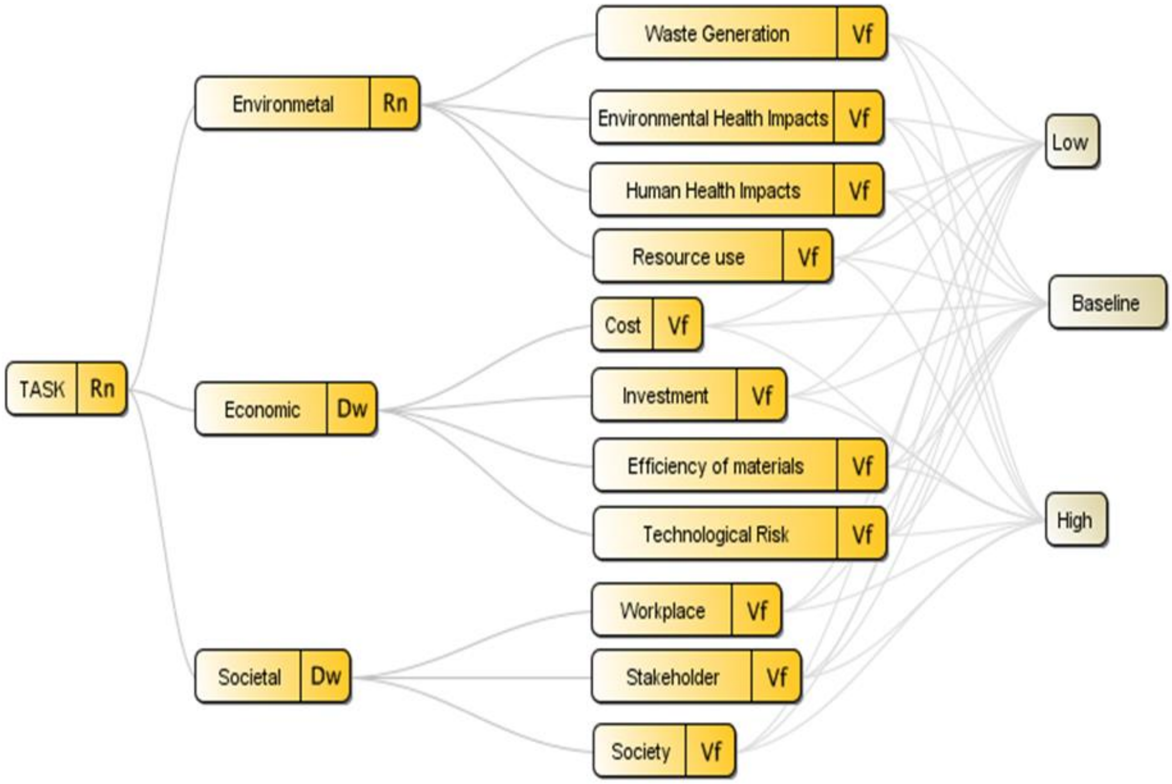


Figure 2.1: Decision Model for Sustainable Nanotechnology

This model serves as the basic conceptual foundation for this PhD thesis, which is further refined through the elicitation of stakeholder needs (described in Chapter 4), development and integration of relevant methodologies (described in Chapter 5, 6 and 7), and testing to case studies (described in Chapter 8).

Some salient features of the sustainable nanotechnology decision model presented in Figure 2.1 are discussed.

The environmental pillar comprises of criteria that are assessed using RA ("Environmental Health Impacts" and "Human Health Impacts") and LCA ("Resource use", "Environmental Health Impacts" and "Human Health Impacts"). Environmental impacts other than (eco)toxicological risks may be included under Environmental Health Impacts and Human Health Impacts. "Waste generation" is measured in the Life Cycle Inventory of a LCA study or exposure assessment of waste, but usually it is the environmental impacts and risks respectively that are of greater interest in these analyses. Further, waste generation pertains to a specific lifecycle stage (i.e. end of life) that tends to be of interest as it is a social externality whose management is resource intensive, expensive and difficult to minimize, although focusing on the entire life cycle can certainly amerliorate waste management issues.

The economic pillar includes microeconomic criteria associated with producing nano-enabled products like fixed costs (“Investment”) and lifecycle costs (“Cost”). “Efficiency of investment” pertains to the cheapest product to deliver a desired functionality. “Technological risk” refers to the monetized risk to human beings from technological systems, and this is partially covered by the “Environmental Health Impacts” and “Human Health Impacts” in the environmental pillar. There may also be additional socioeconomic risks due to technology (e.g. unemployment, inequality), which could potentially fall under the economic (under “Technological risk”) and social (as sub-criteria to specific social groups) pillars.

The societal pillar involves consideration of the key social groups that could be affected by nano-enabled products (e.g. workers, value chain, governments, local community). As social impacts are highly context specific, relevant impacts for each nano-enabled product remain to be defined.

2.2 Ecological and human health risk assessment

Risk is the probability of an adverse effect occurring as a result of specified conditions, which in the context of chemical risk implies exposure to single chemicals or mixtures (van Leeuwen, 1995). RA has been defined as “a process intended to calculate or estimate the risk to a given target organism, system or (sub)-population, including the identification of attendant uncertainties, following exposure to a particular agent, taking into account the inherent characteristics of the agent of concern as well as the characteristics of the specific target system” (OECD Report, 2004). Chemical RA for regulatory purposes, as required by regulations such as EU Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) regulation (EU Regulation 1907/2006) considers two key targets: environment (i.e. the species in relevant ecosystems) and human beings (i.e. workers, consumers and general public). The first group of targets is addressed by Ecological Risk Assessment (ERA) and the second group by Human Health Risk Assessment (HHRA). The key steps in risk assessment are described in Section 2.2.1-2.2.4, including key concepts involved in ERA and HHRA.

RA involves the evaluation of exposure and effect in deterministic (as a point estimate) or probabilistic (as a distribution expressing uncertainty and variability) terms. The advantages of a probabilistic approach include use of all relevant data, explicit consideration of uncertainty and variation, and quantitative estimation of exposure, effect and risk (EPA Report, 2014; 2014b; Wheeler et al., 2002). The disadvantages of a probabilistic approach include more effects and exposure data are needed than a deterministic estimation, it does not address all sources of uncertainty and has not been widely calibrated against field observations (Forbes and Callow, 2002; Solomon and Sibley, 2002).

2.2.1 Problem Formulation

This phase establishes the goal and scope of the RA by identifying potential risks in an environmental or human health context.

In the case of ERA, problem formulation articulates the goals and scope of the RA. Problem formulation entails considerations like suitable representation of the taxonomic diversity, choice of appropriate ecotoxicological endpoints, spatial and temporal scales, mode of exposure, etc. (Traas and van Leeuwen, 1995). In the problem formulation step, a conceptual model of how these stressors and observed effects in an ecosytem is generated (Norton et al., 1992). This conceptual model generates hypothesis, informs choice of assessment endpoints and other aspects of exposure and effect estimation. The assessment of persistent, bioaccumulative and toxic and very persistent and very bioaccumulative substances in ecosystems are required by REACH, even if their ecotoxicity has not been proven (ECHA, 2014).

In the case of HHRA, the first step is usually referred to as “hazard identification”. Data on physicochemical properties and toxicological effects on a chemical of interest are gathered and assessed with regard to their quality. Although data from in vitro, in vivo and in silico (Quantitative Structure Activity Relationships (Organization for Economic Cooperation and Development (OECD) Report, 2007), grouping and read across (ECHA, 2015)) approaches may be used for hazard identification, in vivo animal data from well-designed experiments is preferred for effect assessment (described in Section 2.2.2). The Klimisch score is often used to evaluate the quality of information on the criteria of relevance, reliability and adequacy (Klimisch et al., 1997). Other information criteria frameworks include OECD Guidance Document 34 (OECD Report, 2005) and European Centre for the Validation of Alternative Methods criteria for a pre-validation study (Curren et al., 1995) and test validity (Worth et al, 2004). More generally, the REACH Annexe XI suggests the use of Weight of Evidence (Linkov et al., 2009; Weed, 2005) approach to integrate using expert judgement data from guideline tests, non-guideline tests, and other types of information to make a decision on hazard identification based on criteria based on the above methods (ECHA,2010).

2.2.2 Effect Assessment

Effect assessment characterizes the relationship between the chemical dose and the incidence of adverse effects in the exposed ecological or human targets (van Leeuwen, 1995).

Effect assessment in the case of ERA involves the determination of Predicted No Effect Concentration (PNEC) for an environmental compartment (e.g. aquatic, terrestrial, sewage treatment) during long-term or short-term exposure. PNEC is assessed for deterministic ecological effect assessment by applying suitable assessment factors to the ecotoxicological endpoint concentration of the most sensitive organism within the environmental compartment (Traas and van Leeuwen, 1995). Assessment factors in ERA establish conservative numerical values in order to account for uncertainties in intra- and inter-laboratory variation of ecotoxicity data, intra- and inter-species variations, short-term to long-term toxicity extrapolation, and laboratory data to field impact extrapolation (ECHA, 2008). A conservative approach is recommended in selecting assessment factors given the high uncertainty of ecotoxicological data on ENM and use of data from grouping and read-across approaches (ECHA, 2012b). Further, for highly absorptive ENM, PNEC calculation in certain environmental compartments (e.g. freshwater sediment, marine sediment and soil) by assuming using equilibrium partitioning may not be applicable (ECHA, 2012b). When ecotoxicological datasets are sufficiently abundant, the species sensitivity distribution (SSD) method can be applied, wherein ecotoxicological endpoint data for a species within an environmental compartment is fit to parametric or nonparametric distribution functions (Posthuma et al., 2002). The fifth percentile of the SSD curve is usually assigned as the PNEC (ECHA, 2008).

Effect assessment in the case of HHRA involves the determination of Derived No-Effect Level (DNEL) for threshold effects and Derived Minimal Effect level (DMEL) for non-threshold effects (e.g. carcinogens). DNEL and DMEL are derived for each exposed population (workers, consumers, general population) exposure route (inhalation, oral and dermal), and expected exposure duration (acute, sub-chronic, chronic). The first step involves establishing a dose descriptor in a dose response curve, which is a point of departure (e.g. No observed adverse effect level (NOAEL), No observed adverse effect concentration (NOAEC), lethal dose 50 (LD_{50}), lethal concentration 50 (LC_{50})) (Vermiere et al., 1995). As there is no agreement on appropriate dose metric (e.g. mass concentration, particle number, surface area) for ENM (Hull et al., 2012), it should preferably be expressed in several different metrics. Then assessment factors are applied to establish conservative values to account for intra-species (exposure to workers, sensitive sub-populations) variation, inter- species (metabolic rate and other factors) variation, nature and severity of the effect, duration of exposure, uncertainty in chosen dose descriptor (e.g. NOAEL versus (true) no adverse effect level), data quality and high to low dose extrapolation (ECHA, 2012a; 2012b). For non-threshold effects, as risk is present at any dose, DMEL can be derived using an exposure level that represents a risk level of very low concern (the so-called *de minimis* risk, which is usually set in the order of 10^{-5} and 10^{-6}) (Vermiere et al., 1995). DMEL is based on policy prescription (e.g. As Low as Reasonably Achievable principle that is based on economic considerations) or high to low dose extrapolation (e.g. using linearized multi-stage model). Non-threshold effects can also be assessed using Benchmark Dose (BMD) approach (which can also be used for threshold effects), in which a measurable effect size (differing from controls) is specified and the dose corresponding this effect size i.e. BMD is measured from the dose response relationships. As the upper and lower bounds of BMD are known, uncertainty in dose response relationships can also be quantified (EFSA, 2009). For non-threshold effects, typically the lower bound of 10% response is used as BMD, which is extrapolated to low dose to derive a human health limit or associated risk (Vermiere et al., 1995).

2.2.3 Exposure Assessment

Exposure assessment measures or estimates the intensity, frequency and duration of the ecological or human exposure to the chemical (van Leeuwen, 1995). While precise and comprehensive measurement of exposure in actual contexts is ideal, such data are typically expensive to obtain and hence a tiered approach to exposure assessment is recommended.

Exposure assessment in the case of ERA involves the determination of Predicted Environmental Concentrations (PEC) using actual measurements in environmental matrices or using multimedia fate models simulating release and transfer processes such as direct and indirect emission to air, water, and soil, biotic and abiotic degradation, advective transport, gas absorption and volatilisation processes between compartments (van de Meent and de Bruijn, 1995). The key issues in environmental exposure assessment for nanomaterials are: a) information on amounts and specific nano-forms released into the environment, b) incorporation of nano-specific properties and processes (e.g. aggregation, agglomeration, sedimentation) into the exposure models, c) Methods to detect trace nano-forms in environmental media (Klaine et al., 2012). Probabilistic material flow analysis is one way to estimate PECs and its use has been successfully demonstrated at global and regional scales (Sun et al., 2014; Gottshalck et al., 2015;2013;2009). Other state-of-the-art environmental exposure models estimate environmental exposure through mass-balance models (Mueller and Nowack, 2008; Gottschalk et al., 2009; O'Brien and Cummins, 2010; Arvidsson et al., 2011).

Exposure assessment in the case of HHRA involves the determination of exposure levels for inhalation, dermal and oral routes of exposure. Schneider et al. (2011) consider the potential exposure that could be caused by nano-enabled products through the life cycle and identified four key sources of exposure (1) point source or fugitive emission during the production of nanomaterials (e.g. emissions from the reactor, leaks through seals and connections) ; (2) handling and transfer of bulk manufactured nanomaterial powders (e.g. bag emptying, dumping, scooping), (3) dispersion of either intermediates containing highly concentrated nanoparticles or application of ready-to-use products (e.g. spraying of solutions that will form nano-sized aerosols after condensation) ; and (4) activities resulting in fracturing and abrasion of nano-enabled end products (e.g. sanding, milling, cutting, etc.). Many lower tier tools currently available for exposure assessment of nanomaterials usually follow a control banding approach. Control banding involves a qualitative or semi-quantitative hazard and exposure assessment, and matches a set of control measures to a range or "bands" of hazards and exposures (Brower, 2012). Examples of these tools include Swiss Precautionary Matrix (Höck et al., 2013), NanoRiskCat (Hansen et al., 2014), ANSES Control Banding Tool (Ostiguy et al., 2010), Control Banding Nanotool (Paik et al., 2008) and Stoffenmanager Nano (van Duuren-Stuurman, et al., 2011). Higher tier exposure assessment tools follow source-receptor approach, and examples include NanoSafer (Jensen et al., 2010), Near Field/Far Field model (Cherrie, 1999), ConsExpo (Delmaar et al., 2006) and Advanced REACH tool (Fransman et al., 2011). Particular challenges for exposure assessment of nanomaterials include discrimination from background particles, collection and analysis of particle size information, high spatial and temporal variability, choice of metrics and measurement instruments, and measurement of high aspect ratio nanomaterials (ECHA, 2012b).

2.2.4 Risk characterization

In this step, the results of the exposure and effect assessments are compared (van Leeuwen, 1995). Deterministic risk assessment produces a value for risk characterization ratio (RCR), whereas probabilistic risk assessment yields the probability distribution of exposure exceeding effect. In both cases, risk is considered acceptable when exposure is lower than the no-effect threshold (i.e. RCR<1) (van Leeuwen, 1995).

2.3 Life Cycle Assessment: Environmental, Economic and Social methodologies

Life Cycle Assessment (LCA) is the most extensively used method for assessing the environmental impacts throughout a product's life cycle, and is usually used toward the following ends: a) Guide product and process development toward lower resource intensity, emissions and waste, b) Support product certification (e.g. product footprint), c) Choose between alternative processes, products, and materials to minimize environmental impacts, and d) Support public policy by facilitating the development of regulations and policies for environmental impacts (Huppes and Curran, 2012; Curran, 2006). LCA has been standardised in the 1990s (Heijungs and Guinee, 2012), and the key guidelines for it are International Organization for Standardization (ISO) 14040-44. While the actual practice of LCA is iterative, these four steps can be delineated: a) Definition of the goal and scope of the investigation, b) Life cycle inventory analysis, c) Life cycle impact assessment, and d) Interpretation (ISO 14040, 2006).

In the 2000's, Society for Environmental Toxicology and Chemistry (SETAC) formed two working groups to develop the economic and social counterparts of LCA, namely Life Cycle Costing (LCC) and social Life Cycle Assessment (sLCA) (Curran, 2012; Benoit-Norris, 2012b; Swarr et al, 2011). The idea was that LCA, LCC and sLCA, together known as Life Cycle Sustainability Assessment, could give a systems level view of all aspects of sustainability (Zamagni et al., 2012; Swarr et al, 2011). While attempts have been made to harmonise terminology and methodology of these three lifecycle based methods that cover TBL pillars of sustainability, important differences remain e.g. differing concept of lifecycle and system boundaries, operationalization of functional unit, demarcation of lifecycle stages, nature of models and their aggregation, and scale of the analysis (Zamagni et al., 2012; Swarr et al, 2011). These differences can perhaps only be reconciled in systematic application of the methodology to case studies, and careful interpretation of the results.

LCC is different from other economic assessment methodologies like activity based costing, total cost assessment, full cost accounting as it summarizes the monetary flow within the life cycle of a product that involve several actors (e.g. supplier, product manufacturer, consumer, End-of-Life actor) (Reibitzer and Hunkeler, 2003). Certainly, LCC may be performed from perspective of different actors, by focusing on more detailed cost estimations in lifecycle stages in which they are deeply involved. LCC has narrower system boundaries than environmental and social impacts, and views these as externalities which can be internalized by use of proper policy instruments (e.g. taxes and subsidies) (Hunkeler and Reibitzer, 2003; Reibitzer and Hunkeler, 2003).

sLCA is a relatively younger and less standardized methodology. SLCA can be used to assess social impacts through the product Life Cycle on specific stakeholders (e.g. company, value chain actors, consumer, local community) (Benoit-Norris, 2012b; Althaus et al., 2009). As there is limited literature on sLCA, a bespoke methodology was developed for the framework as described in Chapter 7 of this thesis.

The sub-sections below consider LCA stages as specified by the ISO 14040 series guidelines, and consider how they apply also to LCC and sLCA.

2.3.1 Goal and Scope Definition

The goal of an LCA study involves describing the product system to which the LCA shall be applied and the audience of this application (Heijungs and Guinee, 2012). LCC and sLCA can be performed from the perspective of different actors, by focusing on more detailed cost and social impact estimations in lifecycle stages in which they are deeply involved (Benoit-Norris, 2012b; Althaus et al., 2009). In defining the scope, this description is extended to the functional unit, system boundaries and data requirements.

The functional unit is an operationalisation of the functional performance of the product(s) as a reference to which the inputs and outputs are related. LCA impacts and LCC variables can be linked to a detailed functional unit, but sLCA indicators are typically linked to the social environment (i.e. country or company) in which product manufacturing is located (Benoit-Norris, 2012b; Althaus et al., 2009).

The system boundaries determine which unit processes shall be included within the study. The physical, economic and social lifecycle have important differences. LCC has narrower system boundaries than LCA and sLCA, and may also include different elements (e.g. Research and Development costs) (Hunkeler and Reibitzer, 2003; Reibitzer and Hunkeler, 2003). In conventional LCC, time is considered for long lasting goods by using the concept of discounting i.e. setting the net present value of future costs using a discount rate that depends on inflation, cost of capital, investment opportunities and personal consumption preferences (Gluch and Baumann, 2004). While the physical and economic lifecycle can be partitioned into distinct stages, sLCA includes the whole life cycle by including the value chain and indicators through the life cycle.

Data quality requirements broadly specify the data needed including temporal aspects, geographical aspects, technology coverage and level of detail and data completeness and representativeness (ISO 14040, 2006).

2.3.2 Life cycle inventory analysis

This phase involves the collection, compilation and quantification of inputs and outputs for a product throughout its life cycle (Heijungs and Guinee, 2012; ISO 14040, 2006). For LCA, the Life Cycle Inventory (LCI) is a list of “unit process” included within the system boundary. A “unit process” is the smallest element considered in the life cycle inventory analysis for which input and output data are quantified (Heijungs and Guinee, 2012). Input data includes material and energy consumption data, and output data may include product and emissions (air, water and waste) data. Data is collected for each unit process from LCI databases as well as available information in the literature, patents or expert elicitation. The equations for the unit processes within the system boundaries are balanced in order to arrive at the LCI. In the case of nanomaterials, there is significant knowledge and data gap on releases, particularly nano-specific releases (Hischier and Walser, 2012).

For LCC and sLCA, inventory analysis is less database driven and is usually compiled using peer reviewed literature, internet search and expert interviews (Benoit-Norris, 2012b). LCC can utilise the LCI inventory input items as a checklist for material inputs for which costs have to be calculated as has been done in Open LCA (Ciroth and Eisfeldt, 2016; Zamagni et al., 2012), but this is usually not sufficient for a more comprehensive cost analysis. For sLCA, the Social Hotsposts database (SHDB) provides country data on some social indicators (Benoit-Norris et al, 2012b), but it is paid database and may not be relevant for all types of analysis.

2.3.3 Impact Assessment

For LCA, this phase aims at assessing the magnitude and significance of the potential environmental impacts for a product system by transforming LCI to higher level midpoint and endpoint impact categories. Various available LCA methodologies e.g. International Reference Life Cycle Data System (ILCD) (JRC Report, 2012), methodology of Institute of Environmental Sciences-Leiden (CML) (Guinee et al., 2002), Eco-indicator 99 (Goedkoop and Spriensma, 1999), ReCiPe, (Goedkoop et al., 2012), prescribe specific approaches to impact assessment. The key steps in this phase include classification, characterization, normalization and weighting (the last two steps being optional).

Classification involves the grouping of LCI results to midpoint and endpoint impact categories defined by the LCA methodology (Heijungs and Guinee, 2012). Midpoint impacts focus on environmental consequences immediately downstream from the LCI impacts, e.g. ozone depletion, greenhouse effect. Endpoints are further downstream to midpoints (and thus more uncertain), e.g. resource depletion, ecological health impact, human health impact. Classification is followed by characterization, which is the calculation of midpoint and endpoint impacts by multiplying LCI outputs by the characterization factor based on validated models (Heijungs and Guinee, 2012). In the case of nanomaterials, very few nano-specific characterization factors have been developed, that too in an ecotoxicity impact context (Salieri et al., 2015; Eckleman et al. 2012).

Normalization and weighting are optional steps in the LCA. In normalization, the characterized impact is compared to a reference value (e.g. the average impact of a European citizen for the year) (Heijungs and Guinee, 2012). Weighting is the assignment of weights on impact categories based on different value choices (e.g. personal, social or policy preferences). In lieu of normalization and weighting, the concept of shadow prices can be applied to the characterized midpoint impacts, which express an environmental impact as an economic value based on damage or abatement costs (de Bruyn et al., 2010; Harmelen et al., 2007).

In the case of LCC, classification, characterization, normalization and weighting steps are not required. Costs are easily interpreted as well as aggregated by simple sum as they are in the same monetary unit. On the other hand, most of the steps described for LCA are applicable to sLCA. Analogous to LCA classification, the sLCA framework comprises of two hierarchical levels: impacts and indicators. These impact categories (and sub-categories) are assessed using specific indicators, which is analogous to LCA characterization. Various methodologies exist to aggregate social indicators, including performance reference points (Franze and Ciroth, 2011), life cycle attribute assessment (Norris, 2006) and causal chain modelling (Benoit

-Norris, 2012b; Jorgensen et al., 2010).

2.3.4 Interpretation

In the final phase, the results of the LCA, LCC and sLCA are evaluated with respect to the initial goal and scope of the analysis. While optional, uncertainty analysis and sensitivity analysis are helpful to estimate uncertainty and test the assumptions used to generate the results.

2.4 Decision Analysis

Decision Analysis (DA) is a formal modelling of decision context that helps address complexity, uncertainty, multiple objectives and conflicting viewpoints (Clemen and Reilly, 2014). DA may be used for individual as well as group decisions (based on group decision theory (Carlsson et al., 1992)). DA methods are used to implement software Decision Support System (DSS) that helps decision makers in structuring a complex decision problem by integrating relevant information and tools and evaluating available alternatives (Watkins and McKinney, 1995; Loucks, 1995; Shim et al., 2002; Jensen et al., 2002; Lahmer, 2004). The utility of DSS has been demonstrated for various environmental problems including contaminated sites (Marcomini et al., 2009), water supply systems (Baroudy et al., 2006), flood management (Levy et al. 2007), forest management (Zambelli et al., 2012).

One DA method is MCDA, which comprises a large class of techniques for the evaluation of different alternatives based on relevant criteria, with the possibility to account for decision maker or stakeholder preferences and expert knowledge (Giove et al., 2009; Koksalan et al. 2011, Figueira et al. 2005). Some important examples of MCDA methods include Multi-Attribute Utility/Value Theory (MAUT/MAVT), Outranking, Interactive, Goal aspiration, Analytic Hierarchy Process (AHP), Elimination and Choice Expressing Reality (ELECTRE), Preference Ranking Organization Method for Enrichment Evaluations (PROMETHEE) and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) (Linkov et al., 2011). MCDA methods vary in satisfying various sustainability assessment criteria, but most methods can integrate heterogeneous data types and consider material life cycle (Cinelli et al., 2014). The application of decision analysis to nanomaterials has been reviewed in Chapter 3.

2.5 Regulatory Environmental Health and Safety Context for Nano-enabled products

Several bodies have expressed that the existing horizontal (e.g. European Union (EU)'s Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) regulation; Classification, Labelling and Packaging of substances and mixtures (CLP) regulation, worker protection legislation and environmental legislation on pollution prevention, water and waste) and vertical risk regulation (e.g. general product safety, cosmetics, biocides, plant protection, food, medicines, medical devices, electronic industry, aerosol dispensers) are applicable to ENM (COM/2008/366; COM/2012/572; SCENHIR, 2009; EFSA, 2011; OECD, 2012; SCCS, 2012). However, several case specific technical issues have arisen in almost all aspects of nano-

EHS including physicochemical characterization, environmental release and exposure estimation and hazard estimation (Hristozov et al.,2016), necessitating case-by-case evaluation of ENM risk in terms of specific materials as well as regulatory provisions. Hence, the regulatory focus has been on following scientific developments, prioritizing collection of information that supports regulatory decisions and disseminating information through consumer labels and guidance documents (ECHA, 2015). Table 2 summarizes the nano-specific developments in EU legislation.

In the case of REACH, currently there are no nano-specific requirements in the regulation itself, but the European Chemicals Agency (ECHA) is focusing on the integration of emerging scientific results into appendices to REACH guidance documents. Registration dossiers are required to specify nano-forms of a substance and provide information stipulated by tonnage requirements of REACH. Acknowledging the data gaps and uncertainties inherent in information on ENM, the REACH Annexes permit the use of data from approaches like Weight of Evidence, quantitative structure activity relationship (QSAR), in vitro methods, grouping and read-across approaches. Submission of the standard information requirement can be waived if testing is not scientifically necessary or technically possible, or exposure based risk estimations are acceptable.

As the most comprehensive horizontal chemical regulation for chemicals, mixtures and articles in specific use contexts produced in the EU, an overview of REACH regulatory processes is provided in order to understand how they could apply to sustainable nanotechnology. REACH is implemented through four regulatory processes: Registration, Authorisation, Evaluation and Restriction.

Registration is required for any substance manufactured or imported at or above one tonne per year, and includes: a) a mandatory technical dossier with information on substance identity, manufacture and use, classification and labelling, guidance on safe use, intrinsic properties depending on tonnage band (physicochemical properties, mammalian toxicity, ecotoxicity and environmental fate) and proposals for further testing if relevant, and b) for substances manufactured or imported at over 10 tonnes per year, a Chemical Safety Report (CSR) reporting the results of a Chemical Safety Assessment (CSA) which requires information on intrinsic properties, hazard assessment (physicochemical, human health and environmental), Persistent, Bioaccumulative and Toxic and very Persistent and very Bioaccumulative assessment, Exposure assessment and Risk Characterization. In the case of nanomaterials, each nanoform should be registered separately and information should be provided on its size, shape and surface chemistry (CA/90/2009).

Table 2.2: Summary of EU Legislation applicable to Nanomaterials

Regulatory framework	**Nano-specific provisions in the legal text in relation to:**					**Guidance**
	Definition	Approval procedure	Information requirements	Separate assessment	Labelling requirements	
REACH Regulation 1907/2006						√
Biocidal Products Regulation 528/2012	√	√		√	√	
Cosmetic Products Regulation 1223/2009	√	√	√	√	√	√
Novel food Regulation 258/1997					√	√
Food additives Regulation 1333/2008				√	√	√
Plastic Food Contact Material Regulation 10/2011		√		√		√
Active and Intelligent Food Contact Material Regulation 450/2009		√		√		√
Food Info to Consumers Regulation 1169/2011	√				√	
Novel food Revised Regulation 258/1997	√			√		
Medical Devices Proposal COM(2012) 542	√	√		√	√	

Reproduced from Crutzen, H (2015) EU regulatory perspectives on nanomaterials, presented at the First Sustainable Nanotechnology School, Venice (Italy).

The authorisation process is applicable in case the substance used in industry falls in the candidate list for Substances of Very High Concern (SVHCs, list containing 169 substances in June 2016). REACH authorisation can be granted on two bases: a) Adequate risk control through risk management measures and/or substitution of the chemical with a more benign alternative (known as the adequate control route), and b) Benefits of using the substance significantly outweigh societal costs (known as the socioeconomic route) (ECHA, 2011). Generally, the adequate control route is considered first; only when adequate control cannot be demonstrated a favourable benefit-cost balance is used to make the case for authorisation. Adequate control can be demonstrated a) By reducing risk to below threshold levels using appropriate risk management measures and documenting it in a CSR, and b) By investigating feasible alternatives to the substance (to be documented in an Analysis of Alternatives report) (ECHA, 2011). If suitable substitute is found, then a Substitution Plan, demonstrating its technical and economic feasibility is also required. In the event that risks are not adequately controlled using risk management measures and no feasible alternatives are found, Socioeconomic Analysis (SEA) report demonstrating that benefits significantly outweigh the costs can be used to make the case for an authorisation (ECHA, 2012a). The purpose of a SEA report is to analyse all relevant impacts, at both individual and macro scale, of granting versus refusing an authorisation. Impacts included in an SEA are human health impacts, environmental impacts, economic impacts and social impacts. REACH guidance on SEA favours quantification using Benefit-Cost methodology as far as possible, though multi-criteria methods are mentioned as an alternative when quantification is not possible (ECHA, 2012a).

Restrictions are a tool to limit or ban the manufacture, commercial activity or use of a substance based on inadequate control of its risks and/or unfavourable benefit-risk balance from use of the substance (ECHA, 2008; ECHA, 2007). The intention to prepare a restriction proposal is made public by Member States or ECHA in the registry of intentions at least a year before a restriction dossier is submitted to give advance warning to industry. The restriction dossier may contain information about substance identity, risks, justifications for the proposed restrictions, information on alternatives to the substance and the costs, and environmental and human health benefits resulting from the restriction (ECHA, 2007).

Evaluation involves an assessment of authorisation and restriction dossiers by ECHA and the Member States and judges if a given substance constitutes a risk to human health or the environment.

The key elements from REACH regulation relevant to a sustainable nanotechnology framework are available in the authorization step, namely: a) Assessment and control of ecological and human health risks of ENM through the lifecycle using best available information is a core principle to ensure the sustainability of nanotechnology, as has been echoed by several commentators (Dhingra et al., 2010; Mulvihill et al., 2011; Schulte et al., 2013b), b) ENM should be compared to other alternatives that can provide the same functionality with respect to their risks and economic impacts, and c) The overall sustainability of ENM including environmental, economic and social aspects should be considered.

CHAPTER 3: Review of Tools Applicable to Sustainable Nanotechnology

Ecological and human health RA and LCA have been discussed as relevant tools to support sustainable product design (Linkov and Seager, 2011; Powers et al., 2012; Shatkin, 2012). However, LCA and RA are developed from different perspectives and cannot easily be integrated (OECD, 2015). Traditional risk assessment is normally used for regulatory purposes (National Research Council, 1983) and is specific to substance and exposure route. RA often uses a worst case exposure scenario, and utilizes conservative thresholds to classify occupational and consumer risk. LCA calculates environmental impacts from all released substances through the whole life cycle using average exposure scenarios (United Nations Environment Programme, 2005). LCA has also been extended to (eco)toxicological impacts (Rosenbaum et al., 2008) and occupational exposure impacts (Hellweg et al, 2009; Scanlon et al, 2014). Consumer exposure impacts are more challenging to address using LCA as numerous exposure pathways are possible and need to be included within LCA models.

The application of RA and LCA of ENM and nano-enabled products is hampered by significant uncertainty regarding the physicochemical properties, environmental fate and transport, exposure, biological uptake and end-of-life (Gavankar et al, 2012; Hansen, 2009; Hristozov et al., 2012; Hischier and Walsher, 2012). The lack of nanomaterial-specific characterization factors or reliable and comprehensive LCI data on release for ENM makes it difficult to conduct LCA for nano-enabled products (Gavankar et al, 2012; Hischier and Walsher, 2012). These challenges make decision analytic techniques a viable near-term alternative to integrate RA and LCA to address sustainable nano-enabled product development.

Among decision analytic techniques, this thesis hypothesizes that MCDA is most suitable to integrate RA and LCA and thereby implement sustainable nanotechnology. MCDA involves a large group of methods that collectively synthesize multiple criteria in order to offer a ranked list of alternatives toward a predefined goal (Linkov et al., 2011; Linkov and Seager, 2011) and offers a quantitative approach to assessment of alternatives.

This chapter assesses the potential of RA, LCA, and MCDA toward quantitative sustainability assessment for nanotechnology development through a review of these tools. Previous reviews by Grieger et al. (2012) and Hristozov et al. (2016; 2012) cover frameworks and tools that focus mainly on RA, but do not include frameworks and tools that integrate RA and LCA. Such integration has been previously addressed by frameworks like Comprehensive Environmental Assessment (CEA) (Powers et al., 2012) and Streamlined Life Cycle Risk Assessment (SLCRA) (Shatkin, 2012). However, these frameworks are process-based and, in main parts, are qualitative in nature and do not address the full range of issues linked to safety and sustainability of nanomanufacturing (Bergeson, 2013; Dhingra et al., 2010; Mulvihill et al., 2011; Schulte et al., 2013b). A systematic review of decision analytic tools is required to understand how RA and LCA can be integrated via MCDA into a comprehensive and quantitative framework for Sustainable Nanotechnology.

3. 1. Methods

A state-of-the-application review of RA, LCA and MCDA, with the objective of identifying trends and methods used to aid sustainable nanomanufacturing, was carried out. The Web of Science database (Web of Science, 2014) was queried for 2000-2014 using the following strategy:

- RA: The search strategy used the keywords nano* and risk assessment. The search retrieved 461 records containing various hazard, exposure, and risk assessment tools for nanotechnology. Papers containing an explicit decisional problem context and comparing ENM or exposure scenario were selected for review. 16 papers describing RA tools such as Control Banding (CB), environmental RA, and human health RA tools were selected for review.

- LCA: The search strategy used the keywords ‘nano’ and ‘lifecycle’ OR ‘life cycle’ OR ‘LCA’). The search retrieved 30 records. 18 papers comparing different nanotechnology functionalities, applications, and nanomanufacturing processes were selected for review.

- MCDA: A sequential search strategy was used to find and identify papers pertaining to MCDA and nanotechnology. The first search was done under ‘nano’. The second set of keywords aimed to retrieve research on quantitative decision science approaches, and comprised of ‘decision analysis’, ‘Multi Criteria Decision Analysis’, ‘MCDA’, ‘Multi Criteria Decision Making’, ‘MCDM’, ‘Analytical Hierarchy Process’, ‘AHP’, ‘Outranking’, and ‘Bayesian networks’. The search retrieved 96 records; 15 papers with empirical or hypothetical MCDA applications were selected for review.

For each category of tools, the selected publications were consolidated based on decision context, criteria used for evaluation in the papers, alternatives technologies/materials that are compared, and methods used for analysis. This information was summarized in table format, where rows represent individual papers and columns summarize research done based on criteria listed above. Further, the tools are assessed based on the potential for their contribution to the TBL criteria in the Sustainable Nanotechnology decision tree developed earlier (Figure 2.1). The decision tree comprises of the following criteria: environmental (Waste Generation, Environmental Health Impacts, Human Health Impacts and Resource Use), economic (Cost, Investment, Efficiency of Materials and Technological Risk) or societal (Workplace, Stakeholder and Society) criteria. If any paper included criteria in the Sustainable Nanotechnology decision tree, the category was assigned as “Significant Contribution”, while the category was assigned as “No contribution” if the criteria was excluded in the paper. If no paper reviewed included the Sustainable Nanotechnology decision tree criteria, but it was commonly addressed by the broader literature, the category was assigned as “Potential Contribution”.

3.2 Results

3.2.1 Risk Assessment

The occupational risk context is most studied in the RA tools literature (Table 3.1), which is unsurprising given that occupational health is a pertinent nano-EHS concern (Schulte et al., 2013b). Seven CB tools use risk banding to assess suitable occupational risk management measures (Cornelissen et al., 2011; Höck et al., 2008; Jensen et al., 2013; Ostiguy et al., 2010; Paik et al. 2008; Van Duuren-Stuurman B et al., 2012; Zalk et al., 2009). Table 1 describes three human health RA tools that utilise Weight of Evidence and MCDA approaches for risk ranking, combined with expert elicitation and uncertainty estimation (Hristozov et al., 2012; Hristozov et al., 2014; Tervonen et al., 2009). Tervonen et al. (2009) grouped ENM into relative risk classes using stochastic Multi-criteria Acceptability Analysis (SMAA- TRI), which estimates the uncertainties in the input parameters (Tervonen et al., 2009). Hristozov et al. utilize quantitative MCDA for different human health risk prioritization tools, which account for uncertainty through data quality criteria, input error analysis, sensitivity analysis and Monte Carlo simulations (Hristozov et al.,2012; Hristozov et al., 2014).

Three papers present environmental RA tools (Money et al., 2012; O’Brien, 2011; Sorensen et al., 2010) which apply non-conventional approaches in order to target the knowledge and data gaps about the behaviour of ENM in the environment. Money et al. (2012) used Bayesian networks to combine existing mechanistic, empirical, and expert judgment information to develop a baseline probabilistic model which predicts ENM behaviour, exposure potential, hazard, and risk in environmental settings (Money et al., 2012; Money et al., 2014). Sorensen et al. (2010) proposed a Worst Case Definition model to identify critical epistemic uncertainties in environmental RA, and applied it to nanoscale zero-valent iron used in soil and groundwater remediation as well as to fullerenes used in engine oil lubricants (Sorensen et al., 2010).

3.2.2 Life Cycle Assessment

LCA tools within the reviewed literature collectively evaluated the environmental impacts of various ENM, nano-enabled products, and other nanotechnology applications. A descriptive summary of the literature on LCA tools is presented in Table 3.2. Particularly to compare conventional materials with emerging nanomaterials, a proper and standardized definition of LCA's scope and methods is needed in order to attain meaningful results that take into account different ENM properties and applications. The functional unit of an LCA is specified in the LCA tools for ENM in two ways, including (i) the specification of the ENM mass, and (ii) the specification of the amount of application or service. As dose metrics for nano-EHS impacts include mass, particle number and surface area (Hull et al., 2012), the choice of functional unit must be carefully considered. System boundaries vary in the LCA based tools for ENM, and may be categorized as "within factory gate" (manufacturing process only), "cradle-to-gate" (extraction and manufacturing process) and "cradle-to-grave" (extraction to disposal). Only ten LCA based tools for ENM cover cradle-to-grave phases, while the other studies omit the end-of-life treatment or the use phase.

Two LCA tools estimate uncertainty using Sensitivity Analysis and Monte Carlo simulations (Bauer et al., 2008; Bonton et al., 2012). Bauer et al. (2008) examine the sensitivity of LCI items of three coatings deposited using Physical Vapour Deposition for production and subsidiary processes within the system boundary. Bonton et al. (2012) use Monte Carlo simulations to compare the impact of process variability on environmental impacts in three scenarios with different corrosion control requirements and electric energy source.

3.3 Multi Criteria Decision Analysis

MCDA nanotechnology applications collectively contribute to a small but diverse literature. A descriptive summary of MCDA nanotechnology applications in the literature is presented in Table 3.3.

The literature on MCDA nanotechnology applications illustrates many useful method features to construct a pragmatic framework for Sustainable Nanotechnology. Ten papers developed decision models and tools concerning materials, processes, and occupational practices in industrial (manufacturing and remediation) contexts. Three papers developed decision models about strategic decision-making about which type of nanotechnologies industries or countries should build capability in. Two papers used an MCDA based nanotechnology stakeholder engagement framework for ENM.

A key strength of MCDA lies in its ability to explicitly examine trade-offs, as illustrated in Esawi and Farag's evaluation of the optimum composite material to make tennis rackets (Esawi and Farag, 2007). MCDA nanotechnology applications literature also incorporates stakeholder or expert judgment through eliciting weights for decision tree criteria. Weights can be subjective (obtained through expert/stakeholder elicitation) or objective (obtained through various analytical means). Objective weighting is not always feasible for nanotechnology decision problems due to data gaps and epistemic uncertainties associated with ENM. Expert elicitation seeks the tacit knowledge of experts and can be used to define a feasible range within which technical parameters are likely to lie (Flari et al., 2011; Linkov et al., 2011; Mohan et al., 2012) . Stakeholder elicitation seeks the preference of stakeholders for criteria to construct value profiles of stakeholders that can be integrated with the decision model (Ghazinoory et al., 2013; Kuzma et al., 2008; Tsang et al, 2014). Subjective weighting warrants the application of sensitivity analysis to test if the decision model performs robustly when the weights are varied.

MCDA can also be combined with Value of Information (VoI) to assess potential losses from decision-making errors or to prioritize the future information collection strategy to minimize uncertainty (Linkov et al., 2011; Keisler et al., 2014).

Table 3.1: Applications of Risk Analysis in the context of Sustainable Nanotechnology

The column "RA context" denotes the stage of environmental or human health RA in which the tool is applied. Secondly, the column "Decision Criteria" includes the tool inputs that form the basis to compare different ENM or exposure scenarios. The column "Alternatives" denotes the ENM or exposure scenarios which the tool compares or is applied to. The column "Method Used" describes the established RA procedure that is applied or adapted in the tool.

Journal Article(s)	RA context	Decision Criteria	Alternatives	Method used
Bouillard and Vignes, 2014	Occupational RA	Physicochemical properties, hazard, and exposure in chronic and accidental occupational exposure scenarios	Multi-walled CNT, Aluminium oxide NP	Nano-Evaluris CB Tool coupled with iso-surface toxicological scaling method
Cornelissen et al., 2011	Occupational RA	Physicochemical properties, Occupational hazards, Exposure	ENM in specific exposure scenarios	Guidance on Working Safely with Nanomaterials and Nanoproducts CB Tool with three hazard bands and three exposure bands

Journal Article(s)	RA context	Decision Criteria	Alternatives	Method used
Höck et al., 2008	Occupational RA	Nano-relevant parameters, Lifecycle based parameters, Potential human and environmental effect parameters, Physical surrounding parameters, Human exposure parameters, Environmental exposure parameters	ENM in specific exposure scenarios	Precautionary Matrix CB tool with one hazard band
Hristozov et al., 2012	Hazard screening for human health	Physicochemical characteristics, Toxicity, Data quality criteria	Titanium Dioxide NP	MCDA, Expert judgement, Monte Carlo simulation for uncertainty characterization
Hristozov et al., 2014	Occupational exposure assessment	Material characteristics, Process characteristics, Operational conditions, Risk management measures	Titanium dioxide NP, CNT and fullerenes	MCDA, Expert judgement, Monte Carlo simulation for uncertainty characterization
Jensen et al., 2013	Occupational RA	Hazard, Exposure criteria	ENM in specific exposure scenarios	NanoSafer CB tool with four hazard bands and five exposure bands

Journal Article(s)	**RA context**	**Decision Criteria**	**Alternatives**	**Method used**
Money et al., 2012, Money et al., 2014	Environmental Risk Assessment	Particle behavior, exposure potential, hazard, and risk	Silver NP	Bayesian Belief Modelling, Expert Judgement, Network updating using parameter learning expectation-maximization learning algorithm
O'Brien and Cummins, 2011	Environmental Exposure Assessment	ENM behaviour in aquatic environments, ENM characteristics, Natural aquatic environment characteristics	Titanium dioxide NP, silver NP and cerium dioxide NP	Qualitative RA principles combined with uncertainty and variability estimation
Ostiguy et al., 2010	Occupational RA	Toxicological parameters, Incremental Factors depending on physicochemical properties	ENM in specific exposure scenarios	ANSES CB tool with five hazard and four exposure bands based on response to questions
Paik et al. 2008, Zalk et al.,2009	Occupational RA	Hazard band established based on 13 parameters, Exposure band established based on 5 parameters	Synthesis of nanoporous metal foams, Flame synthesis of ceramic NP, Synthesis of CNT, Consolidation of ceramic NP, Preparation of a single dry bacteriogenic uranium dioxide NP sample	Nanomaterials CB tool with five hazard and exposure bands

Journal Article(s)	RA context	Decision Criteria	Alternatives	Method used
Robichaud et al., 2005	Occupational Hazard screening	Process characteristics, Life cycle characteristics, Volatility, Carcinogenicity, Flammability, Toxicity, Persistence	Single walled CNT (SWCNT), Fullerenes, QD, Alumoxane NP, Titanium dioxide NP	Application of Insurance database methodology
Sørensen et al., 2010	Ecotoxicological RA	Habitat characteristics, Organism characteristics, Vulnerability, Exposure	Zerovalent Iron NP, Fullerene	Worst Case Definition model based on MCDA, Self-organizing mapping
Tervonen et al., 2009	Human health hazard screening	Toxicity, Physicochemical characteristics, Environmental impacts	Fullerenes, Multi-walled CNT (MWCNT), QD, Silver NP and Aluminum NP	Multi-criteria Acceptability Analysis
Van Duuren-Stuurman B et al., 2012	Occupational RA	Product characteristics, Handling/Process characteristics, Working area characteristics, Engineering controls, Personnel Protective Equipment	ENM in specific exposure scenarios	Stoffenmanager Nano CB Tool with five hazard bands and four exposure bands

Table 3.2: Decision analytical LCA Tools for Nanotechnology

The column "Alternatives" denotes the ENM, nano-enabled product, and other nanotechnology applications which the LCA tool compares. The column "Functional unit" is a quantitative performance description of the system whose life cycle is being assessed. The column "Decision criteria" denotes the impacts assessed by the tool, and comprises of midpoint and endpoint indicators. Midpoint indicators are an intermediate point in a cause-effect chain of a particular (endpoint) impact, at which characterization factors can be computed (Goedkoop and Spriensma, 1999). Endpoint indicators are impacts at the end of the cause-effect chain and have an independent value to society (Goedkoop and Spriensma, 1999). There are well established LCA methods that systematically aggregate specific midpoint indicators into endpoint indicators, and if applied, they are mentioned in the "Method used" column.

Journal Article(s)	Alternatives	Functional Unit	Decision Criteria	Method used
Andrae and Andersen, 2011	Nanostructured Polymer based components, Conventional metal components in Ball Grid Array and Chip Scale Packaging	Production of 200 metal solder balls, Production of 1000 metal-plated monodispersed (nanostructured) polymer particle (MPP) balls	Global warming potential, Eco-Indicator'99 scores	Eco-Indicator 99 method (Goedkoop and Spriensma, 1999)
Arvidsson et al., 2014	Graphene produced through ultrasonication, Graphene produced through chemical reduction	1 kg of graphene in solution	Energy Use, Blue Water Footprint, Human Toxicity Potential, Ecotoxicity Potential	USEtox (Rosenbaum et al., 2008)

Journal Article(s)	Alternatives	Functional Unit	Decision Criteria	Method used
Bonton et al., 2012	Nanofiltration plant and enhanced conventional water treatment plant	1 m^3 of nanofiltration grade drinking water	13 Midpoint indicators (Ozone layer depletion, global warming, carcinogens, Mineral extraction, etc.) 4 Endpoint indicators (Human health, ecosystem quality, climate change, resource depletion)	Impact 2002+ method (Jolliet et al., 2003)
Chiueh et al., 2011	Heterogeneous Copper-Palladium/titanate nanotubes, Catalytic hydrogenation Copper-Palladium/titanium dioxide catalysts, Photocatalytic reduction Copper-Palladium-titanium dioxide catalyst), Zerovalent Zinc and Palladium/Zinc bimetallic particles, Catalytic Copper-Palladium bimetallic particles	Removal of 0.325 kg nitrate from groundwater in Taiwan	LCI analysis, 3 endpoint indicators (Human health, Ecosystem quality, Resources), 11 midpoint indicators (Carcinogens, Respiration organics, Respiration inorganics, Climate change, Radiation, Ozone layer)	Ecoindicator 99 method (Goedkoop and Spriensma, 1999)
De Figueirêdo et al., 2012	Cellulose nanowhiskers extracted from unripe coconut fibres, Cellulose nanowhiskers extracted from white cotton fibres	1 gram of extracted cellulose nanowhiskers	Energy, Water, Wastewater emissions, Climate change, Water depletion, Eutrophication, Human Toxicity	ReCiPe method (Goedkoop et al., 2012)

Journal Article(s)	Alternatives	Functional Unit	Decision Criteria	Method used
Dobon et al., 2011a and b	Nanoclay based food packaging system with and without stimuli-sensitive labels	340 grams of pork chops packaged in a nanoclay-based polylactic acid package, with and without a flexible best-before-date (FBBD) communicative device	Carcinogens, Repairable organics, Repairable inorganics, Climate change, Radiation, Ozone layer, Ecotoxicity, Acidification, Eutrophication, Land use, Minerals, Life Cycle Costs	Eco Indicator 99 method (Goedkoop and Spriensma, 1999), Life Cycle Costing, Contingent valuation
Fthenakis et al., 2008; Fthenakis et al., 2009	CdTe NP, Si NP and Ag NP based contact Photo Voltaic (PV) systems	1 m^2 of PV cell	CED	
Hancock et al., 2012	Coupled seawater desalination and water reclamation process alternatives: Sea water reverse osmosis and wastewater discharge;Nano filtration/Reverse osmosis treatment of wastewater and blending with sea water reverse osmosis permeate, Simultaneous osmotic dilution / Sea water reverse osmosis treatment of seawater and wastewater	Production of 1 m^3 of reclaimed water	Abiotic depletion potential, acidification potential,eutrophication potential, fresh water aquatic ecotoxicity potential, global warming potential, human toxicity potential, marine aquatic toxicity potential, ozone layer depletion potential, photochemical oxidation potential, terrestrial ecotoxicity potential	CML method (Guinee et al., 2002)

Journal Article(s)	Alternatives	Functional Unit	Decision Criteria	Method used
Van der Meulen and Alsema, 2011	Amorphous/Nano-crystalline silicon based Photovoltaics	1m^2 PV module area	LCI analysis, Energy inventory, Greenhouse gas emissions	
Meyer et al., 2011	Socks impregnated with Silver NP, Conventional socks	Production and use for 50 wash cycles of a pair ofcotton socks without and with Silver NP (0.2 mg)	Global warming, Acidification, Carcinogenics, Non-carcenogenics, Respiratory effects, Eutrophication, Ozone depletion, Ecotoxicity, Smog	TRACI method (Bare, 2002)
Mohr et al., 2013	Roof integrated amorphous silicon/nanocrystalline silicon photovoltaic system, Roof-mounted multi-crystalline silicon (multi-Si) PV system.	1 kWh electricity supply	18 midpoint categories, 20 end point categories, CED	ReCiPe method (Goedkoop et al., 2012)
Osterwalder et al., 2006	Titanium dioxide NP, Zirconia NP	Synthesis of 1 tonne of NP using dry synthesis	Energy consumed, Carbon dioxide emissions	
Ren et al., 2013	Ceramic filters impregnated with silver nanoparticles, Centralized water treatment and distribution system	37,960 L of water consumed by a typical household over ten years delivered by water treatment system	Energy use, Water use, Global warming potential, Particulate matter emissions, Smog formation potential, Economic Analysis	

Journal Article(s)	Alternatives	Functional Unit	Decision Criteria	Method used
Roes et al., 2007	Polymer nanocomposite on nanoclay base	Amount of packaging film for 1000 bags for 200 grams candies, Amount of fill to cover a standard greenhouse of 650 m3, Body panels to drive 150000 km	CED, Non-renewable energy use, Global Warming, Abiotic depletion, Ozone layer depletion, Photochemical oxidant formation, Acidification, Eutrophication	CML method (Guinee et al., 2002)
Roes et al., 2010	Silica NP, organic montmorillonite, CNT	1 kg of ENM, Material per stiffness	Nonrenewable energy use, Global warming	
Steinfeldt et al., 2004	a) Nano varnish / (b,c) CNT/ (d) QD	(a) Surface treatment of $1m^2$ metal surface / (b) 1 kg Styrol / (c) 17 inch flatscreen / (d) 6.579 million Lumen hours	Various midpoint indicators, CED Values, Cumulative inventory items	
Sengul and Theis, 2011	Quantum Dot PV, Ribbon multi-crystallinesilicon PV, Monocrystalline-silicon PV, Dye sensitized PV, Polycrystalline semiconductors based PV (Copper indium gallium diselenide, Copperindium diselenide), Organic PV	$1m^2$ PV module area	CED, GWP, Aquatic acidification potential, Heavy metal emission, Energy analysis	

Table 3.3: MCDA Applications of Nanotechnology

The column “Decision Problem” describes the nanotechnology decision problem to which MCDA is applied. The column “Decision Criteria” describes the measures used to compare possible courses of action in the decision context. The column “Alternatives” describes the courses of action available to the decision maker. The column “Decision Analytic Approach” lists the mathematical technique applied to the decision problem.

Journal Article(s)	Decision Context	Decision Criteria	Alternatives	Method used
Caliskan, 2013	Material selection decision for multi-component nanostructured boron based hard coatings on cutting tools	Mechanical and tribological properties	Twelve alternatives including multi-component nanostructured TiBN, TiCrBN, TiSiBN and TiAlSiBN coatings deposited by various techniques	EXPROM2, TOPSIS and VIKOR
Chen and Larbani, 2006	Adding air purification functionality through photocatalytic titanium dioxide NP coating	Time to market, ability of acquiring technology to market, cost of technology, forecast of future sales, and compatibility with on-hand technology	Coating titanium dioxide NP on a normal light tube; Coating titanium dioxide NP on toilet devices; Coating titanium dioxide NP on tiles in a house; Coating titanium dioxide NP on air conditioners	MCDA with fuzziness incorporated
Cunningham and van der Lei, 2009	Technology management in a microelectronics supply chain	Native technical and business expertise; Network interests	Network positions to improve product development capability	Exchange modeling analysis

Journal Article(s)	Decision Context	Decision Criteria	Alternatives	Method used
Dabaghian et al., 2008	Choosing the best wastewater treatment for electroplating workshops in Tehran	Economic criteria; Technical criteria	Reverse osmosis, Nanofiltration, Ion exchange,Chemical precipitation	AHP
Esawi and Farag, 2007	Choosing the best CNT-carbon fibre-polymer composite material to make tennis rackets	Cost of the material per unit mass; Benefit	Twelve composite materials with different percentages of CNT, carbon fibre and polymer	AHP
Flari et al., 2011	Build an expert judgement based decision model to evaluate safety of nanotechnology-enabled food products	Ten criteria relevant to potential risk of nano-enabled food products	Twenty six scenarios	AHP
Ghazinoory et al., 2013	Refine the national strategy for nanotechnology in Iran and focus nanotechnology capability building	Social, Technological, Economic, Environmental and Political criteria	List of key nanotechnologies	Capability–Attractiveness matrix, PROMETHEE to prioritize key nanotechnologies
Kuzma et al., 2008	Build an oversight framework for technology	7 development criteria, 15 attribute criteria, 5 outcome criteria, 1 evolution criterion	Risk analysis, social science, public administration, legal, public policy, and ethical perspectives	AHP

Journal Article(s)	Decision Context	Decision Criteria	Alternatives	Method used
Linkov et al., 2011, Canis et al., 2010	Choosing a synthesis process for single-walled CNT	Cost, Material efficiency, Energy consumption, Life cycle environmental impacts, Human health risks	Arc discharge, Chemical vapour deposition, High-pressure carbon monoxide (HiPCO) and Laser vaporization	MCDA and VoI
Mohan et al., 2012	Assessing the legal costs of risk management measures for titanium dioxide NP based sunscreen manufacture	Occupational liabilities, EHS risks across life cycle stages of NMs	Risk management measures	MCDA with probabilistic input
Naidu et al., 2008	Choosing the most sustainable process for silica nanoparticle synthesis	Industrial engineering, Green chemistry criteria, Environmental impact	Sol-gel method, flame based method with tetraethylorthosilicate precursor and flame based method with hexamethyldisiloxane precursor	MCDA
Sudhakaran et al., 2013	Choosing the best technique to remove organic micropollutants in water treatment processes	Treatability, Costs, Technical, Sustainability, Time	Riverbank filtration, Constructed wetlands, Granular activated carbon, Nanofiltration, Reverse osmosis, Ozonation, Advanced oxidation process using oxygen and hydrogen peroxide and Ultraviolet based advanced oxidation using hydrogen peroxide	AHP

Journal Article(s)	Decision Context	Decision Criteria	Alternatives	Method used
Velmurugan and Selvamuthukumar, 2012	Choosing the best procedure for the preparation of nanoparticles for a drug delivery	Process information, operational skill, feasibility, supplier and technical information	Polymer precipitation, interfacial polymer deposition, complex coacervation, cross linking, emulsion solvent diffusion, homogenization and polymerization	AHP
Yu and Lee, 2013	Choosing the best nanotechnology for a Korean company to for capability development	R&D capability, ease of production, urgency, government support, marketability and technical extension	243 nanotechnologies	Analytic hierarchy process (AHP)/Data Envelopment Analysis-Assurance Region (DEA-AR)

3.4. Relevance of Tools to Sustainable Nanotechnology

Table 3.4 visualizes contribution of RA, LCA and MCDA applications to sustainability assessment of nanotechnology. We used sustainable manufacturing criteria recommended by Institute of Chemical Engineers (ICE Report, 2003) and further refined it for nanotechnology applications in Subramanian et al (2014).

Table 3.4 Contribution of Reviewed Tools to Sustainable Nanotechnology TBL Criteria

🟩 Substantial Contribution 🟨 Potential Contribution 🟥 No Contribution

TOOL **PILLAR**	**RA Tools**	**LCA Tools**	**MCDA applications**
Environmental Pillar			
Waste Generation	🟥	🟩	🟨
Environmental Impacts	🟩	🟩	🟩
Human Health Impacts	🟩	🟩	🟩
Resource Use	🟥	🟩	🟩
Economic Pillar			
Cost	🟥	🟨	🟩
Investment	🟥	🟩	🟩
Efficiency of Materials	🟥	🟩	🟨
Technological Risk	🟥	🟥	🟨
Societal Pillar			
Workplace	🟥	🟨	🟨
Stakeholder	🟥	🟨	🟩
Society	🟥	🟨	🟩

RA tools only contribute to the criteria under the environmental pillar of sustainability assessment. Our review of RA tools contains several examples of tools that can guide decision making in occupational, consumer and environmental contexts. While regulatory RA takes a conservative approach to specific environmental and human health risks, sustainability framing allows for comparative evaluation of risks and for explicit trade-offs among a varieties of impacts (National Research Council, 2011).

LCA tools discussed in the literature contribute to the environmental and economic pillars of sustainability assessment, and can potentially contribute to societal pillar (Althaus et al.,2009). USEtox method, which considers (eco)toxicological impacts through the lifecycle, has been applied to ENM (Chiueh et al., 2011). The reviewed LCA studies do not account for consumer and occupational exposure, although these aspects are addressed by the recently developed Life Cycle Approach and Human Risk Assessment tool (van Harmelen et al., 2016).

The LCA tools covered in this review lack nano-specific characterization factors and LCI data on ENM release to air, water, and soil. The input side of LCI in these tools contains fairly detailed information on the energy inputs and material inputs, but the output side of the analysis is sparse due to a poor quantitative understanding and lack of data on emission, transformation, fate, and (eco)toxicity. This lack of reliable LCI data hampers ENM production impact calculation on fairly simple impacts like depletion of abiotic resources, ozone depletion potential, use of fresh water and land, impact on global warming, and other important factors. Though the initial approaches to examine the toxicity of ENM emissions to air and water are reported, it is not clear if nano-specific aspects were taken into account in this analysis.

MCDA applications offer structured approaches to cover all the sustainability pillars, and also examine the trade-offs between criteria included therein. Incorporating uncertainty estimation and stakeholder or expert elicitation with the MCDA model further enhance its utility in dealing with data and knowledge gaps inherent in Sustainable Nanotechnology problems. Uncertainty estimation can pinpoint the most sensitive elements of a Sustainable Nanotechnology decision model, and facilitate better monitoring of these elements (Canis et al., 2010; Mohan et al., 2012). Expert elicitation can extract tacit knowledge of experts on range in which parameter values are likely to lie (Caliskan, 2013; Chen and Larbani, 2006; Hristozov et al., 2014), which can be valuable in narrowing the range in which parameter values lie. Stakeholder elicitation can extract normative beliefs of stakeholders and support decision making on Sustainable Nanotechnology (Malsch et al., 2015a; Malsch et al., 2015b).

Section B: Methodological development

CHAPTER 4 – SUNDS Framework

The aim of this chapter is to present and discuss SUN conceptual decision framework (Section 4.1) and how it addresses needs of stakeholders in regulatory, industry and insurance sectors (Section 4.2). Framework development was carried out in collaboration with LICARA NanoSCAN developers at TNO during a period abroad in December 2014.

4.1 Description of SUNDS Conceptual Decision Framework

SUNDS conceptual decision framework aims to address the lacunae in existing frameworks. Comprehensive nanosafety research exists in the public domain for few ENMs like nanosilver and nano titanium dioxide, and even for these there are several permutations of physicochemical characteristics (e.g. size, coatings) for which specific data may not be available. Further, several innovative nano-enabled products are developed in SMEs where significant research expenditure and analytical capacity to understand results is not available. In these situations, a lower tier sustainability analysis gives a clue on potential hotspots. If exhaustive data is available or can be generated for a nano-enabled product, there is potential for detailed analysis and more definitive conclusions on product sustainability. With these considerations, a two-tiered framework was designed to address differing data availability and expertise of stakeholders to handle analytical complexity. This framework is described in the sub-sections below.

4.1.1 SUNDS Tier 1

SUNDS Tier 1 comprises of LICARA NanoSCAN, a tool developed within the FP7 LICARA project (www.licara.eu) specifically for SMEs. As SMEs have limited time and internal expertise to carry out complex analyses, LICARA NanoSCAN is designed as a user-friendly, screening-level tool that assists SMEs in checking supplier risks, competing products, market opportunities or making an internal risk and benefit analysis. To achieve this, the tool integrates RA and LCA using MCDA to provide a semi-quantitative evaluation of the environmental, social and economic benefits and the ecological, occupational and consumer health risks of nano-enabled products from life cycle perspective in comparison to conventional products with similar uses and functionality (van Harmelen et al., 2016, Som et al, 2014). The conceptual framework of LICARA NanoSCAN is provided in Figure 4.1.

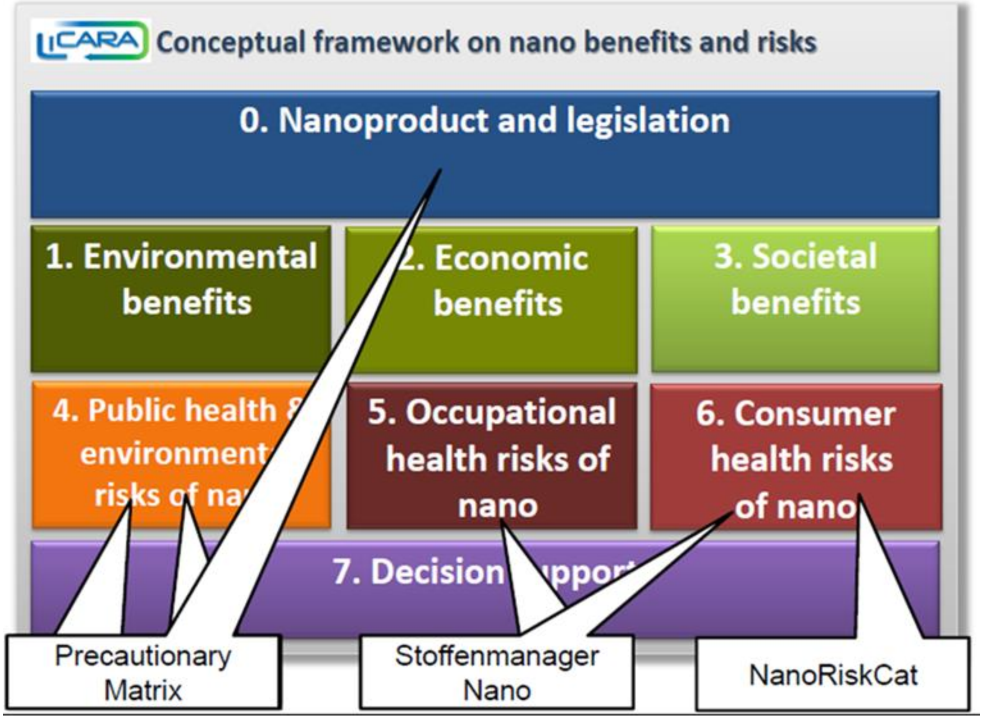


Figure 4.1: Conceptual Framework for LICARA NanoSCAN

LICARA NanoSCAN is modular and contains eight sections. The questions involved in each section are qualitative and semi-quantitative and can thus be answered without detailed data (e.g. yes, no, unknown). Uncertainty is estimated by user input (selecting ‘unknown’) or unanswered questions; in which case a worst case scenario is used (specifying the most negative answer).

Module 0 assesses the nano-relevance of the product that is being evaluated in terms of whether it contains nanomaterials and provides current EU and International Standards Organisation (ISO) definitions of ENM.

Modules 1–3 aim to compare environmental, economic and societal benefits between nano-enabled products and conventional products. Results of these modules are presented on a scale from -1 to 1. A score close to -1 indicates that the nano-enabled product is worse than a conventional product; a score close to 0 indicate that they are similar; while a score close to 1 indicates that the nano-enabled product is better than the conventional product.

Modules 4–6 aim to assess public health and environmental risks, occupational health risk and consumer risks of the nano-enabled products. Module 4 utilises Precautionary Matrix (Höck et al, 2013), Module 5 utilises Stoffenmanager Nano (van Duuren-Stuurman et al, 2012), and Module 6 utilises Stoffenmanager Nano (van Duuren-Stuurman et al, 2012) and NanoRiskCat (Hansen et al, 2011). The results of these modules are not comparative and presented on a scale of 0 to 1. Scores below 0.3 indicate low risks; scores between 0.3-0.7 indicate moderate risks, and a score higher than 0.7 indicates a high risk.

Module 7 synthesizes the results of Modules 1-6 into a two-dimensional risk-benefit space that is divided into four quadrants with respect to nano-enabled product development: Go ahead, Cancel/Rethink, Further research needed, and Other benefits required. Especially in the case that the results are located in the centre (“Undecided”), the user is advised to move to SUNDS Tier 2.

LICARA NanoSCAN has been tested to the case of four nano-enabled products, with additional corroboration from in depth RA and LCA: (1) A Polymer Electrolyte Membrane fuel cell containing multiwalled carbon nanotubes, (2) an antibacterial nanosilver coating for door handles in hospitals, (3) nanosilver in a microfiber cloth, and (4) a façade coating containing nanotitanium dioxide. Van Harmelen (2016) report that there is good agreement of LICARA NanoSCAN and in depth assessment for the fuel cell and façade coating. For the other two case studies, LICARA produced results that were more positive (in the case of anti-microbial fiber cloth due to detailed information on reference product) or negative (in the case of antibacterial coating due to magnitude of social benefit). The reliability of the results of LICARA NanoSCAN can be improved using corroboration with in depth assessment (van Harmelen et al, 2016), and these measures can be easily implemented within SUNDS Tier 2. Application to case studies and stakeholder feedback suggested that significant value of the LICARA NanoSCAN framework lies in the facilitation of discussion on the sustainability of nano-enabled products and an indication of how it can be potentially improved.

4.1.2 SUNDS Tier 2

SUNDS Tier 2 comprises of more advanced tools to support sustainable nanotechnology. A stand-alone module based on CENARIOS standard has also been included in order to enable users to assess the effectiveness of their organizational risk management practices (CENARIOS standard, 2013; Widler et al., 2016). Figure 4.2 presents the conceptual framework for SUNDS Tier 2.

Figure 4.2: SUNDS Tier 2 Conceptual Decision Framework

SUNDS Tier 2 has the following sub-modules:

Ecological Risk Assessment (ERA) sub-module derives ecological risk by integrating outputs from: a) an environmental exposure model that estimates Predicted Environmental Concentrations (PECs) in different environmental compartments (e.g. water, soil), and b) deterministic procedures or Species Sensitivity Distributions (SSDs) (ECHA,2012) that estimate Predicted No Effect Concentrations (PNECs) for various species in the ecosystem in these compartments. Resulting ecological risk will be either deterministic (i.e. PEC/PNEC > 1) or probabilistic (i.e. Potentially Affected Fraction of species > 0.05) depending on the nature of exposure and effect input data. The methodology for exposure and effect estimation and its application to case studies can be found in other publications (Gottshalck et al, 2015, 2013, Semenzin et al, 2015, Sun et al, 2014).

Public Health Risk Assessment sub-module estimates the risks for humans exposed to nanomaterials via the environment by integrating outputs from: a) the environmental exposure model described above, and b) deterministic and probabilistic procedures for dose-response assessment and intra/inter-species extrapolations. The resulting estimation of human health risk will be always quantitative, but either deterministic (Exposure dose/Derived No-Effect Level (DNEL) >1) or probabilistic (e.g. 5% of the population has at least a 10% response with 95% confidence) depending on the nature, quantity and quality of the input exposure and effects data.

Occupational and Consumer Human Health Risk Assessment (HHRA) sub-module derives occupational and consumer health risk by integrating outputs from: a) Human health exposure model that assesses relevant occupational and consumer exposure scenarios according to three tiers (i.e. qualitative, semi-quantitative and quantitative) and taking into account the effect of applied risk management measures (RMMs), and b) the above deterministic and probabilistic procedures for dose-response assessment and intra/inter-species extrapolations.

Life Cycle Impact Assessment (LCA) sub-module uses tools that employ LCA midpoint methods for each life cycle stage (e.g. ReCiPe (Goedkoop et al, 2013)). These indicators will be weighed using shadow prices (van Harmelen et al, 2007, Bruyn et al, 2010) or national level statistical data and subsequently aggregated in order to obtain a final score.

Economic Assessment (EA) sub-module assesses microeconomic impacts for each life cycle stage of a nano-enabled product. This module implements a cost evaluation methodology that considers the cost of capital, material, manufacturing inputs, regulatory compliance, risk management and benefits at the individual company level for the functional unit under consideration.

Social Impact Assessment (SIA) sub-module assesses social impacts through the life cycle due to a nano-enabled product (UNEP SETAC Report, 2009). This sub-module will focus upon quantitative evaluation of social impacts, classified as benefit or cost, to workers and community stakeholders.

Like SUNDS Tier 1, SUNDS Tier 2 is based on the integrated evaluation based on Risk control (RC) (ECHA 2011a) and Socioeconomic Analysis (SEA) (ECHA 2011b). In the RC module in Tier 2, the best risk control strategies will be assessed for scenarios of nano-enabled product development. Toward this end, outputs of ERA and HHRA sub-modules will be ranked according to efficiency and cost using an inventory that includes safety-by-molecular design solutions, personnel protective equipment and engineering controls. An inventory of technological alternatives and risk management measures (TARMM) ranks TARMM relevant to specific exposure scenarios according to their efficiency and cost using questionnaire and data from literature and ongoing projects (Oksel et al, 2016).

The SEA module in Tier 2 will integrate outputs of ERA, HHRA, LCA, EA and SIA sub-modules using user preference profiles to compare scenarios of nano-enabled products with each other or conventional product. While mathematical integration to produce a single score is possible, the interpretation of such an output is not clear or theoretically supported by the sustainability literature. Thus, the SEA module provides a snapshot of various sustainability criteria, classified according to users' preference profiles, to support decision-making.

4.2 SUNDS Framework and Stakeholder Needs

The proposed framework was presented at a stakeholder workshop held at Utrecht (NL) in October 2014 to representatives of potential users of SUNDS. The workshop included twenty four participants, and attendance by core stakeholders was as follows: six regulator representatives (risk assessors and policymakers), three representatives from industry and three representatives from insurance sector. The remaining participants comprised of researchers and tool developers. Arguably, sustainability of the nanotechnology sector is dependent on a broader range of stakeholders (e.g. workers, consumers and the general public). We focussed upon regulators, industry (small and large) and insurance sector representatives as they are the intended users of the SUNDS tool. The stakeholders recognized the potential utility of the SUN conceptual decision framework and offered feedback on the decision analytic framework and other tools proposed to be included in SUNDS (http://www.sun-fp7.eu/summary-report-on-sun-stakeholder-workshop/).

Based on thematic analysis of transcript of workshop discussions, it was possible to extract the stakeholder preferences for the following sustainability assessment methods: screening and advanced RA (RA(s) and RA(a)), screening and advanced LCA (LCA(s) and LCA(a)), Benefit Cost Assessment (BCA), Insurance Cost Assessment (ICA), Social Impact Assessment (SIA) and alternatives assessment based on Risk Management Measures efficiency and cost (RMM (e) and RMM (c)).Specifically, stakeholder preferences were assigned to selected methods in the categories of "no preference" (score=0), "medium preference" (score=0.5) and "high preference" (score=1). Figure 3 presents needs of regulators, SME, large industry and insurance sector with respect to sustainability assessment methods represented as force diagrams. The visualization was built using JSFiddle software. Averages across nodes (TBL and Alternative Assessment criteria) and sub-nodes (specific methods) to calculate distance from the outermost orbit. In other words, the closer the node is to the centre, the greater is the interest of the stakeholder in the method.

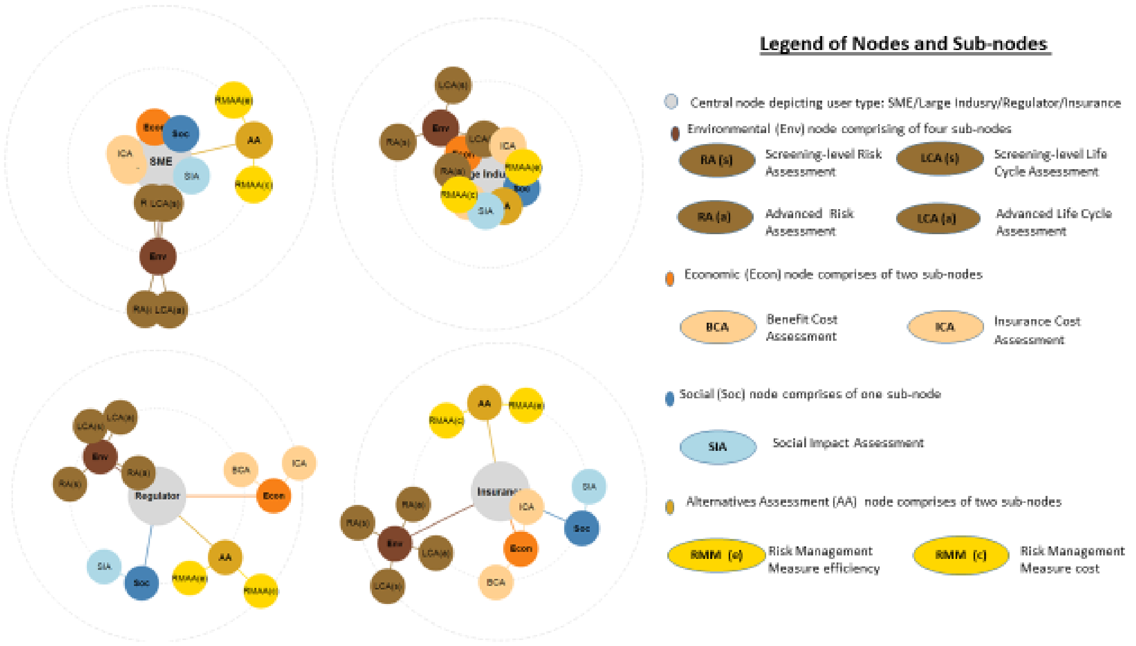


Figure 4.3: User Needs with respect to sustainability assessment methods

Stakeholders from industry are interested in a tool that supports safe and sustainable nanomanufacturing (Malsch et al., 2015b), but large industry and SME have different needs for such a tool. Large Industry users have an interest in proactively tailoring their products-in-development toward safety and sustainability, and have dedicated Research and Development (R&D) units to address these needs. On the other hand, while SMEs are interested in sustainability, they are limited in capacity to handle complex analyses and data generation. Due to this difference, large Industry is more interested in RA (a) and LCA(a), while SMEs are more interested in RA (s) and LCA (s). However, large industry may also use screening level tools for prioritizing (or flagging) product development. Similarly, SMEs can use advanced tools and interpret its output with the assistance of consultants.

Regulators at the workshop included individuals who support the implementation of regulation like REACH. While existing RA frameworks are considered to cover ENM (SCENHIR, 2009; OECD, 2012; EC, 2012), regulatory agencies are making efforts to address case-specific aspects of ENM dossiers. In the case of REACH regulation, European Chemicals Agency (ECHA) requires that the nano-form of the substance needs to be registered separately from the bulk form. It participates in two working groups to improve the application of RA to ENM: nanomaterials working group (NMWG) and group assessing already registered nanomaterials (GAARN). ECHA and regulators expressed preference for SUNDS to be tailored to REACH guidelines. Quantitative ecological and human health risk assessment and the implementation of suitable risk management measures are mandatory for REACH registration and authorization dossiers. Regulators favor absolute assessment for both threshold (i.e. substances with a linear dose-response up to a particular limit) and non-threshold effects (i.e. substances with a linear dose-response e.g. endocrine disrupting chemicals and carcinogens), with appropriate uncertainty analysis methods. In the event that applicants are making a socioeconomic argument for authorization, regulators also require to review LCA, BCA, SIA as well as RMM (c).

The insurance sector is extremely concerned about knowledge gaps in nanosafety, potential liability claims as they are called upon to accept nanotechnology production risk in a field with high scientific and economic uncertainty and no actuarial data (Mullins et al, 2013). Development of actuarial protocols and other ICA tools was deemed by the insurance sector stakeholders as a pressing need to ensure the long term sustainability of the nanotechnology. As these needs are being addressed, the insurance industry has emerged as an effective lobby for improved risk management practices in industry. Insurance providers present at the stakeholder workshop expressed a willingness to offer discretionary premium discounts if industry demonstrated an understanding of risk, regulation and Standard Operating Procedures. Insurance providers are not interested in assessment of alternatives according to efficiency and cost, and hence the AA node has not been shown in the insurance diagram in Figure 4.3.

CHAPTER 5: Risk Control Methodology

This chapter outlines the RC methodology that supports the control of human health and ecological risks by assessing risk control strategies (e.g. safety-by-molecular design solutions, personnel protective equipment and engineering controls) along nano-enabled product lifecycle (Oksel et al., 2016; Subramanian et al, 2016). There are two key challenges to be addressed in implementing risk control through the nano-enabled product lifecycle. The first issue concerns the application of appropriate Technological Alternatives and Risk Management Measures (TARMM) (Oksel et al., 2016) to address the risk posed by a specific nano-form in an exposure context. Much of the available literature on risk management of ENM is qualitative, and is focused with disseminating best practice recommendations to control workplace exposure (Schulte et al., 2013a; Kuempel et al, 2012). Even though there is quantitative information on TARMM efficiency for bulk materials, information on specific nano-forms is limited, as recently reviewed by Oksel et al. (2016). The other issue concerns implementation of risk control in a cost effective manner, as even explicitly recognized by regulations (e.g. REACH Authorisation's Analysis of Alternatives and Socioeconomic Analysis) and policy prescriptions (e.g. European Commission's Precautionary Principle, UK Health and Safety Executive's As Low as Reasonably Practicable (ALARP) principle). It is not surprising that Helland et al. (2008) report cost as the biggest barrier to occupational risk management for small nanotechnology firms. Fleury et al. (2012) pinpoint the uncertainties in risk assessment of nanocomposites, and propose risk management and cost evaluation based on the ALARP principle.

In this chapter, Section 5.1 sketches the general idea behind the risk control methodology, and Section 5.2 details how risk assessment is linked to TARMM.

5.1 Outline of risk control methodology

The RC methodology highlights human health and ecological risks deemed "not acceptable" (i.e. hotspots) along the life cycle of nano-enabled product (i.e. synthesis of functional components, manufacturing of nano-enabled product, consumer use and product end of life including disposal, recycling and reuse) and guide the selection of relevant, efficient and least expensive TARMM to reduce them to acceptable levels. A detailed description of Human Health Risk Assessment (HHRA) and Ecological Risk Assessment (ERA) methodologies implemented in the RC module is out of the scope of this chapter and is provided in some publications (Tsang et al., submitted; Pang et al., 2016; Semenzin et al., in preparation); this chapter focusses on the aggregation and classification of their results in order to link them to TARMM.

The HHRA methodology assesses risk along the life cycle of a nano-enabled product to workers, consumers and general population. Human health risk for each life cycle stage is calculated by integrating outputs from: a) models applying deterministic or probabilistic procedures for toxicological effect assessment, and b) occupational and consumer exposure models or environmental exposure models calculating Predicted Environmental Concentrations (PECs) in different environmental compartments (for public health risks). The HHRA output for a probabilistic risk assessment is a probabilistic distribution of risk (Tsang et al, submitted; Pang et al., 2016), whereas deterministic risk assessment produces a single risk value (ECHA, 2015). In both cases, risk is considered not acceptable when exposure exceeds prescribed no-effect threshold (i.e. the risk characterization ratio (RCR) is greater or equal than 1).

The ERA methodology assesses risk along the life cycle of a nano-enabled product to key environmental compartments e.g. surface water, soil (natural and urban or sludge), sediments, waste water treatment plant (WWTP) effluent. Ecological risk for each life cycle stage is calculated by integrating outputs from: a) the same environmental exposure model used in Public Health Risk Assessment and b) deterministic procedures or Species Sensitivity Distributions (SSDs) (ECHA, 2012a) that estimate Predicted No Effect Concentrations (PNECs) for various species in the specific environmental compartment. Resulting ecological risk is either deterministic (i.e. PEC/PNEC) or probabilistic (i.e. percentage of RCR distribution greater or equal than 1) depending on the nature of exposure and effect input data (Semenzin et al, in prep).

For both HHRA and ERA, a single output is presented for the four life cycle stages and the global scenario, which may be classified as Acceptable/Not Acceptable (in the case of deterministic risks) as Acceptable/Needs further consideration/Unacceptable (in the case of probabilistic risks). These outputs are produced by the aggregation and classification of several individual risk values or what is referred to as the lowest unit of assessment (LUA). An example of LUA for HHRA is the combination of a lifecycle stage (synthesis/production/use/end of life), a specific target (workers/consumers/general population), a specific activity (applicable to occupational exposure scenarios) and a defined route of exposure (inhalation/dermal/oral).

Each LUA corresponds to a single nano-form, but the transformation of engineered nanomaterials (ENM) through the life cycle (i.e. pristine nanomaterial, fragment with embedded nanomaterial, fragment with protruding nanomaterial, nanomaterial agglomerate) is allowed. An aggregation step is therefore required to produce a single risk value for each lifecycle stage as well as for the entire lifecycle from all assessed LUAs. Aggregated outputs are then classified with communicative labels based on the acceptability of risk to offer guidance to the non-expert.

Aggregation and classification steps were developed by using a web-based questionnaire to experts. Twenty experts (ten for HHRA and ten for ERA) were chosen from personal networks and contacted by email in December 2015 with a request to participate in methodology development by completing a questionnaire implemented in the Surveymonkey platform. Eight responses were received for HHRA, including two regulators (one from US and one from Canada) and six researchers (from EU), and three for ERA, including two regulators and one researcher (both from EU). Data collection through the questionnaires was closed in February 2016 and results were used to finalise the aggregation methods as well as classification profiles for HHRA and ERA as described below.

Aggregation in HHRA may be additive (in the case of risks related to the same target) or non-additive (in the case of risks related to different targets for the same lifecycle stage). The instances of additive integration include a worker exposed to more than one exposure route (e.g. inhalation and dermal contact), or a worker involved in more than one activity within a single lifecycle stage (e.g. weighing nanomaterials and mixing within the synthesis or production phase). The risk value for a lifecycle stage involving more than one exposure route is calculated by summing the risk for all exposure routes. In the case of a single worker involved in different activities, the risk is calculated by summing the contribution of the different activities on the same worker weighted by the exposure duration. In order to produce a single HHRA output for each lifecycle stage and the entire lifecycle, aggregation of non-additive risks (i.e. risk to different targets) also needs to be addressed. According to the findings of the questionnaire, each life cycle stage is represented by the maximum risk value within that stage (i.e. a single not acceptable risk for a lifecycle stage is sufficient to classify the risk for the lifecycle stage as not acceptable).

In HHRA acceptability of risk (i.e. the risk characterization ratio (RCR) is lower than 1) has been used for results classification, according to an approach based on confidence intervals.

Specifically, in case a deterministic risk is calculated (as ratio between exposure levels and suitable hazard values such as Derived No Effect Levels or Derived Minimum Effect Levels), two classes are identified: Acceptable (ratio below one) and Not Acceptable (ratio above one). Probabilistic risk can be obtained if either exposure or effect values (or both) are represented by a probability curve (EPA, 2012). As probabilistic risk distributions typically follow a right-skewed log-normal distribution, it is too rare to have a completely acceptable risk. Literature suggests that the risk is acceptable if the 90th percentile of the population is characterized by an acceptable risk, but conservative values can also be selected (i.e. the 95th percentile or the 99th percentile) (US-EPA, 2001; US-EPA, 2014). The default classification profile for probabilistic Human Health risk includes the following three classes: Acceptable (when the threshold of one (i.e. the acceptable risk) is over the 99th percentile of the risk characterization ratio distribution), Needs further consideration (threshold of one between 90th and 99th percentile) and Not acceptable (threshold of one below the 90th percentile). The selection of the percentiles for the classification profile can be changed depending on expert evaluations, assessment needs and data availability.

Aggregation of LUA in ERA is always non-additive, because PEC and PNEC are highly dependent upon physicochemical transformation, fate, transport, exposure and species within an environmental compartment and thus risks for different environmental compartments cannot be added. According to the questionnaire results and in agreement to the HHRA methodology, the approach consists of selecting the maximum risk to represent each life cycle stage and the entire life cycle.

As far as ERA classification is concerned, similar to the HHRA methodology, an approach based on confidence intervals are followed. In case a deterministic risk is calculated (as ratio between exposure levels (PECs) and suitable hazard values (PNECs)), two classes are identified: Acceptable (ratio below one) and Not Acceptable (ratio above one). Probabilistic ecological risk can be obtained if either exposure (e.g. based on probabilistic material flow analysis) or effect values (e.g based on SSDs), or both, are represented by a probability curve (Gottshalck et al, 2013). As for HHRA, the default classification profile for probabilistic ecological risks include three classes (though with different values, agreed with questionnaire's respondents): Acceptable (when the threshold of one is over the 99th percentile), Needs further consideration (threshold of one between 95th and 99th percentile), and Not acceptable (threshold of one under the 95th percentile).

RC methodology is implemented starting from the single lifecycle stage outputs for HHRA and ERA. If these outputs contain an “Unacceptable risk”, it is traced back to the LUA. Risks can be reduced through TARMMs that lower either hazard or exposure, although a strict distinction between these categories is not always possible in specific cases. A database of TARMM with their efficiency and cost is currently being constructed from three sources: Exposure Control Efficacy Library (ECEL) 1.0 (Fransman et al, 2008), Advanced REACH tool (ART) (Tielemans et al., 2011) and TARMM inventory (Oksel et al., 2016). These sources were assessed for their applicability for exposure control of nano-enabled products through the life cycle based on study design of measurement (in case of data derived from literature or real exposure measurements), data quality, ENM type, exposure route (inhalation/dermal/oral), physical state (solids/liquids), lifecycle stage, workplace control measures (divided into categories described next), sampling (stationary sampling or normal) and source domain (e.g. powder , solid matrix, suspension, on surface) . The resulting database contains the following kinds of TARMM: engineering controls, respiratory protective equipment, dermal protective equipment and protective clothing. As no information on technological alternatives was found, it is not currently included in the database but this can be included once the information is available.

The conceptual schematic for risk control is shown by Figure 5.1.

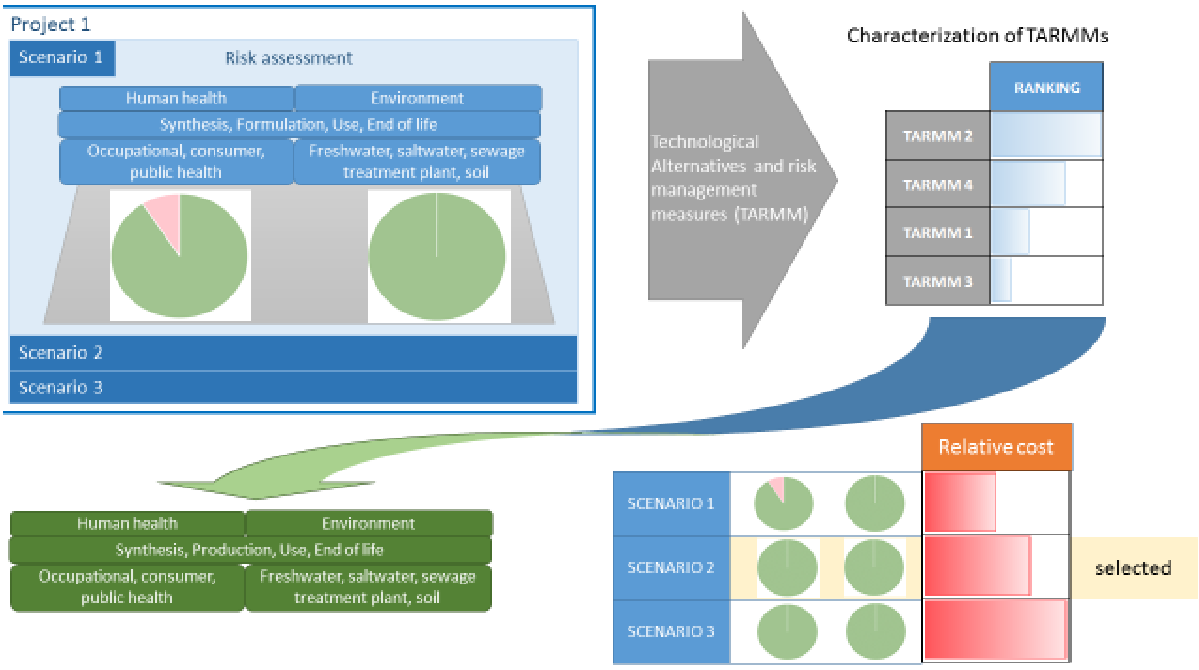


Figure 5.1: Conceptual Schematic for Risk Control

5.2 Linking TARMM database to risk assessment

The TARMM database can be linked to RA in slightly different ways depending on if risk reduction is targetted through hazard or exposure. One approach to reduce the hazard of nano-enabled products is by safety-by-design (S-by-D) technological alternatives that modify nanomaterial properties (e.g. to reduce nanomaterial release from products, induce their accelerated alteration/degradation, change their biological interactions in order to affect their persistence, bioaccumulation and hazard) while maintaining their intended functionality. Examples of S-by-D strategies at the level of nanomaterial chemistry include physicochemical property modification (e.g. change in nanomaterial size, shape, properties influencing aggregation), surface modification (e.g., coating, surface functional groups) and embedding in matrix (Costa, 2013; Morose, 2010; Caruso, 2001). If S-by-D based technological alternative is available to reduce the hazard (in ecological or human health terms) for the nano-form involved in producing the unacceptable risk for a LUA, a hazard and risk re-estimation is perfomed (using HHRA or ERA methodology as the case may be) to check if it brings risk down to acceptable levels. If this is successful, its cost effectiveness is considered in comparision with other relevant TARMM.

Exposure reduction is the more common and generic circumstance. It is approached for ecological and public health risks in RC methodology by selecting applicable TARMMs based on emission control e.g. engineering controls, and using efficiency to re-estimate environmental exposure and ecological risks. To find the most cost-effective solution, the cost of TARMMs successful at reducing ecological risk to below threshold levels are compared. Thus, the following attributes are required to model environmental exposure control: nanomaterial type including identity and lifecycle stage (i.e. pristine nanomaterial, fragment with embedded nanomaterial, fragment with protruding nanomaterial, nanomaterial agglomerate), particle size distribution, efficiency (single value or range) and cost (single value or range). For unacceptable occupational risks, TARMM need to be linked to the exposure activity corresponding to unacceptable risk. The following attributes are required to model occupational exposure control: activity/process, source domain (solid matrix, on surface, suspension, powder, spray, mechanical, dispersion/formulation, material contact, food), nanomaterial type including identity and lifecycle stage (i.e. pristine nanomaterial, fragment with embedded nanomaterial, fragment with protruding nanomaterial, nanomaterial agglomerate), particle size distribution, efficiency (single value or range), cost (single value or range), task frequency, task duration, number of persons involved in the task. The key TARMM to mitigate consumer risk are consumer information labels; their effectiveness can possibly be operationalized by studying consumer risk perception but this cannot be currently included in the TARMM database. However, some occupational TARMM (e.g. specialized spray cans to control release, gloves, protective clothing, etc.) may be applicable in the consumer context for specific nano-enabled products and these will be linked to consumer scenarios. Efficiency of TARMM for exposure control is defined in different ways in the literature, and also depends on exposure assessment methodology used. In the TARMM database, efficiency is defined as follows:

Engineering controls

1) Reduction (efficacy) factor = $C_{control\ on}$ / $C_{control\ off}$; **OR** $C_{after/with}$ / $C_{before/without}$
2) For Effectiveness (%) = 1 – Efficacy factor * 100, **OR** ($C_{without/off}$ – $C_{with/on}$) / $C_{Without/off}$ × 100

Respirators, gloves, protective clothing

1) Protection factor, PF = $C_{outside}$ / C_{inside}; **OR** $C_{upstream}$ / $C_{downstream}$, **OR** $C_{without}$ / C_{with}
2) Penetration/migration (%) = C_{inside} / $C_{outside}$ *100, **OR** $C_{upstream}$ / $C_{downstream}$ *100
3) Effectiveness (%) = 1 – (C_{inside} / $C_{outside}$) * 100

Where C=exposure concentration

Costs of TARMM may be highly variable, and ranges of cost included in the database were collected through internet search.

CHAPTER 6: Socioeconomic Assessment Methodology

The socioeconomic assessment (SEA) methodology compares scenarios of nano-enabled products to relevant alternatives with respect to their sustainability aspects (environmental, economic and social costs and benefits) through the lifecycle (Subramanian et al, 2016a). This chapter aims to describe the SEA methodology, and is organized as follows: Section 6.1 describes key concepts included in the SEA methodology. Aggregation methods and classification profiles to be applied to the different assessment methodologies in SEA were developed by internal discussion for LCIA, EA and SIA methodologies, and are described in Section 6.2, 6.3 and 6.4 respectively. The reader is referred to Section 5.1 for aggregation and classification methodologies for HHRA and ERA.

6.1 Outline of Socio-Economic Assessment methodology

The SEA methodology aims to pinpoint hotspots (i.e. high risks and impacts or low benefits) that allow the user to see in which ways the sustainability profile of a nano-enabled product can be improved. Each scenario covers the whole life cycle of a nano-enabled product i.e. synthesis of functional components, product manufacturing, consumer use and product end of life (disposal, recycling and reuse). The SEA methodology aims to account for salient sustainability aspects such as transformation of pristine nanomaterial to diverse nano-forms (which constitute different exposure agents), environmental (including human) targets, material and energy fluxes contributing to environmental impacts, economic inputs and social context.

Aligned with the Triple Bottom Line (TBL) formulation of sustainability, the SEA includes the three sustainability pillars through the integration of the following components (Subramanian et al., 2016a):

- Human Health Risk Assessment (HHRA), Ecological Risk Assessment (ERA) and Life Cycle Impact Assessment (LCIA) methodologies are included in the environmental pillar,
- Economic Assessment (EA) methodology is included in the economic pillar, and
- Social Impact Assessment (SIA) methodology is included in the social pillar.

For a description of HHRA and ERA methodologies, the reader is referred to Section 5.1.

The LCIA in SEA methodology assesses the environmental impacts for each lifecycle stage of a nano-enabled product for the defined functional unit based on the fluxes of material and energy in the scenario. The LCIA methodology accepts the outputs of LCIA software which utilize specified life cycle assessment methodologies (e.g. ILCD, ReCiPe, CML, Ecoindicator 95 and 99, TRACI) to calculate midpoint and endpoint impacts in prescribed units of measure. For example, ReCiPe allows to calculate midpoint impacts in points which can be further aggregated into three endpoint impacts viz damage to resources, damage to ecosystem diversity and damage to human health (Goedkoop et al., 2012), while according to the concept of shadow prices, which are constructed prices for environmental quality based on abatement or damage (de Bruyn et al, 2010; van Harmelen et al., 2007), midpoint impacts can be conveniently expressed in monetary terms and further aggregated into a single final score.

The EA in SEA methodology assesses costs for the defined functional unit within each life cycle stage of a nano-enabled product from the perspective of the manufacturer. The inputs to this methodology include microeconomic variables for synthesis, production, use and end of life lifecycle stages. Variables for synthesis and production phases include material costs (nanomaterials and other production inputs), labour costs, worker training costs, maintenance and purchasing cost of plant, machinery and equipment. Variables for the use phase include maintenance and operating costs. Variables for the end of life phase include disposal and recycling costs. Two key points are to be borne in mind in implementing the EA methodology: a) Double counting should be avoided across life cycle stages. Examples where double counting can occur include nanomaterial cost in synthesis and production stage and nano-enabled product cost in production and use stage, and b) The direction of flow of costs in EA should be aligned with the LCA and the real scenario. For example, recycling is always a beneficial environmental impact in a global sense but as EA is performed from the perspective of the manufacturer, it makes a difference whether the monetary benefit of recycling flows to the manufacturer or not. The variables within each lifecycle stage are summed to obtain a single final cost score for each lifecycle stage in monetary units, as well as a global cost score (which is a sum of all lifecycle stages).

The SIA in SEA methodology assesses yearly social impacts produced by a nano-enabled product through the lifecycle, with reference to the context of the company producing it, located within a specific country. The SIA methodology integrates Social Life Cycle Assessment (sLCA) and Multi-Criteria Decision Analysis (MCDA), and comprises of normalization, weighting and aggregation steps (Subramanian et al., 2016b). Normalized and weighted social indicators are aggregated as overall benefit and cost scores as per the benefit and cost conceptual framework (Subramanian et al, 2016b). Then, the net benefit score is calculated as the difference between benefit and cost scores. As the SIA methodology characterizes the social context and cannot be split into discrete lifecycle stages, the output of the SIA methodology is a single score representing the net benefit of a nano-enabled product.

As it is clear from the above description, the different methodologies included in SEA provide heterogeneous results, consequently the integration of their outputs toward a final sustainability assessment score is not straightforward. The option of integrating these outputs to a single scale e.g. in monetary units or non-dimensional index was discussed with the group of stakeholders (i.e. industries, regulators and insurance companies) involved in SUNDS design (http://www.sun-fp7.eu/wp-content/uploads/2015/02/SUN-user workshopsummaryfinal.pdf). Stakeholders felt that an integrated sustainability score could only pinpoint a better scenario in comparative analysis, but could not prescribe how product sustainability could be further improved. Therefore, it was decided to use HHRA, ERA, LCIA, EA and SIA results to create a sustainability portfolio as depicted in Figure 6.1.

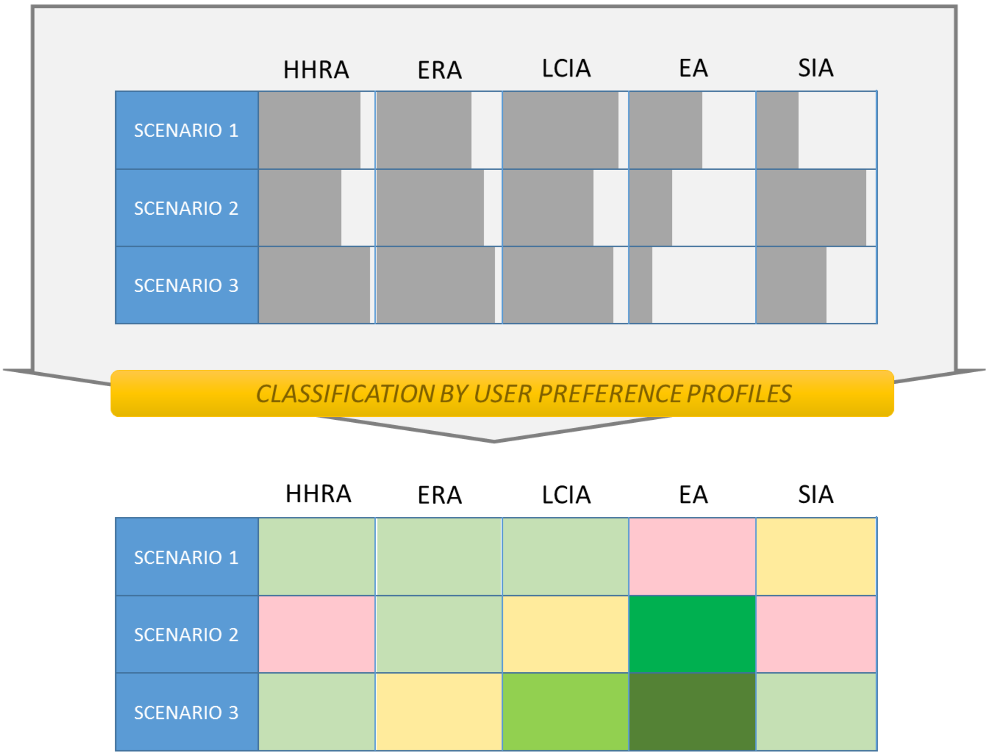


Figure 6.1: Representation of SEA sustainability portfolio

A sustainability portfolio comprises of single outputs for global and lifecycle stage scores for all methodologies which are assigned communicative labels to provide further guidance to the user. The combination of classifications for each scenario can be considered on its own; for example, a nano-enabled product with low risks and environmental impacts, low costs and high benefits could be innovative and commercially profitable. In the case of more than one scenario, sustainability portfolio provides the framework for systematic as well as detailed comparison of results of each methodology.

To this end, for each scenario and each assessment methodology, results are first aggregated (where needed) to a single numerical value for each lifecycle stage and to a global value including all lifecycle stages, which in turn can be classified. Aggregated outputs from HHRA, ERA and EA methodologies are always negative impacts or costs, whereas outputs from LCIA and SIA methodologies may be benefits (positive impacts) or costs (negative impacts).

6.2 Derivation of life cycle impact classification profile

Aggregation of LCIA results into life cycle stage and global scores first requires the normalization of results to a single scale. Normalization is an optional step in LCA and can be performed by expressing the contribution of a midpoint relative to a reference, which is often performed using country level statistical data (Goedkoop et al., 2012), or by associating a cost to each midpoint unit of measure in order to translate impacts into monetary value, as it is done in the shadow prices method (de Bruyn et al, 2010; van Harmelen et al, 2007). In the first case, midpoints should be aggregated into endpoints before further aggregation into life cycle stage and global scores and the first aggregation step usually includes the application of a weighting scheme (Heijungs and Guinee, 2012). This does not apply to the shadow prices method, as costs are directly applied to midpoint scores which are subsequently summed up into life cycle stage and global scores.

In the classification step, the four lifecycle stage scores and the global score are classified as High/Medium/Low costs or benefits to offer additional guidance to the user. Costs include endpoints or midpoint (expressed as shadow prices) scores with a positive sign, which represent a negative environmental impact due to the product. Benefits include endpoints or midpoint (expressed as shadow prices) scores with a negative sign, which represent a positive environmental impact due to the product (e.g. recycling may improve resource use). Costs and benefits may be classified using two methods: Reference method in case normalization was performed relative to a reference, and Eco-efficiency method (Saling et al, 2002) when sum of midpoint impacts expressed as shadow prices are compared to the market price of the functional unit.

In the Reference method, LCIA global score, lifecycle stage scores (obtained from aggregating endpoints or midpoints as shadow prices) are classified by comparing them with those obtained for a reference product with the same functionality. Given the uncertainty and variability in the underlying data, the LCIA experts suggested that differences between alternative scenarios should be at least 20% to be significant. Therefore, thresholds for Low/Medium and Medium/High classes for costs and benefits are set, as default, at 80% and 120% of the reference specified by the user, and life cycle stage and global scores obtained for the scenario under consideration are classified accordingly. In the case of a negative reference ratio, only simple classification is provided i.e. a benefit changing into a cost is always classified as high cost and a cost changing into a benefit is always classified as high benefit.

According to the Eco-efficiency method, the eco-efficiency ratio is calculated between the environmental performances (midpoint results expressed as shadow prices and summed up in lifecycle stage scores and global scores) and the market price (actual or expected) of the product included in scenario under consideration. It should be noted that in the case of lifecycle stage eco-efficiency ratios, the market price is split in proportion of the contribution of each positive lifecycle stage score to the global score (i.e. negative lifecycle stage scores are excluded as they do not affect market price). As default, it is proposed to set classification thresholds based on calculation of country level mean eco-efficiency ratios. For example, the mean eco-efficiency ratio for the Netherlands in 2013 was calculated as a ratio between country level environmental impacts for key industries (including data from Dutch environmental accounts on steel, steel industry, copper industry, aluminium industry and zinc industry) expressed in shadow prices to the Gross Domestic Product at around 5%. Low/Medium and Medium/High thresholds for classification of eco-efficiency ratios were then set at 2.5% (half of the mean eco-efficiency ratio) and 7.5% (half over the mean of eco-efficiency ratio), respectively. A negative lifecycle stage score is always classified as high benefit.

6.3 Derivation of economic impact classification profile

As aggregation of variables' results into lifecycle stage and global scores is already included in the EA methodology, the SEA methodology involves only the classification step. Here, the four lifecycle stage scores and the global score are classified as High/Medium/Low to offer additional guidance to the user. Similar to LCIA, classification profiles are based on two methods: Reference method and Efficiency method.

In the Reference method, the user specifies a reference product and provides its lifecycle stage and global cost scores. Thresholds for lifecycle stages and global score are calculated for Low/Medium and Medium/High at 80% and 120% of the reference respectively and scenario's scores are classified accordingly. If the synthesis stage of the product cannot be compared to a reference scenario (e.g. in the case of a conventional product that does not possess the functionality conferred by the nanomaterial), these alternative thresholds, set using expert elicitation, are used: ratio between synthesis and global costs under 0.33 (Low), between 0.33 and 0.66 (Medium) and over 0.67 (High).

In the Efficiency method, preliminary thresholds are set based on discussion with experts. For the synthesis and production phases, the market price is split in the ratio 1/12 for the synthesis phase, 1/6 for the production phase and ¾ for the profit margin. Low/Medium and Medium/High thresholds are established for the first two fractions of the market price provided by the user at 80% and 120%. The use phase includes the market margin, maintenance cost and operational cost. From the user's perspective, it is not desirable that the use phase cost is greater than the market price (for a product that is for utility and not for hobby). Therefore, Low/Medium and Medium/High thresholds for the use phase are defined at 75% and 100% of the market price, respectively. The end of life phase includes the cost of disposal of the product as well associated material related to its functionality and use. These costs are highly variable ranging from fairly low (e.g. paper and organic waste) to medium (e.g. glass, wood, plastic) to high (e.g batteries, hazardous waste). Low/Medium and Medium/High thresholds for the end of life phase are defined at 10% and 100% of the market price respectively.

Application of efficiency method needs to be developed further by application to case studies, particularly with products that are representative of low and high costs for particular lifecycle stages. The reference method should be preferred if information on reference scenario is available as the interpretation is clearer.

6.4 Derivation of social impact classification profile

As for the EA methodology, an aggregation step is not required to incorporate SIA output to the SEA hotspot portfolio as the SIA methodology already provides a single output (i.e. the net benefit score).

The classification implemented for the net benefit score classifies it as low, medium or high. This classification is based on the assumption that size of the industrial enterprise affects the social impacts (Subramanian et al, submitted). Thresholds of High, Medium and Low classes for Small and Medium Sized Enterprises (SME) and Large Industries (LI) are developed using country level data using employment and value added as proxies for specific indicators (Subramanian et al, submitted). First, the “relative potential” of an SME or LI company to create a social impact in a country is derived using either a) average number of employees for SME and LI, and b) average value added for SME and LI. Each social indicator is linked to one of these relative potentials based on if it is more closely linked to employment (a) or value added (b). Both these relative potentials are used to derive the adjusted total number of companies, which in turn is used to derive the mid-level value for the social indicator for a SME and LI. The mid-value of the social impact is divided by the social indicator data at country level to obtain benchmarks for SME and LI. Low/Medium and Medium/High thresholds are defined using 80% and 120% of benchmark’s value. Classification thresholds for net benefit scores are calculated for SME and LI at company level by following the weighting and aggregation of benchmarks. A negative net benefit is classified as a High/Medium/Low cost whereas a positive net benefit is classified as High/Medium/Low benefit. It should be noted that while two scenarios can be compared at unit’s level within a company (e.g. sub-division level) using their net benefit scores, classification of scenarios is currently only possible at company level, because available national statistics allow development of thresholds (e.g. employment, value added, number of companies) only at company level.

CHAPTER 7: Social Impacts Assessment Methodology

It is widely agreed that the entire Life Cycle of nano-enabled products is the appropriate unit of analysis for to manage the nanotechnology Environmental Health and Safety and sustainability (Greiger et al, 2012a; Shatkin et al., 2008; Som et al., 2010; Sweet and Strohm, 2006), and social impacts of nano-enabled products should also cover the entire Life Cycle. Social Life Cycle Assessment (sLCA), an approach to assess social impacts associated with the product Life Cycle on specific stakeholders (Althaus et al., 2009), is suitable for this purpose. The sLCA framework comprises of two hierarchical levels: impacts and indicators. Social impacts can be defined as the consequences of social relations or interactions in the context of the Life Cycle of an activity and/or by preventive or reinforcing actions taken by stakeholders (Althaus et al., 2009). They may be caused by specific behaviours and socioeconomic processes, and are related to human, social and cultural capitals (Althaus et al., 2009). SIA impact categories (and sub-categories) are assessed using specific indicators, which are qualitative, semi-quantitative or quantitative variables associated with measurement units (Althaus et al., 2009). sLCA for products has been implemented within SEEBALANCE sustainability assessment tool (Schmidt et al., 2004), Social Hotspots Database (SHDB) scoping assessments (Benoit-Norris et al, 2012a) and LICARA NanoSCAN tool (Som et al, 2014), the last one being the only existing nano-specific tool. However, LICARA NanoSCAN compares the manufacturer’s perception on social impacts of nano-enabled products and conventional products through semi-quantitative indicators (Som et al, 2014) and therefore, there is interest in developing a quantitative methodology to assess the social impact of nano-enabled products in order to support risk governance, in particular by offering salient indicators to be used for monitoring and a basis for stakeholder dialogue.

This chapter proposes a quantitative sLCA methodology to be included in SUNDS. First, a list of social impacts that can be used for sustainability evaluation of products was developed from available sources e.g., guidelines pertaining to industry/manufacturing, product sLCA tools (Section 7.1). In the next step, the key social impacts relevant to nanotechnology bare reviewed review (Section 7.2). Then, statistical databases were reviewed to find available indicators that could be classified under the social impacts (Section 7.3). Finally, a MCDA methodology was developed to integrate the selected indicators into a final social impact score (Section 7.4).

7.1 Impacts for Social Life Cycle Assessment of Products

This section aims to compile a list of social impacts of products to be utilized within an sLCA framework. Sources which comprise of social impacts of products and manufacturing contexts include: a) Guidelines like Corporate Social Responsibility (CSR) guideline (ISO 26000, 2010), Global Reporting Initiative (GRI) Sustainability Reporting guidelines (GRI, 2014), REACH Socioeconomic Analysis (SEA) Authorization guideline (ECHA, 2011) and SEA dossiers found by searching ECHA website (http://echa.europa.eu/), European Commissions' (EC) Impact Assessment (IA) guideline (EC Report, 2009) and United Nations Environmental Programme (UNEP)- Society for Environmental Toxicology and Chemistry (SETAC) sLCA guidelines (Althaus et al., 2009), and b) Tools for sustainability assessment of products (Benoit-Norris et al, 2012a, Schmidt et al, 2004, Som et al, 2014), also including reviews of sustainable development literature to build these tools (Schmidt et al., 2004).

The selection of social impacts from these sources entailed harmonization due to several reasons. Firstly, in nearly all sources, social impacts are not explicitly defined and terminology with decisions needed to be made whether to combine or keep as separate similar sounding terms. In accordance with their approach, the broadest category was adopted to define the impact. For example, child labour and forced labour could be considered as part of the broader category human rights. Secondly, social impacts in these sources are at different levels of analysis (i.e. impacts and indicators) and classified as being relevant to different stakeholders (e.g. gender equality may be relevant to both workers and community). Further, there is varying classification of which impacts count as “social”; environmental and economic impacts also have important social dimensions. Examples include toxicity potential and Foreign Direct Investment. Indeed, a strict division between environmental, economic and social dimensions may not be possible in some cases. The Roundtable of Product Social Metrics (2014) harmonizes the definitions of social impacts and served as a valuable guide in resolving these issues in this chapter

Two chosen sources comprised of indicators (instead of impacts): GRI metrics and REACH SEA dossiers. They were mapped under existing social impacts (e.g. number of jobs can be classified under employment) or new social impact categories were defined for them (e.g. impact of critical supply losses in the value chain).

The sub-sections below briefly summarize the sources based on which the list of social impacts for products/manufacturing reported in Table 7.1 is compiled and the rationale behind the selection of the 9 impacts each for workers, consumers and community and the 6 impacts for value chain actors.

Table 7.1 Social impacts for products through their Life Cycle

Stakeholder category	**Social Impact**	**Reference**
Workers	Freedom of Association and Collective Bargaining	Althaus et al. (2009), Schmidt et al (2004), RPSM (2014), Benoit-Norris et al (2012a)
	Education and training	GRI (2014) , Seear et al. (2009), EC IA (2009), Schmidt et al (2004), RPSM (2014)
	Human Rights (including child labour and forced labour)	Althaus et al. (2009), GRI (2014), RPSM (2014), Benoit-Norris et al (2012a)
	Wages	Althaus et al. (2009), SEA submissions(ECHA website, 2015) , Benoit-Norris et al (2012a), Scmidt et al (2004), RPSM (2014)
	Working Hours	Althaus et al. (2009), RPSM (2014)
	Equal opportunity/Discrimination (including gender and other social distinctions)	Althaus et al. (2009), GRI (2014), RPSM (2014)
	Occupational Health and Safety (occupational diseases, accidents, etc)	Althaus et al. (2009), GRI (2014), EC IA (2009), SEA submissions (ECHA website), Schmidt et al (2004), RPSM (2014)
	Social Benefits/Social Security	Althaus et al. (2009), Schmidt et al (2004), RPSM (2014)
	Employment type and quality	GRI (2014), Seear et al. (2009), SEA submissions (ECHA website), RPSM (2014)
Consumer	Consumer Health & Safety	Althaus et al. (2009), EC IA (2009), Schmidt et al (2004), RPSM (2014)
	Quality of health and safety labelling and other information on other risks	sLCA Consumer Health and Safety Sheets (2010), GRI (2014), Schmidt et al (2004)
	Consumer Satisfaction	GRI (2011), SEA submissions, sLCA Consumer Health and Safety Sheets (2010), Schmidt et al (2004), RPSM (2014)
	Complaints and Feedback Mechanism	Althaus et al. (2009), sLCA Consumer Health and Safety Sheets (2010)
	Legal issues and Compliance	GRI (2014)
	Consumer Privacy	Althaus et al. (2009), GRI (2014)

Stakeholder category	Social Impact	Reference
	Ethical issues	GRI (2014), Seear et al. (2009), EC IA (2009)
	Transparent Marketing Communications	Althaus et al. (2009), sLCA Consumer Health and Safety Sheets (2010)
	End of life responsibility	Althaus et al. (2009)
Community	Local engagement	Althaus et al. (2009), EC IA (2009), RPSM (2014)
	Employment	Althaus et al. (2009), EC IA (2009), Schmidt et al (2004), ECHA (2011), RPSM (2014), Benoit-Norris et al (2012a)
	Technology development	Althaus et al. (2009), Som et al (2014)
	Crime and Security	Althaus et al. (2009), EC IA (2009)
	Access to material resources	Althaus et al. (2009), RPSM (2014)
	Social diversity	Althaus et al. (2009), EC IA (2009), ECHA (2011), Benoit-Norris et al (2012a)
	Delocalization and Migration	Althaus et al. (2009), EC IA (2009)
	Contribution to sustainable development goals	Som et al (2014)
	Cultural Heritage	Althaus et al. (2009), EC IA (2009)
Value chain	Fair treatment	Althaus et al. (2009), GRI (2014)
	Human rights enforcement through the supply chain	Scmidt et al (2004), GRI (2014)
	Respect of intellectual property rights	Althaus et al. (2009)
	Collective governance	GRI (2014)
	Non-EU country impacts	EC IA (2009)
	Impact of critical supply losses	SEA submissions (ECHA website)

The column "stakeholder category" lists one of four categories: worker, consumer, community and value chain actor. The column "social impact" specifies a word or phrase to describe the social impact chosen from our review. The column "reference" provides the sources where the social impact is mentioned, as described in sub-section 7.2.1-7.2.4.

7.2.1 Corporate Social Responsibility Guidelines and Global Reporting Initiative Metrics

The key guideline available for CSR is ISO 26000 Guidelines on Social Responsibility, which defines this concept as follows: "Responsibility of an organization for the impacts of its decisions and activities on society and the environment, through transparent and ethical behaviour that contributes to sustainable development, including health and the welfare of society; takes into account the expectations of stakeholders; is in compliance with applicable law and consistent with international norms of behaviour; and is integrated throughout the organization and practiced in its relationships.” (ISO 26000, 2010). While ISO 26000 elucidates the general principles of social responsibility in organizational culture and processes, GRI Sustainability Reporting guidelines provide practical principles and indicators for companies to report on their implementation of ISO 26000 (GRI, 2014). GRI comprises of two categories of indicators: general standard disclosures and specific standard disclosures. Specific standard disclosures are divided into the three sustainability dimensions. The social category among these is further divided into four sub-categories for which metrics are proposed: Labor Practices and Decent Work, Human Rights, Society, and Product Responsibility. Table 7.1 covers social specific standard disclosures (impacts) covered under GRI.

7.2.2 Social Life Cycle Assessment

UNEP-SETAC report “Guidelines for Social Life Cycle Assessment of Products” (Althaus et al., 2009), the key report which contains guidelines to implement an sLCA, contains a list of social and socioeconomic impacts for five categories of stakeholders: workers, local community, society, consumers and value chain actors. This list of social impacts has been compiled from various sources including international conventions and treaties, CSR initiatives and social impact assessment literature. A related sLCA document contains a list of social impacts for consumers with respect to health and safety impacts across the Life Cycle (sLCA Consumer Health and Safety Sheets, 2010). Table 7.1 covers these lists of social impacts covered by the Althaus et al. (2009).

7.2.3 Social Impact Assessment Methodologies

Social impacts associated with product Life Cycles are also available in some relevant regulatory and technical guidelines. We focussed upon the social impacts mentioned in two sources: SEA Authorization guideline (ECHA, 2011) and six SEA authorization dossiers available by searching the ECHA website (http://echa.europa.eu/) and European Commission’s guidelines for Impact Assessment (EC Report, 2009). SEA is a route to REACH authorization that requires companies to demonstrate that the benefits of using a specific chemical in a manufacturing context significantly outweigh the costs (ECHA, 2011). The REACH SEA authorization guideline emphasizes two social impacts: employment and social inclusion, and refers to the EC Impact Assessment (IA) guideline for additional impacts (ECHA, 2011). EC’s

IA guideline lists potential social impacts related to the following areas: employment, job quality, social inclusion, gender equality, culture, public health and safety, crime and security, impacts on non-European countries, family life and privacy, governance and education (EC IA, 2009). Social impacts in these guidelines are not explicitly associated with specific stakeholders. Table 7.1 covers social impacts covered by the SEA Authorization guideline and IA guideline and indicators from SEA authorization dossiers.

7.2.4 Social Impacts from existing Product Sustainability Assessment tools

There are three tools that focus upon the social sustainability of products: SEEBALANCE, LICARA NanoSCAN and SHDB. BASF developed the SEEBALANCE tool to assess the sustainability footprint of products (https://www.basf.com/us/en/company/sustainability/management-and-instruments/quantifying-sustainability/seebalance.html). The social indicators included in SEEBALANCE were developed based on a review of 60 sustainable development documents from which 3200 social impacts were extracted, and further narrowed down to 33 impacts for the chemicals manufacturing sector (Schmidt et al., 2004). SEEBALANCE social profile is divided by impacts on five “stakeholders”: Employees, International community, Future Generations, Consumers and Local and national community. LICARA NanoSCAN uses social indicators like technological breakthrough, qualified labour force and global health or food situation (Som et al, 2014). SHDB contains country and sector-specific indicators for the themes of Human Rights, Labor Rights and Decent Work, Governance and Access to Community Services (Benoit-Norris et al, 2012a). Table 7.1 covers social impacts and indicators used in these tools.

7.3 Salient Social Impacts for Nano-enabled Products

In addition to extracting social impacts of products, the literature on social impacts of nanotechnology was also reviewed in order to understand which impacts were most relevant for nano-enabled products. The ELSI literature on nanotechnology is largely focused on risk perception, governance and ethical implications of nanotechnology, and only few publications focus on specific social impacts of nano-enabled products. While this is a large literature, Seear et al (2009) provides a comprehensive review of social and economic impacts of nanotechnology. This literature provides insight on social impacts that could be relevant to nano-enabled products.

Nano-enabled products may have features such as novel functionality, greater efficacy and lower cost over their conventional counterparts. These features may be linked to downstream end of the value chain and result in greater consumer satisfaction and provide solutions to pressing global problems (e.g. as operationalized in the sustainable development goals (SDG)) (Salamanca-Buentello et al, 2005; Cozzens et al, 2013; Som et al, 2014). These issues could be captured by social impacts mentioned under stakeholder categories of consumer (consumer satisfaction, ethical issues), community (contribution to SDG) and value chain (human rights enforcement through the supply chain, non-EU country impacts) in Table 7.1.

Proactive communication with workers, supply chain and consumers about nanosafety and other risks are emphasized by voluntary codes of conduct for nanotechnology (e.g. Responsible Code of Conduct (NIA Report, 2006) and BASF's Nanotechnology code of conduct(http://www.nanotechnology.basf.com/group/corporate/nanotechnology/en/microsites/nanotechnology/safety/code-of-conduct). Due to the significant uncertainty associated with nano-enabled products, it is important the latest information on occupational, consumer risks and environmental risks of ENM are shared within the value chain in a timely manner. Key forums to communicate risks may include a) direct communication with downstream value chain on ENM hazard and exposure, and b) informative consumer labels about the ENM used in the product and its known risks. These issues could be captured by social impacts mentioned under stakeholder category of consumer (consumer Health & Safety, quality of health and safety labelling and other information on other risks, complaints and feedback mechanism, transparent marketing communications) in Table 7.1.

Moreover, there may be more or different educational needs and in-house technical expertise involved in producing nano-enabled products than conventional products, and this expertise may need to be updated frequently (Malsch, 2013). These issues could be captured by social impacts mentioned under stakeholder category of worker (education and training) in Table 7.1.

Finally, loss of privacy and ethical implications may be associated with specific nanotechnology applications e.g. nanomedicine (Spagnolo and Daloiso, 2009, Kuiken, 2011). These issues could be captured by social impacts mentioned under stakeholder categories of consumer (ethical issues, consumer privacy, end of life responsibility), community (social diversity, cultural heritage, access to material resources, delocalization and migration) and value chain (respect for intellectual property rights) in Table 7.1.

This appraisal of the nanotechnology ELSI literature, while not specific to nano-enabled products, enables us to pinpoint some social impact categories that could be relevant to nano-enabled products (Section 7.4).

7.4 Selection of Quantitative Indicators

After compiling a list of social impacts for nano-enabled products (Table 7.1), the next step was to define indicators that could be used to build a quantitative methodology. One way to build a quantitative sLCA methodology is to create scores for each indicator in which data at the level of production line or company level are normalized to the same data at region or country level (Schmidt et al, 2004). These scores are dimensionless and enable aggregation of social impacts with heterogeneous units to consider the overall social profile of the product. To find region or country-level data that could be used to operationalize into indicators the social impacts listed in Table 7.1, the following sources were reviewed:

- OECD Science and Technology indicators database (http://www.oecd-ilibrary.org/science-and-technology/data/oecd-science-technology-and-r-d-statistics/main-science-and-technology-indicators_data-00182-en)
- World Bank Database (http://databank.worldbank.org/data/databases.aspx)
- International Labour Organization (ILO) Labour statistics database (http://www.ilo.org/inform/online-information-resources/databases/stats/lang--en/index.htm)
- United Nations Statistical Databases (http://unstats.un.org/unsd/databases.htm)
- World Health Organization (WHO) database (http://www.who.int/gho/publications/world_health_statistics/en/)
- Eurostat database (http://ec.europa.eu/eurostat/statistics-explained/index.php/Europe_in_figures_-_Eurostat_yearbook)
- Recent Company Annual Reports containing data on social impacts

Fifteen indicators were selected for inclusion and each indicator was classified in terms of stakeholder and Benefit/Cost. These indicators selected covered two stakeholders, namely worker (8 indicators) and community (7 indicators). The coverage in terms of classification as benefits and costs is as follows: 10 benefit indicators (6 indicators for workers and 4 indicators for community) and 5 cost indicators (2 indicators for workers and 3 indicators for community). Expert assessment deemed five indicators to be particularly relevant for nano-enabled products (shown in bold in Table 7.2). Two indicators in the community cost category are relevant only to developing countries (indicated in text in Table 7.2).

Table 7.2 Social Indicators in SIA methdology

Worker Benefits	Worker Costs
- Social Benefits and Pension **-Professional training** **-Tertiary education** -Female employees -Trade union membership -Collective agreements	-Strikes and lockout **-Non-fatal occupational injuries**
Community Benefits	**Community Costs**
-Employment -Employment to handicapped persons **-Patent applications** -Employees in Research and Development	-Poverty (if product is developed in a developing country) **-Research and Development (R&D) investment** -Child labour (if product is developed in a developing country)

7.5 Social Impact Assessment Methodology

The sLCA framework was linked to an MCDA method which comprises of the following steps: a) Normalization, b) Weighting, c) Aggregation, and d) Classification. MCDA comprises a large class of methods for the evaluation of different alternatives based on relevant criteria (Giove et al., 2009). In the Multi Attribute Value Theory (MAVT), a value function is specified for each criterion (Giove et al., 2009) and modified according to normalization and user weights and finally integrated into a common domain. The classification step proposes a method to derive benchmarks according to which outputs of the SIA sub-module can be compared to provide guidance to the user of DSS.

In environmental LCA, impacts can be clearly linked to functional unit but the cause and effect relationship is more ambiguous in the case of sLCA (Swarr, 2009; Klopffer, 2008; Dreyer et al, 2005). Ideally, the unit of analysis for the production scenario should be fairly specific but the appropriate level is not always easy to pinpoint, obtain data for, or interpret. For example, perhaps the most discrete unit of analysis for a production scenario is the manufacturing production line in which the product is manufactured. Having annual data for the production line allows the analysis of a decision context where a manufacturer can manufacture two types of products with similar functionality. However, the same production line is used to manufacture more than one product (particularly in medium and large industry) and hence the social indicator score in such contexts cannot be viewed as strictly associated with a single product. Due to the dynamic nature of the company context (e.g. mergers, data collection processes, etc.), data aggregated at higher units of analysis over the year is viewed as more reliable, meaningful and typically used in reporting. The explanatory value of the analysis results is a further test of the use of the appropriate unit of analysis.

7.5.1 Normalization

Social indicator scores represent the product development's annual share contribution to the country level social impact. Product development's social impact is defined in terms of the annual contribution of the chosen unit of analysis within the company. As available social indicator data for countries is not disaggregated in terms of Small and Medium Sized Enterprises (SME) and Large Industry (LI) contributions, country-level proxies for which data is classified as SME/LI are used to derive proxies. The "relative potential" of an SME or LI company to create a social impact in a country was derived using a) average number of employees for SME and LI, and b) average value added for SME and LI. Relative potential index was calculated for 22 EU countries and EU-28 group. Each social indicator is linked to one of these relative potentials based on if it was more closely linked to employment or value added. In the case of the 15 social indicators listed in Table 7.1, two are classified as linked to value added (i.e. Social Benefits & Pension and Research & Development investment), and the rest are classified as linked to employment. Both these relative potentials are used to derive the adjusted total number of companies, which in turn is used to derive the mid-level value for the social indicator for a SME and LI.

7.5.2 Weighting

Weighting involves the assignment of an importance value to social indicator scores based on personal, social or policy preference, mathematical properties, panel weighting approaches based on polls, etc. sLCA categorizes social impacts as being relevant to stakeholders like worker, consumer, value chain, legal framework, community or society. The SUNDS user may attach different value to different social indicators, as well as stakeholders through the Life Cycle. The SIA sub-module method accounts for this by using a nested weighing scheme.

Users are asked to define weights on a scale of 1-5 first at stakeholder level and then at social indicator level. MAVT value functions for both sets of weights are normalized in order to have a sum of one. Stakeholder and indicator weights are integrated with each (normalized) social indicator value function.

7.5.3 Aggregation

Normalized and weighted social indicator value functions are aggregated as overall benefit and cost scores using weighted sum of the social indicator scores classified as benefit and cost respectively. Net benefit score is the difference between benefit and cost score. In addition, stakeholder percentage of impacts calculate the relative share of benefits and costs generated by each stakeholder.

7.5.4 Classification

Social indicator and aggregated scores are closely tied to the relevant social context and can vary significantly even in the same country in terms of social values, type of industrial structure, laws and regulations, preferences and other factors. To guide the user, a classification system was developed and implemented as default option in SUNDS. It is based on the assumption that one of the key factors that can cause social impacts or benefits are significantly different for companies of different sizes. The overall social impact in a country is composed of different activities within that country (including industry), and the size of the industrial enterprise influences its capacity to create social impacts at country level. We therefore explored the idea to develop thresholds of High, Medium and Low classes for SME or LI.

The mid-value of the social impact (obtained as described in Section 7.5.1) is divided by the social indicator data at country level to obtain benchmarks for SME and LI. Low/Medium and Medium/High thresholds are defined using 80% and 120% of benchmark’s value. Thresholds for aggregated scores are calculated for SME and LI by following the same process of weighting and aggregation.

Section C: Application to case studies

CHAPTER 8: SUNDS Application

This chapter demonstrates the application of SUNDS methodology (described in Chapters 4, 5 and 6) to two case studies of real nano-enabled industrial products: nano-copper oxide based wood preserving biocidal paint (Section 8.1) and two kind of pigments: nano-sized organic pigment (n-OP) and nano-sized carbon black (n-CB) used to colour a plastic automotive part (bumper) (Section 8.2). First, the case study is described (Section 8.1.1 and Section 8.2.1 for paint and pigments respectively), followed by description of input data used (Section 8.1.2 and Section 8.2.2 for paint and pigments respectively). Then, the results of application of Tier 1 are presented (Section 8.1.3 and Section 8.2.3 for paint and pigments respectively), followed by the decision support outcome on nano-enabled product development (Section 8.1.4 and Section 8.2.4 for paint and pigments respectively). Tier 2 application is presented first for RC methodology (Section 8.1.4 and Section 8.2.4 for paint and pigments respectively), followed by SEA methodology (Section 8.1.5 and Section 8.2.5 for paint and pigments respectively). The results of case study application are then discussed (Section 8.1.6 and Section 8.2.6 for paint and pigments respectively).

8.1 Nano-copper based biocidal paint case study

8.1.1 Description of case study

Wood preservation treatment is indispensable to increase the service life of timber by imparting it with bactericidal, fungicidal and insecticidal properties (Freeman and McIntyre, 2008; Lebow et al., 2004). Improving the efficacy of wood preservation treatments and ability to use a variety of timber species can limit deforestation and also save human labour to build essential infrastructure (http://www.wei-ieo.org/woodpreservation.html). While impregnation of wood with chemical preservatives using pressure treatment is the most effective way to achieve good penetration and retention, superficial treatments may also be used when lesser protection is required, if pressure treatment is not practicable for any reason or for consumer based applications. Non pressure treatments include non-pressure impregnation (e.g. brief dipping, cold soaking and steeping, diffusion processes, vacuum processes) and in situ treatments (e.g. surface treatments using spraying, brush and paste application, installation of internal diffusible chemicals, internal fumigant treatments) (Lebow et al., 2004).

Copper based formulations have been widely used for several years particularly in ground contact applications to treat timber due to their effectiveness as a biocide and low mammalian toxicity (Lebow et al., 2004; Freeman and McIntyre, 2008). The biocidal mechanism of copper based formulations is based upon the cupric ion's interference with homeostatic processes and cell membrane functions, protein and enzyme damage and precipitation, production of reactive oxygen species and DNA disruption. Copper is the only biocide that successfully inhibits wood decomposition by soft rot fungi (Civardi et al., 2015a). Key limitations of copper based wood preservation formulations include lack of efficacy to treat some copper tolerant wood destroying fungi (*Basidomycetes*, fungi included in genera *Serpula* and some fungi species once included within the genus *Poria*), refractory wood species (e.g. several species of fir) (Civardi et al., 2015b; Freeman and McIntyre, 2008) and aquatic toxicity (Freeman and McIntyre, 2008).

This case study assesses through the life cycle a hypothetical n-CuO-based biocidal paint manufactured in Germany by comparing it to a conventional acrylic paint (CAP) applied to a wooden garden fence. The function of both paints is to protect a wooden fence consisting of poles and boards in ground contact and fully exposed to the weather. In addition to weathering protection provided by CAP, the n-CuO paint also provides a biocidal functionality (decay by micro-organisms especially soft rot fungi) to the softwood cladding. The following functional unit is specified for this case study: The provision of a physical and visual boundary by a square meter of softwood fence for one year. It should be noted that while a square meter of painted wood is specified as the functional unit, as emissions occur over all painted surfaces, a painted wood volume of 0.016 cubic meter is considered (assuming 16 mm plank thickness). Two coats of paint are applied to the wood, resulting in a paint consumption of 0.203 liter/square meter. The wooden fence is re-painted every five years and the cladding is reinstalled every 20 years in the case of n-CuO paint and every 10 years in the case of CAP.

Both paints are produced using similar manufacturing processes, except the manufacture and use of n-CuO. n-CuO is made from a copper inorganic precursor (copper carbonate) which is freshly synthesized and dried at ca. 100°C. The dried milled precursor is then decomposed at ca. 350°C for several hours with periodical slight mixing during the decomposition. n-CuO used in the paint has a particle size of 3-35 nm. It is mixed with an acrylic base to produce the nano-enabled paint according to composition specified in Table 8.1. CAP contains the same components except n-CuO, which is replaced with additional titanium dioxide. The density of both paints is assumed as 1.3 kg/liter.

Table 8.1 Composition of n-CuO wet and dried paint in percentage by mass

Component	Wet paint (%)	Dried paint (%)
Binder	24.0	51.7
TiO_2	19.7	42.5
Organics	1.7	3.8
Biocide (to preserve paint against microbial attack)	0.2	0.5
n-CuO	0.7	1.5

8.1.2 Input data

Inputs to produce benefit, risk and decision graphs in Tier 1 was solicited from an industrial expert in wood preservation in Germany who had amateur (consumer) experience in painting wooden fences. The inputs to Tier 1 provided by the expert is presented in Appendix 1. The interpretation of the graphical results are provided in 8.1.3.

The input data required for applying Tier 2 HHRA consists of occupational and consumer risks occurring within the four lifecycle stages. The number of human health risks estimated per lifecycle stage for this case study were as follows: two for synthesis stage (1 occupational risk via inhalation, 1 occupational risk via dermal contact), six for production stage (3 occupational risk via inhalation, 3 occupational risks via dermal contact), four for use stage (2 consumer risks via inhalation, 2 consumer risks via dermal contact) and two for end of life stage (1 occupational risk via inhalation and 1 dermal contact).

For the Tier 2 ERA methodology application, the input data for the case study consists of ecological risks in different environmental compartments investigated for each of the four lifecycle stages. Deterministic PNEC for pristine n-CuO was derived for species representing terrestrial and aquatic ecosystems. PNEC for terrestrial systems (0.19 mgCu/kg soil) was based on a single effect concentration 10% (EC_{10}) available for an *Enchytraeidae* divided by an assessment factor (AF) of 100. PNEC for aquatic systems (0.003 µg/L water) was based on a single EC_{10} available for *Lymnaea stagnalis* divided by an AF of 1000. Table 8.2 lists mean values of PEC distributions for the environmental compartments considered in this assessment. Probabilistic RCR were calculated for 24 relevant cases (i.e. 6 for each life cycle stage). For the global ecological risk, the highest calculated life cycle stage risk was used.

Table 8.2 Mean values of Predicted Environmental Concentrations (PEC) distributions used for n-CuO paint ERA

Environmental Compartment	Unit of measure	Global	Synthesis	Production	Use	EoL
Soil (Natural and Urban)	µg/kg·y	1.03E-02	0.00E+00	1.78E-06	2.98E-03	7.36E-03
Soil (Sludge treated)	µg/kg·y	2.35E-01	0.00E+00	1.42E-01	9.30E-02	0.00E+00
Surface water	µg/L	1.49E-04	0.00E+00	8.33E-05	5.78E-05	8.08E-06
WIP waste	mg/kg	8.46E-01	0.00E+00	0.00E+00	1.59E-02	8.30E-01
WWTP effluent	µg/L	1.92E-03	0.00E+00	1.16E-03	7.57E-04	0.00E+00
WWTP sludge	mg/kg	1.65E-01	0.00E+00	9.99E-02	6.54E-02	0.00E+00

To apply risk control methodology to unacceptable risks, TARMM relevant to exposure scenarios were collected from industry and exposure assessment experts. Efficiency for these TARMM was derived by calculating average of literature values for each TARMM. Cost ranges were derived wherever possible using internet search.

Reference method using endpoints (human health, ecosystem and resources) was applied to obtain the classification of Tier 2 LCIA results, which are provided in Table 8.3 below. Reference method was also applied to 12 ReCIPe midpoints (Climate change, Ozone depletion, Terrestrial acidification, Freshwater eutrophication, Marine eutrophication, Human toxicity, Photochemical oxidant formation, Particulate matter formation, Terrestrial ecotoxicity, Freshwater ecotoxicity, Marine ecotoxicity, Ionising radiation, Agricultural land occupation, Urban land occupation, Natural land transformation, Water depletion, Metal depletion and Fossil depletion) expressed as shadow prices to support the interpretation of results (results not presented).

Table 8.3 LCIA endpoint scores for n-CuO paint (nCuO) and conventional paint (CAP) scenarios

	Global		Synthesis		Production		Use		End of Life	
	CAP	nCuO	CAP	nCuO	CAP	nCuO	CAP	nCuO	CAP	nCuO
Aggregated scores	1.07E+01	1.54E+01	9.62E+00	1.40E+01	5.39E-01	6.74E-01	6.56E-04	6.06E-02	5.06E-01	6.51E-01
Human Health	5.27E+00	7.69E+00	4.27E+00	6.60E+00	2.61E-01	3.28E-01	5.33E-05	1.91E-03	7.39E-01	7.58E-01
Ecosystems	2.45E+00	2.83E+00	1.86E+00	2.02E+00	1.34E-01	1.48E-01	6.02E-04	5.87E-02	4.61E-01	6.02E-01
Resources	2.94E+00	4.89E+00	3.49E+00	5.40E+00	1.43E-01	1.98E-01	0.00E+00	0.00E+00	-6.93E-01	-7.09E-01

Reference method was applied to obtain classification for Tier 2 EA results for this case study, which are provided in Table 8.4 below. These aggregated scores were obtained by eliciting data from industrial experts familiar with manufacturing processes and with amateur (consumer) experience in painting wooden fences. Publically available information on prices for disposal of wooden waste for Germany was used to calculate end-of-life costs for the functional unit.

Table 8.4 Aggregated EA scores in unit Euros for n-CuO paint and conventional paint (CAP) scenarios

	n-CuO paint	**CAP**
Global	2.224	1.777
Synthesis	0.099	0
Production	0.259	0.207
Use	1.841	1.520
End of Life	0.025	0.05

Tier 2 SIA aggregated scores are calculated for the nano-enabled products i.e. n-CuO paint, n-OP bumper and n-CB bumper are identical as they are proposed to be manufactured in the same company. The input data for SIA for these case studies comprises of aggregated scores not split by lifecycle stage and include net benefit, benefit and cost scores. They are provided in Table 8.5 below.

Table 8.5 Aggregated SIA scores for n-CuO paint, n-OP bumper and n-CB bumper scenarios

Aggregated Score	**n-CuO, n-OP and n-CB Score**
Cost score	6.7E-02
Benefit score	2.5E-01
Net Benefit Score	1.7E-01

8.1.3 Application of SUNDS Tier 1 to nano-copper based biocidal paint case study

The methodology used in Tier 1 has already been described in Section 4.2.1. Briefly, there are three benefit modules (Modules 1-3) and three risk modules (Modules 4-6), which are integrated on a two dimensional Benefit-Risk scale divided into four quadrants (Module 7).

The single score for each benefit and risk module (except Module 5) is an average of all criteria that it includes. In the occupational risk module, the single score is based on the worst case exposure chosen from manufacturing of nanomaterial, processing of nanomaterial and application of nano-enabled product.

The results for application of Tier 1 methodology for the n-CuO paint are presented in this section. Module 0 assessed that the nano-copper oxide based paint is a nano-enabled product, and n-CuO as well as the paint itself would need to be approved under Biocidal Products Regulation (BPR). This information has an economic implication: regulatory approval involves significant costs and affects the time to market.

Figure 8.1 shows the relative benefits of the n-CuO paint obtained from application of Modules 1-3. Compared to CAP, the n-CuO paint had positive environmental (average score = 0.11) and economic benefit (average score = 0.33), while social benefits of both paints were identical (average score= 0).

While the average environmental benefit was positive (Module 1), the manufacturing stage of the n-CuO paint was worse than CAP (normalized score = -0.62) in terms of consumption of energy and hazardous materials. n-CuO paint had a better use (normalized score = 0.46) and end of life stage (normalized score = 0.50) profile than CAP. The uncertainty in environmental benefits (shown by the error bars) is due to lack of information about the waste generated in the manufacturing stage and the effectiveness of the End-of Life treatment.

The economic benefit of the n-CuO paint (Module 2) was due to foreseen market potential (normalized score = 0.50) in a medium sized market and profitability (normalized score = 0.50) due to lower operational costs during use stage. There are no advantages in terms of time to market the n-CuO paint due to the need to get BPR approval.

The three social benefits considered for n-CuO paint (Module 3) viz. technological breakthrough, highly skilled labour force and improvements to food/health are identical to CAP.

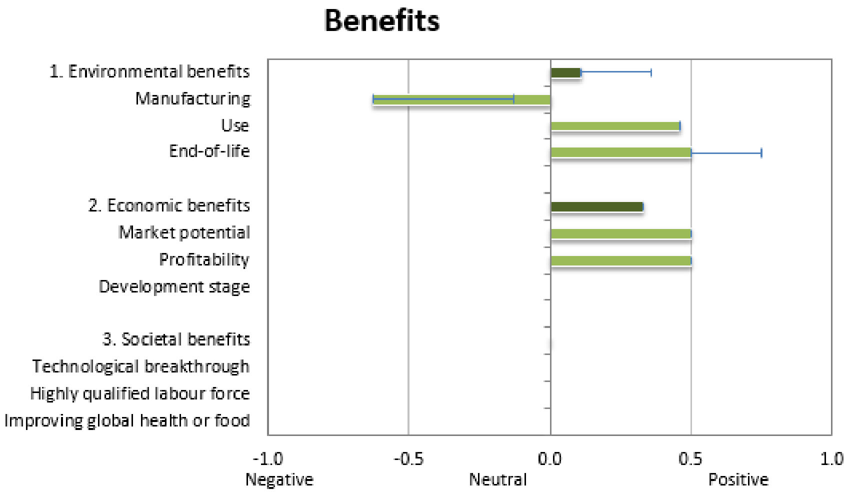


Figure 8.1 Results of application of benefit modules of Tier 1 to n-CuO paint scenario

Figure 8.2 shows the risks of the n-CuO paint obtained from application of Modules 4-6. Risks for n-CuO paint were greatest for public health and environment (average score=0.65), followed by equal scores for occupational health and consumer health (score for each=0.43). The scores for the public health and environmental risks approaches the threshold for the class of high (around 0.67), while the other risks are medium. There are no uncertainties in risk estimation for n-CuO paint (which can occur only in public health and environmental risk module and consumer risk module).

In the case of public health and environmental risks (Module 4), the most significant contributor to the average score was potential effect based on free radical activity and oxidative stress (normalized score=1.0), followed by potential input into the environment through the life cycle (normalized score=0.63) and system knowledge (normalized score= 0.33).

In the case of occupational risks (Module 5), the greatest occupational risk was caused by nanomaterial manufacture (normalized score=0.43), which corresponds to a Stoffenmanager Nano control banding classification of C2 (classified as medium risk). Nanomaterial processing and nano-enabled product application had equal occupational risk with normalized score for each=0.29 (Stoffenmanager Nano control band C1 classified as low risk). In the case of consumer risks (Module 6), while exposure potential existed due to surface bound particles (n-CuO dispersed in paint and applied to wood), the size of the consumer population was low (fraction of households less than 5%). The combination of these criteria corresponds to an exposure band of 2 (on a scale of 1-4). The worst hazard score from Module 6 is C, corresponding to a consumer risk control banding classification of C2 (normalized score=0.43).

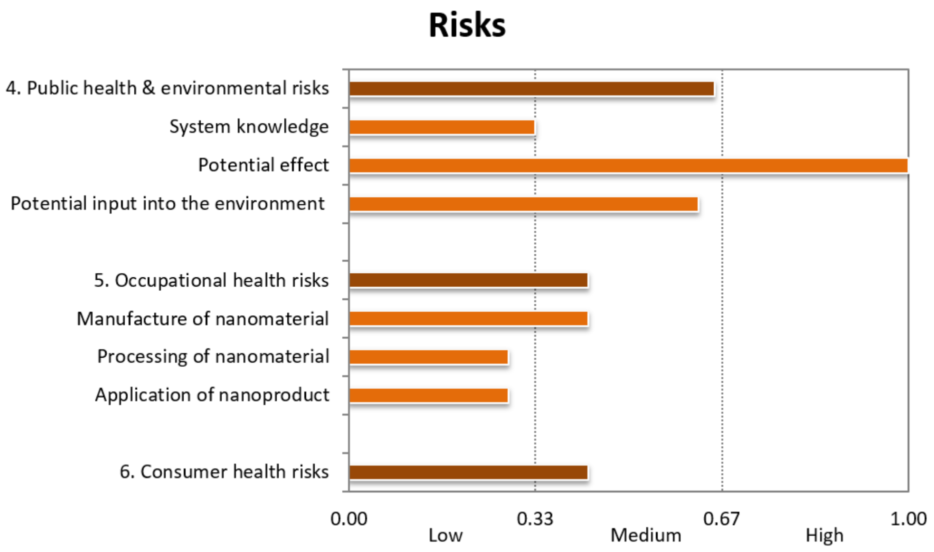


Figure 8.2 Results of application of risk modules of Tier 1 to n-CuO paint scenario

Figure 8.3 shows the two-dimensional space where benefit and risks are integrated for n-CuO paint, and the result lies in the quadrant “Cancel/Rethink”. Although the result is somewhat closer to the yellow "undecided" area, this first tier assessment suggests that given significantly higher risks over benefits n-CuO paint is not likely to be a commercially successful product. The highest risk module score is for public health and environmental risks with an average score equal to 0.65 (which is quite close to the high risk threshold of 0.67). Even lowest risk module scores (i.e. occupational and consumer risks at 0.43) are higher than the highest overall benefit score (i.e. average economic benefit score at 0.33) and there are no social benefits.

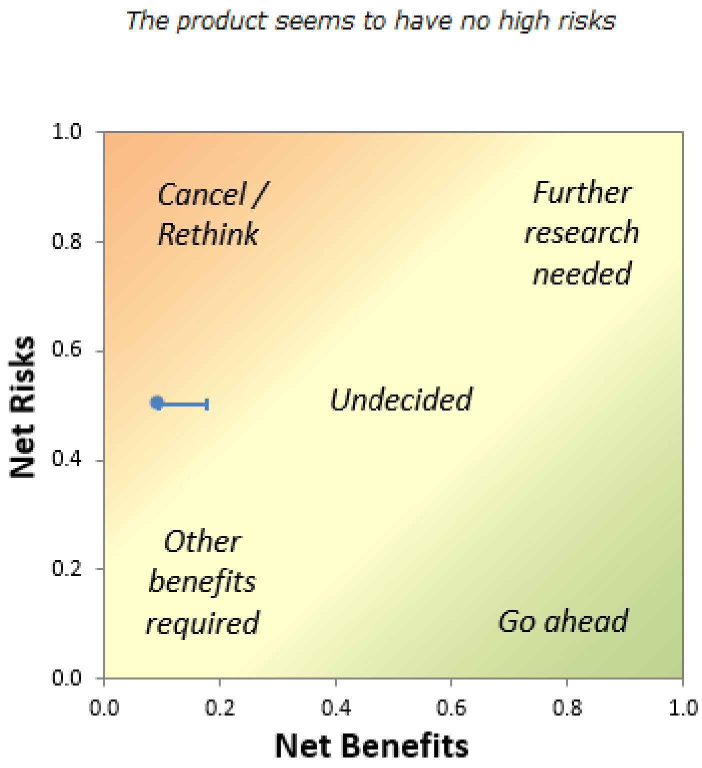


Figure 8.3 Result of the application of the decision support module of Tier 1 to n-CuO paint scenario

8.1.4 Application of n-CuO biocidal paint case study to SUNDS Tier 2 Risk Control Methodology

Application of Tier 2 ERA classification methodology yielded a global score classified as unacceptable (Figure 8.4a). This was mainly due to the unacceptable risk of WIP waste in the end of life stage (Figure 8.4b). Other ecological risks needing further consideration regarded production stage and use stage (both due to the risks estimated for the compartments WWTP effluent and WWTP sludge) (Figure 8.4b). Currently, in the TARMM database there are not solutions applicable for the control of ecological risks and therefore it was not possibile to build alternative scenarios to address the estimated unacceptable ecological risks for this product.

Application of Tier 2 HHRA classification methodology yielded a global score classified as unacceptable (Figure 8.4a) due unacceptable risks in production and use stages (Figure 8.4b). In the case of human health risks that need further considerations (two) or are unacceptable (three), industry and exposure assessment experts were consulted about suitable TARMM to reduce them. Reduced exposure concentrations resulting from TARMM application are used to re-estimate risks and assess if they are controlled. Table 8.6 illustrates the application of the RC methodology to n-CuO paint using a variety of suitable TARMM. The initial risk and re-estimated risk are colour coded according to the HHRA classification methodology (described in Section 5.1).

Table 8.6 Application of TARMM to unacceptable human health risks in n-CuO paint lifecycle

LCA stage	**Target**	**Exposure scenario**	**Exposure route**	**Initial exposure concentration**	**Initial Risk estimation**	**Relevant TARMM with efficiency**	**Exposure concentration with TARMM application**	**Risk re-estimation**	**TARMM cost**
Production	Occupational	Incorporating n-CuO to the paint matrix	Inhalation	Near Field (NF) 9.7 mg/m^3	100% (Near Field)	Local exhaust ventilation = 90%	NF 0.97 mg/m^3	99.99%	Local Exhaust Ventilation (LEV, vertical/horizontal laminar flow hood): €3280 to €5818
Production	Occupational	Sanding wood treated with n-CuO paint (estimation through Scanning Mobility Particle Sizer (SMPS))	Inhalation	0.015 mg/m^3	5.86%	FFP3=96.88%	0.0005mg/m^3	0%	FFP3 mask: €5
Production	Occupational	Sanding wood treated with n-CuO paint (estimation through Optical Particle Sizer (OPS))	Inhalation	0.32 mg/m^3	99.46%	FFP3=96.88%	0.01 mg/m^3	1.75%	FFP3 mask: €5
Use	Consumer	Airborne particles released due to sanding or sawing wood treated with n-CuO paint (estimation through SMPS)	Inhalation	0.015 mg/m^3	5.86%	Reusable Cloth mask=20.08%	0.012 mg/m^3	3.12%	Respro Bandit mask =€22.50 Breathe Healthy Cloth mask=€14.50

LCA stage	**Target**	**Exposure scenario**	**Exposure route**	**Initial exposure concentration**	**Initial Risk estimation**	**Relevant TARMM with efficiency**	**Exposure concentration with TARMM application**	**Risk re-estimation**	**TARMM cost**
Use	Consumer	Airborne particles released due to sanding or sawing wood treated with n-CuO paint (estimation through SMPS)	Inhalation	0.015 mg/m^3	5.86%	FFP2 mask= 92.59%	0.001 mg/m^3	O%	Disposable FFP2 mask=€0.25
Use	Consumer	Airborne particles released due to sanding or sawing wood treated with n-CuO paint (estimation through OPS)	Inhalation	0.32 mg/m^3	99.46%	Reusable Cloth mask=20.08%	0.256 mg/m^3	98.83%	Respro Bandit mask =€22.50 Breathe Healthy Cloth mask=€14.50
Use	Consumer	Airborne particles released due to sanding or sawing wood treated with n-CuO paint (estimation through OPS)	Inhalation	0.32 mg/m^3	99.46%	FFP2: 92.59%	0.002 mg/m^3	0.001%	Disposable FFP2 mask=€0.25

Table 8.6 shows TARMM application for risks that are unacceptable or needing further consideration. In the production stage, risk was successfully controlled to acceptable thresholds in all cases except incorporation of n-CuO to the paint matrix. Despite investing in a sophisticated TARMM like LEV, risk could not be controlled. This suggests that in the paint formulation it is difficult to control the risks of a hazardous nanomaterial to acceptable levels using currently available TARMM. The risk assessment is strongly affected by a very low DNEL of CuO for inhalation, which is based on a lower confidence level of benchmark dose (BMDL)= 0.16 mg/m^3. This will produce unacceptable risks, even at very low exposure estimations. In this specific aspect, Safety by Design (S-by-D) strategies that control exposure to powders may be relevant, provided they are feasible in other respects (e.g. retaining functionality, affecting release in other scenarios).

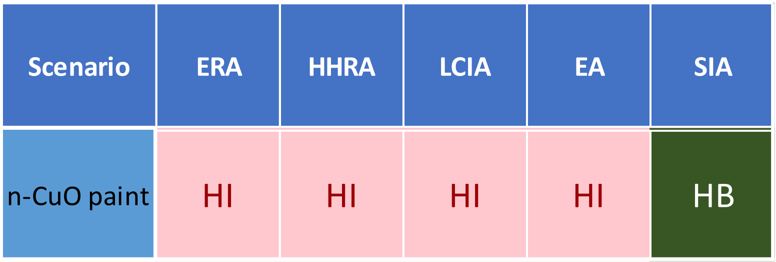
In the case of occupational and consumer risks due to exposure to airborne particles released due to sanding or sawing wood treated with n-CuO paint, some respiratory protective equipment are implemented for risk control of a single worker or consumer including FFP3 mask in occupational setting and FFP2 mask and cloth masks (detailed in Rengasamy et al. (2010)) in consumer setting. FFP3 and FFP2 masks were successful in controlling sanding/sawing risks derived using SMPS and OPS measurements. Cloth masks were successful in controlling sanding/sawing risk derived using SMPS measurement, but they could not control risk derived using OPS measurement. In addition to evaluated TARMM, Rengasamy et al. (2010) examine also the use of other fabric materials like sweatshirts, T-shirt, scarf and towels which provide some protection and may serve risk management purpose at an even lower cost. Here, however, assume the fabric will be washed, nano-wastes be transferred to waste treatment, and n-CuO paint ecological risks for waste in the use stage are already unacceptable. Hence, in the interest of environmental protection, the masks (in particular FFP3 and FFP2 masks) may be a better option to protect consumers in vicinity of sanding or sawing operations. Among the TARMM effective in control of sanding/sawing risks, FFP2 is the cheapest. In addition to these personnel protective equipment, sanding devices are equipped with air suction and filter bags, which are expected to further reduce exposure.

8.1.5 Application of n-CuO biocidal paint case study to SUNDS Tier 2 Socioeconomic Assessment methodology

The SEA sustainability portfolios for n-CuO paint are provided in Fig 8.4 a and b, according to the classification of obtained global scores and lifecycle stage scores, respectively.

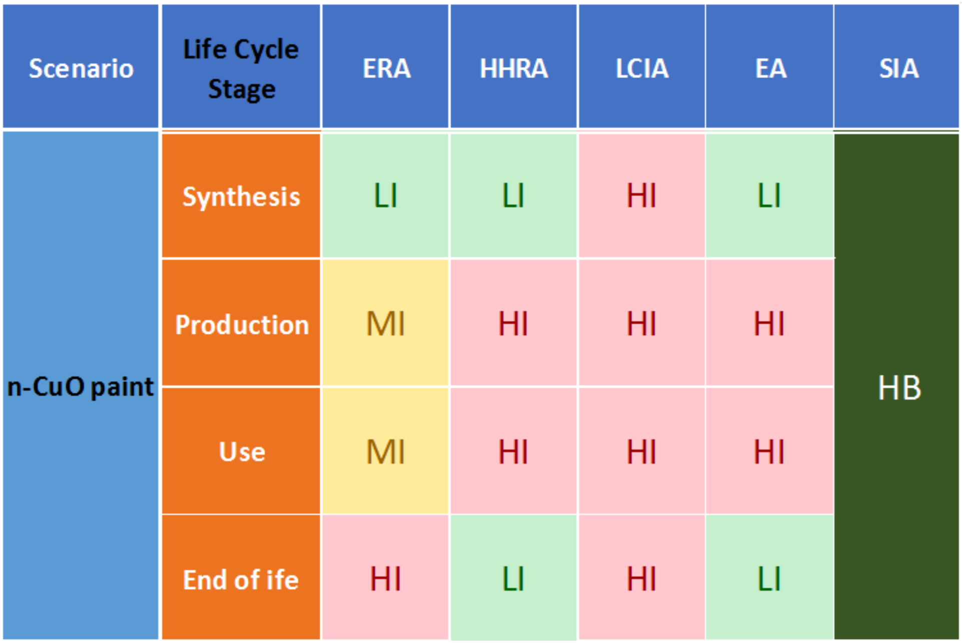
The application of Risk Control for n-CuO paint (Table 8.6) did not change the SEA global portfolio (Figure 8.4c) but it changed the HHRA use stage in the lifecycle portfolios (Figure 8.4d).

a)



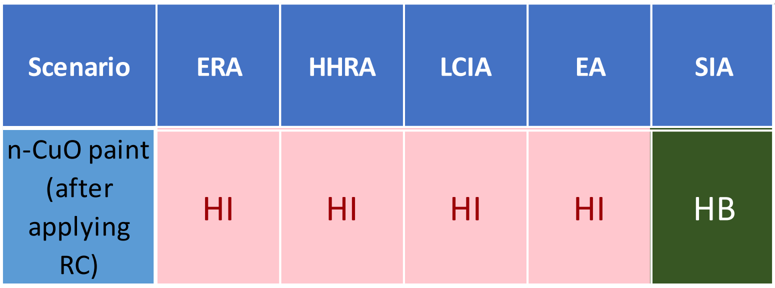
Scenario	ERA	HHRA	LCIA	EA	SIA
n-CuO paint	HI	HI	HI	HI	HB

b)



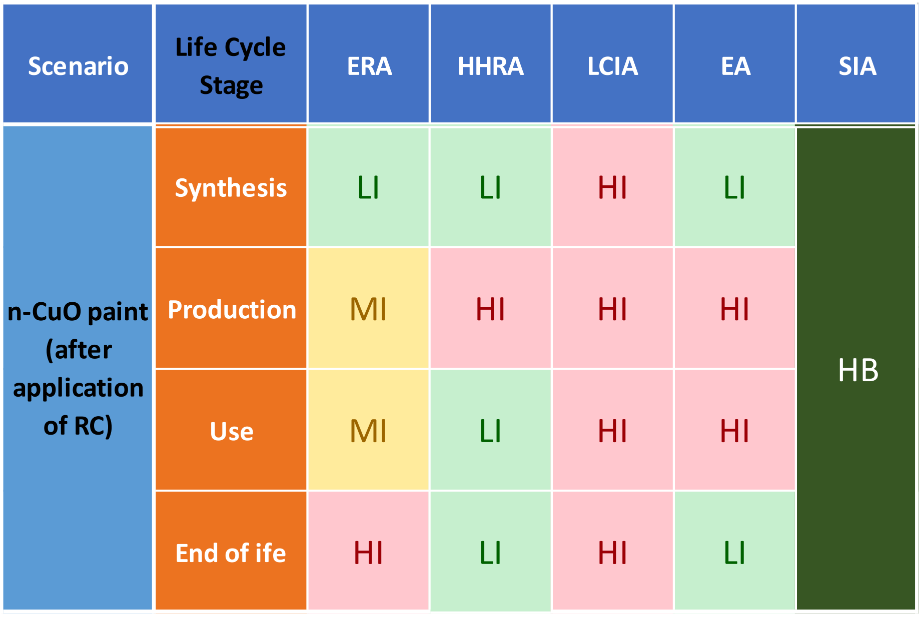
Scenario	Life Cycle Stage	ERA	HHRA	LCIA	EA	SIA
n-CuO paint	Synthesis	LI	LI	HI	LI	HB
	Production	MI	HI	HI	HI	
	Use	MI	HI	HI	HI	
	End of ife	HI	LI	HI	LI	

c)



Scenario	ERA	HHRA	LCIA	EA	SIA
n-CuO paint (after applying RC)	HI	HI	HI	HI	HB

d)

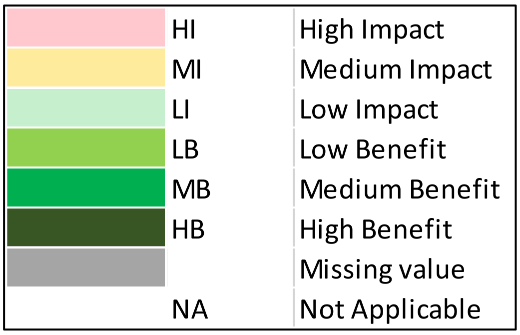


Scenario	Life Cycle Stage	ERA	HHRA	LCIA	EA	SIA
n-CuO paint (after application of RC)	Synthesis	LI	LI	HI	LI	HB
	Production	MI	HI	HI	HI	
	Use	MI	LI	HI	HI	
	End of ife	HI	LI	HI	LI	

Figure 8.4: SEA global sustainability portfolio for n-CuO paint before (a) and after (c) RC application, and SEA lifecycle stage sustainability portfolio for n-CuO paint before (b) and after (d) RC application.

S: Synthesis, P: Production, U: Use; E: End of Life.

LEGEND



🟥	HI	High Impact
🟨	MI	Medium Impact
🟩	LI	Low Impact
🟩	LB	Low Benefit
🟩	MB	Medium Benefit
🟩	HB	High Benefit
⬜		Missing value
	NA	Not Applicable

According to the global SEA classification, only SIA shows high benefits (Figure 8.4c).The lifecycle sustainability portfolio (Figure 8.4d) informs us that the synthesis stage has the best sustainability portfolio. End-of-life portfolio has two high impacts and two low impacts. The sustainability portfolio of production and use are initially similar, but use stage improves on applying RC. SIA classification is high benefit but not split by lifecycle stage. Lifecycle classification for each Tier 2 methodology is discussed below.

Application of ERA classification methodology yielded an unacceptable risk due to WIP waste in the end of life stage and two risks in production and use stages needing further consideration. The ERA global classification (Figure 8.4c) is in agreement with Tier 1 Public health and environmental risks (Module 4) analysis, which shows overall high risks. Tier 1 Public health and environmental risks are not split by lifecycle stage and the criteria potential effect and potential input into the environment correspond to a semi-quantitative evaluation of PNEC and PEC respectively. A high score for potential effect and a medium score (close to high threshold) for potential input into the environment suggests that at least some unacceptable ecological risks would be present, as found in Tier 2.

Application of HHRA classification methodology yielded unacceptable risks in production stage, and low risks for synthesis, use (after applying RC) and end of life stages. Tier 1 Occupational risks (Module 5) evaluates risks in synthesis and production stages using a control banding approach, and yielded two low risks (processing and application of nanomaterial) and one medium risk (manufacture of raw material). Tier 1 Consumer risks (Module 6) evaluates risk in use stage, and yielded medium risk. Tier 1 application has thus correctly identified scenarios which show unacceptable risks in Tier 2 HHRA analysis, although classification labels (i.e. low, medium and high) between the two tiers are not precisely aligned. Exhaustive testing to case studies is required to validate if this is globally true.

According to LCIA classification, n-CuO paint results in high environmental impacts compared to the CAP, according to the reference method (Fig 8.4d). However, by applying reference method to shadow prices (results not shown), a low benefit was seen in the end of life stage. Detailed results on reference method applied to midpoints and endpoints (results not shown) show a corresponding medium benefit in the endpoint “resources” which is the outcome of energy recovery in the municipal solid waste incinerator (as modelled in the LCA). In terms of shadow prices (results not shown), n-CuO paint translates into medium benefit for ozone depletion, terrestrial acidification, freshwater eutrophication, marine eutrophication, human toxicity, particulate matter formation, terrestrial ecotoxicity, ionising radiation, agricultural land occupation, natural land transformation and water depletion. These results are in broad agreement with Tier 1 Environmental Benefits (Module 1) analysis for the manufacturing and end-of-life stages, where high impact and medium benefit can be seen seen respectively. However, Tier 1 analysis shows a medium benefit in the use stage , while the classification in Tier 2 analysis is high impact. Tier 1 is semi-quantitative and its criteria do not correspond exactly to those within Tier 2, hence the exact cause for this cannot be pinpointed. It should be noted that none of the criteria for Environmental Benefits for Tier 1 (Appendix 1) perform worse for n-CuO paint in comparison to CAP. Four out of the seven criteria perform identically for both scenarios (e.g. hazardous substance used for maintenance, amount of wastewater, hazardous emissions and efficiency of use), while the rest are better for n-CuO paint (e.g. product lifetime, need for maintenance, amount of solid waste).

According to EA classification, n-CuO paint results in high costs for global as well as production and use stages compared to CAP. Synthesis cost for n-CuO paint cannot be classified with respect to synthesis cost for CAP (which is zero). As the synthesis cost for n-CuO paint is lower than 33% of the market price, it classified as low cost. End of life cost for n-CuO paint results in low classification as it required only single disposal over twenty years, as compared to two disposal events for CAP. While comparing these findings with Tier 1 Economic Benefits (Module 2) results, it must be noted that Tier 1 criteria (market potential, profitability and development stage) are comparable to Tier 2 use stage score (which may also include operational and maintenance cost if applicable). For this case study, the high impact for the Tier 2 use stage includes aspects represented by Tier 1 score (classified as medium) for the manufacturer as well as maintenance cost to the consumer for the functional unit.

The SIA classification for n-CuO paint in the specific company and country context shows high net benefit, which is composed of high benefits and costs. The social indicator which has the most significant magnitude in cost category is research and development expenditure. n-CuO paint is particularly favourable to workers, with high benefits and low costs (Subramanian et al, submitted). These results are not in agreement with Tier 1 Social Benefits (Module 3) analysis, which shows no benefit for the criteria mentioned (and equal benefit due to n-CuO paint and CAP). As Tier 1 is semi-quantitative, comparative and its criteria are different from those used within Tier 2, results from the two tiers are not comparable.

From the sustainability pillars view, environmental and economic aspects of n-CuO paint need improvement. Detailed results for each methodology offer further prescription in how this can be done, particularly in the case of HHRA where RC is directly implemented through TARMM (Table 8.6). Here it must be noted that only occupational and consumer risks (as per SMPS exposue estimate) of sanding could be controlled. The risk of incorporting n-CuO into paint, which is a key step in imparting biocidal property to a coating using nanomaterial, could not be adequately controlled.

Tier 1 analysis of the n-CuO paint indicate that n-CuO paint is not a very promising commercial prospect with a medium-sized market (sales between €1000 and €1000,000), significant time to market, and high costs for BPR approval. The risks are also not insignificant, which is reiterated by Tier 2 risk assessment results. There are unacceptable ecological risks in waste, and risks needing further consideration in production and use stages. There are unacceptable occupational and consumer risks in production and use stages, and only use stage risks can be controlled to acceptable levels using FFP2 masks.

Industrial experts conveyed the opinion that the biocidal performance of the n-CuO paint and its physicochemical parameters to be modified in an S-by-D approach to control the release of copper ions and/or particles are likely to be in conflict. S-by-D design strategies were investigated in SUN project through development of different surface coatings for n-CuO that decrease the hazard and consequently the risk. Nevertheless, to overcome conflict between desired mitigation of risk and the preservation of toxicity against bacteria is necessary to identify and properly modify physicochemical properties that can improve antibacterial properties, minimising human or environmental potentially adverse effects. Such challenging goal that can be extended to any other nanomaterial designed and used in antibacterial application can be won only if different mechanisms of action drive the two biological effects and if there are properties that can maximise one despite to the other. From evidence collected in EU FP7 Sanowork project and SUN project, ion speciation and bioavailability seem to be the key metrics to play with, in order to discriminate in a beneficial way between toxicological and antibacterial reactivities (Blosi et al., submitted). In summary, the development of a S-by-D strategies for n-CuO is still in development and could not be currently implemented in this thesis. When an S-by-D development is completed, ERA and HHRA will be performed again according to new (eco)toxicological information, and RC will be implemented if necessary.

To conclude, it appears that while n-CuO paint is an innovative product there is a lack of enough benefits to warrant proceeding with its commercial production (also in light of existing wood preservative products in the market).

8.2 Nano-pigment coloured automotive part case study

8.2.1 Description of case study

Automobile weight reduction is a known strategy to address growing concerns about greenhouse gas emissions and fuel use by passenger vehicles, with a 10% reduction in vehicle weight cutting fuel consumption by about 7% (Cleah, 2010). The growing use of plastics in interior, exterior, and under bonnet components of automobiles reduce automobile weight, improve aesthetics, vibration and noise control, and cabin insulation (Research and Markets Report, 2015). Among all the automotive plastics, polypropylene is the most used (with a market share of 37%), followed by polyurethane, acrylonitrile-butadiene-styrene, high density polyethylene, composites, polycarbonate and polymethyl methacrylate (Research and Markets Report, 2015). The automotive plastics market for passenger cars is projected to be a 40.1 billion market by 2020 (Research and Markets Report, 2015). Nano-enhanced functionalities to automotive plastics include abrasion resistance (e.g. using metal oxide coatings), protection from ultraviolet radiation (e.g. nano-zinc oxide and nano-titanium dioxide), anti-fogging functionality (e.g. nano-titanium oxide coating, silica nanoparticles and polyallylamine hydrochloride composite coating), self-cleaning functionality (e.g. nano-titanium dioxide) and aesthetic functionality based on optical effects (e.g. iron oxide nanoparticles) (Mohseni et al.,2012; Stauber, 2007).

Plastics may be coloured using dyes or pigments. Dyes are soluble, interact chemically with the medium and transmit light through it (Christie, 1998). Common examples of dyes include reactive dye, disperse dye, sulfur dye, vat dye, acid dye, direct dye and basic dye. Pigments, on the other hand, have low solubility, and dispersed within matrix can both absorb or scatter light (Christie, 1998). Pigments may be classified as organic (e.g. azo, phthalocyanines blues and greens, diketopyrrolopyrroles (DPP)) or inorganic (e.g. titanium dioxide, iron oxide, chromates, carbon black). Organic pigments generally show an increase in color strength as the particle size is reduced, while with many inorganic pigments there is an optimum particle size at which the colour is saturated (Christie, 1998). Pigments can have several advantages as colorants in polymers, including: a) high brightness and good color strength, b) superior fastness properties (especially migration resistance and mechanical reinforcement), and c) inhibition of polymer degradation (Christie, 1998).

DPP is highly insoluble and extremely resistant to temperature and pressure, and is typically used in paints for luxury cars (Norman, 2007), plastic colourant, high quality printing, fluorescence dyes (Fischer, 2010) and solar cells (Chandran and Lee, 2007). Chemically, DPP is a nitrogenous heterocyclic compound comprising of two five-ring pyrrole and two carbonyl groups (chemical formula: $C_{18}H_{10}Cl_2N_2O_2$). It was first known to have been synthesized in 1974 by chemist Donald G. Farnum (Farnum et al., 1974). Ciba-Geigy Ltd. (then Ciba Specialty Chemicals, then acquired and integrated in BASF) patented the first known method of producing the pigment in 1983 (henceforth “organic pigment Red 254”, Iqbal and Cassar, 1983). Earlier, red paint used by auto manufacturers tended to fade and develop a dusty look known as "chalking”, but organic pigment Red 254 was extraordinarily bright, stable and resistant to ultraviolet light and extremes of heat and cold. (Norman, 2007). Nicknamed "Ferrari Red," the pigment was used on all solid-red Ferraris from 2000 to 2002, and on all solid-red Alfa Romeos, BMWs, Corvettes, Volkwagen GTI models and the Lexus Soarer (SC

430) from 2000 to 2006 (Norman, 2007). The DPP pigment makes it possible to achieve high transparency with low light scattering as is normally achieved only for molecularly dissolved dyes, while retaining the fastness and light stability advantages of pigments. Chemical modifications to DPP can also yield pigments of other colours (e.g. alkylation leads to greater solubility and orange to green colour palette).

While the primary role of pigments is as a colorant, it can (along with other additives) influence the chemistry of the oxidation, degradation and stabilization process of the polymer. Photostability of plastics is influenced by several factors like light source, humidity, atmosphere, temperature and aggregation, chemical structure of both the colorant and polymer (Marzec, 2014). Absorption of light by pigments can lead to pigment molecules being promoted to an excited state, which can give rise to subsequent physical and chemical interactions. Through these interactions, pigments can promote or deter the degradation of polymers, and this property is utilized in different applications. Polymers intended for outdoor use involving sun exposure can be rendered photostable by the use of carbon black, benzotriazoles, benzophenones, and phenyl esters (Marzec, 2014). Organic pigments can act as photosensitizers or photodegradants, generally achieving light absorption by means of conjugated aromatic system (Marzec, 2014). Weathering of plastics combines the photophysical and photo-chemical effects of ultraviolet radiation with the oxidative effects of the atmospheric oxygen and hydrolytic effects of water (Marzec, 2014). Additionally, humidity, temperature, geographic location, mechanical stresses, abrasion and biological attack can also affect the degradation rate (Marzec, 2014).

The case study on automotive plastics simulates the decision context of a manufacturer choosing to colour a plastic bumper with one of two nano-sized pigments: n-OP or n-CB. n-OP comprises of nano-sized (size range of 14-151 nm) DPP pigments that are used to impart red colour (colour index is Pigment Red 254 | 56110). n-CB comprises of nano-sized (size range of 10-100 nm) rubber grade pigments that are used to impart black colour. Both pigments do not have conventional counterparts that impart functionality of the same quality and aesthetics. The conventional technology for colouring plastics date back to the 20th century and involve dyes molecularly dissolved in the plastic, but dyed plastics were prone to leaching and are not stable to weathering. In the case of n-OP, non-nano DPP pigments are available but these are opaque and less efficient to filter light. Further, they do not constitute a good comparative scenario as most of the assessments of the non-nano DPP are expected to be identical to the nano version. With this caveat of different quality functionality, n-OP and n-CB are compared to dyes in Tier 1 and assessed independently in Tier 2.

n-OP and n-CB pigments are used to colour plastics with a content of 0.2% and 1% in the polymer matrix respectively. The polymer used is Polypropylen KSR 4525 (Borealis), which is a reactor elastomer modified polypropylene intended for injection moulding automotive applications. Polypropylen KSR 4525 has excellent balanced mechanical properties and gives a good surface quality, and has been developed especially to be used in automotive exterior parts. The functional unit of this case study is the lower rear bumper of the Alfa Romeo MITO, and is a plastic car part weighing 1.54 kg.

8.2.2 Input data

For Tier 1 application , an industrial expert who is involved in the pigments business was asked to provide inputs that produced benefit, risk and decision graphs. The inputs to Tier 1 for automotive part with n-OP and n-CB provided by the expert are presented in Appendix 2 and 3 respectively. The interpretation of the graphical results are provided in 8.2.3.1.1 and 8.2.3.1.2 for n-OP and n-CB bumpers respectively.

The input data required for Tier 2 HHRA methodology application consists of occupational and consumer risks occurring within the four lifecycle stages. The number of human health risks estimated per lifecycle stage for this case study were as follows: one for synthesis stage (1 occupational risk via inhalation), two (n-OP) and three (n-CB) for production stage (2 occupational risk via inhalation for n-OP and 3 occupational risks via inhalation for n-CB), four for use stage (1 consumer risk via inhalation, 3 consumer risks via dermal contact) and one for end of life stage (1 occupational risk via inhalation). In the case of n-CB, no toxicological or exposure assessment experiments were conducted in the SUN project. A literature review was used to collect hazard and exposure information, and derive risks. Toxicological data in Elder et al. (2005) was used to derive a DNEL distribution. Exposure was calculated in two ways: a) Exposure measurements and estimates derived in the SUN project for n-OP were extrapolated to n-CB by considering their relative concentration in the plastic matrix, and b) Some exposure estimates available in the literature for production of n-CB (Kuhlbusch et al.,2004), production of masterbatch (Kuhlbusch et al., 2004) and bagging (Kuhlbusch et al., 2006) were used by considering the highest single measurement.

Ecological risk estimation for n-CB bumper was not possible because PEC are not available in the literature (nano-sized carbon black is produced by various natural and anthropogenic sources and is highly variable in space and time). For the n-OP, the input data for the case study consists of ecological risks in different environmental compartments investigated for each of the four lifecycle stages. Deterministic PNECs for pristine (for synthesis and production stages) and fragmented n-OP (for use and end of life stages) were derived for species representing terrestrial and aquatic ecosystems. PNEC for pristine material for terrestrial systems (16 mg DPP/kg soil) was based on the lowest EC_{10} available for an *Enchytraeidae* divided by an assessment factor (AF) of 100. PNEC for fragmented material for terrestrial systems (3.2 mg fragmented product/kg soil) was based on the highest-observed-no-effect concentration (HONEC) available for an Enchytraeidae divided by 10 to get a NOEC and then by an AF of 100. PNEC for pristine material for aquatic systems (0.015 µg DPP/L water) was based on the lowest EC_{10} available for *Daphnia magna* divided by an AF of 1000 (all ecotoxicological data were generated in WP4). Mean values of probabilistic PEC distributions used in the assessment are shown in Table 8.7 below. Probabilistic RCR were calculated for relevant cases. For the global ecological risk, the highest risk estimated at life cycle stage level was used.

Table 8.7 Mean values of Predicted Environmental Concentration distributions for n-OP bumper scenario

Environmental Compartment	Unit of measure	Global	Synthesis	Production	Use	EoL
Soil (Natural and Urban)	µg/kg·y	4.30E-05	1.83E-08	1.86E-09	1.86E-11	4.30E-05
Soil (Sludge treated)	µg/kg·y	0.006501	1.65E-06	0.002574	4.07E-05	0.003885
Surface water	µg/L	4.13E-06	1.10E-09	1.51E-06	2.38E-08	2.59E-06
WIP waste	mg/kg	0.015469	1.76E-05	0.000643	6.03E-06	0.014802
WWTP effluent	µg/L	5.29E-05	1.35E-08	2.09E-05	3.32E-07	3.16E-05

To apply risk control methodology to unacceptable risks in the n-OP and n-CB scenarios, TARMM relevant to exposure scenarios were collected from industry and exposure assessment experts. Efficiency for these TARMM was derived by calculating average of literature values for each TARMM. Cost ranges were derived wherever possible using internet search.

Eco-efficiency method using shadow prices (in Euros) was applied to classify Tier 2 LCIA results for n-OP and n-CB, which are provided in Table 8.8 below. The scores for both pigments differ only in the synthesis stage. The market price for the functional unit used for classification is provided by experts as €144 and €138 for red and black bumpers respectively.

Table 8.8 Aggregated LCIA scores in shadow price for n-OP and n-CB bumper scenario

	n-OP	n-CB
Global	7.53E-03	7.55E-01
Synthesis	3.60E-01	3.62E-01
Production	3.59E-01	3.59E-01
Use	0.00E+00	0.00E+00
End of Life	3.38E-02	0.0338

Efficiency method was applied to classify EA results for this case study, which are provided in Table 8.9 below. Aggregated scores for the first three lifecycle stages were obtained by eliciting data for four lifecycle stages for both scenarios from industrial experts in the pigments and injection moulding sector. Due to non-availability of data for the synthesis stage cost for n-CB bumper, this nanomaterial cost is directly included in the production stage (and not reported in the synthesis stage). End-of-life scores were calculated using publically available prices for incineration and landfilling for Germany over the funcational unit of the case study (EC, 2012; CEWEP Country Report, 2010).

Table 8.9 Aggregated EA scores in Euros for for n-OP and n-CB bumper scenarios

	n-OP	n-CB
Global	138.43	156.61
Synthesis	0.03	0.00
Production	12.40	12.45
Use	131.60	125.55
End of Life	0.13	0.13

Tier 2 SIA aggregated scores for both scenarios are identical to each other as well as to the n-CuO paint case (not split by lifecycle stage). The reader is referred to Table 8.5 for these data.

8.2.3 Application of SUNDS Tier 1 to automotive case study

8.2.3.1 Nano-Organic Pigment bumper

The reader is referred to the description of Tier 1 methodology in Section 4.2.1. Briefly, there are three benefit modules (Modules 1-3) and three risk modules (Modules 4-6), which are integrated on a two dimensional Benefit-Risk scale divided into four quadrants (Module 7). The single score for each benefit and risk module (except Module 5) is an average of all criteria that it includes. In the occupational risk module, the single score is based on the worst case exposure chosen from manufacturing of nanomaterial, processing of nanomaterial and application of nano-enabled product.

The results for application of Tier 1 methodology for the automotive part containing n-OP are presented in this section. Module 0 assessed that the nano-enabled product was compliant with current regulation. ECHA recently stipulated that ENM has to be registered separately from its bulk counterparts if its use triggers REACH registration tonnage limits (over one tonne/year), which is applicable to the company in which this case study is based. While this additional registration cost is not considered in the economic assessment in Tier 1 or Tier 2, it should be considered in the final assessment (though REACH registration costs are significantly lower than BPR approval for n-CuO paint).

Figure 8.5 shows the benefits of the n-OP automotive part relative to conventional alternatives from application of Modules 1-3. Compared to the conventional alternative, the n-OP had positive environmental benefit (average score= 0.11) and economic benefit (average score= 0.67), while social benefits of both paints were identical (average score= 0).

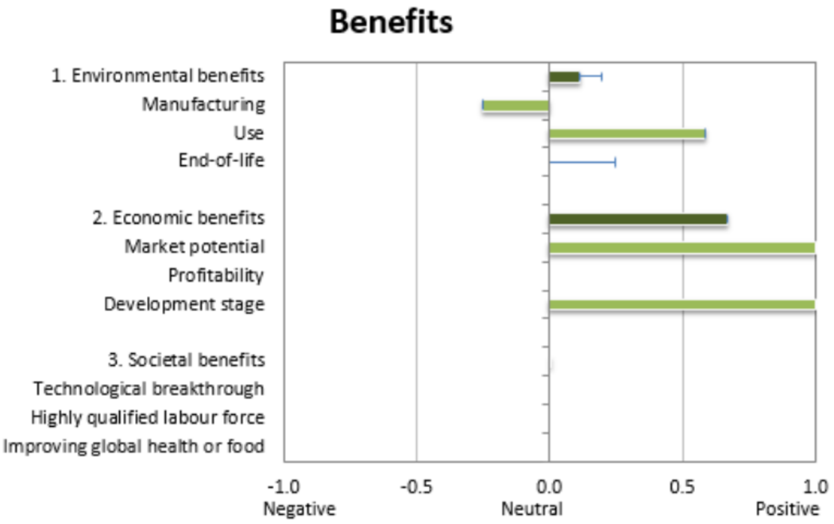


Figure 8.5 Results of application of benefit modules of Tier 1 to nano-organic pigment bumper

While the average environmental benefit was positive (Module 1), the manufacturing stage of the n-OP scenario was worse than conventional alternatives (normalized score= -0.25) due to higher energy consumption. There was moderate benefit in the use stage (normalized score= 0.58) due to higher product life time, lower emissions of hazardous substances and effectiveness of use, while end of life benefits for all scenarios were identical (normalized score= 0). The uncertainty in environmental benefits (shown by the error bars) is due to lack of information on the effectiveness of the End-of Life treatment.

The highest economic benefit of the n-OP (Module 2) was due to high foreseen market potential in a large market (normalized score= 1) and low time to market (normalized score= 1). n-OP did not confer any cost savings in the use stage compared to the conventional counterpart (normalized score= 0).

The three social benefits considered for n-OP (Module 3) viz. technological breakthrough, highly skilled labour force and improvements to food/health are identical to conventional alternatives.

Figure 8.6 shows the risks of the n-OP automotive part obtained from application of Modules 4-6. Risks for n-OP automotive part were greatest for public health and environment (normalized score=0.49), followed by occupational health (score =0.29) and no consumer risks (score= 0).

In the case of public health and environmental risks (Module 4) of n-OP automotive part, the biggest contributor to the average score was potential input into the environment through the life cycle (normalized score=0.63), followed by potential effect based on free radical activity and oxidative stress (normalized score=0.5), and system knowledge (normalized score= 0.33). Uncertainties arise in public health and environmental risks due to lack of information on stability of nanomaterial and potential input of nanomaterials in the environment.

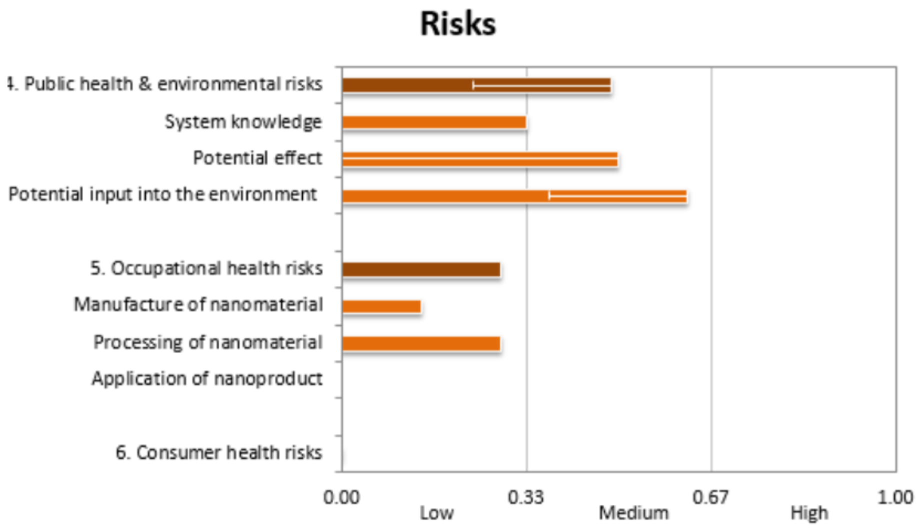


Figure 8.6 Results of application of risk modules of Tier 1 to nano-organic pigment bumper

In the case of occupational risks (Module 5) of n-OP automotive part, the worst case occupational risk was caused by nanomaterial processing (normalized score =0.29), which corresponds to a Stoffenmanager Nano control banding classification of A3 (classified as low risk). Nanomaterial manufacture and nano-enabled product application had Stoffenmanager Nano control banding classification of A2 (normalized score=0.14 and classified as low risk) and A1 (normalized score= 0 and classified as low risk) respectively.

As there was no exposure potential of n-OP from the plastic matrix and no hazard potential, consumer risks (Module 6) are not expected (normalized score= 0).

Figure 8.7 shows the two-dimensional space where benefit and risks are integrated for n-OP automotive part, and the result lies in the quadrant “Other Benefits needed” with some uncertainty bars extending from the “yellow” into the “green” regions. According to this first tier assessment, the n-OP automotive part is a good commercial proposition with high economic benefits with an overall score touching the high threshold. The risks are low as well, with highest risk score being for public health and environment (average score= 0.49) and no consumer risks. However, as the environmental benefits are comparatively low (average score=0.11) and there are no social benefits (average score=0), n-OP automotive part has the profile of a conventional product.

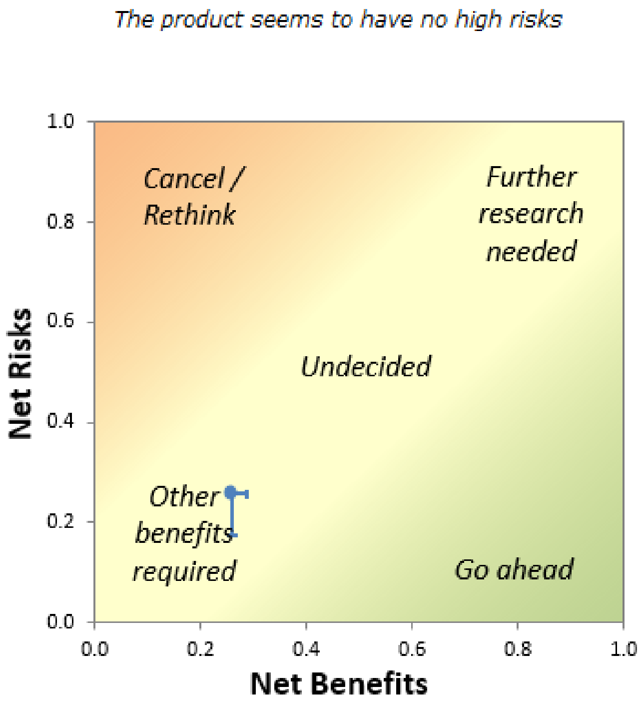


Figure 8.7 Result of the application of the decision support module of Tier 1 to nano-organic pigment bumper.

8.2.3.2 Nano Carbon Black bumper

The application of Tier 1 methodology to the n-CB bumper involve mostly identical inputs as the n-OP scenario except two changes in the risk modules. In Module 4 (Public Health and Environmental risks), a higher hazard is indicated for n-CB in Q 4.4 (Appendix 3) leading to a higher score for potential effect (normalized score=1.0). This leads to a higher score of 0.65 for Module 4 of n-CB, which is much closer to the threshold of high risk than the n-OP score.

In Module 5 (occupational risks), the risk for manufacture of nanomaterial is different due to higher hazard of n-CB and different manufacturing process (Chemical Vapour Deposition) (Kuhlbusch et al., 2006; Kuhlbusch et al., 2004). The worst case occupational risk was caused by nanomaterial manufacturing (normalized score =0.43), which corresponds to a Stoffenmanager Nano control banding classification of D1 and is classified as medium risk. Risks for nanomaterial processing and nano-enabled product application were similar to n-OP. As the pigment is well contained in the matrix, the consumer risks was also identical to n-OP (normalized score= 0).

Figure 8.8 shows that overall results of Tier 1 application is also similar to n-OP sceanario, and the result lies in the quadrant “Other Benefits needed”.

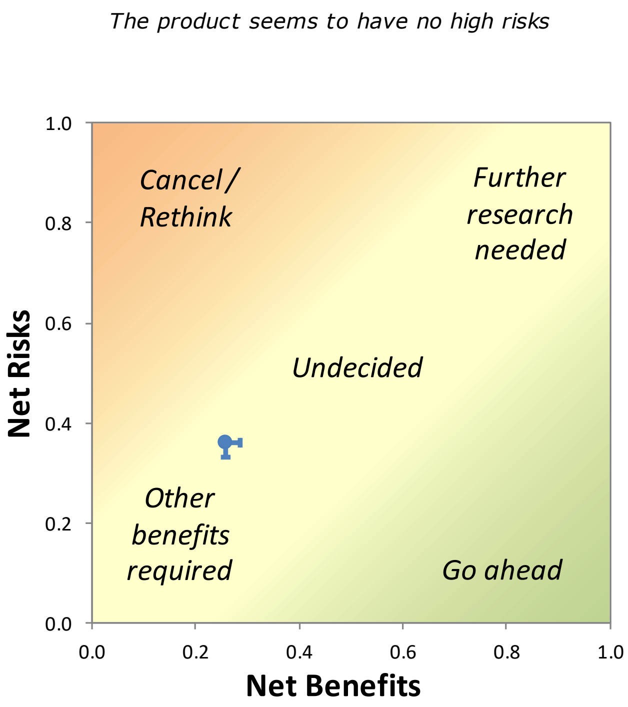


Figure 8.8 Result of the application of the decision support module of Tier 1 to nano-carbon black bumper

8.2.4 Application of automotive case study to SUNDS Tier 2 RC Module

8.2.4.1 Nano organic pigment bumper

Application of Tier 2 ERA classification methodology to n-OP bumper yielded a global score classified as acceptable (Figure 8.9a).

Application of Tier 2 HHRA classification methodology to n-OP scenario yielded a global score classified as unacceptable (Figure 8.9a), due to a single unacceptable risk related to production of pigment in the synthesis stage (Figure 8.9b). The application of RC methodology to this risk is shown in Table 8.10. The initial risk and re-estimated risk are colour coded according to the HHRA classification methodology (described in Section 5.1).

Table 8.10: Application of TARMM to unacceptable risks in n-OP bumper lifecycle

Exposure scenario	**LCA stage**	**Target**	**Exposure route**	**Initial exposure concentration**	**Risk classification**	**Relevant TARMM with efficiency**	**Exposure concentration with TARMM application**	**Risk re-estimation**	**TARMM cost**
Production of organic pigment	Synthesis	Occupational	Inhalation	5 mg/m^3 (very conservative estimation)	99.27%	Containment (closed process)= 90%	Containment =0.5 mg/m^3	39.23%	Difficult to estimate
						LEV (Horizontal/downward laminar flow booth and Other enclosing hoods)= 90%	LEV (vertical/horizontal laminar flow hood)= 0.5 mg/m^3	39.23%	LEV (vertical/horizontal laminar flow hood): €3280 to €5818
						LEV (Movable capturing hoods)= 50%	LEV (Movable capturing hoods)= 2.5 mg/m^3	94.91%	LEV (Movable capturing hoods)= €890 to €2676

Table 8.10 shows that despite investing in a sophisticated TARMM like LEV and developing an efficient containment (closed process) strategy, risk could not be controlled for the production of the organic pigment. The hazard of n-OP for inhalation is quite high (NOAEC = 30 mg/m^3), however, the risk estimation is based on very conservative assumptions at the basis of the exposure estimation, and the actual risk is likely to be lower (though it is not known if a more realistic risk assessment will be acceptable). All other risks through the lifecycle of n-OP scenario are acceptable.

8.2.4.2 Nano Carbon black bumper

Tier 2 ERA classification methodology could not be applied to n-CB because ERA results were not available (due to missing exposure data).Application of Tier 2 HHRA classification methodology to n-CB scenario yielded a global score classified as High (Figure 8.13a), due to high risks in synthesis and production stage (Figure 8.13b). The application of RC methodology to these risks is shown in Table 8.11. In the case of two scenarios i.e. production of n-CB and production of masterbatch, both extrapolated exposure estimates from SUN project and literature have been used to derive risks. Using the worst case exposure estimate in Kuhlbusch (2006) for production of n-CB already shows low risk (3.36%) and no TARMM needs to be applied. Similarly, in the case of masterbatch production using SUN exposure estimates, there is no risk and hence TARMMs do not need to be applied. Hence, only the worst case risks among these (production of n-CB as per SUN estimate and masterbatch production as per Kuhlbush et al. (2006) are shown in Table 8.11. The initial risk and re-estimated risk are colour coded according to the HHRA classification methodology (described in Section 5.1).

Table 8.11: Application of TARMM to unacceptable risks in n-CB bumper lifecycle

Exposure scenario	**LCA stage**	**Target**	**Exposure route**	**Initial exposure concentration**	**Risk**	**Relevant TARMM with efficiency**	**Exposure concentration with TARMM application**	**Risk re-estimation**	**TARMM cost**
Production of n-CB (SUN exposure estimate)	Synthesis	Occupational	Inhalation	5 mg/m^3 (very conservative)	99.99%	Containment at source= 90%	0.5 mg/m^3	90.29%	Difficult to estimate
						LEV (Horizontal/downward laminar flow booth and Other enclosing hoods)= 90%	0.5 mg/m^3	90.29%	€3280 to €5818
						LEV (Movable capturing hoods)= 50%	2.5 mg/m^3	99.97%	€890 to €2676
Bag filling	Synthesis	Occupational	Inhalation	0.258 *mg*/m3(worst case in Kuhlbusch (2004))	65.202%	LEV (Horizontal/downward laminar flow booth and Other enclosing hoods)= 90%	0.0258 mg/m3	0.32%	€3280 to €5818
						LEV (Movable capturing hoods)= 50%	0.129 mg/m3	29.17%	€890 to €2676
						LEV (Canopy hood)= 50%	0.129 mg/m3	29.17%	€63 to €1972
Manufacture of Master-batch (Kuhlbusch et al. (2006 worst case single measurement)	Production	Occupational	Inhalation	4 mg/m3	99.99%	LEV (Horizontal/downward laminar flow booth and Other enclosing hoods)= 90%	0.4 mg/m3	84.05%	€3280 to €5818
						LEV (Movable capturing hoods)= 50%	2 mg/m3	99.92%	€890 to €2676
						LEV (Canopy hood)= 50%	2 mg/m3	99.92%	€63 to €1972

In the case of production of n-CB, using very conservative SUN project estimate (same as one used for n-OP), risks cannot be controlled to below acceptable thresholds even with the use of three types of high efficiency TARMM. The NOAEL for inhalation by rats is 1 mg/m^3 which determines a DNEL described by a low confidence interval (LCL) equal to 0.001 and an upper confidence interval (UCL) equal to 0.365.

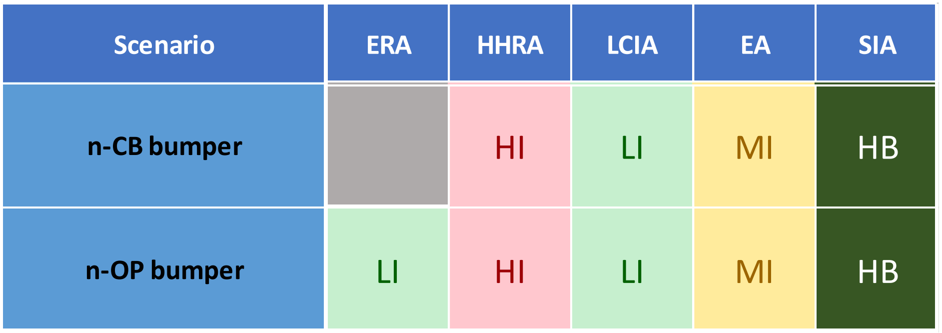
In the case of bag filling scenario, LEV (vertical/horizontal laminar flow hood, cost range=€3280 to €5818) is successful in reducing risk to acceptable levels, whereas movable capturing and canopy hoods are not.

In the case of masterbatch production, Kuhlbusch et al. (2006) exposure estimate yield unacceptable risks that could not be reduced to acceptable risks with all three TARMM considered.

8.2.5 Application of automotive case study to SUNDS Tier 2 SEA Module

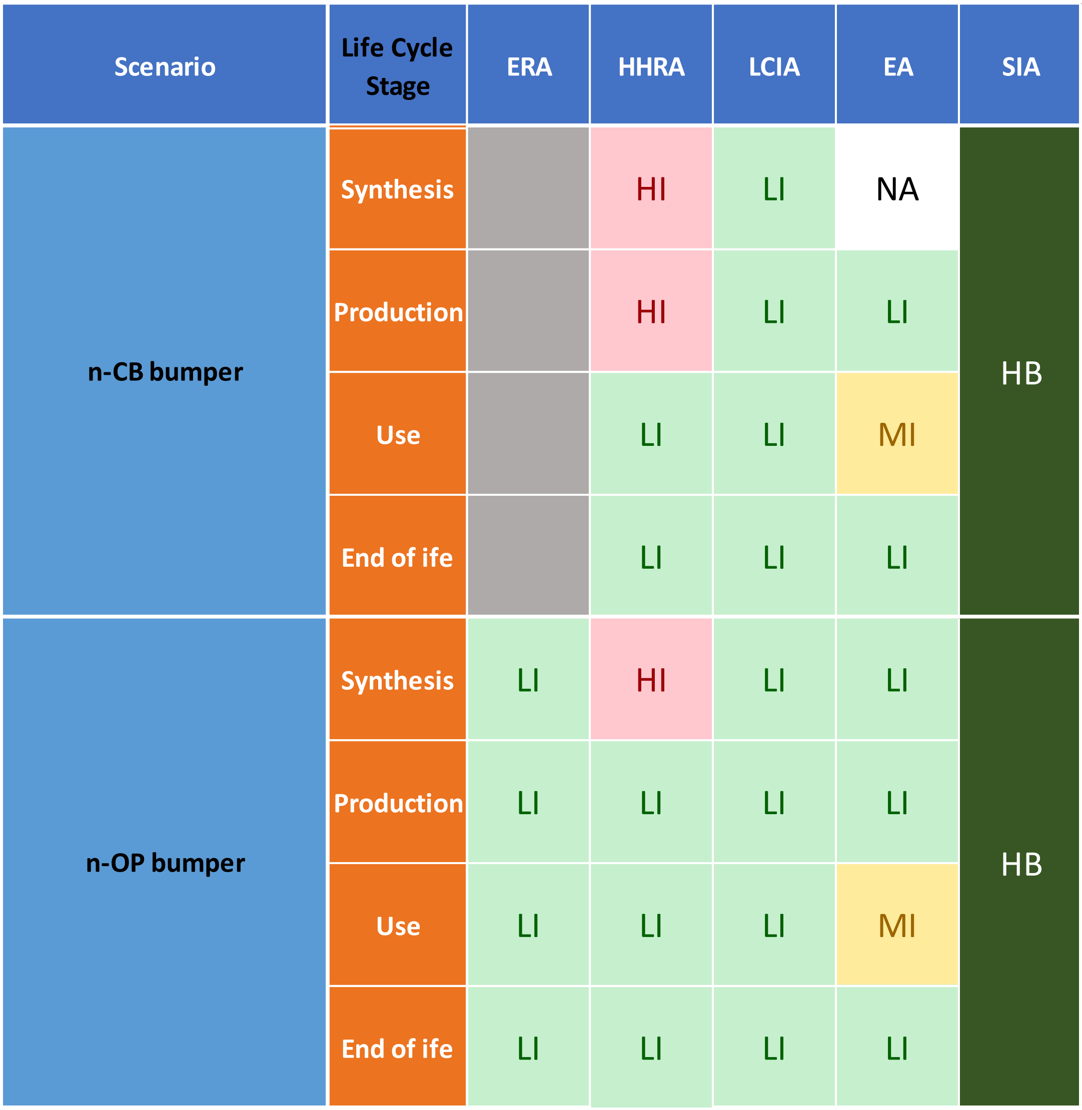
The SEA sustainability portfolios for automotive part with n-OP and n-CB are provided for global scores and lifecycle stage scores in Fig 8.9 a and b respectively, and results after RC application are provided in Fig 8.9 c and d respectively. The application of RC did not change the global or lifecycle portfolio of n-OP or n-CB. n-OP and n-CB scenarios have a similar profile, except for the human health risks in the production stage are high for n-CB and low for the n-OP bumper.

a)



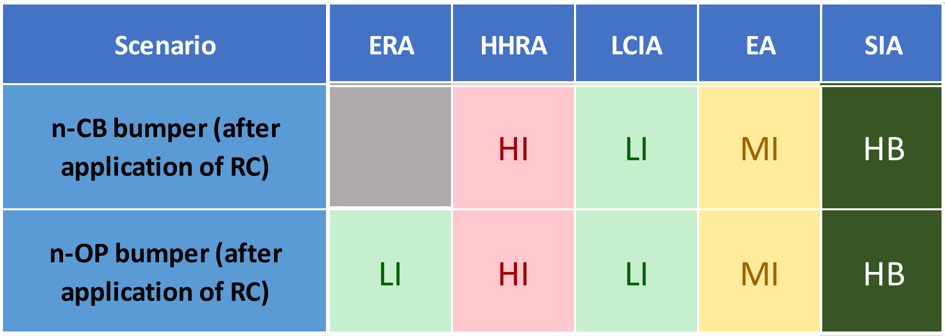
Scenario	ERA	HHRA	LCIA	EA	SIA
n-CB bumper		HI	LI	MI	HB
n-OP bumper	LI	HI	LI	MI	HB

b)



Scenario	Life Cycle Stage	ERA	HHRA	LCIA	EA	SIA
n-CB bumper	Synthesis		HI	LI	NA	HB
	Production		HI	LI	LI	
	Use		LI	LI	MI	
	End of ife		LI	LI	LI	
n-OP bumper	Synthesis	LI	HI	LI	LI	HB
	Production	LI	LI	LI	LI	
	Use	LI	LI	LI	MI	
	End of ife	LI	LI	LI	LI	

c)



Scenario	ERA	HHRA	LCIA	EA	SIA
n-CB bumper (after application of RC)		HI	LI	MI	HB
n-OP bumper (after application of RC)	LI	HI	LI	MI	HB

d)

Scenario	Life Cycle Stage	ERA	HHRA	LCIA	EA	SIA
n-CB bumper (after application of RC)	Synthesis	▨	HI	LI	NA	HB
	Production	▨	HI	LI	LI	
	Use	▨	LI	LI	MI	
	End of ife	▨	LI	LI	LI	
n-OP bumper (after application of RC)	Synthesis	LI	HI	LI	LI	HB
	Production	LI	LI	LI	LI	
	Use	LI	LI	LI	MI	
	End of ife	LI	LI	LI	LI	

Figure 8.9: SEA global sustainability portfolio for n-CB and n-OP bumper scenarios before (a) and after (c) RC application, and SEA lifecycle stage sustainability portfolio for n-CB and n-OP bumper scenarios before (b) and after (d) RC application

S: Synthesis, P: Production, U: Use; E: End of Life.

LEGEND

🟥	HI	High Impact
🟨	MI	Medium Impact
🟩	LI	Low Impact
🟩	LB	Low Benefit
🟩	MB	Medium Benefit
🟩	HB	High Benefit
▨		Missing value
	NA	Not Applicable

According to the global SEA classification for automotive part, only SIA for both n-OP and n-CB scenarios shows high benefits (Figure 8.9c). The lifecycle sustainability portfolio (Figure 8.9d) for n-CB informs us that the order of lifecycle stages from best to worst is end-of-life, use, synthesis and production. In the case of n-OP, the order of lifecycle stages from best to worst is end-of-life, production, use and synthesis (Figure 8.9d). The lifecyle stage classification results are discussed for each methodology below.

The ERA classification all lifecycle stages for n-OP was Acceptable Risk. ERA classification was not performed for n-CB due to non-availability of data. The ERA global classification (low impact, as shown in Figure 8.9c) is lower than Tier 1 Public health and environmental risks (Module 4) analysis for n-OP, which shows medium risk. Tier 1 Public health and environmental risks are not split by lifecycle stage and the criteria potential effect and potential input into the environment correspond to a semi-quantitative evaluation of PNEC and PEC respectively. A medium score for potential effect and potential input into the environment suggests that there could be some ecological risks, but this is not the case in Tier 2 analysis, according to available exposure and effect estimations.

The HHRA classification for n-OP is acceptable for all lifecycle stages except synthesis (using very conservative exposure estimate on production of pigment). The risk for synthesis of n-OP could not be controlled with the prescribed TARMM for the worst case exposure (Section 8.2.4.1). For Tier 1 occupational risks (Module 5) and consumer risk (Module 6) of n-OP bumper, all risks were low. In the case of n-CB, both synthesis and production stages contained unacceptable human health risks. These worst case exposure n-CB risks in synthesis and production stages could not be fully controlled (Section 8.2.4.2). For Tier 1 occupational risks (Module 5) of n-CB bumper, there was a medium risk for nanomaterial manufacture, while the other risks were low. Consumer risk (Module 6) for n-CB was low as well.

The LCIA classification for both n-OP and n-CB for all lifecycle stages was low impact as calculated using eco-efficiency method. These results are in agreement with Tier 1 Environmental Benefits (Module 1) analysis for the manufacturing stage, where low impact is also seen. Tier 1 analysis shows a medium benefit for the use stage for n-OP and n-CB bumper scenarios as opposed to low impact in Tier 2 analysis. Tier 1 is semi-quantitative and its criteria do not correspond exactly to those within Tier 2, hence the exact cause for this cannot be pinpointed. It should be noted that none of the criteria for Environmental Benefits for Tier 1 perform worse for n-OP and n-CB bumpers than the conventional molecular plastic dyes (Appendix 2 and 3). Four out of the seven criteria perform identically for both scenarios (e.g.

need for maintenance, hazardous substances used for maintenance, amount of wastewater and amount of solid waste), while the rest perfom better for n-OP and n-CB bumpers (e.g. product lifetime, efficiency of use, hazardous emissions). Tier 1 End-of-Life scores for n-OP and n-CB bumpers are identical to their conventional counterparts, while they are classified as low impact in Tier 2 LCIA. Tier 1 End-of-Life analysis balances the higher volume of waste generated in the novel scenarios with their less hazardous nature, whereas Tier 2 involves specific End-of-Life scenarios (shredding, downcycling, landfill and incineraration) of which only a portion is capable of generating benefit (downcycling).

The EA classification for n-OP and n-CB for production and end-of-life stages was low as calculated using efficiency method. The synthesis stage for n-OP was low, and classification could not be applied to synthesis stage for n-CB as nanomaterial was directly included as a cost in production. Use stage for both bumpers was classified as medium impact, which is resulting from the significant market margin of the automotive part carried by the consumer. While comparing these findings with Tier 1 Economic Benefits (Module 2) results, it must be noted that Tier 1 criteria (market potential, profitability and development stage) are comparable to Tier 2 use stage score (which may also include operational and maintenance cost if applicable). For this case study the medium classification for the Tier 2 use stage corresponds to a medium benefit to the manufactuer (there are no operational and maintenance costs applicable in this case study), while Tier 1 classifies the same functionality as high benefit.

The SIA classification for n-OP and n-CB in the specific company and country context shows high net benefit, which is composed of high benefits and costs. The social indicator which has the most significant magnitude in cost category is research and development expenditure. n-OP and n-CB are particularly favourable to workers, with high benefits and low costs (Subramanian et al, submitted). These results are not in agreement with Tier 1 Social Benefits (Module 3) analysis, where there is no social benefit for the criteria mentioned (and there is equal benefit to conventional dyed plasics). As Tier 1 is semi-quantitative, comparative and its criteria are different from those used within Tier 2, results from the two tiers are not comparable.

Overall, the current sustainability portfolio for n-OP and n-CB bumpers informs us that these nano-enabled products have low impacts, with the exception of some unacceptable human health risks. Human health risks are unacceptable for both scenarios for synthesis stage using very conservative SUN estimate. For the production stage, risk for production of n-CB pigment is acceptable using literature estimate (Kuhlbusch et al. , 2006) and unacceptable using SUN project estimate (shown in Table 8.11). Further, risk for production of n-CB masterbatch are acceptable using SUN project estimates and unacceptable using literature estimate (Kuhlbusch et al., 2006, shown in Table 8.11). Hence, it may be worthwhile to measure real time exposure concentrations for exposure estimations resulting in high risks. Human health risks in production stage of n-CB are unacceptable using (single) highest measurement, but here again a conservative approach is used (PM_{10} exposure concentrations are used instead of nano fraction and single highest measurement is used from a broad range). In summary, the human health risks for both scenarios may not be as high with more realistic exposure measurements.

Further, there is a medium impact classification for use stage in EA owing to the market margin of the automotive part carried by the consumer.

This combination of low impacts and high profits makes both n-OP and n-CB automotive parts similar to parts coloured with conventional pigments i.e they use a well-established technology and while they are commercially profitable, they do not have additional benefits. This was also confirmed by the Tier 1 application of these scenarios.

CHAPTER 9: Conclusions and further developments

This thesis presents the doctoral research performed during three years of doctoral studies in Environmental Sciences. The activities also aimed to contribute to the goals of the EU FP7 SUN project and had three main objectives:

1. Review the needs of stakeholders in addressing the complex risks associated with nano-enabled products through the lifecycle, including industry, regulators and the insurance sector in the literature and by employing a user elicitation process;
2. Develop a conceptual decision framework for risk management and sustainability assessment of nano-enabled products based on stakeholders' needs and a methodology to implement such a framework;
3. Apply the framework to commercially available nano-enabled products to assess their sustainability.

All the above objectives have been achieved. The value of this research is most evident in case study application, where trade-offs between innovation, risks and impacts could be better understood and prescription for improving the sustainability of nano-enabled products could be gleaned. The summary interpretation of the case studies is in agreement with the intuition of product experts, and a systematic approach to case study application is demonstrated that would enable stakeholders to achieve important insights during early product development.

The results of this research have been widely disseminated to the scientific community (through nine publications and three oral platform presentation to conferences; few others planned in the near future) which highlight its impact. The software implementation of the above research is ongoing in the SUN project and a fully functional version is expected to be presented to stakeholders in March 2017.

Sustainable nanotechnology continues to evolve rapidly resulting in new scientific issues (e.g. development of nano-specific assessment factors and exposure models) and changing needs of stakeholders (e.g. need to calculate insurance cost for manufacturing nano-enabled products). SUNDS conceptual decision framework and methodology is adaptive to new knowledge and stakeholder perspectives. There are several directions in which this preliminary work can be continued, some of which are planned in future projects by the research group in which the PhD research has been conducted, and are briefly presented below.

Apart from nanotechnology risk management and sustainability assessment, SUNDS conceptual decision framework and methodology is suitable for further development into a tool that can support the broader aims of risk governance. Risk governance is defined as a unifying approach to decision making that involves the actors, conventions, rules and processes concerned with how relevant risk information is collected, analysed and communicated in order to enable more effective risk management that is convergent with other public and private policies (IRGC, 2012). Renn (2008) relates risk governance and sustainability by positing sustainability as the outcome of successful risk governance process over longer time scales. The specific near term activities to develop SUNDS conceptual decision framework and methodology may include collecting SUNDS user experience feedback, application to numerous case studies and utilization in various risk governance application contexts (e.g. international governance of nanotechnology as proposed by Malsch et al. (2016c), multi-stakeholder online platform, etc.).

Sustainability of innovation is addressed at the levels of product (Raza et al. 2014; Zhang et al. 2014), production process (Kumaraguru et al. 2014; Kurdve et al. 2014; Porzio et al. 2014), program or project (Teng et al. 2012; Jansujwicz and Johnson 2015; Wu and Issa 2014), industry (Hsu et al. 2015), supply chain (Devika et al. 2014; Govindan et al. 2014; Azadnia et al. 2015; Boukherroub et al. 2015), sector (Gazquez-Abad et al. 2015), and industrial policy (Popescu et al. 2015). The definition of sustainable nanotechnology proposed in this thesis (Figure 2.1) is focussed on product, process and nanotechnology value chain (in the mentioned order of focus). Organizational risk management has also been included in the SUNDS tool through an adaptation of CENARIOS risk management system (Widler et al., 2016), and some important elements of policy are included in the conceptual decision framework by alignment with EU REACH regulation. However, the definition of sustainable nanotechnology adopted in this thesis is deficient in macroeconomic factors that come into play at industry and sector level. Given that nanotechnology is not a well-defined industrial sector and only preliminary steps have been made toward its commoditization (e.g. INSCX exchange tracks trade in ENM since 2009), this is more a reflection of the current state-of the-art rather than a limitation of this work.

Another aspect that could be developed in the definition of sustainable nanotechnology is a measure of performance of the proposed functionality and how this is affected by the adoption of technological alternatives. If physicochemical parameters influencing functional performance and intended S-by-D strategy are the same, technological alternatives cannot be used for risk control.

This thesis proposes a conceptual decision framework has a two-tier structure comprising of screening and advanced tools to address varying data availability and stakeholder needs. Currently, data may not be available to apply the SUNDS Tier 2 to all nano-enabled products.

In these situations, Tier 1 results can provide some insight on nano-enabled products to the user to support decision-making. Further, in terms of Benefit-Risk or Benefit-Cost assessment, the framework is not balanced as it has more risk and costs than benefits partly due to case-specific nature of benefits. Benefits are currently available in the LCIA and SIA methodology, and should be developed further.

Specifically, as far as SIA is concerned, the framework and methodology developed in this research currently has some limitations like few nano-specific indicators, no indicators associated with use and end-of-life phase and indicators relevant to several stakeholders (Subramanian et al., 2016b; Lehmann et al, 2013). Without precise nano-specific indicators, nano-enabled products cannot be compared with conventional alternatives. However, these limitations are due to the state-of the-art and the methodology offers a flexible structure that can be revised and extended as more knowledge and data on assessment of nano-enabled products becomes available. The simple conceptual framework is also an advantage as it allows value-laden conceptual categorization (i.e. benefits and costs or stakeholder categories) to be easily changed in the analysis.

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Appendix 1: Tier 1 Input data for Nano Copper oxide paint

Conventional product: Conventional acrylic paint (white) for weathering protection

Nano Product and Legislation

	Type of nano material and application	Please select or specify
Q 0.1	Which nanomaterial will be used?	Other
	Please specify additional nano subtype or indications / properties:	The nanoCuO (along with co-biocides) is added to an acrylic paint base which is applied to the softwood.
Q 0.2	In which type of application is the nanomaterial be used?	Softwood preservative paint used in exterior cladding
Q 0.3a	Is this a completely new product with a new functionality (which cannot easily be compared with a conventional product)?	No
Q 0.3b	If not, what conventional product is being replaced by the new nanoproduct? (this can also be 'doing nothing')	Conventional acrylic paint (white) for weathering protection
Q 0.4	The product under evaluation is:	A product for consumer and professional markets
Q 0.5	What is the main function that the nanomaterial provides in your application?	Biocide
Q 0.6	What is the appropriate unit to compare the nanoproduct with the conventional product? (It is only correct to compare the same functionality)	Other
	In case you have selected 'Other' please specify:	1m2 per year

	Nano-relevance	Please select
Q 0.7	Approach 1 (precautionary approach): Ranges of sizes of primary particles contained in the materials (free, bound or as aggregates or agglomerates)?	1-500 nm

Q 0.8	Approach 2 (EU-proposed definition 2011/696/EU): Material containing primary particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50% or more of the primary particles in the number size distribution, one or more external dimensions is in the size range 1 nm - 100 nm or (if the number size distribution is unknown) Material where the specific surface area by volume is greater than 60m2/cm3 or Material consists of fullerenes, graphene flakes or single wall nanotubes.	Yes

	Legislation	**Please select or specify**
Q 0.9	Are you aware of existing legisation (e.g. EU Nr. 1907/2006 (REACH), The EU Biocides Regulation 528/2012 (EU BPR), Regulation (EC) No 1223/2009 on cosmetic products …)	Yes
Q 0.10	Is your nanomaterial approved or notified according to relevant EU-legislation (e.g. EU Nr. 1907/2006 (REACH), The EU Biocides Regulation 528/2012 (EU BPR), Regulation (EC) No 1223/2009 on cosmetic products …)	No
Q 0.11	Do you use the nanomaterial below its specific concentration limits recommended in the legal framework (e.g. http://ec.europa.eu/environment/chemicals/biocides/active-substances/approved-substances_en.htm)	Yes

Environmental Benefits

	Manufacturing phase of the nanoproduct versus conventional product	**[Better/Equal/Worse/Unknown]**
Q 1.1	Energy consumption of the manufacturing process?	Worse
Q 1.2a	Materials consumption in this manufacturing process?	Equal
b	Amounts of hazardous substances used in the manufacture?	Worse

Q 1.3	Efforts needed to produce the product using the nanomaterial?	Equal
Q 1.4a	Amount of solid waste from the manufacturing process?	Unknown
b	Amount of waste water from the manufacturing process?	Unknown
c	Emissions to the air or (waste) water from the manufacturing process itself?	Unknown

	Use phase (only for final products and articles)	**[Better/Equal/Worse/Unknown]**
Q 1.5	Product life time (use phase)?	Better
Q 1.6a	Need for maintenance?	Better
b	Amounts of hazardous substances used in maintenance?	Equal
Q 1.7a	Amount of solid waste from using the product?	Better
b	Amount of waste water resulting from use of the product?	Equal
c	Emissions of hazardous substances to air, water and/or solid?	Equal
Q 1.8	Efficiency of use?	Equal

	End-of-life (only for final products and articles)	**[Better/Equal/Worse/Unknown]**
Q 1.9	Volume of waste (due to e.g. longer lifetime, less weight, less material used)?	Better
Q 1.10a	Amounts of other hazardous substances released from the waste water treatment?	Better
b	Amounts of other hazardous substances released during incineration?	Better
Q 1.11	Established recycling systems (glass, PET, paper, carton, batteries, biowaste, electronic devices, etc.) exposed to the nanomaterial in the product?	Equal
		[Yes/No/Unknown]
Q 1.12a	Can the waste water treatment facility eliminate the nanoproduct's emissions?	Unknown
b	Can the waste incineration facility eliminate the nanoproduct's emissions?	Yes

Economic Benefits

	Market potential	Please select
Q 2.1	Does the nanoproduct have increased marketability due to an improved functionality or a new functionality (for example: UV-protection, enhanced photolytical self-cleaning/ self-cleaning capacity/property, conductible, antimicrobial function), or a clear image advantage compared to the conventional product (e.g.: more resistant to environmental effects, prolonged lifetime/persistence, reduced weight or increased strength)?	higher
Q 2.2	What is the foreseen market potential of the nanoproduct or -application in Europe?	medium (1 k€ - < 1 M€ sales)

	Profitability	[higher / equal / lower / unknown]
Q 2.3	What is the (expected) purchase price per unit of the nanobased product or material compared to the conventional one?	higher
Q 2.4	What are the operational costs (i.e. maintenance, energy use etc) during the use phase of the nanobased product or application compared to the conventional one? (Think of advantages due to nanoproperties in the manufacturing process)	lower

	Development stage	Please select
Q 2.4	What is the time-to-market to manufacture the nanoproduct on a commercial scale?	medium (1 - <5 year)

Societal Benefits

	Societal aspects	Please select
Q 3.1	Could the use or application of the nanoproduct be considered a technological breakthrough (in general, but particularly in energy systems and Information and Communication Technologies, ICT) compared to the conventional alternative?	more or less equal

Q 3.2	Does the production of the application lead to a substantial improvement in the development of a highly qualified labour force compared to the conventional alternative?	more or less equal
Q 3.3	Compared to the conventional alternative... Does the use or application of the nano-based product lead to improvements in feeding the world's population, a marked increase in food production and the nutritional value of food? OR Does the use or application of the nano-based product lead to improvements in people's health, particularly the direct user, e.g. by improvements in water purity, sanitation or medicines and pharmaceuticals?	more or less equal

Public Health & Environmental Risks

	System knowledge	**[Yes/Partly/No]**
Q 4.1	Is the origin of the (nanoscale) starting materials known?	Yes
Q 4.2	Are the next users of the nanomaterials under consideration known?	No
Q 4.3	How accurately is the material system known or can disturbing factors (e.g. impurities) be estimated?	Accurately

	Potential effect	**[Low/Medium/High/Unknown]**
Q 4.4	Do the nanomaterials cause redox activity, catalytic activity or have a potential for oxygen radical formation or to induce inflammation reactions? (The drop-down menu gives clues which forms of nanoproducts have a low, medium or high potential effect.)	High, all other nanoparticles (excl. nanorods), <10nm
Q 4.5	What is the stability (half-life) of the nanoparticles present in the nanomaterial under ambient environmental conditions?	Months

	Potential input into the environment	**Please select**
Q 4.6	What is the annual quantity of nanoparticles from the ***manufacturing phase*** that reaches the environment via wastewater, exhaust gases or solid waste?	5 - <500 kg

Q 4.7	What is the physical surrounding or carrier material of the nanoparticles in the product during the ***use phase***?	Liquid media
Q 4.8	What is the annual quantity of nanoparticles in products that reaches from production or use phase the environment via utility products, waste water, exhaust gases or solid waste?	5 - <500 kg
Q 4.9	What is the annual quantity of disposed nanomaterial (from the production or use phase)?	5 - <500 kg

Occupational Health Risks

	Hazard & exposure during manufacture of the nanomaterial	Please select
Q 5.1a	Hazard score from Stoffenmanager	C
Q 5.2a	Exposure score from Stoffenmanager	2
	Resulting category	**C2**

	Hazard & exposure during processing the nanomaterial	Please select
Q 5.1b	Hazard score from Stoffenmanager	C
Q 5.2b	Exposure score from Stoffenmanager	1
	Resulting category	**C1**

	Hazard & exposure during application of the nanoproduct	Please select
Q 5.1c	Hazard score from Stoffenmanager	C
Q 5.2c	Exposure score from Stoffenmanager	1
	Resulting category	**C1**

	Hazard & exposure during manufacture (worst case)	Maximum risk score
	Maximum hazard score from Stoffenmanager	**C**
	Maximum exposure score from Stoffenmanager	**2**
	Maximum risk category	**C2**

Consumer Health Risks

	Hazard & exposure by consumers during use phase	**Please select**
Q 6.1	At what location is the nanoelement situated in the article or the product?	The product:
-	contains nanostructured particles that are surface bound (IIIa): may cause exposure	
Q 6.2	What is the size of the consumer population using the nanoproduct and hence which may be exposed?	Low (fraction of households <5%)
	The hazard score (worst hazard score taken from Stoffenmanage Nano, see sheet 5. Occupational Health Risks)	**C**
	Resulting category	**C2**

Appendix 2: Tier 1 Input data for Nano-Organic Pigment

Conventional product: Red dye, molecularly dissolved in the plastic, but these leach and are not weathering-stable and thus does not deliver the same performance.

Nano Product and Legislation

	Type of nano material and application	**Please select or specify**
Q 0.1	Which nanomaterial will be used?	Other
	Please specify additional nano subtype or indications / properties:	the nanoform of Diketokyrrolo-Pyrrole (DPP transparent) pigment is a high-performance pigment required for bright red color in plastics or coatings.
Q 0.2	In which type of application is the nanomaterial be used?	colored plastic parts
Q 0.3a	Is this a completely new product with a new functionality (which cannot easily be compared with a conventional product)?	No
Q 0.3b	If not, what conventional product is being replaced by the new nanoproduct? (this can also be 'doing nothing')	alternative "particulate, non-nano" is given by larger DPP particles, but these are then opaque in visual appearance and less efficient to filter light; Another alternative "non-particulate" is by using red dyes, molecularly dissolved in the plastic, but these leach and are not weathering-stable. Thus both alternatives do not deliver the same performance.
Q 0.4	The product under evaluation is:	A product for the professional market only
Q 0.5	What is the main function that the nanomaterial provides in your application?	Color
Q 0.6	What is the appropriate unit to compare the nanoproduct with the conventional product? (It is only correct to compare the same functionality)	1 kg
	In case you have selected 'Other' please specify:	

	Nano-relevance	Please select
Q 0.7	Approach 1 (precautionary approach): Ranges of sizes of primary particles contained in the materials (free, bound or as aggregates or agglomerates)?	1-500 nm
Q 0.8	Approach 2 (EU-proposed definition 2011/696/EU): Material containing primary particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50% or more of the primary particles in the number size distribution, one or more external dimensions is in the size range 1 nm - 100 nm or (if the number size distribution is unknown) Material where the specific surface area by volume is greater than 60m2/cm3 or Material consists of fullerenes, graphene flakes or single wall nanotubes.	Yes

	Legislation	Please select or specify
Q 0.9	Are you aware of existing legisation (e.g. EU Nr. 1907/2006 (REACH), The EU Biocides Regulation 528/2012 (EU BPR), Regulation (EC) No 1223/2009 on cosmetic products …)	Yes
Q 0.10	Is your nanomaterial approved or notified according to relevant EU-legislation (e.g. EU Nr. 1907/2006 (REACH), The EU Biocides Regulation 528/2012 (EU BPR), Regulation (EC) No 1223/2009 on cosmetic products …)	Yes
Q 0.11	Do you use the nanomaterial below its specific concentration limits recommended in the legal framework (e.g. http://ec.europa.eu/environment/chemicals/biocides/active-substances/approved-substances_en.htm)	Yes

Environmental Benefits

	Manufacturing phase of the nanoproduct versus conventional product	**[Better/Equal/Worse/Unknown]**
Q 1.1	Energy consumption of the manufacturing process?	Worse
Q 1.2a	Materials consumption in this manufacturing process?	Equal
b	Amounts of hazardous substances used in the manufacture?	Equal
Q 1.3	Efforts needed to produce the product using the nanomaterial?	Equal
Q 1.4a	Amount of solid waste from the manufacturing process?	Equal
b	Amount of waste water from the manufacturing process?	Equal
c	Emissions to the air or (waste) water from the manufacturing process itself?	Equal

	Use phase (only for final products and articles)	**[Better/Equal/Worse/Unknown]**
Q 1.5	Product life time (use phase)?	Better
Q 1.6a	Need for maintenance?	Equal
b	Amounts of hazardous substances used in maintenance?	Equal
Q 1.7a	Amount of solid waste from using the product?	Equal
b	Amount of waste water resulting from use of the product?	Equal
c	Emissions of hazardous substances to air, water and/or solid?	Better
Q 1.8	Efficiency of use?	Better

	End-of-life (only for final products and articles)	**[Better/Equal/Worse/Unknown]**
Q 1.9	Volume of waste (due to e.g. longer lifetime, less weight, less material used)?	Worse
Q 1.10a	Amounts of other hazardous substances released from the waste water treatment?	Better
b	Amounts of other hazardous substances released during incineration?	Better
Q 1.11	Established recycling systems (glass, PET, paper, carton, batteries, biowaste, electronic devices, etc.) exposed to the nanomaterial in the product?	Equal
		[Yes/No/Unknown]
Q 1.12a	Can the waste water treatment facility eliminate the nanoproduct's emissions?	Unknown
b	Can the waste incineration facility eliminate the nanoproduct's emissions?	Yes

Economic Benefits

	Market potential	**Please select**
Q 2.1	Does the nanoproduct have increased marketability due to an improved functionality or a new functionality (for example: UV-protection, enhanced photolytical self-cleaning/ self-cleaning capacity/property, conductible, antimicrobial function), or a clear image advantage compared to the conventional product (e.g.: more resistant to environmental effects, prolonged lifetime/persistence, reduced weight or increased strength)?	higher
Q 2.2	What is the foreseen market potential of the nanoproduct or -application in Europe?	high (> 1 M€ sales)

	Profitability	**[higher / equal / lower / unknown]**
Q 2.3	What is the (expected) purchase price per unit of the nanobased product or material compared to the conventional one?	higher
Q 2.4	What are the operational costs (i.e. maintenance, energy use etc) during the use phase of the nanobased product or application compared to the conventional one? (Think of advantages due to nanoproperties in the manufacturing process)	equal

	Development stage	**Please select**
Q 2.4	What is the time-to-market to manufacture the nanoproduct on a commercial scale?	low (< 1 year)

Societal Benefits

	Societal aspects	**Please select**
Q 3.1	Could the use or application of the nanoproduct be considered a technological breakthrough (in general, but particularly in energy systems and Information and Communication Technologies, ICT) compared to the conventional alternative?	more or less equal
Q 3.2	Does the production of the application lead to a substantial improvement in the development of a highly qualified labour force compared to the conventional alternative?	more or less equal
Q 3.3	Compared to the conventional alternative... Does the use or application of the nano-based product lead to improvements in feeding the world's population, a marked increase in food production and the nutritional value of food? OR Does the use or application of the nano-based product lead to improvements in people's health, particularly the direct user, e.g. by improvements in water purity, sanitation or medicines and pharmaceuticals?	more or less equal

Public Health & Environmental Risks

	System knowledge	**[Yes/Partly/No]**
Q 4.1	Is the origin of the (nanoscale) starting materials known?	Yes
Q 4.2	Are the next users of the nanomaterials under consideration known?	No
Q 4.3	How accurately is the material system known or can disturbing factors (e.g. impurities) be estimated?	Accurately

	Potential effect	**[Low/Medium/High/Unknown]**

Q 4.4	Do the nanomaterials cause redox activity, catalytic activity or have a potential for oxygen radical formation or to induce inflammation reactions? (The drop-down menu gives clues which forms of nanoproducts have a low, medium or high potential effect.)	Low, unfunctionalised polymer
Q 4.5	What is the stability (half-life) of the nanoparticles present in the nanomaterial under ambient environmental conditions?	Unknown

	Potential input into the environment	**Please select**
Q 4.6	What is the annual quantity of nanoparticles from the ***manufacturing phase*** that reaches the environment via wastewater, exhaust gases or solid waste?	5 - <500 kg
Q 4.7	What is the physical surrounding or carrier material of the nanoparticles in the product during the ***use phase***?	Solid matrix, stable under conditions of use, nanoparticles not mobile
Q 4.8	What is the annual quantity of nanoparticles in products that reaches from production or use phase the environment via utility products, waste water, exhaust gases or solid waste?	Unknown
Q 4.9	What is the annual quantity of disposed nanomaterial (from the production or use phase)?	>500 kg

Occupational Health Risks

	Hazard & exposure during manufacture of the nanomaterial	**Please select**
Q 5.1a	Hazard score from Stoffenmanager	A
Q 5.2a	Exposure score from Stoffenmanager	2
	Resulting category	**A2**

	Hazard & exposure during processing the nanomaterial	**Please select**
Q 5.1b	Hazard score from Stoffenmanager	A
Q 5.2b	Exposure score from Stoffenmanager	3
	Resulting category	**A3**

	Hazard & exposure during application of the nanoproduct	**Please select**

Q 5.1c	Hazard score from Stoffenmanager	A
Q 5.2c	Exposure score from Stoffenmanager	1
	Resulting category	**A1**

	Hazard & exposure during manufacture (worst case)	**Maximum risk score**
	Maximum hazard score from Stoffenmanager	**A**
	Maximum exposure score from Stoffenmanager	**3**
	Maximum risk category	**0**

Consumer Health Risks

	Hazard & exposure by consumers during use phase	**Please select**
Q 6.1	At what location is the nanoelement situated in the article or the product?	The product:
-	contains nanostructured particles suspended in solids (IIIc): no expected exposure	
Q 6.2	What is the size of the consumer population using the nanoproduct and hence which may be exposed?	High (fraction of households > 5%)
	The hazard score (worst hazard score taken from Stoffenmanage Nano, see sheet 5. Occupational Health Risks)	**A**
	Resulting category	**A1**

Appendix 3: Tier 1 Input data for Nano-Carbon Black

Conventional product: Black dye, molecularly dissolved in the plastic, but these leach and are not weathering-stable and thus does not deliver the same performance.

Nano Product and Legislation

	Type of nano material and application	**Please select or specify**
Q 0.1	Which nanomaterial will be used?	Other
	Please specify additional nano subtype or indications / properties:	nano carbon black of size range in the size range of 15–500 nm
Q 0.2	In which type of application is the nanomaterial be used?	colored plastic parts
Q 0.3a	Is this a completely new product with a new functionality (which cannot easily be compared with a conventional product)?	No
Q 0.3b	If not, what conventional product is being replaced by the new nanoproduct? (this can also be 'doing nothing')	Black dye molecularly dissolved in the plastic, but these leach and are not weathering-stable. Thus this alternative does not deliver the same performance.
Q 0.4	The product under evaluation is:	A product for the professional market only
Q 0.5	What is the main function that the nanomaterial provides in your application?	Color
Q 0.6	What is the appropriate unit to compare the nanoproduct with the conventional product? (It is only correct to compare the same functionality)	1 kg
	In case you have selected 'Other' please specify:	

	Nano-relevance	**Please select**
Q 0.7	Approach 1 (precautionary approach): Ranges of sizes of primary particles contained in the materials (free, bound or as aggregates or agglomerates)?	1-500 nm

Q 0.8	Approach 2 (EU-proposed definition 2011/696/EU): Material containing primary particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50% or more of the primary particles in the number size distribution, one or more external dimensions is in the size range 1 nm - 100 nm or (if the number size distribution is unknown) Material where the specific surface area by volume is greater than 60m2/cm3 or Material consists of fullerenes, graphene flakes or single wall nanotubes.	Yes

	Legislation	**Please select or specify**
Q 0.9	Are you aware of existing legisation (e.g. EU Nr. 1907/2006 (REACH), The EU Biocides Regulation 528/2012 (EU BPR), Regulation (EC) No 1223/2009 on cosmetic products …)	Yes
Q 0.10	Is your nanomaterial approved or notified according to relevant EU-legislation (e.g. EU Nr. 1907/2006 (REACH), The EU Biocides Regulation 528/2012 (EU BPR), Regulation (EC) No 1223/2009 on cosmetic products …)	Yes
Q 0.11	Do you use the nanomaterial below its specific concentration limits recommended in the legal framework (e.g. http://ec.europa.eu/environment/chemicals/biocides/active-substances/approved-substances_en.htm)	Yes

Environmental Benefits

	Manufacturing phase of the nanoproduct versus conventional product	**[Better/Equal/Worse/Unknown]**
Q 1.1	Energy consumption of the manufacturing process?	Worse
Q 1.2a	Materials consumption in this manufacturing process?	Equal
b	Amounts of hazardous substances used in the manufacture?	Equal
Q 1.3	Efforts needed to produce the product using the nanomaterial?	Equal

Q 1.4a	Amount of solid waste from the manufacturing process?	Equal
b	Amount of waste water from the manufacturing process?	Equal
c	Emissions to the air or (waste) water from the manufacturing process itself?	Equal

	Use phase (only for final products and articles)	**[Better/Equal/Worse/Unknown]**
Q 1.5	Product life time (use phase)?	Better
Q 1.6a	Need for maintenance?	Equal
b	Amounts of hazardous substances used in maintenance?	Equal
Q 1.7a	Amount of solid waste from using the product?	Equal
b	Amount of waste water resulting from use of the product?	Equal
c	Emissions of hazardous substances to air, water and/or solid?	Better
Q 1.8	Efficiency of use?	Better

	End-of-life (only for final products and articles)	**[Better/Equal/Worse/Unknown]**
Q 1.9	Volume of waste (due to e.g. longer lifetime, less weight, less material used)?	Worse
Q 1.10a	Amounts of other hazardous substances released from the waste water treatment?	Better
b	Amounts of other hazardous substances released during incineration?	Better
Q 1.11	Established recycling systems (glass, PET, paper, carton, batteries, biowaste, electronic devices, etc.) exposed to the nanomaterial in the product?	Equal
		[Yes/No/Unknown]
Q 1.12a	Can the waste water treatment facility eliminate the nanoproduct's emissions?	Unknown
b	Can the waste incineration facility eliminate the nanoproduct's emissions?	Yes

Economic Benefits

	Market potential	**Please select**
Q 2.1	Does the nanoproduct have increased marketability due to an improved functionality or a new functionality (for example: UV-protection, enhanced photolytical self-cleaning/ self-cleaning capacity/property, conductible, antimicrobial function), or a clear image advantage compared to the conventional product (e.g.: more resistant to environmental effects, prolonged lifetime/persistence, reduced weight or increased strength)?	higher

Q 2.2	What is the foreseen market potential of the nanoproduct or -application in Europe?	high (> 1 M€ sales)

	Profitability	**[higher / equal / lower / unknown]**
Q 2.3	What is the (expected) purchase price per unit of the nanobased product or material compared to the conventional one?	higher
Q 2.4	What are the operational costs (i.e. maintenance, energy use etc) during the use phase of the nanobased product or application compared to the conventional one? (Think of advantages due to nanoproperties in the manufacturing process)	equal

	Development stage	**Please select**
Q 2.4	What is the time-to-market to manufacture the nanoproduct on a commercial scale?	low (< 1 year)

Societal Benefits

	Societal aspects	**Please select**
Q 3.1	Could the use or application of the nanoproduct be considered a technological breakthrough (in general, but particularly in energy systems and Information and Communication Technologies, ICT) compared to the conventional alternative?	more or less equal
Q 3.2	Does the production of the application lead to a substantial improvement in the development of a highly qualified labour force compared to the conventional alternative?	more or less equal

Q 3.3	Compared to the conventional alternative... Does the use or application of the nano-based product lead to improvements in feeding the world's population, a marked increase in food production and the nutritional value of food? OR Does the use or application of the nano-based product lead to improvements in people's health, particularly the direct user, e.g. by improvements in water purity, sanitation or medicines and pharmaceuticals?	more or less equal

Public Health & Environmental Risks

	System knowledge	**[Yes/Partly/No]**
Q 4.1	Is the origin of the (nanoscale) starting materials known?	Yes
Q 4.2	Are the next users of the nanomaterials under consideration known?	No
Q 4.3	How accurately is the material system known or can disturbing factors (e.g. impurities) be estimated?	Accurately

	Potential effect	**[Low/Medium/High/Unknown]**
Q 4.4	Do the nanomaterials cause redox activity, catalytic activity or have a potential for oxygen radical formation or to induce inflammation reactions? (The drop-down menu gives clues which forms of nanoproducts have a low, medium or high potential effect.)	Low, unfunctionalised polymer
Q 4.5	What is the stability (half-life) of the nanoparticles present in the nanomaterial under ambient environmental conditions?	Unknown

	Potential input into the environment	**Please select**
Q 4.6	What is the annual quantity of nanoparticles from the ***manufacturing phase*** that reaches the environment via wastewater, exhaust gases or solid waste?	5 - <500 kg
Q 4.7	What is the physical surrounding or carrier material of the nanoparticles in the product during the ***use phase***?	Solid matrix, stable under conditions of use, nanoparticles not mobile
Q 4.8	What is the annual quantity of nanoparticles in products that reaches from production or use phase the environment via utility products, waste water, exhaust gases or solid waste?	Unknown

Q 4.9	What is the annual quantity of disposed nanomaterial (from the production or use phase)?	>500 kg

Occupational Risk

	Hazard & exposure during manufacture of the nanomaterial	**Please select**
Q 5.1a	Hazard score from Stoffenmanager	D
Q 5.2a	Exposure score from Stoffenmanager	1
	Resulting category	**D1**

	Hazard & exposure during processing the nanomaterial	**Please select**
Q 5.1b	Hazard score from Stoffenmanager	A
Q 5.2b	Exposure score from Stoffenmanager	3
	Resulting category	**A3**

Consumer Risk

	Hazard & exposure by consumers during use phase	**Please select**
Q 6.1	At what location is the nanoelement situated in the article or the product?	The product:
-	contains nanostructured particles suspended in solids (IIIc): no expected exposure	
Q 6.2	What is the size of the consumer population using the nanoproduct and hence which may be exposed?	High (fraction of households > 5%)
	The hazard score (worst hazard score taken from Stoffenmanage Nano, see sheet 5. Occupational Health Risks)	**D**
	Resulting category	**A1**

ACKNOWLEDGEMENTS

First and foremost, I am deeply grateful to my supervisor, Dr. Elena Semenzin for her excellent mentorship. She has been extremely kind and supportive and at the same time set a high standard of research conduct through personal example and instruction. Without her guidance, this work could certainly not have achieved the breadth and quality it has and I would be a less competent researcher.

Next, I acknowledge the support of other researchers involved in the Nanosafety group for their contribution to my PhD research, particularly Dr. Alex Zabeo, Dr.Danail Hristozov, Dr.Lisa Pizzol and Gianpietro Basei. I thank Prof. Antonio Marcomini for hosting me in his research group and being supportive of my PhD.

This highly multidisciplinary research would not be possible without the significant contributions of several experts within the SUN project consortium. It has been a significant advantage to be able to conduct research in the company of the most respected experts in nanosafety field, and I thank all of them for being so generous with their time and expertise. In addition, I thank Prof. Igor Linkov for his guidance and collaboration on framework development.

I am grateful to the the Italian Ministry of Education, Universities and Research for granting me a three year scholarship to pursue my PhD. I acknowledge support of the Department of Environmental Sciences, Informatics and Statistics at the University Ca' Foscari Venice for hosting me as a PhD student.

I thank Prof. Fabrizio Passarini and Prof. Finbarr Murphy for their valuable feedback on the first draft of the thesis.

Finally, I am forever indebted to my family and friends for their faith in me and significant support in the completion of the PhD.