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Safe by Design: Guidance for combining RA and LCA at TRL 1-6

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Contents

Glossary of Acronyms

ACQ: Alkaline copper quaternary

CCA: Chromated Copper Arsenate

CB: Control Banding

CAP: Conventional Acrylic Paint

ECHA: European Chemicals Agency

EHS: Environmental Health and Safety

ERA: Ecological Risk Assessment

EU: European Union

GSD: Goal and Scope Definition

HHRA: Human Health Risk Assessment

ILCD: International Reference Life Cycle Data System

ISO: International Standards Organisation

LC: Life Cycle

LCA: Life Cycle Assessment

n-CuO: Nano copper oxide

pZZS: Potentieel Zeer Zorgwekkende Stoffen

RA: Risk Assessment

REACH: Registration, Evaluation, Authorisation and Restriction of Chemicals

SbD: Safe by Design

SSbD: Safe and Sustainable by Design

TRL: Technological Readiness Level

US: United States

ZZS: Zeer Zorgwekkende Stoffen

1.Introduction

The Safe by Design (SbD) approach aims to identify and mitigate chemical risks to the environment and human health through the life cycle during early product development. SbD approach to achieve chemical safety is fairly new and there is limited knowledge about applicable methods and their implementation in a product development context.

This guidance document is composed to aid product designers by explaining how and existing practical risk assessment (RA) and life cycle assessment (LCA) tools could be combined in product design practice. This document is based on a literature review (Subramanian and Guinee, 2021) investigating the combination of RA and LCA at low technology readiness levels (TRL): concept stage (TRL 1-4) and laboratory scale (TRL 4-6). The key findings of the literature review are summarized in Appendix 1 of this document.

This guidance document is structured as follows. After the Introduction (Section 1), a workflow for using RA and LCA together at different TRLs is elaborated (Section 2). This workflow is illustrated by applying it to a case study of nano copper oxide based biocidal paint for wood preservation (Section 3)[1]. The guidance document is concluded with summary conclusions (Section 4).

2. Safe by Design Approach through Technological Readiness Levels 1-6

Subramanian and Guinée (2021) found ten publications with a product development application suitable for assessing combination of RA and LCA or life cycle thinking (LCT) at low TRL. Based on this review, we formulate a working approach for product design teams to implement SbD at a certain design stage varying from TRL 1 to 6 (Figure 1). Given the limited literature reviewed, the preliminary nature of the workflow is strongly emphasized. It is expected that, as more studies including joint application of RA and LCA at low TRLs in product development contexts will be carried out, the workflow and practical tools will also evolve.

The steps of the workflow are explained below. Three steps of the workflow are elaborated separately in detail: Step 5 (input chemicals), Step 6 (emissions)and Step 7 (wastes). See Figure 2, 3 and 4 respectively.

[1] Information to apply the case study was obtained from the EU FP7 Sustainable Nanotechnology project (http://www.sun-fp7.eu/), where nano copper oxide paint was one of the case studies.

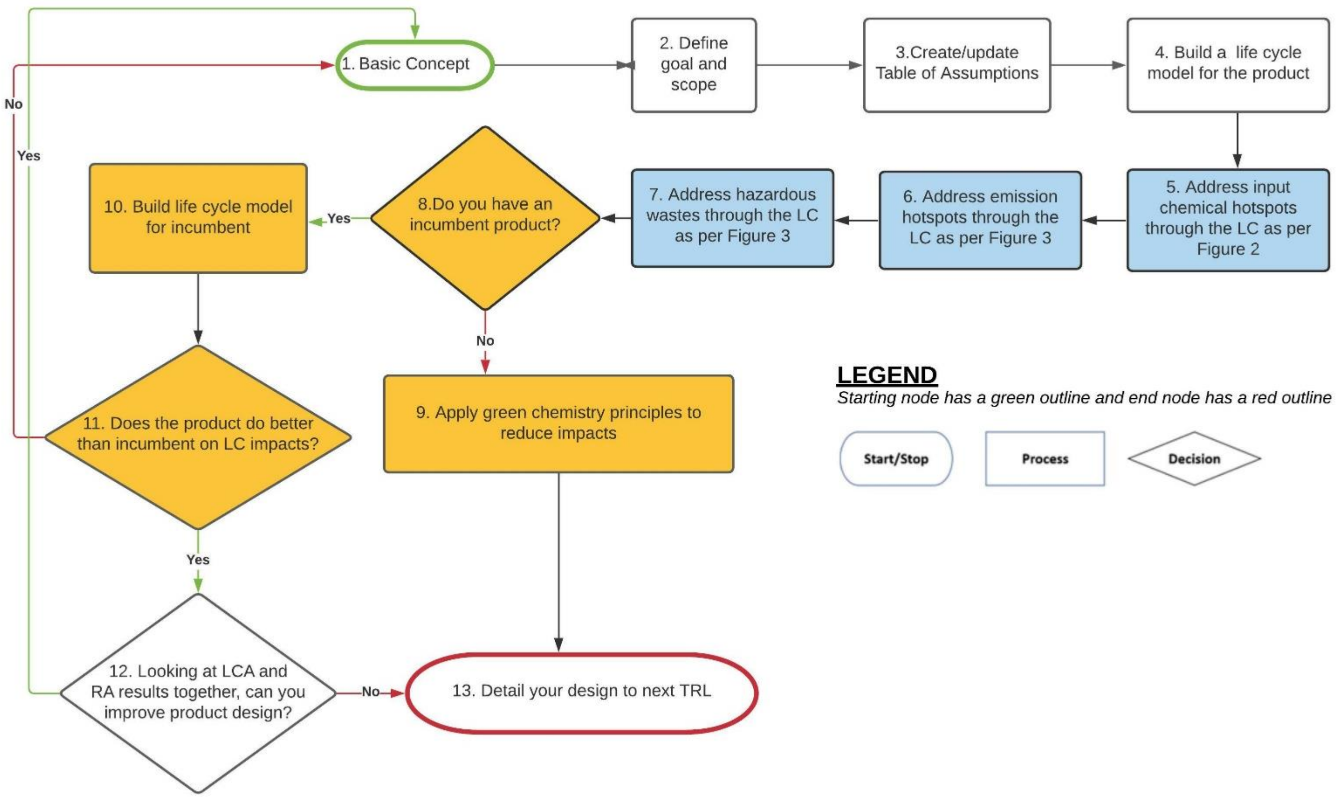

Figure 1 SbD Workflow for each TRL level

Step 1: Formulate a concept of an innovative product in as much detail as possible to which the SbD approach could be applied. This so-called basic concept is modified iteratively when it turns out that risks are not adequately controlled and/or a better environmental impact profile is possible (Steps 5, 6, 7, 11 and 12).

Step 2: Perform the Goal and Scope Design (GSD) for the product. While a comprehensive GSD as required by International Standard organization (ISO) 14041 (2015) or International Reference Life Cycle Data System (ICLD) guidelines (2010) may not be possible at lowest TRLs, the GSD should focus upon the salient aspects e.g., functionality , technical performance, target market and price and other quality characteristics. It could be attempted to define functional units and identify incumbent market alternatives with the same functionality which will be used in Step 8. Functional unit is a quantification of the identified function of the product or incumbent, that helps define the amount of product needed to achieve this functionality and subsequently the inputs and the outputs. The case study (Section 3) used in this guidance document defines functional unit in terms of square meter of wood protected against microbial attack.

Step 3: Create or update the Table of Assumptions, which documents any assumptions that will be used in the subsequent steps. These include economic, product quality aspects, or any assumptions used in RA/LCA so that explicit trade-offs can be made, and scope and interpretation of the analysis becomes clear.

Step 4: Apply LCT and build a model of the product's life cycle (LC). The product LC includes the synthesis of primary chemicals used in the product (Synthesis), the formulation of the product (Production), the use in a consumer context (Use) and the waste treatment or recycling (End of Life). Identify, within each LC stage, key unit processes and activities that mediate flows that may create risk hotspots.

Unit processes are characterized by input (e.g., chemicals, energy) and output (e.g., emissions, waste) flows. Safety issues in a unit process can be related to input chemicals, emissions and/or waste. Input chemicals can be addressed through hazard-based approaches (detailed in Figure 2), that mitigate the inherent hazard of the product constituents or the product as a whole. Risk-based approaches can be used for addressing safety issues regarding emissions and waste (detailed in Figure 3 and Figure 4 respectively).

Product design teams with LCA modelling experience can even try to set up a flowchart of the novel product system using existing flows and unit processes from Life Cycle Inventory databases. It should be noted that unit processes in LCA databases may not fully cover the activities that cause human health risk, especially in the use phase. This gap can be filled by considering activities that constitute human exposure. The European Chemicals Agency (ECHA) offers guidance documents for setting up basic occupational and consumer exposure scenarios (ECHA, 2017; ECHA, 2015), which may be useful in this regard.

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The working approach now explores RA (Steps 5-7 Figure 1 in blue) and LCA (Steps 8-11 Figure 1 in yellow) and how they may impact the design process independently, and subsequently how combining the outputs of both methods (Step 12) can offer additional insights.

Step 5: Address the risk hotspots due to input chemicals through the product LC (Figure 2), based on the inherent hazard of input chemicals and of the overall product. A two-step approach is followed. The first step involves checking the hazards of all input chemicals constituting the product independently. The second step involves checking for aggregate effects (hazard) through product (eco)toxicological screening. For the first step Subramanian and Guineé (2021) found some useful approaches:

- Checking if input chemicals occur in various environmental regulation lists as confirmed or suspected hazardous. Resources for doing this check include the Dutch 'Zeer Zorgwekkende Stoffen' (ZZS, hazardous chemicals compiled from fifteen environmental regulations)[2] and 'Potentieel Zeer Zorgwekkende Stoffen' (PZZS, chemicals suspected of being hazardous)[3].
- Checking hazard statements associated with input chemicals based on the Classification, Labelling and Packaging regulation. Hazard statements may be based on

[2] https://www.infomil.nl/onderwerpen/lucht-water/zeer-zorgwekkende/
[3] https://rvs.rivm.nl/onderwerpen/Zeer-Zorgwekkende-Stoffen/Potentiele-ZZS

physical hazards (e.g. a H284 chemical under pressure may explode if heated), health hazards (e.g. a H314 chemical causes severe skin burns and eye damage), and environmental hazards (e.g. a H420 chemical harms public health and the environment by destroying ozone in the upper atmosphere). Manufacturers of chemicals are obliged to communicate information on hazard statements. This information can be found in Safety Data sheets (ECHA, 2020), which are also uploaded online by several primary chemical providers.

- Using the Environmental Health and Safety tool developed by Koller et al. (1999) to estimate risks of specific volumes of chemicals for the environment and in occupational settings (also addressing accidental release).

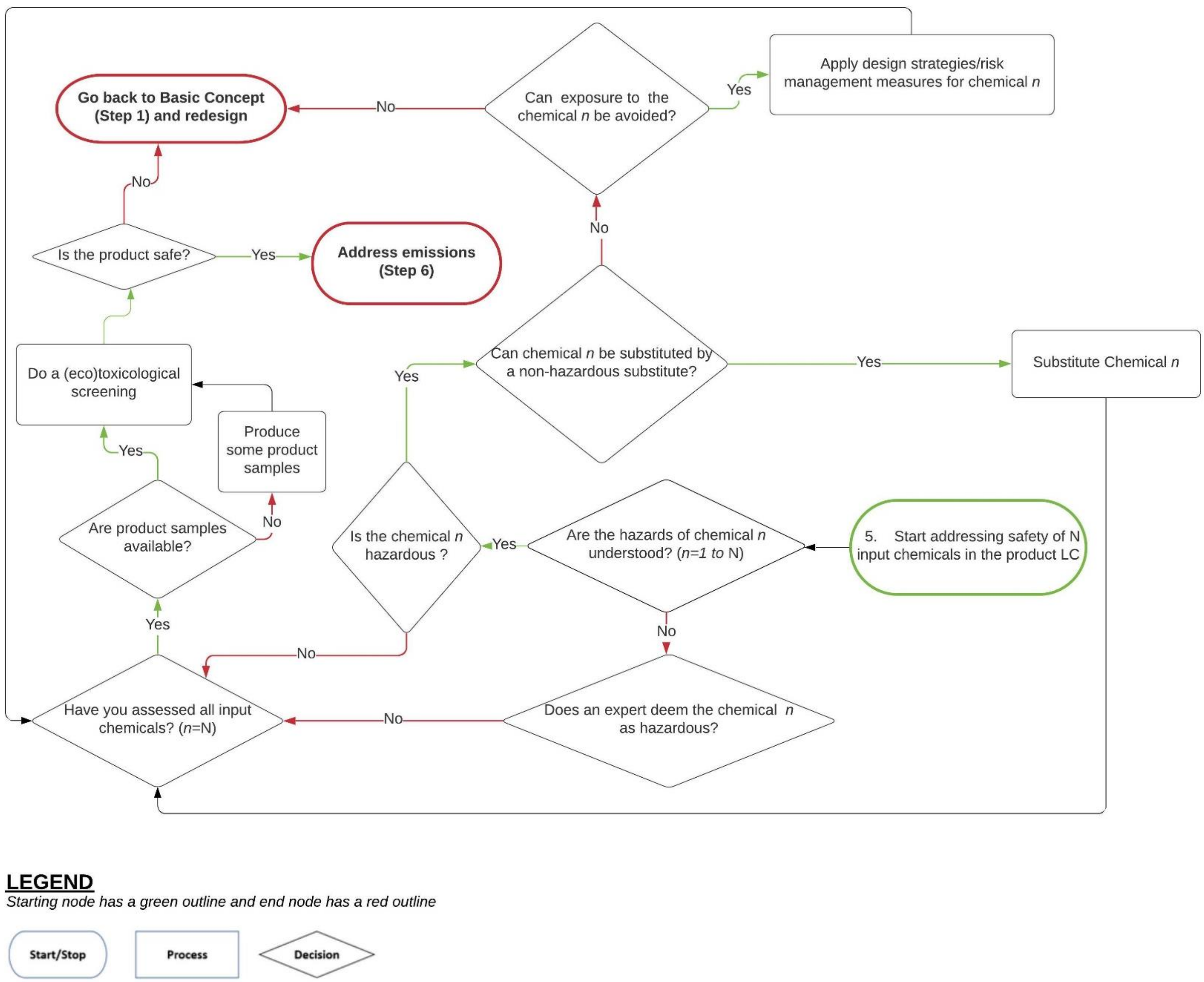

Figure 2 Sub-workflow to address input chemicals through product LC (Step 5)

Once the hazard of all product constituents has been addressed, and if product samples are available (TRL 4-5), (eco)toxicological screening could also be applied to the whole product.

At laboratory scale (TRL 5-6), product design teams could also collaborate with experts to apply methods like Alternatives Assessment (OECD, 2021) and In Silico approaches (e.g., Grouping and read across, Quantitative Structure Activity Relationships)[4].

Step 6: Address risk hotspots due to emissions to air, water and soil through the LC (Figure 3). An example of such a risk hotspot is the incomplete combustion of carbon black and petroleum derivatives, which can lead to the emission of Polyaromatic hydrocarbons to air that may cause acute and chronic respiratory and cardiovascular effects in human beings.

Control Banding (CB) approach uses prior experiences on hazard and exposure to develop classification systems or bands. Combinations of hazard and exposure bands are associated with an evaluation of risk and (often) risk management that has been used successfully for the specific combination of hazard and exposure (Zalk and Nelson, 2008). Hazard bands may include hazard statements or potential effects, and exposure bands may include ranges of emissions quantities for various types of emissions (e.g. aerosol, droplets, powder, gas). For example, one of the simplest CB tools for nanomaterials is the Swiss Precautionary Matrix (Hock et al, 2008), with a hazard band based on redox activity (present/not present) and an exposure band based on quantity of nanomaterials entering the environment (tonnage bands associated with Low, Medium, High).

The risk modules of the LICARA Nanoscan tool use three CB tools: Precautionary Matrix (Hock et al, 2008, for environmental and public health risks), Stoffenmanager Nano (van Duuren-Stuurman et al, 2012, for occupational and consumer risks), and NanoRiskCat (Hansen et al, 2011, for consumer risk). The Nanoscan tool has been generalized for all innovative products and is known as LICARA Innovation Scan, and contains more CB tools applicable to all innovative products.

Product design teams need to consider the scope of CB tools and chose the appropriate one for their context. Seeking expert input for choosing hazard or exposure bands may be done if designers do not understand hazard and exposure characteristics of a potential risk hotspot. Expert elicitation has even been used in the reviewed literature to build a CB system (Shatkin and Kim, 2008; Wardak, 2008). If needed, product designers can collaborate with RA experts and define hazard and exposure bands to evaluate their products.

[4] See OECD QSAR toolbox for some methods: https://qsartoolbox.org/support/

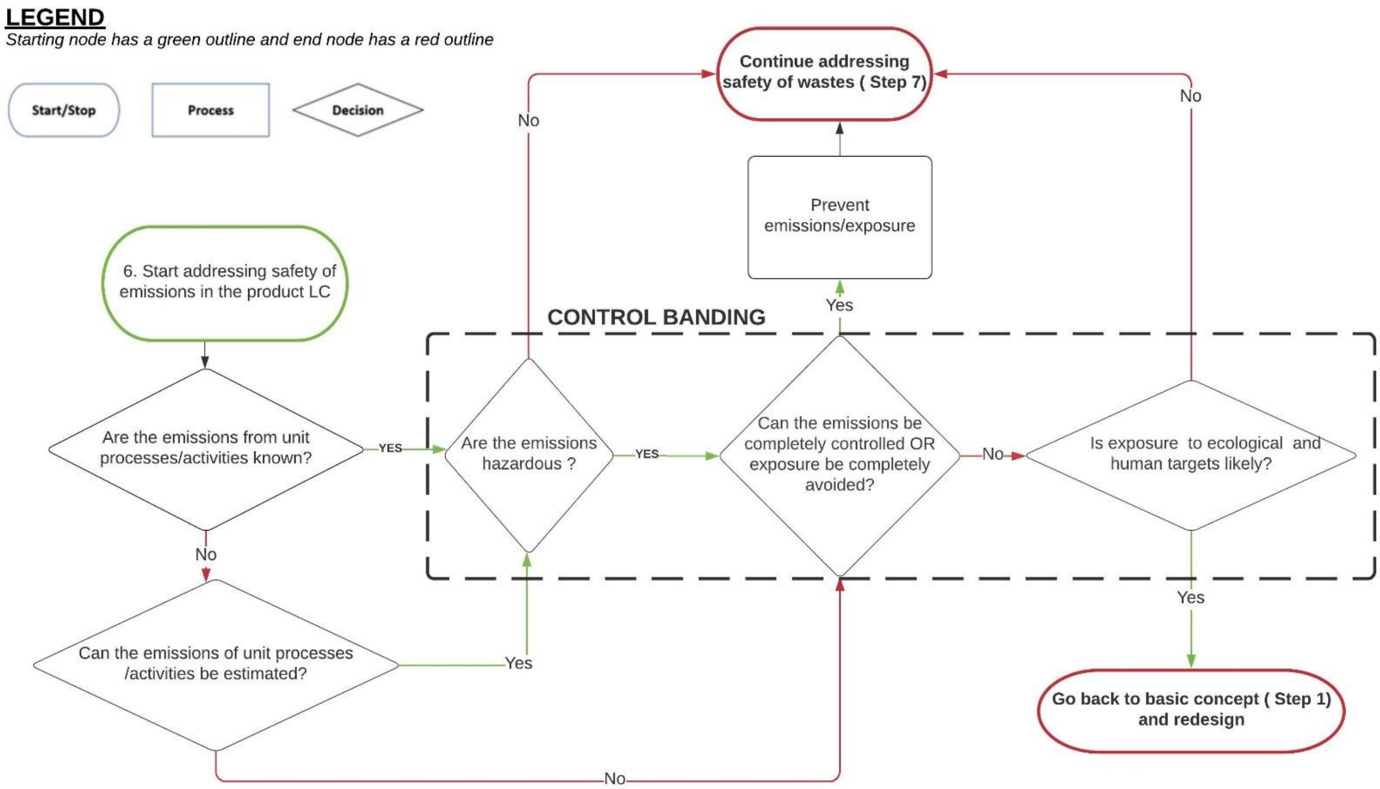

Figure 3 Sub-workflow to address emissions through product LC (Step 6)

Step 7: Address risk hotspots due to wastes through the LC (Figure 4). Risks from wastes are less understood and often become a source of pollution and environmental and health risks. Any analysis of safety issues of wastes should also consider that materials should sustain multiple cycles to meet circular economy aspirations. Literature review and expert elicitation are used in the reviewed literature (Subramanian and Guinée, 2021), and CB tools for environmental and occupational exposure could also be used.

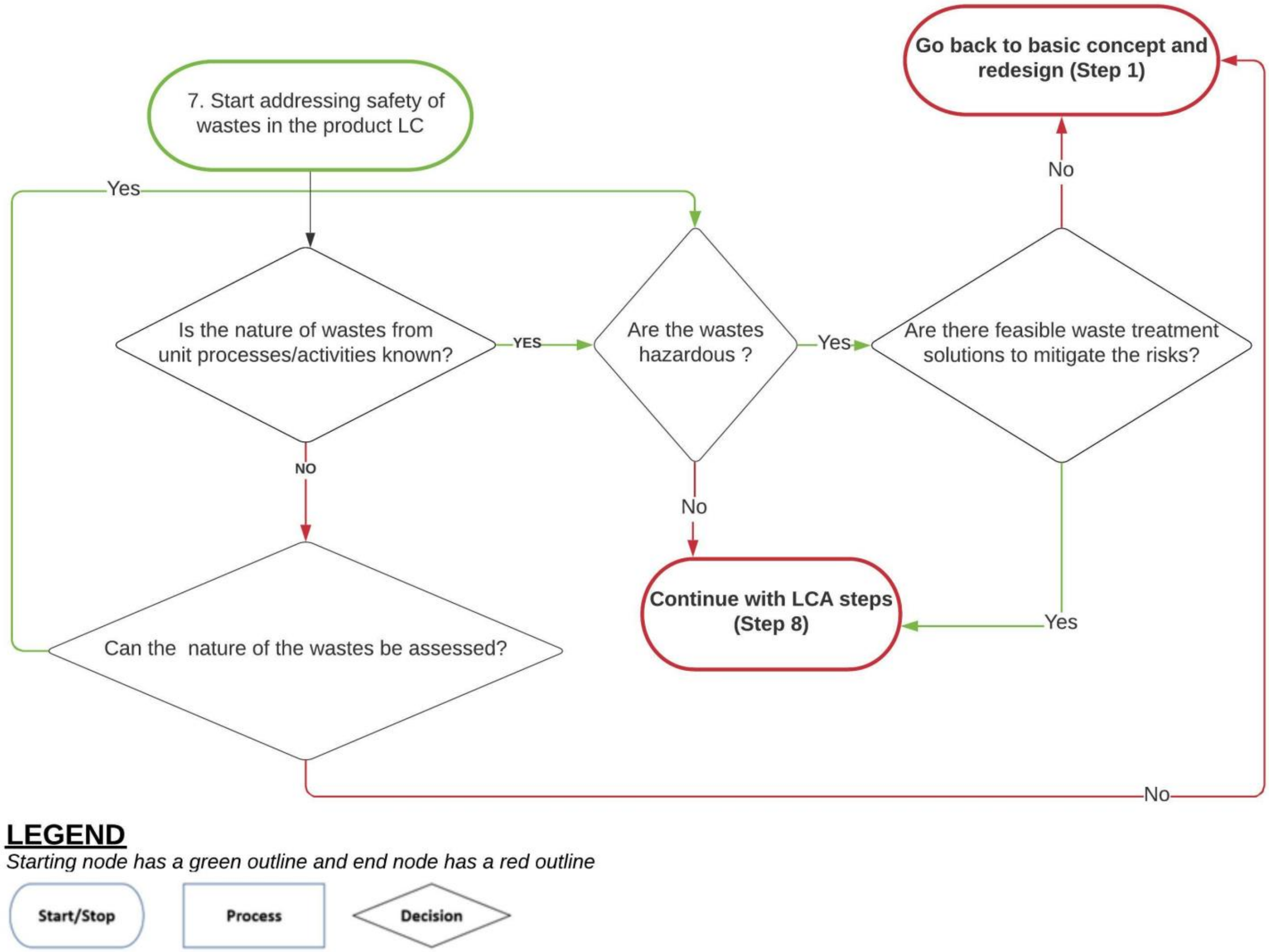

Figure 4 Sub-workflow to address wastes through the product LC (Step 7)

Step 8-10: If it was possible to identify an incumbent alternative that provides the desired functionality (Step 2), build the LC model of the incumbent (Step 10, as described in Step 4 for building the LC model for the product under design).

If the functionality of the product being designed is novel or unclear (e.g. a new material), it is not possible to use LCA to compare the impacts of the product with the incumbent (Step 11). In this case, it can be checked if green chemistry principles can be applied to improve the product's environmental impact profile. With risks addressed (Step 5-7) and product at its best possible environmental impact profile (outcome of Step 9), the working approach can be followed again when the product design has been detailed further to the next TRL (Step 13).

Step 11: Compare the environmental impacts of the product (result of Step 4) and the incumbent (Step 9), and check if the product is (overall) better (Step 11).

The LICARA Innovation Scan can be used to compare the impacts of the product and incumbent at low TRLs with inputs from experts if needed. , and collaboration with LCA experts can also be used to set up an ex-ante LCA (Step 11). The LCA modules of the LICARA NanoScan (comprising of environmental, economic and social benefits) compare the product and its existing alternative for each lifecycle stage by comparing potential environmental impacts (e.g., energy consumption, materials consumption, water use, waste generation).

If it is possible to collaborate with an LCA expert, ex ante LCA can also be applied in which the future, upscaled version of the product and its incumbent are compared at a specified point in the future. Ex-ante LCA can suggest areas where greatest improvements are needed, and also allows for comparison of the impact of material (Tan et al., 2018) and process changes (Kralisch, 2013).

Step 12: After completing the SbD workflow at a particular TRL, consider the RA and LCA results together (Step 4). If any improvements to product safety and sustainability are possible, adjust your basic concept (Step 1), if not, detail your design concept further and move to a higher TRL evaluation (Step 13).

The purpose of considering RA and LCA together can differ with context and how methods are applied. Researchers have combined them to avoid problem shifting across life cycle, risk receptors and/or geographical boundaries. In the LICARA Innovation Scan, the positive environment, economic and social impacts of the product over the incumbent are considered as benefits, and are compared with risks of the new product to assess implications for product development.

3.The Case of Nano Copper oxide based Biocidal Paint for Wood

The case study of a hypothetical nano copper oxide-based biocidal paint (n-CuO paint) for light outdoor applications will be used to illustrate some parts of working approach (Section 3). The section starts with establishing a realistic design context (Section 3.1) followed by an illustration of key insights from the application of the working approach (Section 3.2). LICARA Nanoscan tool is used in Sections 3.2.3-3.2.5. A description of the methodology used in LICARA Nanoscan is provided in Appendix 2 and the inputs provided for the n-CuO paint case study are provided in Appendix 3. For details on the application of the LICARA Nanoscan to the n-CuO paint case study, the reader is referred to Subramanian (2017); here we focus on the insights for product development from the results.

The steps demonstrated include performing a GSD (Section 3.2.1, Step 2), building a LC model (Section 3.2.2, Step 4), assessing risk hotspots due to emissions (Section 3.2.4, Step 6), and comparing RA and LCA results (Section 3.2.5, Step 9).

3.1 Product Design Context

In this section, a short background is provided on wood preservation (Section 3.1.1) and development goals are formulated (Section 3.1.2).

3.1.1 Background

Wood preservation treatment is essential for increasing the service life of timber in many applications by imparting it with fungicidal and insecticidal properties. Two types of wood pressure treatments exist: pressure injection (where pressure is used to force an antimicrobial coating into wood) and coating (applying a preservative coating on wood).

Pressure injection treatments are used to strengthen weaker species of wood to be used for heavy duty applications. The first copper based wood preservative, chromated copper arsenate (CCA), was an inexpensive broad-spectrum biocide with copper providing protection against fungi, chromium fixing copper and arsenic in the wood, and arsenic providing supplemental protection against copper-tolerant fungi and insects (Lebow et al. 2004). CCA was less corrosive to brass and steel (used as fasteners) than the other copper formulations (Zhang and Jiang 2006). CCA was discontinued after concern on exposure of children to arsenic. Further, the robust fixing mechanism of CCA to the wood led to waste with high concentration of metals that needed special management. CCA use in US and EU was henceforth restricted to heavy duty applications with limited potential for exposure (e.g., utility poles, railway sleepers).

To avoid the toxicity of preservatives like CCA, Chemical formulations using ionic copper as the primary insecticide and fungicide were developed next, which also included a co-biocide to provide additional resistance. The US Environmental Protection Agency awarded its U.S. Environmental Protection Agency's Presidential Green Chemistry Challenge Award in 2002 to the company Chemical Specialties, Inc. (now Viance) for commercial introduction of Alkaline copper quaternary (ACQ) to replace CCA[5]. While ionic copper-based formulations were less toxic and effective in timber preservation, increased release of ionic copper into the surrounding environment resulted in the degradation of metal fasteners and subsequent structural failure (Forest Products Laboratory, 2000).

Coatings are not likely to be suitable for wood subjected to extreme weathering (where pressure treatment is appropriate), but they can provide sufficient protection for short lived wooden structures with low to moderate weathering (e.g., exterior cladding).

It can be seen from the above brief context that certain conditions should be met for a viable wood preservation treatment: effective against a range of microbes and fungi but low toxicity to human health and environment, less leaching and/or corrosivity to metals and durability of treatment.

3.1.2 Development goal

The product development team aims to develop a wood preserving coating for consumer use for non-treated wood (or added protection to pressure treatment). In addition to wood preservation, the coating also provides an aesthetic functionality (as a paint). The paint should be free from safety issues and have low environmental impacts, and also economic and social benefits.

[5] https://www.epa.gov/greenchemistry/presidential-green-chemistry-challenge-2002-designing-greener-chemicals-award

3.2 Application of Working approach to nano copper oxide biocidal paint case

In this section, we discuss the key results and insights from applying key steps (Step 2, 4, 6, 11, 12) of the working approach (Figure 1).

3.2.1 Working approach Step 2 -Goal and Scope Definition

Here we describe a GSD for the n-CuO paint based on a basic concept and preliminary information that may be available to a product design team.

While there can be many uses for a biocidal paint, a promising use case to consider is painting a house fence. A surface area based functional unit seems appropriate to quantify the area of wood protected or given a certain aesthetic finish e.g., provision of one square metre of an exposed softwood exterior cladding during a year. The incumbent product is a conventional acrylic paint (CAP), without n-CuO (i.e biocidal functionality is absent). Note that pressure treated wood would not be a good incumbent as the application and LC aspects vary substantially. Hence the market is niche and the price point should be determined in reference to CAP and not pressure treated wood.

The n-CuO paint has a relatively simple formulation and could be commercialized within two years by a company already in the paints and coatings business.

The product LC of the n-CuO paint is relatively simple. n-CuO is made from a copper inorganic precursor (copper carbonate) which is freshly synthesized and dried at 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 thus produced is mixed with an acrylic base to produce the nano-enabled paint according to specified composition in Table 1. The entire production (synthesis of n-CuO and production of paint) is performed in the same country, and there are no scarce resources, transportation or trade related impacts.

Table 1 n-CuO paint composition

Component	Wet Paint (%)
Binder	24
Titanium Dioxide	19.7
Organics	1.7
Didecyldimethylammonium chloride (DDAC)[6]	0.2
Nano copper oxide	0.7

Customers can buy this paint from the hardware store and paint wooden planks that are used to make the house fence through spray or coating application of the paint. It will be recommended that painting is done every five years, and the wood is sanded every third repainting.

At the end-of-life the treated wood is incinerated with energy recovery, but they could also in principle be placed in a landfill or composted.

[6] Biocide to prevent degradation of paint

3.2.2 Working approach Step 4 -Life Cycle Model

We now build a LC model for the n-CuO paint by focussing on the unit processes and activities, and identifying the input chemicals, emissions and waste. Here we illustrate the case LC model for only n-CuO paint for a focussed discussion.

Process engineers and chemists in the manufacturing unit were asked to identity emissions and waste, along with their relative strength for the unit process/activities identified for the n-CuO paint (Figure 6). Information that is not known was marked with "?"

In terms of life cycle stages, the highest emissions are to air and water in the use and end of life stages. Thus assessing the extent of the emissions to air and water is important and it should be ensured that these release quantities are not hazardous to the environment and human beings.

Two types of consumer application of paint are compared: spraying and coating. Spraying has low releases to air and waste, whereas coating has high releases to water and soil. This is just a qualitative comparison, but the toxicity of n-CuO in these environmental compartments and even risk management and design modification costs could also be compared to see if spraying or brushing may have lower risks.

The end of life emissions should be clarified with waste management experts as there is significant uncertainty with regard emissions of nanomaterials on incineration, landfill and composting.

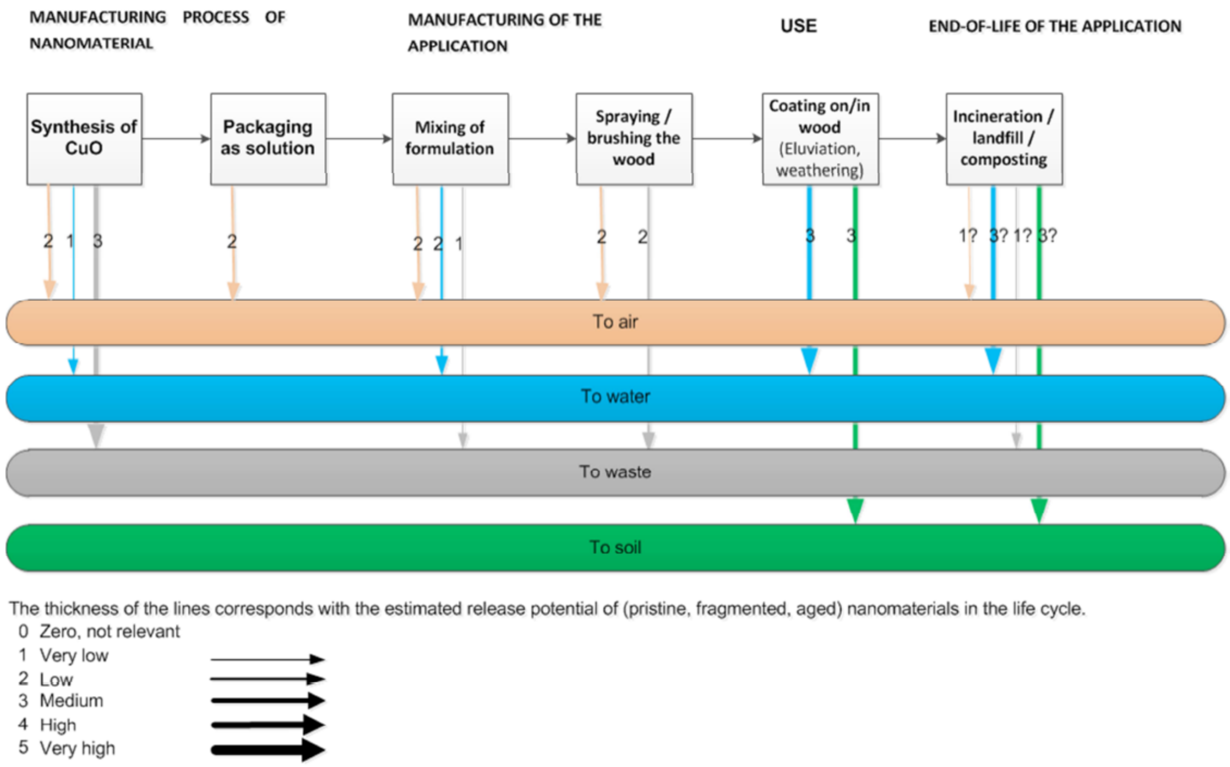

Figure 6 Life cycle thinking applied to n-CuO paint[7]

[7] This figure is extracted from SUN Project Deliverable 2.1 *Life cycle model for Nanoproducts/materials*

3.2.3 Working approach Step 6: Assessing Risk hotspots of Emissions of n-CuO paint

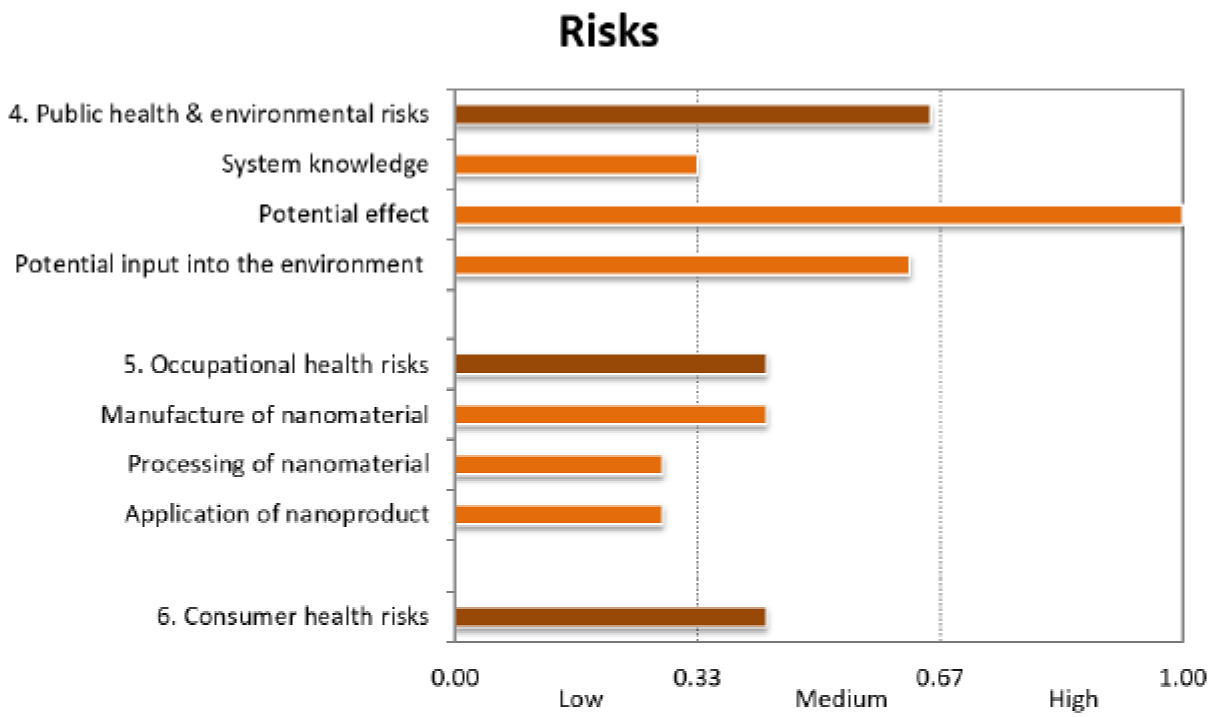

Figure 8: Risks from emissions for n-CuO paint

Scores on X axis correspond to Control Banding results translated to scores in 0-1 range (see Appendix 2)

Here CB tools included within LICARA Nanoscan are used to consider public health and environmental risks, occupational risks and consumer risks of n-CuO paint. Risks for n-CuO paint were greatest for public health and environment, followed by equal scores for occupational health and consumer health.

In the case of public health and environmental risks, the most significant contributor to the average score was potential effect based on free radical activity and oxidative stress (hazard), followed by potential input into the environment (exposure) and system knowledge (uncertainty). In the case of occupational risks, the greatest occupational risk was caused during nanomaterial manufacture, which corresponds to a Stoffenmanager Nano risk band assigned to medium risk. In the case of consumer risks, while exposure potential existed due to surface bound particles (n-CuO dispersed in paint and applied to wood), the fraction of exposed consumer population was less than 5%.

Hence SbD strategies to control hazard of n-CuO as well as exposure during n-CuO manufacture and use may be relevant.

3.2.4 Working approach Step 11: Assessing Impacts of n-CuO paint compared to CAP

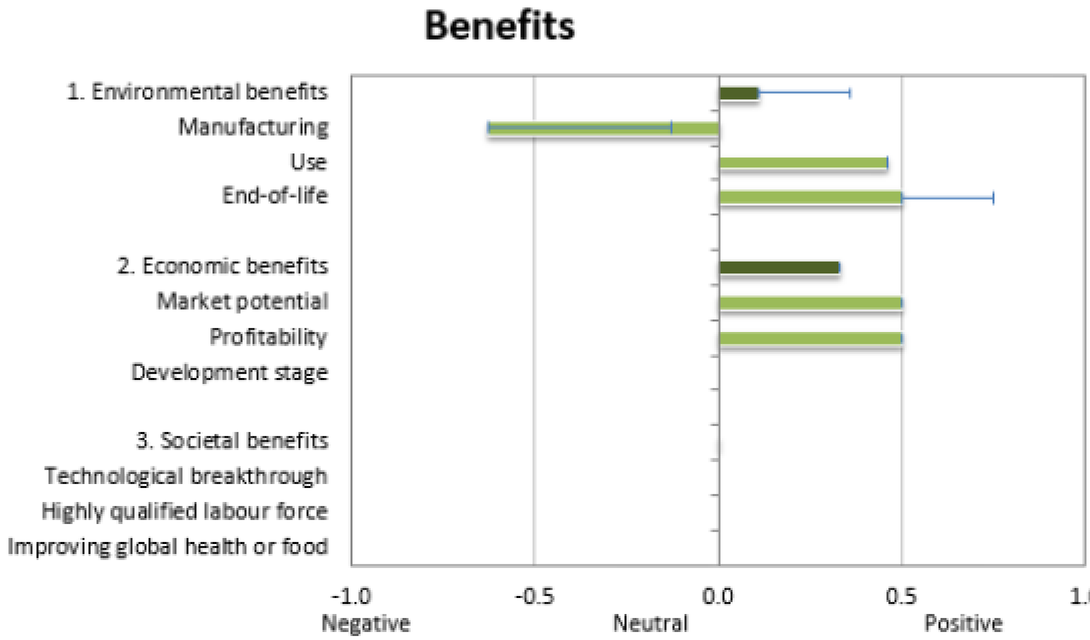

Figure 7: Impact of n-CuO paint compared to CAP

Scores on X axis correspond to sum of scores ranging from (minus)1 to 1 (see Appendix 2)

Here the environmental, economic and social benefits of the product are compared with the incumbent. While the average environmental benefit of n-CuO paint was positive in comparison to CAP, the manufacturing stage of the n-CuO paint was worse than CAP in terms of consumption of energy and hazardous materials. n-CuO paint had a better use and end of life stage 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 was due to foreseen market potential in a medium sized market and profitability 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 Biocidal Product Review approval. n-CuO paint has no social benefits over CAP.

For the novel n-CuO paint to be beneficial over the incumbent CAP paint, the manufacturing process has to be redesigned to decrease environmental impact and social impacts should be strengthened.

3.2.5 Working approach Step 12-Comparing RA and LCA results

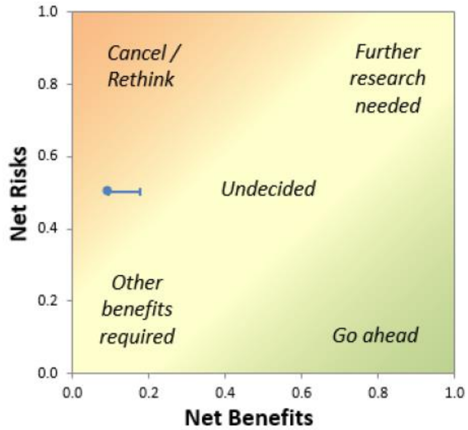

Figure 9 Benefit Risk for n-CuO paint

Blue dot with error bar indicates the benefit-risk profile of n-CuO paint

LICARA Nanoscan tool integrates LCA and RA into a two dimensional benefit-risk matrix that provides guidance on product development (Go ahead, Cancel/Rethink, Further research needed, and Other benefits required). On integrating the risk and benefit quadrants (Figure 9), the result lies in the quadrant "Cancel/Rethink". In the SbD workflow (Figure 1), the risks would already be mitigated by this stage and net benefits would also have been considered. But the above benefit risk framework guides the product to lie as high in net benefits and as low in risks as possible. Even as the product lies in the "Go ahead" green zone, marginal improvements to the safety and sustainability may be possible.

The blue dot of indicates the benefit-risk profile of n-CuO paint *without* revision of the basic concept in response to the risks (Step 6) and impacts (Step 11). Even if risks of n-CuO paint are mitigated, significant benefits would be needed to make the n-CuO paint a viable product.

4.Summary Conclusions

The working approach described in this document comprises of preliminary guidance drawn from a limited review of currently existing literature combining RA and LCA at low TRL. The approach can certainly further evolve and improve in the next years with more SbD studies. For now, we found some hazard-based methods and risk-based methods fostering SbD at TRL 1-6, but envision a larger role for ex ante LCA in facilitating SbD in the future.

SbD in practice can best be fostered in a collaborative and interdisciplinary culture within companies, and between product design teams and RA/LCA experts. Design, technical and marketing functions within a company need to closely collaborate applying these methods on their own and mobilize information that can support application of other LCA and RA approaches. LCA and RA experts can facilitate application of more complex approaches across the TRLs.

Results from the application of RA/LCA methods at various TRL levels may vary. SbD within the design process should be viewed as an iterative evaluation of a product development scenarios based on best available knowledge and data at that point, thus improving their safety and sustainability.

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Appendix 1

Key findings on combining Risk Assessment and Life Cycle Assessment at low TRL

We present a short summary of the literature review from Subramanian and Guinée (2021). The number of essential papers found was reduced to ten papers combining RA and LCA/LCT at TRL 1-6, and these were characterized by a predefined set of criteria. Of the ten studies reviewed, four were found to be the most useful for product designers who would like to combine RA and LCA or aspects thereof:

1. Study by van Harmelen et al. (2016) comprehensively combining RA and LCA for nanomaterials on two tiers depending on data availability;

2. Study by Tan et al. (2018) performing a two-step hazard screening and combining it with ex ante LCA at two different TRLs;

3. Study by Kralisch et al (2013) applying screening for ecological and human health hazards and combining it with an ex ante LCA to improve process design;

4. Study by Shatkin and Kim (2015) using expert knowledge to prioritize data gaps on a novel cellulosic nanomaterial.

The research questions and key findings for each are summarized below.

Research question 1: What approaches and methods for combining RA and LCA at TRL 1-6 can designers currently use?

For low TRL technologies and materials, product designers can immediately apply the following practical insights without further consultation of outside experts :

- Avoid the use of substances in products of which the hazards are sufficiently known (Zeer Zorgwekkende Stoffen (ZZS)) or are suspected (Potential ZZS (PZZS)).

- Apply life cycle thinking (LCT) to identify potential risk hotspots in the different life stages of a material or product.

- Reduce the use of energy, water and scarce resources in the design as much as possible.

Product designers, in collaboration with outside experts, can adopt the following approaches:

- Assess uncertainties, prioritize data gaps, perform control banding and other screening RA approaches

- Perform predictive toxicological screening tests using in vitro or in vivo approaches

- Perform an ex-ante LCA of the application (product, material)

Research question 2: What is the scope and quality of what designers can currently accomplish with these methods and approaches?

- For low TRL technologies and materials using known substances, product designers can perform a simplified assessment of potential risk hotspots across the different phases of a product/material life cycle, and can apply generic principles such as avoiding of the use of hazardous substances (ZZS and PZZS), minimizing energy/water consumption, minimizing emissions and waste, to minimize potential risks and environmental impacts. All of these simplified approaches cannot replace a quantitative LCA/RA (which often only becomes possible at higher TRLs), but they can help avoid some obvious sources of risk and impact.

- For low TRL technologies and materials using novel substances, product designers can gain general ideas for estimating potential risks from case studies applying LCT, such as in the studies of Som et al. (2010) and Sweet & Strohm (2006). However, a more complete and substance-specific mapping of potential risks of new substances (RA and LCA) requires expertise from external experts.

Research question 3: What gaps and challenges remain to be addressed to (better) facilitate RA and LCA application by product design teams?

RA and LCA are comprehensively combined in van Harmelen et al. (2016) and Tan et al. (2018), and these studies demonstrate that RA and LCA can be combined at low TRL even with significant uncertainties. All other reviewed studies predominantly focused more on either RA or LCA, not exploiting the full potential of combining RA and LCA.

- The Goal and Scope Design (GSD) phase of an LCA offers a good starting point for incorporating SbD into product design through collaboration between design, technical and marketing teams, but this option has not been applied so far.

- LCT is frequently applied in the reviewed studies (Subramanian and Guinee, 2021), but the performance of full ex ante LCA studies is still the exception rather than the rule. Although ex ante LCAs have already been extensively applied in studies outside the SbD field to materials and technologies starting at TRL 2, ex ante LCA in the reviewed SbD literature has so far only been applied from TRL 4-5.

- By focusing SbD not only on the safe use of chemicals but on a wide range of environmental, economic and social impacts during the life cycle (LC), an even more comprehensive preventive analysis for Safe & Sustainable by Design (SSbD) can be made.

To further promote the joint use of ex ante LCA and RA for SbD, the following issues need to be addressed:

- The review showed that SbD studies are still scarce at the moment. More studies should therefore be conducted in which both LCA and RA are applied at low TRL in order to build a knowledge base in practical SbD methods for product designers.

- The collaboration between researchers and companies in SbD studies is currently limited. Of the reviewed studies, only Van Harmelen et al. (2016) collaborated with Small and Medium Enterprises (SMEs). At the same time, it is known from the ex ante LCA literature that collaboration between companies and LCA at an early stage in the development of new materials and products stimulates designers to develop more sustainable materials, products and technologies.

- The GSD phase of an LCA could be better utilized to establish good collaboration between design, technical and marketing teams for SbD studies. There is no single discipline that can tackle the SbD challenge alone.

- Preferably, there should be pooled and user-friendly sources of information on risk information (information on risks, hazards, baseline exposure scenarios) about chemicals, which designers can understand and apply in their daily practice. There is some information available on the European Chemicals Agency (ECHA) website, but it is not tailored to the knowledge and perspective of the product designer (e.g. including function of substances, costs, examples of life cycle thinking and risk identification for product types). This information is currently too fragmented across different sources or is even missing altogether.

- Complete data sets are often not available for new materials and products. That is the challenge of ex ante analyses. Usually it is possible to obtain the material and energy data with the help of companies and technology experts, but what is lacking is insight into potential emissions from new material technologies. It is recommended, where possible, to develop generic estimation methods for potential emissions from such new technologies.

- Assessment of risks of exposure to substances for human health is usually done for the production phase of substances but much less for the use and disposal phases of the same substances, and this gap should be filled. Furthermore, there is a gap in estimation of emissions of novel substances.

- Most of the reviewed publications focus on the risks of one substance (group) from a product life cycle. That is already a broadening from doing just an RA or just an LCA, but ultimately product design teams should focus on the risks of all relevant substances from a product life cycle so that different applications, chemicals and derived exposure scenarios can be involved. Such a comprehensive assessment of all chemical risks in a product context is so far lacking and it is necessary to explore how to extend the scope of current approaches in this direction.

Appendix 2

Background on methodology of LICARA Nanoscan

The conceptual framework of LICARA NanoSCAN is provided in Figure 1. This excerpt has been extracted from Subramanian et al. (2016).

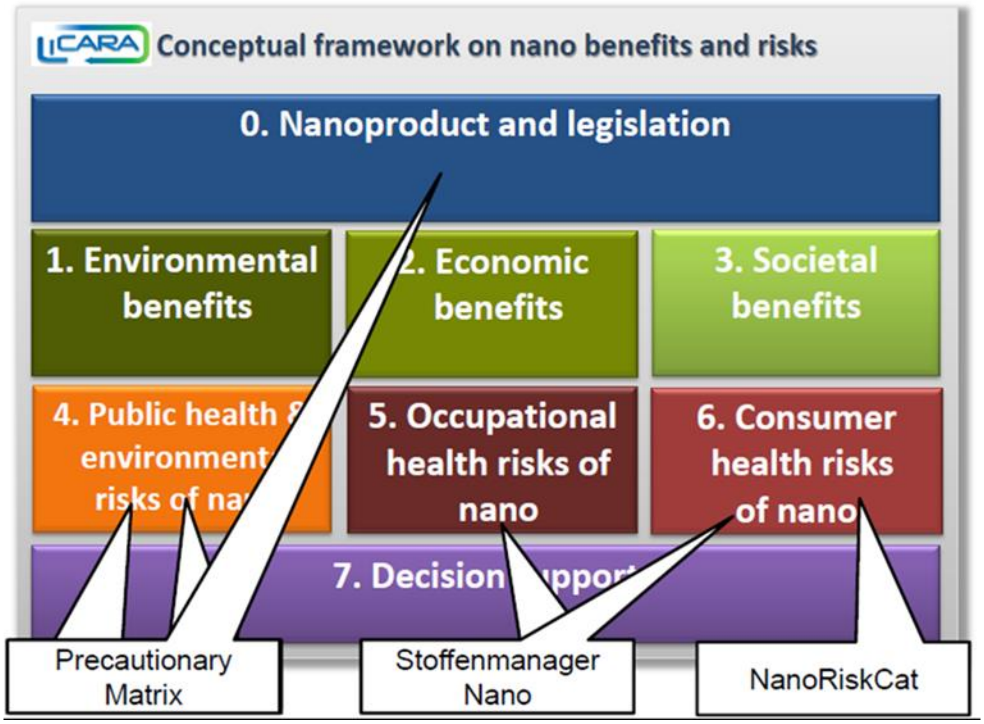

Figure 10: Conceptual Framework for LICARA NanoSCAN

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 ISO definitions of nanomaterials.

Modules 1–3 implement screening level socioeconomic assessment, and 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 implement screening level risk control, and aim to assess public health and environmental risks, occupational health risk and consumer risks of the nano-enabled products. Module 4 utilises Precautionary Matrix (Hock et al, 2008), 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 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 MCDA based 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.

Appendix 3

Inputs to Licara Nanoscan for n-CuO case study

The inputs used to apply LICARA Nanoscan to the n-CuO paint case study are extracted from Subramanian (2017).

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